DOE/MC/16220-1306
(DE83003821)

EVALUATION OF GASIFICATION AND GAS CLEANUP
PROCESSES FOR USE IN MOLTEN CARBONATE FUEL
CELL POWER PLANTS

Final Report

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Work Performed Under Contract No. AC21-81MC16220

For
Morgantown Energy Technology Center
Morgantown, West Virginia

Westinghouse R&D Center
Pittsburgh, Pennsylvania

TECHNICAL INFORMATION CENTER
UNITED STATES DEPARTMENT OF ENERGY

DOE/MC/16 220--1306

DE83 003821

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ACKNOWLEDGMENTS

In addition to the principal investigators listed on the title page, V. P. Kothari, METC's Project Officer, and T. Grindley, also of METC, have provided invaluable guidance and assistance.

EXECUTIVE SUMMARY

This report satisfies the requirements for DOE Contract DE-AC21-81MC16220 to:

- List coal gasifiers and gas cleanup systems suitable for supplying fuel to molten carbonate fuel cells (MCFC) in industrial and utility power plants (Section 2).
- Extensively characterize those coal gas cleanup systems rejected by DOE's MCFC contractors for their power plant systems by virtue of the resources required for those systems to be commercially developed (Section 2).
- Develop an analytical model to predict MCFC tolerance for particulates on the anode (fuel gas) side of the MCFC (Section 3).
- Develop an analytical model to predict MCFC anode side tolerance for chemical species, including sulfides, halogens, and trace heavy metals (Section 3).
- Choose from the candidate gasifier/cleanup systems those most suitable for MCFC-based power plants (Section 4).
- Choose a reference wet cleanup system (Section 4).
- Provide parametric analyses of the coal gasifiers and gas cleanup systems when integrated into a power plant incorporating MCFC units with suitable gas expansion turbines, steam turbines, heat exchangers, and heat recovery steam generators, using the Westinghouse proprietary AHEAD computer model (Section 5).
- Provide efficiency, investment, cost of electricity, operability, and environmental effect rankings of the systems (Section 6).
- Provide a final report incorporating the results of all of the above tasks.

Section 7 of this final report provides general conclusions for the required tasks. The reader is encouraged to explore each section of this report for more specific, detailed results.

ABSTRACT

This report in satisfaction of the requirements for DOE Contract DE-AC21-81MC16220, lists coal gasifiers and gas cleanup systems suitable for supplying fuel to molten carbonate fuel cells (MCFC) in industrial and utility power plants. It extensively characterizes those coal gas cleanup systems rejected by DOE's MCFC contractors for their power plant systems by virtue of the resources required for those systems to be commercially developed. It develops an analytical model to predict MCFC tolerance for particulates on the anode (fuel gas) side of the MCFC and to predict MCFC anode side tolerance for chemical species, including sulfides, halogens, and trace heavy metals and selects from the candidate gasifier/cleanup systems those most suitable for MCFC-based power plants as well as a reference wet cleanup system. Coal gasifiers and gas cleanup systems, when integrated into a power plant incorporating MCFC units with suitable gas expansion turbines, steam turbines, heat exchangers, and heat recovery steam generators, are analyzed parametrically using the Westinghouse proprietary AHEAD computer model. Systems are ranked by efficiency, investment, cost of electricity, operability, and environmental effect.

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Section 1

INTRODUCTION

The U.S. Department of Energy (DOE) has funded two major programs for the development of molten carbonate fuel cell (MCFC) power systems for utility and industrial applications. While the high-temperature MCFC is a promising concept for future power generation, especially when fueled from an integrated low- or medium-Btu coal gasifier, it is sensitive to coal-derived contaminants such as sulfur, halogens, and particulates. These contaminants may poison catalysts, damage electrodes and electrolytes, and clog passages. In view of the above, projecting MCFC tolerance of coal-derived contaminants and assessing the ability of existing and developing cleanup technology to meet these tolerances were considered to be mandatory.

The objective of this program was to evaluate and compare coal gasification and gas cleanup processes systematically for use in advanced MCFC-based power plants including topping and/or bottoming cycles. Specifically, the goals were to:

- Predict MCFC tolerance of contaminants found in coal
- Identify gasifier/cleanup combinations suitable for application to MCFC-based power plants
- Develop parameterizations that accurately describe the overall performance and cost of alternative integrated MCFC plant subsystems.
- Select optimal power plant configurations with emphasis on efficiency, operability, cost, and effluents.

The Westinghouse Electric Corporation, with Davy McKee Corporation and Energy Research Corporation (ERC), undertook a 12-month evaluation of gasifier/cleanup processes for application to MCFC. The

evaluation work can be described by means of the Work Breakdown Structure derived for it.

This final report contains the results of Tasks A through D, plus the additional analytical model Tasks A2a(1) and A2a(2), which were authorized by contract modification during the performance of Task A.

Section 2

DEFINITION OF PROCESS/INFORMATION

2.1 INTRODUCTION

Definition of this process information includes a listing of candidate gasifiers for use in a coal gasifier/gas cleanup/MCFC power facility; discussion of MCFC operating characteristics and contaminants and particulate tolerances; a listing of advanced cleanup systems, both high and low temperature; a study of design constraints on heat recovery equipment to provide a basis for design of a cost-effective, reliable heat recovery apparatus; and a set of facility criteria that bear directly on cleanup system selection.

The section lists, as exhaustively as possible, all gasifiers that could be candidates for use in a coal gasification/gas cleanup MCFC power facility. It includes gasifiers in each of the following categories: fixed-bed, fluidized-bed, entrained-flow, and a miscellaneous category covering gasifiers such as the molten salt reactor.

The following information, as available in the public domain, has been generated for each gasifier:

- State of commercial development and availability
- Time-scale and resource requirements for commercial development
- Characteristics of output -- major and minor gas constituents as functions of input variables
- Operational characteristics and limitations
- Environmental effluents
- Reliability
- Applicability to a gasifier/gas cleanup/MCFC facility.

Following the gasifier listing is a description of MCFC operating characteristics and contaminant tolerances, using existing

fuel cell performance models and other information sources in the public domain, such as the DOE-MCFC development work. Specific information includes,

- Cell pressure and temperature
- Fuel composition
- Limits on major gas stream contaminants, e.g., H_2S , COS , NH_3 , NO_x , SO_x , tars, etc.
- Limits on particulates and trace elements.

The information definition continues with an exhaustive list of advanced cleanup systems, covering both high- and low-temperature systems. The cleanup system lists produced by General Electric and by United Technologies, Inc., for the DOE-MCFC power-plant technology development program have also been considered. These lists have been critically evaluated and amended where necessary. Those systems not chosen by those DOE contractors for further consideration by virtue of their resource requirements for commercial development and those systems specifically defined by the DOE Technical Project Officer have been characterized extensively. The characterization includes, but is not limited to, the following information, as available in the public domain:

- State of commercial development, availability
- Operational characteristics
- Environmental effluents
- Waste-product or recycle requirements
- Form in which sulfur is rejected
- Contaminants in the effluent streams
- Thermal efficiency
- Utility requirements
- Reliability.

Finally, design constraints on heat recovery equipment are discussed in such a way as to provide a design basis for cost effective, reliable, heat recovery apparatus for use in cooling the raw fuel gas down to the temperature level required for low-temperature fuel gas

cleanup or to the MCFC operating temperature, when high-temperature fuel gas cleaning processes are used. Consideration has been given to:

- Corrosion
- Erosion
- Deposition.

2.2 GASIFIERS FOR MOLTEN CARBONATE FUEL CELL (MCFC) APPLICATION

This section provides a comprehensive list of gasifier systems that could qualify for use in a coal gasification gas cleanup MCFC power facility. The coal gasification systems investigated include the fixed-bed, fluidized-bed, entrained-flow systems, and miscellaneous systems of which the molten salt reactor is the most prominent.

In fixed-bed processes the sized coal is fed into the top of the gasifier and moves down through the gasifier countercurrent to the hot product gases as the coal is reacted and consumed. Ash is discharged from the bottom, and coal-derived synthesis gas flows out the top. The fixed-bed gasifier is commercially available but has relatively low gas production, thermal efficiency, high costs per unit of capacity, and a limited range of acceptable feed coals plus tar/oil disposal requirements.

In fluidized-bed processes the coal is kept in a constant state of agitation by a stream of hot, fluidizing gases flowing up from the bottom. The resulting mixing, swirling behavior of the solids provides superior solids/gas contact and a relatively high specific throughput, with only traces of tar/oil production. Some fluidized-bed units cannot directly handle caking coals.

In entrained-flow processes finely pulverized coal is carried into the reaction chamber by a stream of reaction gases (i.e., oxygen and steam). The gasification of the coal occurs as the mixture is swept through the reaction vessel. The entrained-flow design offers the highest specific throughput and the ability to handle nearly all coal

types but requires slag handling and an extensive cleanup train because of high temperature and solids carry-over.

In molten salt systems coal is gasified in a bath of molten sodium (Na_2CO_3) or potassium carbonate (K_2CO_3). The molten salt process incorporates many desirable characteristics for MCFC applications but requires a complex system for ash removal and sulfur recovery. The subsequent selection and use of one (or several) of these four basic systems in a MCFC application results in a trade-off of the comparative advantages and disadvantages of each system, as shown in Table 1.

Table 1
RELATIVE ADVANTAGES/DISADVANTAGES OF SELECTED SYSTEMS

	Fixed Bed	Fluidized Bed	Entrained Bed	Molten Salt
Cold Gas Efficiency	Low	High	High	High
Tar & Oil Concentration	High	Low	Low	Low
Coal Processing Capability	Limited*	Limited** (mildly caking)		
Capital Cost	Highest	Moderate	Moderate	Lowest
Ash Disposal	Moderate	Moderate	Simple	Complex
In-Situ Desulfurization	No	Possible	No	Yes
Reactor Capacity	Low	High	Highest	High
Reliability & Stability	Moderate	High	Low	High
Entrainment	Low	High	High	Low
Steam Consumption	High	Medium	Low	Low

* Requires noncaking and double-screened coals.

** Westinghouse pressurized, fluidized system handles caking coals.

The results of initial screening studies indicate that all gasification categories could be used with a MCFC system. In order to select the most suitable coal gasification system (or systems) from each of the four categories, however, a specific set of evaluation criteria must be established. As the Institute of Gas Technology (IGT) noted,¹ the optimum gasifier for integration with MCFC must:

1. Produce a gas with the required composition
2. Be highly efficient
3. Be able to use nearly all types of coals
4. Be economically attractive
5. Have load-following capability.

Each suitable gasifier has been investigated in terms of the following:

- State of commercial development and availability
- Time-scale and resource requirements for commercial development
- Characteristics of output major and minor gas constituents as functions of input variables
- Operational characteristics and limitations
- Environmental effluents
- Reliability.

To compile this list, 40 gasifiers were studied. The history leading to the present state of commercial development and the availability of each coal gasification system have been itemized. Because the up-to-date published data are incomplete, we have attempted to indicate the relative position that a particular gasifier system occupies. A "commercial" process designates state-of-the-art technology that exists and can be purchased from some company that will sell the gasifier for commercial operation and provide some degree of warranty related to its performance. "Demonstration" is used to indicate those gasification systems currently in the advanced developmental stage or ready for demonstration as a commercial unit. The "pilot plant" refers to those systems currently in the pilot-plant stage of development and designates the newer, advanced concepts that are either at the bench-scale level of

development or in the early process development (PDU) phase. The term "availability" refers to all commercial gasifier systems.

Information on the time-scale and resource requirements for commercial development is highly subjective and, in most cases, unavailable.

The characteristics of output are given as a function of input variables. Gas compositions are indicated for gasifiers after cooling and before acid gas removal. Representative cases of coal gasification product streams are characterized with respect to their:

- Major constituents, e.g., CO, H₂, CO₂, CH₄, N₂, H₂O
- Minor constituents, e.g., H₂S, COS, particulates, halogens, tar.

In most cases operating conditions for each gasification system are based on reported ranges of temperature and pressure. Because of the effects of gasifier type, operating conditions, and coal type on the product gas composition, however, general data reported as N/A (not available) could be obtained only with a more exhausting search than time permitted; N/A does not indicate that the data are absolutely unavailable.

We have considered all major environmental effluents (where available) up to the point at which the gas is suitable for a low-temperature acid gas removal system. In most cases the gasification effluents result from producing a cool, clean, raw product gas suitable for some undesignated sulfur removal system.

Finally, we have indicated the reliability of a gasifier from a commercial or demonstration operation viewpoint, based on information available in the literature.

Of the 40 gasifiers investigated, 32 were found to be suitable for utilization with a MCFC fuel system. Table 2 lists the acceptable gasifiers by process, and Table 3 summarizes them by developer, reactor type, coal type, pressure, and current operating status. Table 4 lists the 8 gasifiers rejected for our purposes and why. The detailed

Table 2

LIST OF SUITABLE MOLTEN CARBONATE FUEL CELL GASIFIERS BY PROCESS

<u>Fixed-Bed Processes</u>	<u>Fluidized-Bed Processes</u>
Lurgi (Dry Ash)	Winkler
British Gas/Lurgi Slagging	Rheinbraun High Temperature Winkler
METC Stirred Bed	Westinghouse Pressurized
Slagging Fixed-Bed	Carbon Dioxide Acceptor
Wellman-Galusha	Synthane
Foster Wheeler-Stoic	BCR Tri-Gas
Woodall Duckham/Gas Integrale	U-Gas
Riley-Morgan	Battelle/Carbide
Wilputte	
Wellman Incandescent	
<u>Entrained-Bed Processes</u>	<u>Miscellaneous</u>
Texaco	Rockwell Molten Salt
Koppers-Totzek	Pullman Kellogg
Combustion Engineering	Otto-Rummel
Bi-Gas	Atgas
Babcock & Wilcox	Saarberg/Otto
Foster Wheeler	Kiln Gas
Shell/Koppers	Hitachi

compilation can be found, for each acceptable gasifier, in Appendix A of Reference 2.

This study indicates that a wide variety of gasifier systems are available for use in an MCFC power facility.

2.3 COAL GAS CONTAMINANT EFFECTS ON MCFC COMPONENTS

This subsection presents information in the public domain on the effects of coal-gas contaminants on the performance of a molten carbonate fuel cell. Literature data from various sources, including

Table 3

SUMMARY OF MOLTEN CARBONATE FUEL CELL/GASIFIER LISTING

<u>GASIFICATION PROCESS</u>	<u>DEVELOPER</u>	<u>REACTOR TYPE</u>	<u>COAL</u>	<u>PRESSURE, (kPa) psig</u>	<u>STATUS</u>
Lurgi (Dry Ash)	Lurgi Mineralo- technik Gmbh	Fixed bed	Noncaking, lump coal, no fines	2515-3204 (350-450)	Commercial
British Gas/Lurgi Slagging	British Gas Corp. Lurgi Mineralotechnik	Fixed Bed	All types, no fines	2101-2687 (290-375)	Demonstration
METC Stirred Bed	Morgantown Energy Tech. Ctr.	Agitated fixed bed	All types, no fines	101-2066 (0-285)	Pilot
Slagging Fixed Bed	Grand Forks Energy Research Center	Fixed bed slagging	All Types	653-2859 (80-400)	Pilot
Wellman-Galusha	McDowell-Wellman Eng. Co.	Fixed bed w/wo stirring	All types no fines	101 0	Commercial
Foster Wheeler Stoic	Foster Wheeler Energy Corp.	Two-stage fixed bed	Noncaking, lump coal, no fines	101 0	Commercial
Woodall Duckham/Gas Integrale	Woodall Duckham (USA) Ltd.	Two-stage fixed bed	Noncaking, lump coal, no fines	101 0	Commercial
Riley-Morgan	Riley Stoker Corp.	Fixed bed	All types, no fines	101 0	Commercial
Wilputte	Wilputte Corp.	Fixed bed	Lignite or bitu- minous	101	Commercial
Wellman Incandescent	Wellman Incandescent Ltd.	Two-stage fixed bed	Noncaking, lump coal, no fines	101 0	Commercial
Winkler	Davy Powergas Inc.	Fluidized bed	All types with pretreatment	101-1377 (0-185)	Commercial
Rheinbraun High Temperature Winkler	Rheinische Braun- Kuhlenwerke AG	Fluidized bed	All types	584-2170 (70-300)	Pilot

Table 3 (Cont'd)

<u>GASIFICATION PROCESS</u>	<u>DEVELOPER</u>	<u>REACTOR TYPE</u>	<u>COAL</u>	<u>PRESSURE, (kPa) psig</u>	<u>STATUS</u>
Westinghouse Pressurized	Westinghouse Electric Corp.	Fluidized bed	All types	998-1480 (130-200)	Demonstration
Carbon Dioxide Acceptor	Conoco Coal Development Co	Fluidized bed	Lignite subbituminous	1136 (150)	Pilot
Synthane	ERDA & Pittsburgh Energy Research Ctr.	Fluidized bed	All types with pretreatment	3549-6996 (500-1000)	Pilot
BCR TRI-Gas	Bituminous Coal Research	Three-Stage fluidized bed	All types	101-1722 (0-235)	Pilot
U-Gas	Institute of Gas Technology	Fluidized bed	All types with pretreatment	446-2515 (50-350)	Demonstration
Battelle/Carbide	Battelle Memorial Institute	Fluidized bed ash agglom.burn.	All types with pretreatment	791 (100)	Pilot
Texaco	Texaco Development Corp.	Entrained bed, slagging	All types	2170-8375 (300-1200)	Commercial
Koppers-Totzek	Koppers Co., Inc.	Entrained bed, slagging	All types	101 0	Commercial
Combustion Engineering	Combustion Eng. Inc.	Entrained bed, slagging	All types	101 0	Demonstration
BI-Gas	Bituminous Coal Research	Entrained bed, slagging	All types	3549-10443 (500-1500)	Pilot
Babcock and Wilcox	Babcock & Wilcox Co.	Entrained bed, slagging	All types	101-2170 (0-300)	Demonstration
Foster Wheeler	Foster Wheeler Energy Corp.	Entrained bed, slagging	All types	2515 (350)	Pilot
Shell-Koppers	Sheel International Petroleum	Engrained bed, slagging	All types	1894-3101 (260-435)	Demonstration

Table 3 (Cont'd)

<u>GASIFICATION PROCESS</u>	<u>DEVELOPER</u>	<u>REACTOR TYPE</u>	<u>COAL</u>	<u>PRESSURE, (kPa) psig</u>	<u>STATUS</u>
Rockwell Molter Salt	Rockwell International Corp.	Molten salt	All types	101-2032 (0-280)	Demonstration
Pullman-Kellogg	MW Kellogg Co.	Molten salt	All types	2032-2859 (280-400)	Pilot
Otto-Rummel	Dr. C. Otto and Comp. GmbH	Slag bath	All types	101-2583 (0-360)	Pilot
Atgas	Humboldt-Wedag AG	Molten iron bath	All types	136 (5)	Pilot
Saarberg/Otto	Saarberg-Dr. C. Otto	Entrained-flow slag bath	All types	1825-2583 (250-360)	Demonstration
Kiln Gas	Allis-Chalmers	Rotary ported kiln	All types	515 (60)	Demonstration
Hitachi	Babcock Hitachi Co. Ltd.	Two-stage fluidized bed	Most types	618-3066 (75-430)	Pilot

major fuel cell developers [United Technology Corporation (UTC), ERC, General Electric (GE), IGT] have been compiled. Possible deleterious effects of a given contaminant and its tolerance limit, wherever available, have been presented. To supplement these published contaminant effects, in Section 3 we have provided analytical results from our thermodynamic equilibria and particulate deposition computer models.

Operating an MCFC stack with coal-derived fuels requires careful consideration of the effect of impurities on its performance. Practically all the elements in the periodic chart and many of their compounds are present in coal and, hence, in coal-derived gas. Many of these elements and compounds may damage the cell by degrading power output or causing mechanical failure.

The contaminants significant to fuel cell performance are those introduced by the coal and gasifier and not removed in the gas cleanup system, plus those contaminants that come from the cleanup system itself. Since the anode exhaust is recycled to the cathode side for CO_2 transfer, some of the contaminants are carried further on into the cathode side. Additional contaminants may also be introduced by the CO_2 transfer device. The effect of contaminants, therefore, becomes important for the anode as well as for the cathode side.

The primary categories of contaminants considered and the constituents of major concern are:

- Sulfur compounds - H_2S , COS , CS_2 , SO_2 , mercaptans, thiophene
- Halogen compounds - Cl_2 , HCl , HF , alkali halides
- Nitrogen compounds - NH_3 , NO_x , HCN , HCNS
- Metals and trace elements - As, Se, Te, Hg, Cd, Pb, Sn, Ge
- Hydrocarbons - Tars, oils, phenol, benzene, toluene, ethylene, etc.
- Particulates - Ash, char, solid compounds of volatile metals and halides.

A theoretical as well as an experimental evaluation of possible deleterious effects of these contaminants is being performed by

Table 4
LIST OF UNSUITABLE MCFC GASIFIERS

<u>Process</u>	<u>Reason</u>
CoGas	Fluidized-bed pyrolyzers designed to produce oil, gas, and char. The char is then fed to a fluidized-bed gasifier for production of syn-gas. Eliminate it because syncrude is a major product, i.e., 52.5 kg/s (5000 tons/d) plant produces 52 m ³ /s (159 mm scfd) of 12,502 KJ/m ³ (335 Btu/scf) gas and 795 m ³ /d (5000 bbl/d) of syncrude.
Hydrane	Gasification produces gas with high methane content, i.e., (57-79 mol % CH ₄) @ 29,860 KJ/m ³ (800 Btu/scf)
HyGas	Designed for high methane content.
Exxon Catalytic	Designed for high methane content.
Bell	Designed for high methane content.
Avco	Designed for high methane content.
Rockwell Short Residence Time	Designed for high methane content.
Gegas	Data unavailable; See METC Process

various organizations under DOE- and EPRI-sponsored programs. Significant progress has been made in understanding the behavior of some contaminants such as sulfur and halogen compounds, whereas very little knowledge exists for other contaminants such as particulates, metals, and trace elements. Table 5 summarizes the effect of impurities and their tolerance limits. A detailed description of various contaminant effects is presented in the sections following the table.

2.3.1 Literature Review

2.3.1.1 Sulfur Compounds

Sulfur compounds are considered to be the most obvious contaminants, causing significant performance as well as endurance penalty to the MCFC stack. Depending on the gas cleanup processes used, varying amounts of sulfur will be present as H_2S and COS in the anode feed gas. Because the CO_2 requirements of the cathode are satisfied by combusting and recycling, the spent anode effluent will appear as SO_2 in the cathode inlet gas. Thus, both the electrodes are exposed to sulfur-containing gases. Sulfur compounds have also been found to react with the molten carbonate electrolyte to form alkali sulfides at the anode and a mixture of alkali sulfates and sulfides at the cathode. As a result, all the cell components are exposed to a combination of sulfur species, with a consequently negative effect on the power output of the cell and also on its endurance because of:

- Electrode corrosion and structural changes
- Current collector corrosion
- Wet-seal corrosion
- Separator plate corrosion
- Carbonate loss resulting from compositional changes in the electrolyte
- Lithium aluminate changes.

The effects of sulfur on cell performance can be characterized by the following losses:

Table 5

SUMMARY OF THE EFFECT OF IMPURITIES AND TOLERANCE LIMITS

Impurity	Possible Effect	Operating Limits
Sulfur compounds (H_2S , COS, CS_2 , SO_2)	<ul style="list-style-type: none"> • Sulfation of carbonates and increase in overpotentials • Deactivation of anode by chemisorption • Sulfation of anode materials • Sintering • Sulfidation of cell hardware • loss of strength and increase of ohmic resistance 	Less than 1 ppm
Halogen Compounds (Cl_2 , HCl, alkali halides)	<ul style="list-style-type: none"> • Severe performance loss at cathode • Formation of chlorides and hardware corrosion 	100 ppm in fuel 10 ppm in oxidant(a)
Nitrogen Compounds (NH_3 , NO_x)	<ul style="list-style-type: none"> • Electrolyte composition changes 	Very large for NH_3
Metals (Fe, Cu, As)	<ul style="list-style-type: none"> • Deactivation and plugging 	(b)
Heavy metals (Hg, Sn, As)	<ul style="list-style-type: none"> • Corrosion, alloying and structural damages 	(b)
Tar and Oil	<ul style="list-style-type: none"> • Deactivation, mechanical problems 	(b)
Particulates	<ul style="list-style-type: none"> • Diffusion problems, blockage of flow passages 	$0.8 \text{ lb}/10^6 \text{ ft}^3$
Hydrocarbons	<ul style="list-style-type: none"> • Carbon formation 	Less than 1 mol%

(a) TRW analysis shows 0.2 ppmV tolerance for HCl and 100 ppmV for HF.³

(b) Very low tolerance expected in IGT's handbook of fuel cell performance.

- Reversible - caused by chemisorption of the sulfur species on the metallic surfaces. This mainly reduces the catalytic surface of the nickel electrode, increasing its overpotential and poisoning catalysis for the water gas shift reaction.
- Irreversible - caused by reaction of the sulfur species with the metallic components (Ni, Co, Cr, Fe, etc.), to form corresponding sulfides. This reaction promotes large structural changes in the anode and corrosion of cell hardware.

Two general approaches in solving the sulfur problem in the molten carbonate fuel cell are possible. The first approach is to remove the sulfur species to very low levels before the gas enters the fuel cell anode. The second approach is to identify the sulfur tolerance of the fuel cell components currently in use and, if degradation in performance and materials stability becomes evident, to develop sulfur-tolerant components that show acceptable long-term electrochemical performance and/or corrosion stability. This review emphasizes the latter approach. The results of experimental studies as well as theoretical work to explain sulfur effects on various fuel cell components are summarized below. Because of the extreme importance of experimental techniques employed in studying sulfur effects, a brief description covering this aspect is also presented. Without sulfur-tolerant fuel cell components, highly efficient and, therefore, expensive fuel gas cleanup is required.

Experimental Techniques. A study of sulfur effects on fuel cell performance can be conducted in a conventional MCFC equipped with a reliable reference electrode and appropriate instrumentation. Great care should be exercised, however, in conducting experiments with small quantities of active species such as sulfur. The sulfur species H_2S , COS , and SO_2 in premixed form with other fuel cell gases tend to be absorbed in the system plumbing and vessels. They also have significant stability problems. If these factors are not properly addressed, they can lead to confusing experimental results and erroneous conclusions. A description of these factors and the corresponding required design features in the test facility are given below.⁴

The loss of sulfur-containing components of the anode feed gas that occurs prior to reaching the fuel cell and between the cell exit and the sampling port is a major source of error in determining the sulfur balance across the fuel cell. Such losses can be minimized by:

- Keeping to a minimum the stainless steel (SS) surface of the system plumbing exposed to H_2S , especially at temperatures below $450^{\circ}C$. This can be done by using alumina and Teflon® tubing and Teflon® fittings wherever possible (Figure 1).
- Humidifying the fuel gas prior to introducing H_2S , since H_2S injected prior to humidification can partly dissolve in the humidifier water bath.
- Joining the alumina to the SS tubing using a "soft" sealant
- Adequately preheating the fuel gas to $650^{\circ}C$ before it enters the cell.

The supply of premixed gases containing low-level sulfur contaminants can be stabilized by employing permeation tubes to feed the contaminants.⁵ A permeation tube of a given length, under controlled temperature conditions, provides a very uniform, stable, and measurable flow of the selected compound (H_2S , COS, or SO_2) into a carrier stream (fuel or oxidant). In measuring sulfur concentrations with a gas chromatograph, for example, similar care should be observed. Presaturation of the system plumbing with a similar sulfur-containing gas, prior to injecting the gas sample, is normally required to provide reproducible measurements

Anode. The effect of exposure to sulfur is a decrease in cell voltage of some 60 to 90 mV at normal power levels, primarily at the anode. From the in-cell and out-of-cell tests performed with sulfur-containing anode gas by major fuel cell developers, we can conclude the following:

- Short-term exposure to low-level (1-10 ppm) sulfur contaminants in the fuel (as H_2S or COS) increases the anode polarization but has no significant effect on open-circuit potentials (OCP) or cell resistance.
- With low-Btu fuel, 1 to 10 ppm H_2S cause a cell performance loss of approximately 10 mV/ppm H_2S at 160 mA/cm^2 and $650^{\circ}C$.⁵

Figure 1 -- Design of Test Facilities for Reliably Evaluating Sulfur Tolerance of the Anode

- Cobalt-containing anodes display a resistance to sulfur superior to that of nickel or nickel-chromium anodes.^{6,7} In addition to the initial 60 mV loss with 10 ppm H_2S , cells using nickel anodes show a continuous decay (Figure 2). In similar tests, however, cobalt-containing anodes were more stable, as would be expected from thermodynamic calculations. The ratio of $\text{H}_2\text{S}/\text{H}_2$ required for sulfide formation is 5.0×10^{-3} for cobalt and 1.8×10^{-3} for nickel.
- Screening tests showed that magnesium-doped lanthanum chromite ($\text{Mg}_{0.05}\text{La}_{0.95}\text{CrO}_3$) can tolerate significantly higher concentrations of sulfur (up to 1000 ppm).

Figure 2 -- Comparative Endurance of MCFC Using Cobalt and Nickel Anodes and Low-Btu Fuel Gases Containing 10 ppm H₂S at 650°C⁷

- The greater performance loss is due to a higher anode polarization, even when sulfur is introduced into the cathode.
- Half-cell electrochemical tests have shown the kinetics of anode reaction to be unaffected by H₂S in the anode feed gases up to a sulfur level of 50 ppm. The cause of the higher anode polarization observed in cell tests, therefore, may be related to changes in mass transfer characteristics of the sulfur-contaminated melts and/or to structural changes in the electrode.^{7,8}
- The effect of COS in low-Btu fuel on the cell performance at 650°C is similar to that of H₂S (47 mV loss with 5 ppm COS in low Btu-fuel at 160 mA/cm²).
- The cell performance loss due to H₂S/COS (<10 ppm) contaminant can be recovered completely after the removal of H₂S/COS from the fuel (contamination exposure period up to two weeks).

- At higher cell temperatures (up to 700°C), the nickel-based anode appears to be more tolerant of sulfur contaminants than at 650°C, and more tolerant of H₂S than of COS.⁵
- The cell performance loss due to sulfur contamination increases sharply as the hydrogen level in the fuel decreases from 21% (inlet) to 4% (fuel outlet condition).
- The cell performance losses due to H₂S, COS, or SO₂ increase with the current density.^{4,5}
- The mechanism of anode performance loss from 1 to 10 ppm H₂S is attributed to absorption of sulfur species onto the nickel anode surface, reducing the concentration of available nickel surface sites for adsorption of hydrogen. The sulfur adsorption step appears to be coupled with a Faradaic effect the transport of sulfur-containing ions in the carbonate electrolyte. At large concentrations of H₂S (10 ppm) the sulfidation effect also becomes prominent, due particularly to the formation of a molten eutectic phase (Ni₃S₂).
- In the operation of a MCFC power plant, we recommend that sulfur contaminants in the fuel gas be reduced to low levels of less than 1 ppm and that SO₂ be completely removed from the spent fuel recycled to the cathode. An increase in nominal cell temperature from 650 to 700°C will increase the sulfur tolerance level, although other cell performance/endurance trade-offs need to be considered.

Cathode. Sulfur dioxide at the cathode is readily absorbed into the molten carbonate mixture present both at the porous nickel oxide cathode and within the tile, by the equilibrium reaction (M represents any metallic component):

The equilibrium constant for this reaction is very high (10^{15} to 10^{17}), and, hence, SO₂ absorption is almost quantitative. Data in the literature on the stability of NiO in the presence of SO₂ are very limited. The concentration of SO₂ required to form NiSO₄ is indicated to be around 120 ppm.⁹ In the ideal case, however, the porous NiO electrode is covered with a thin film of molten carbonate, a factor that

makes it difficult to predict readily the electrode material stability by directly extrapolating Ellingham-type plots.¹⁰

- Only small changes in cathode polarization are observed when SO₂-containing cathode feed gases are used up to a 50 ppm level.
- Sulfur species are transported from the cathode to the anode when SO₂-containing feed gases are used. This transport, coupled with the equilibrium existing between the carbonate and the feed gases at each electrode, results in a sharp concentration gradient of sulfur species in the electrolyte tile between the cathode and the anode. The average, or bulk concentration of sulfur species in the tile is low - less than 10⁻¹² mol fraction.
- An additional performance loss is caused by SO₂ in the oxidant (with simultaneous contamination in the fuel); the performance becomes unstable and shows a slow continuous decay. After exposure to 10 ppm SO₂ in the oxidant for 150 hours, losses are about 15 to 20 mV/ppm SO₂ at 160 mA/cm² and 650°C.

Electrolyte. The molten alkali carbonates readily convert to sulfates and sulfides in the presence of SO₂ at the cathode or H₂S at the anode. SEM-EDAX analysis of posttest electrolyte tiles show significant sulfur intake (Figure 3). The presence of sulfates in the tile may alter conductivity, coal gas solubility, and diffusivity properties, and will affect the electrolyte inventory in the electrodes.

A method of mixed potential analysis has been used by Townley et al. to explain an increase in cell overpotentials.¹¹ The following discussion deals with the sulfide/sulfate/carbonate equilibria and a mechanism to explain loss in cell performance due to compositional changes in the electrolyte. The important reactions for the system are those of sulfide, sulfite, and sulfate conversion of the carbonate:

Figure 3 -- Composite SEM and Sulfur Concentration Map of Anode + Tile Composite¹²

where M is 0.62 Li/0.38 K in most cases. The thermodynamic data required to evaluate the equilibrium for these reactions are known, except for the free energy of formation of M_2SO_4 $\{\Delta G_f (M_2SO_4)\}$, M_2SO_3 $\{\Delta G_f (M_2SO_3)\}$, and M_2S $\{\Delta G_f (M_2S)\}$, and the activities of the species in the melt. These values were determined experimentally.⁸

Using experimental values, known thermodynamic data, and the equations:

$$\Delta G_{\text{reaction (2)}} = -RT \ln \frac{[M_2S] P_{H_2O} P_{CO_2}}{[M_2CO_3] P_{H_2S}} \quad (5)$$

$$\Delta G_{\text{reaction (3)}} = -RT \ln \frac{[M_2SO_3] P_{H_2}^3 P_{CO_2}}{[M_2CO_3] P_{H_2S} P_{H_2O}^2} \quad (6)$$

$$\Delta G_{\text{reaction (4)}} = -RT \ln \frac{[M_2SO_4] P_{H_2}^4 P_{CO_2}}{[M_2CO_3] P_{H_2S} P_{H_2O}^3}, \quad (7)$$

we calculated effective ΔG_f . Bracketed terms represent component activities. These data can then be manipulated to map a concentration profile of M_2S and M_2SO_4 from fuel inlet to outlet (Figure 4). The results indicate that the conversion of carbonate to sulfate and other as yet unidentified sulfur compounds occurs to a considerable degree with relatively low H_2S levels in the fuel, particularly near the cell exit. The sulfation, however, has not been shown to be the only mechanism causing loss of performance. A likely possibility remains that adsorption of sulfur compounds formed concurrently with the sulfate, e.g., thionates, thionites, thiosulfates, and thiocarbonates, contributes to the problem.

Although the situation at the anode is not completely clear, the reactions of SO_2 at the cathode are straightforward. The equilibrium constant for the family of reactions represented by

is 10^{15} to 10^{17} , depending on the data source and identity of the cations. From this result it is clear that in a system where the fuel exhaust is burned and fed into the cathode stream to provide CO_2 , essentially all of the sulfur will be scrubbed by the cell, depending on the cell's mass transport limitation. Molten carbonate cells can tolerate some level of sulfur in the fuel gas if the effect of the sulfur compounds on the electrode performance is small, since the percentage of electrolyte conversion at low fuel sulfur levels is not large, as shown in Figure 5. In addition, the sulfur could be removed from the cells periodically by purging the anode side at open circuit reversible losses only.⁴

Bipolar Hardware. The effect of sulfur on the anode or cathode current collector has been studied in both in-cell and out-of-cell tests. Very high corrosion rates were observed with Type 316 stainless steel anode current collectors with 10 ppm sulfur-containing gases.

The data in Table 6 show that the corrosion of the cathode current collector is virtually unaffected by cathode gases containing SO_2 . On the other hand, because of the transport of sulfur through the tile, the corrosion of the anode increases by 66% when these same SO_2 -containing cathode gases are used in conjunction with clean anode fuels. When clean cathode gases are used with sulfur-containing fuel gases, the corrosion of the anode current collector is even more severe, and the cathode current collector is virtually unaffected.

Figure 4 -- Approximate Concentration of S and SO_4 Predicted across a Subscale M/C Cell

Figure 5 -- Rate of Carbonate Conversion by H_2S (SO_2) at Design Current Density and Utilization

Table 6

THICKNESS OF OXIDE SCALES ON TYPE 316 SS
CURRENT COLLECTOR MATERIALS AT 650°C

Cell No.	Anode			Cathode		
	Gas Side	Electrode Side	Total	Gas Side	Electrode Side	Total
EPRI-3, μm *	5	30	35	5	10	15
EPRI-7, μm **	28	30	58	10	10	20

*Cell operated 1562 hours under sulfur-free gases with reformed natural gas fuel.

**Cell operated 1104 hours total, 620 hours with a 50 ppm SO_2 oxidant flowing (low-Btu fuel used for 240 hours, high-Btu for 380 hours).

Screening studies to evaluate other candidate materials for bipolar hardware showed that Types 446, 410, and 310 stainless steels have better initial corrosion resistance than the standard Type 316 stainless steel used in all cell testing. Longer-term testing of these materials in laboratory cells is required to verify these initial trends.

2.3.1.2 Halogen Compounds

Hydrogen chloride and HF are known catalyst poisons expected to be present in the coal gas; HCl is a known promoter of stress-corrosion cracking. The effects of exposure to these contaminants on various fuel cell components are described below.

Anode. Nickel is highly resistant to chloride formation, so no immediate performance degradation for the anode can be expected.³ This assumption was confirmed by short-term tests with HCl concentrations from 10 to 100 ppm (Table 7). No significant corrosion was observed on the nickel anode or wet seal area. With an HCl level of 100 ppm, however, a slight corrosion of stainless steel hardware at the anode exit was observed. While HCl up to 100 ppm poses no apparent

serious problem during short-term tests, long-term trends have yet to be established.

Cathode. The effect of HCl in the oxidant stream has been found to be catastrophic.¹³ With 100 ppm HCl in the cathode gas, the power output of a cell decreased by more than 70% during 300 hours of test duration. This decrease was accompanied by deterioration and buildup of corrosion products in several areas of the cathode compartment. The corrosion was very extensive at the inlet side of the cathode chamber. The stainless steel current collector, along with the entire stainless steel cathode chamber, had experienced severe corrosion. The nickel oxide cathode showed a loss of structural integrity, along with signs of changes in morphology.

Tile. Hydrogen chloride can be expected to react with the alkali carbonates, converting a portion of the electrolyte to a chloride. Out-of-cell tests with electrolyte tiles exposed to 100 ppm HCl did show chlorine take-up (Table 8). The chlorine take-up was significantly higher with the low-Btu fuel than with the standard oxidant containing air-CO₂. The chlorination of tile occurring under anode conditions can significantly affect cell performance during long-term operation. TRW analysis shows that for a HCl level of less than 1 ppm, the activity of HCl is below the threshold for formation of chloride from carbonates.³ Thus, by setting the maximum allowable HCl concentration below 1 ppm, long-term chemical degradation of the electrolyte can be eliminated. A similar analysis for HF showed a maximum allowable concentration limit of 100 ppm.

2.3.1.3 Mechanisms to Explain Loss in Performance

The main effect of HCl on cell performance comes from its presence in the cathode gas. Four major reactions may be causing this loss in performance. The first involves take-up of the chlorine by the tile by the reaction:

Table 7

EFFECTS OF EXPOSURE TO HCl ON MCFC PERFORMANCE¹³

Conc. of HCl, ppm		Test Duration, hr	Comments
In Fuel	In Oxidant		
10	-	500	<ul style="list-style-type: none"> • No decay in cell performance • Presence of HCl, LiCl and LiAlOCl₂ in the tile
-	10	120	<ul style="list-style-type: none"> • No deterioration in cell performance
75	10	120	<ul style="list-style-type: none"> • No deterioration in cell performance
100	100	250	<ul style="list-style-type: none"> • Rapid and steady decay in cell performance • Severe corrosion of cathode hardware

Table 8

CHLORINE TAKE-UP BY ELECTROLYTE TILES¹³

Gas Atmosphere	Electrolyte Tile Exposed to		Chlorine Take-up by Electrolyte Tile, wt%
	HCl Conc., ppm	Test Duration, hr	
Low Btu	100	30	6
Std. Oxidant Air/CO ₂	100	58	3

Although no thermodynamic data are available at present for the eutectic melts, substantial take-up of the chlorine by the electrolyte would result in a change in cell potential caused by the difference in activity of the carbonate at the two electrodes. Since no such difference was apparent, either the eutectic reactions are closer to the Li_2CO_3 chlorination reaction

than to reaction 9, or the chlorine was taken up by the hardware prior to contacting the electrolyte. Analysis of the tile for chlorine was not reported.

The second possible effect of HCl at the cathode is chlorination of the stainless steel by the reaction:

For an oxidant containing 15% oxygen it would take only 0.2 ppm HCl to cause chlorination of the stainless steel, well below the 100 ppm value used.

The third possible reaction of HCl at the cathode is chlorination of the nickel oxide by:

For the cathode operating on an oxidant gas containing 2.2% H_2O , it would require an HCl concentration of 23%, far above the 100 ppm HCl employed.

A final possible reaction of the HCl at the cathode is the formation of FeOCl by the reaction:

For the standard cathode gas composition (70% air, 30% CO_2) this would require a chloride concentration greater than 10^{-15} .

Thus, chlorination of the stainless steel and chloride formation in the tile are possible causes of the catastrophic effect of HCl in the cathode gas. We do not know at this time which mechanisms are responsible for this performance decay.

2.3.1.4 Nitrogen Compounds

Molecular nitrogen at the anode or cathode acts as a diluent. It can also be present as ammonia at the anode and as NO_x at the cathode. No experimental data on the effect of these impurities on cell performance are available. Ammonia may tend to increase the volatility of carbonates, thereby increasing the evaporative losses of electrolyte. At normal fuel cell operating temperatures, however, the nickel anode should promote decomposition of ammonia to N_2 and H_2 , with the H_2 being removed by electrochemical oxidation.¹⁴

The concentration of NO_x at the cathode depends upon the type of product exchange device, particularly the combustor. The $\text{K}_2\text{CO}_3/\text{Li}_2\text{CO}_3/\text{Na}_2\text{CO}_3$ eutectic is known to absorb NO ,¹⁵ but catalytic combustors employing platinum do not introduce a significant amount of NO_x if a large excess of oxygen is not present.

If any NO_x is present, it can react with the electrolyte to form the alkali nitrate. For example:

Equilibrium considerations indicate that at the MCFC operating temperature of 650°C , there will be no loss of electrolyte by nitrate

formation from NO_2 if the NO_2 concentration is below 15 ppb by volume.³ Note, however, that the presence of NO_x depends on the operation of the power production section and not on the feed fuel gas.

2.3.1.5 Metals and Trace Elements

While more than 20 trace elements are consistently detected in coal gas,¹⁶ no experimental data are available on their possible effects on the catalytic activity and/or stability of MCFC components. Some understanding, however, can be derived from thermodynamic considerations and analogy with operating limits of methanation catalysts. A brief description of theoretical analyses available in the literature is presented in this section. In Section 3, a model is derived from these thermodynamic considerations.

The metallic compounds, if absorbed at the electrode surface, can make the electrode an insulator or a semiconductor, adversely influencing the ohmic overpotential of the fuel cell. In the reduced form many of the trace metals would also degrade performance of the electrode for the oxidation of fuel ($\text{H}_2 + \text{CO}$) and for the reduction of the oxidant CO_2 , because these metals have a higher activation barrier than Ni or NiO for various electrode reactions, not because they are poor conductors.¹⁷

Out of various trace elements present in coal gas, a study of five potentially detrimental contaminants on electrolytes and electrode materials is available.¹⁷ These contaminants are cadmium, lead, titanium, mercury, and tin. Some of their thermodynamically stable forms in the effluent streams of gasifiers are CdS , PbS , TiO_2 , Hg/HgS , and $\text{Sn/SnCl}_2/\text{SnCl}_4$, respectively. The effects of these compounds and of some other metal compounds on fuel cell anode, cathode, and electrolyte are presented below.

Anode. Possible electron transfer reactions of trace contaminants with the anode nickel, along with their free energy of reaction, are presented in Table 9. We can see that reactions 15, 18,

20, and 21 are thermodynamically favored. The results of these reactions would be the deposition of the metallic tin [reaction (15)], coating the electrode surface with sulfides [reactions (18) and (20)], or the dissolution of the anode into the solution [reaction (21)]. While all these reactions would be detrimental to the electrode operation, the reaction with HgS [reaction (18)] seems particularly damaging to the electrode surface. As pointed out earlier, reactions (15), (18), and (20) would reduce the electrode activity by blocking the approach of H₂ molecules to the anode (catalyst poisoning) through formation of thin films, by making the electrode either a semiconductor or an insulator (NiS films) or by raising an activation barrier for an electrode reaction (Sn and Hg films). The NiS film will increase the ohmic loss whether it is a semiconductor or an insulator. The formation of tin films will lower the exchange current density for the hydrogen

Table 9

POSSIBLE ELECTRON TRANSFER REACTIONS OF TRACE CONTAMINANTS WITH ANODE¹⁷

oxidation by at least four orders of magnitude; the mercury film will lower the oxidation efficiency by about seven orders of magnitude.¹⁸

Arsenic can be present in the fuel gas as the element or as AsH₃. The hydride, which is stabilized by the presence of hydrogen and is decomposed by hot water vapor,³ can deactivate the anode by decomposing on the nickel. The decomposition would be highly favored at anode outlet conditions, where the H₂O/H₂ ratio is the highest. The maximum

limit of arsenic at the anode can be obtained by the equilibrium consideration of the following reaction:

This limit is 0.05 ppm by volume $\text{AsH}_3(\text{g})$ in the feed fuel gas.

Selenium and tellurium from the sulfur group exhibit similar catalyst poisoning behavior. They may be present as hydrides in the feed gas (H_2Se and H_2Te). The limiting concentrations for these elements were estimated by analogy to sulfur, assuming that selenium and tellurium will degrade the performance of the nickel anode through chemisorbed H_2Se and H_2Te , leading to formation of NiSe and NiTe . Based on limited thermodynamic data, the TRW study¹⁷ estimated 80 ppm by volume for both H_2Se and H_2Te as maximum allowable limits.

Mercury may be absorbed with the nickel anode to form amalgam, i.e.,

The ΔG^0 value for this reaction was estimated to be -38 kcal/mol at 900 K. This number indicates that the absorption process of mercury at the nickel surface is essentially encounter controlled.

Cathode. The elemental contaminants tin and mercury can undergo electron transfer-type reactions with the NiO -cathode as follows:

Of these two reactions, only reaction (24) appears to be important, if there are not any physical interactions. The effect of the resulting SnO_2 film is unknown. When heavily doped, n-SnO_2 is a good semiconductor with a high oxygen overpotential. Also, since the nickel oxide is of a p-type and SnO_2 is of an n-type, a power loss due to the p-n junction formation is possible.³

At the cathode, where negatively charged atoms are exchanged, simple exchange reactions appear to be more important. These reactions are illustrated in Table 10.

Table 10

SIMPLE EXCHANGE REACTIONS OF TRACE CONTAMINANTS WITH CATHODE

As we can see from free energy values, only the last three reactions in Table 10 are important. Again, these reactions will cause either the dissolution of the electrode material [reactions (28) and (30)] or the formation of the NiS film on the cathode [reaction (29)]. The reaction with TiO_2 has not been considered, since the only effect would be the exchange of oxygen atoms.

At the cathode, out of various contaminants only Sn(IV) is expected to be reduced to Sn(II) . This Sn(II) may dissolve and accumulate in the electrolyte solution.

Electrolyte. Possible reactions of the contaminants with the electrolyte, along with their free energy changes, are listed in Table 11.

Table 11

POSSIBLE REACTIONS OF THE TRACE CONTAMINANTS WITH THE ELECTROLYTE

As before, a similar reaction with TiO_2 is impossible. Also, no reactions of alkali cations with the contaminants were considered. Of the reactions listed in Table 11, reactions (34), (35), and (37) are important because of their large negative free energies. As we can see, the effect of these reactions on the electrolyte would be the loss of electrolyte and the introduction of a new ionic species (SO_4^{2-}) or a new phase (SnO_2). This could change physical properties such as viscosity and conductivity, leading to decreased cell performance.

2.3.1.6 Hydrocarbons

Hydrocarbons can deactivate electrodes or can lead to carbon formation under certain thermodynamic conditions. While no direct in-cell data are available, light hydrocarbons such as ethane, ethylene, propane, methanol, and benzene have been tested for deactivation of nickel methanation catalysts.¹⁹ For the light hydrocarbons at concentrations of 0.1 to 0.5 mol%, there was a depression of catalyst activity and indication that the nonolefinic compounds were reforming to CO and H_2 . For methanol at 0.1 to 1.0 mol%, there was no measured change in catalyst activity. There was an indication that the methanol was reformed to methane. For benzene at 1.0 mol%, catalyst activity was depressed with reforming to methane, carbon monoxide, and hydrogen. Carbon formation was observed at 5 mol% in the catalyst. If the methane is not reformed, fuel cell efficiency will decrease. Methane in small

quantities can be reformed by adding sufficient water to the fuel gas. Olefins require substantially more water to avoid carbon formation, but at low concentrations the effect is not assessed as a major additional water requirement.

The conclusion is that, at these moderate concentrations, light hydrocarbons, methanol, and benzene are not catalyst poisons. At most, they depress catalyst activity reversibly, and care must be taken to avoid carbon deposition and anode plugging.

2.3.1.7 Particulates

Coal gas may contain significant quantities of fine particulates. The pore diameter for the fuel cell porous nickel anode is likely to be between 5 and 10 μm . The smaller particles ($<5 \mu\text{m}$) would then be able to diffuse into the pores and eventually lead to partial plugging. No experimental data on particle settling rates and active site coverage are available.

The application of coal gas for methanation also poses similar problems. The particulate concentration level for the methanation application, however, is not known quantitatively. The multiple-stage liquid scrubbing actions used in conventional low-temperature processes for quenching and acid-gas removal are estimated to reduce the particulate concentration to low levels. Westinghouse has estimated that a total particulate loading of $8.5 \text{ lb}/10^6 \text{ ft}^3$, all below $1.0 \mu\text{m}$, is achievable for a Selexol desulfurization system.²⁰ For the combined-cycle application another engineering estimate of $0.8 \text{ lb}/10^6 \text{ ft}^3$ has been proposed, with all particles smaller than $2 \mu\text{m}$.

The concern is that the safe operating particulate concentration level for fuel cell applications may be very low, as for the methanation application. We have explored this subject in depth and discuss it in Section 3 of this report.

2.4 GAS CLEANUP SYSTEMS

This subsection presents a comprehensive list of cold and hot gas cleanup systems. Cleanup systems mentioned by General Electric and United Technologies, Inc., in their reports for the DOE MCFC power plant technology development program are included. The list provides the following information from sources in the public domain:

- State of commercial development
- Operation characteristics
- Environmental effluents
- Waste-product or recycle requirements
- Form in which sulfur is rejected
- Contaminants in the effluent streams
- Thermal efficiency
- Utility requirements
- Reliability.

Typical modes of occurrence of trace and minor elements in coal are identified, where such data are available,* and qualitative results from coal-fired power plants are reviewed. The concept of efficiency, as applied to the cleanup system's ability to remove sulfur, is also discussed. Finally, the entrainment and vaporization losses of the gas cleanup solvent are considered. Fuel gas cleanup systems for MCFC application are characterized by their principal duty: desulfurization. Ancillary gas cleanup equipment for control of particulates and of trace elements, such as chlorine and heavy metals, will be added as required.

* N/A (not available) is used wherever the required information could not be obtained within the time available constraints imposed on this task.

2.4.1 Cold Gas Cleanup Systems

2.4.1.1 Background

Gas cleanup systems required for gases used in MCFC must be able to remove sulfur compounds [(H_2S) and (COS) in coal gas] to 0.1 ppm. Current systems are capable of reducing the H_2S concentration only to less than 1 ppm. Carbonyl sulfide, which is more difficult to absorb than H_2S , must be catalytically converted to H_2S before it enters the gas cleanup system. Zinc oxide sorbents are used downstream of the system and reduce the balance of the sulfur concentration to below 0.1 ppm. Although many systems do not absorb COS, both Rectisol and Benfield HiPure claim to absorb both H_2S and COS to low concentrations. Along with sulfur, there are other potentially harmful contaminants in the untreated gas. These are the trace elements, alkali metals, nitrogen oxide formers, and halides. Table 12 lists the potential concentrations of the untreated effluents of Illinois No. 6 coal.

Ammonia, often found in large quantities in coke-oven gas and in low-temperature gasification, is usually removed by scrubbing it with water. Higher volumes of water and higher pressures lead to increased ammonia removal but at the same time to costlier operation. The gas scrubbing system is suitable for removing ammonia. Partially removed from the raw gas, also, are HCN and HCl , which easily form aqueous solutions when contacted with water.

2.4.1.2 Characteristics

TRW Study of Trace Elements. Those trace elements that occur in coal are given in Table 13. Modes of occurrence are common associations rather than exact compounds.

Little quantitative work has been done on trace elements in coal gas. First attempts to follow trace elements in HyGas and Synthane bench-scale tests found imbalances in following the elements and

Table 12
ESTIMATED POTENTIAL CONSTITUENTS IN UNTREATED FUEL GAS²¹
(Illinois No. 6 Coal)

<u>Constituent</u>	<u>Notes</u>	<u>(lb/10⁶/Btu)</u>
Ammonia	b,f	0.99
Antimony		0.00003
Arsenic	b,e,f	0.0015
Beryllium	b,c	0.00002
Boron		0.0017
Cadmium	b,e,f,k	0.00004
Chlorine	b,e,f	0.17
Chromium	b,e,f	--
Fluorine	b,d,e,f	0.0005
Lead	b,e,f	0.0003
Mercury	b,c,e,f,g	0.000009
Nickel	b,f	0.0003
Potassium		0.059
Selenium	b,e,f	0.0008
Sodium		0.0064
Sulfur	a,b,d,e,f	3.02
Titanium		0.0058
Vanadium		0.0004
Zinc	b,e,f	0.0004

NOTES: Federal Regulations Applying Quantitative Limitations to
Potential Environmental Pollutants

- a. National Primary and Secondary Ambient Air Quality Standards
- b. Occupational Safety and Health Administration Standards for Air Contaminants
- c. National Emission Standards for Hazardous Air Pollutants
- d. New Stationary Source Performance Standards
- e. National Interim Primary Drinking Water Regulations
Supplement: 1962 Public Health Service Regulations on Drinking Water
- f. EPA Effluent Standards
- g. Criteria for the Evaluation of Permit Applications for Ocean Dumping of Materials

produced unreliable data. In these tests all the effluent streams usually were analyzed for trace compounds and were compared to the feed coal. Other attempts at analysis have been made at the University of North Dakota and at the No. 13 Lurgi gasifier of the Sasolburg plant, but because of private funding, information was not made available. TRW's study of trace elements in gasifier ash, oil, tar, and quench liquor obtained data reported to be slightly better than that from Synthane bench-scale tests.³ Other experimental data from industrial-sized gasifiers were available from the Lurgi fixed-bed gasifier at Sasolburg, South Africa, using South African subbituminous coal, and the Lurgi dry bottom gasifier in Westfield, U.K., using Illinois Nos. 5 and 6. Radian Corporation also released limited experimental data from samples of gasifier ash, cyclone dust, by-product tar, and quench liquor from an atmospheric fixed-bed gasifier. No published data exist on trace elements for entrained-bed and molten-salt coal gasification.

A number of studies have been performed on the behavior of trace elements of coal-fired power plants. These studies divide the elements into three groups, depending on distribution among bottom ash, fly ash, and combustion flue gas.

Group I. Elements in this group form compounds with very high boiling points and are not volatilized in the combustion zone [(1315-1593°C (2400-2900°F)]. Concentrations of these elements in the fly ash tend to equal the concentrations in the bottom ash. Elements in this group are Al, Ba, Ca, Eu, Fe, Hf, K, La, Mg, Mn, Rd, Sc, Si, Sn, Tu, Th, and Ti.

Group II. These elements tend to volatilize in the combustion zone and condense on the fly ash as it cools. Concentrations in the fly ash are several times greater than in the main ash flow. Elements in this group are As, Cd, Cu, Ga, Mo, Pb, Sb, Se, and Zn.

Group III. These elements volatilize and remain in the gas phase. Elements in this group include Br, Cl, F, Hg, and, in some compounds, Se.

Table 13
TYPICAL MODES OF OCCURRENCE OF TRACE AND MINOR ELEMENTS IN COAL

<u>Element</u>		<u>Element</u>	
Sb	Sulfide	Mo	Sulfide
As	Oxide, sulfide	Ni	Sulfide
Ba	Carbonate, sulfate with Ca	N	OC
Be	OC	K	KCl, carbonate
Bi	Sulfide	Sm	SQ
B	OC, borate	Sc	Oxide
Cd	Sulfide	Se	POC, sulfide, iron selenides
Ca	Oxide, carbonate, sulfate	Si	Oxide, SQ
Cl	POC, sodium chloride	Ag	Element, sulfide, Sq
Cr	POC, oxide	Na	POC, carbonate
Co	POC, sulfide	Sr	POC, with Ca
Cu	CuFeS ₂ , sulfide	S	POC, sulfides, sulfates
F	CaF ₂	Te	Iron tellurides
Ge	POC, carbonate	Th	SQ
Fe	Carbonate, sulfide oxide	Sn	Carbonate, sulfide
Pb	Sulfide	Ti	POC, SQ
Li	SQ	V	OC
Mg	POC, carbonate, SQ	Yb	SQ
Mn	Carbonate in CaCO ₃ , SO	Zn	Sulfide
Hg	POC, element sulfide	Zr	Oxide, SQ

** OC - Organic contribution.
POC - partial organic contribution.
SQ - silicates, clay, quartz.

Characteristics intermediate between Groups I and II include Be, Cr, Cs, Na, Ni, U, and V, and are found only slightly concentrated in fly ash.

TRW's study developed a qualitative rationale to identify elements consistently appearing in product raw gas. If an element appearing as 10% or more of the amount in coal feed or recovered in effluents such as ash in the raw gas is found in more than 50% of the cases studied for that element, then that element is identified as one consistently appearing in the gas. These elements are As, B, Be, Cd, Ce, Cl, F, Ge, Hg, Mo, Pb, S, Sb, Se, Te, Ti, V, Zn, and Zr. Not considered, however, were elements that did not meet the criteria but are in large concentrations in the feed coal. These elements would end up with concentrations of 50 ppm or more in the raw gas. Those elements consistently identified are Al, Ca, Fe, Mg, Na, and S. A second group not identified by the original criteria but which would also provide 50 ppm or more in the raw gas are B, Cl, F, K, Te, Ti, V, Zn, and Zr.

The two groups found consistently in the data combined would then be likely to be present in the gasifier gas. Most of the elements form nonvolatile compounds and would be caught by the wet scrubbing system. Only volatile, water-insoluble compounds such as As, B, Ge, Se, and Te should be present in the cleaned gas.

Particulates that usually carry trace elements also may cause plugging in the fuel cell. Removal devices such as Venturi and packed-bed scrubbers are found to be efficient and to have low exit dust loadings, which may or may not affect operations. Figure 6 shows the effect of scrubbing devices in cold gas cleanup processes. Hydrophobic dust particles, such as soot, are usually not removed effectively by these devices.

2.4.1.3 Efficiency

Efficiency applies to the cleanup system's ability to remove sulfur compounds and to conserve energy during sulfur removal operation.

To define efficiency, using published operating data of the various cleanup systems, we used a simple ratio of sulfur removed to energy used. The units of the ratio are kilograms of sulfur removed per an arbitrary unit of power. The unit of power equals the steam consumption, expressed in kWh, plus the kWh of electrical power (both converted to a factor by multiplying by 0.04).

After the ratios were found, each system was compared with other systems of the same amount of feed gas sulfur (see Table 14). The comparison demonstrates that the ratio increases for increasing acid gas concentration and that, except for the Stretford Process which is completely selective towards H_2S , low acid gas concentrations give low ratios. Obviously, the higher the ratio, the better the sulfur removal efficiency. These results can be misleading, however, since it is at low concentration that absorption becomes difficult. A low level sulfur concentration in the feed gas will require more power per kilogram sulfur than high concentrations. For this reason, in Table 14 the various systems grouped have been by progressively increasing sulfur concentration for equivalence of comparison.

In consideration of the above information, when we compare cold gas cleanup systems the sulfur concentrations in each feed gas must be close to each other. Of course, the system's selectivity towards H_2S would also play an important part in efficiency since there is no mention of CO_2 in efficiency. The purpose of this exercise is to rank the cleanup systems approximately by their ability to remove sulfur with the least power consumption.

2.4.1.4 Entrainment and Vaporization

Final consideration in cold gas cleanup is the entrainment and vaporization loss of the solvent. Such loss can be minimized by several different methods, e.g., washing with water. The method used on most acid gas absorbers consists of washing the gas in the top section of the absorber. The wash water is transported to the regenerator with the

Case A

Case B

Figure 6 - Projected Particle Size Distribution at Various Stages in the Cold Gas Cleanup Process

Table 14
DESULFURIZATION EFFICIENCY OF CLEANUP SYSTEMS

	<u>Ratio</u>	<u>H₂S, % in feed gas</u>
MDEA	4	0.6
Alkazid "DIK"	3	0.7
Selexol	6	0.5
Rectisol	16	1.0
Stretford	82	1.0
MEA	2	1.7
Sulfinol	11	1.6
Purisol	96	6
ADIP	28	10
Estasolvan	195	10
DEA	15	15
Benfield Hi Pure	58	15

rich solvent and can subsequently be converted to steam and used to de-absorb gases. The washing can also take place in a separate wash tower. Vaporized absorbents also can be recovered by absorption on bauxite or similar solids, followed by steam conditioning to recover the solvent.

2.4.1.5 Approach

Cold gas cleanup systems have been selected for this study by virtue of their ability to remove sulfur compounds from feed gas streams. Acceptable systems are assumed to have the following characteristics:

- The ability to produce a Claus quality acid gas or elemental sulfur
- Established commercial acceptability
- Ability to reduce H₂S and COS levels to 1 ppm total.

Five categories of cold gas cleanup systems were established in this study. The categories are defined in the following manner:

- Absorption by chemical reaction with ethanolamines
- Absorption by chemical reaction with alkaline salts

- Physical absorption by organic solvents or methanol
- Both physical absorption by solvent and chemical absorption by ethanolamines
- Direct liquid phase oxidation of H_2S to elemental sulfur.

Category 1, ethanolamines, includes the MEA, DEA, SNPA-DEA, DGA, DIPA (Adip), and MDEA systems. The first system, MEA, is a primary amine and the most reactive of the ethanolamine systems. DEA, SNPA-DEA, DGA, and DIPA are secondary amines, and MDEA is a tertiary amine. A basic sketch of an ethanolamine system is shown in Figure 7. As mentioned above, the primary amines are the most reactive, a disadvantage in selectivity for H_2S and CO_2 . The primary amines react directly with CO_2 . Secondary amines react more slowly but undergo reactions similar to those of MEA, and tertiary amines absorb CO_2 much more slowly in a series of complicated reaction steps. In regeneration the most reactive amines tend to require more energy to reverse the reactions and desorb H_2S and CO_2 . Also, some ethanolamine systems react irreversibly with COS, CS_2 , or HCN. In addition, other losses can occur through evaporation. Corrosion occurs in places of high acid gas concentration. A highly reactive amine, therefore, tends to be more corrosive because the acid gases are held longer through incomplete stripping. The degree of amine tends to rule the reactivity, or selectivity, for H_2S , corrosion, and steam consumption in the stripper.

Category 2 covers the alkaline salt absorption medium, also illustrated by Figure 7. The most commonly used are the potassium carbonate systems, although some use activators plus amine systems to enhance H_2S removal. Generally, these systems were developed to remove CO_2 from synthesis gases but, owing to the alkaline nature of the salts, were found to remove H_2S . The ability to absorb H_2S and CO_2 , a diminished corrosiveness to carbon steel, and lower steam consumption depend on proprietary advancements made by developers of alkaline salt systems.

Category 3 covers physical absorption, which includes the Estasolvent, Fluor Solvent, Purisol, Rectisol, and Selexol systems (see Figure 8). Unlike the chemical absorption systems, where the

Figure 7 -- Chemical Absorption

L.P. Flash and Recompression

Figure 8 - Physical Absorption

circulation rate depends on the number of moles of acid gases in the feed stream, physical absorbents rely on the partial pressures of the acid gases. A physical solvent, therefore, is used best at high pressure and usually is ineffective at low pressures. Since little absorption takes place at low pressures, to desorb acid gases usually requires only low pressure flashing or inert gas stripping. If high purity is required, however, steam stripping may be used, but usually much less than in chemical absorption systems. Because absorption is physical, in some systems hydrocarbons, including H_2 and CO , become coabsorbed with the acid gases, requiring intermediate flashing to release hydrocarbons. Aromatics are sometimes retained and come out in the stripped gases. A special filter may be needed to remove hydrocarbons from recovered acid gases that enter sulfur recovery systems. Physical solvents are usually more selective than chemical absorption and can absorb H_2S and leave CO_2 in the feed gas. Many other impurities are generally absorbed by physical systems.

The physical absorption system usually operates at high pressures and low temperatures (substantially lower than ambient, subzero), and if high purity of the purified gas stream is not required, the absorbent can be regenerated by flashing solvent at low pressure.

Category 4 describes the Amisol and Sulfinol systems. These are both physical and chemical absorption systems and add flexibility to operating conditions. Of course, disadvantages such as higher utility consumption than in physical absorption and higher hydrocarbon losses than in pure amine systems occur. The basic flow for these systems is similar to that in Figure 7.

Cleanup systems in Category 5 include Stretford, Giammarco-Vetrocoke, Perox, Konox, Takahax. A basic sketch is shown in Figure 9. These systems absorb and directly oxidize H_2S to elemental sulfur by an agent that can be reoxidized by air. The sulfur product usually is processed within the system. Operating conditions are close to ambient temperature and atmospheric pressure. The systems mainly produce small

amounts of sulfur, which can be sold or thrown away. For comparison, a Claus plant produces in the range of 500 tons per day of sulfur in a single train, whereas the largest Stretford process in the United States produces 30 tons per day in a single train. These direct oxidation systems are highly selective for H_2S , and their solutions react with other impurities, such as HCN. Hydrogen sulfide can be reduced to a low level, less than 1 ppm, but the Category 5 systems do not efficiently remove COS. Table 15 summarizes the cold gas systems accepted for compilation. A detailed compilation appears as Appendix B of Reference 2.

2.4.1.6 Rejected Systems

Cold Gas Cleanup Systems. Several cold gas cleanup systems under study either have not demonstrated previously listed acceptable characteristics or have been found to be obsolete. These systems are listed below, with a brief description of those qualities found to be undesirable.

Burkheiser uses ammonia, iron oxide, and elemental sulfur to oxidize H_2S to elemental sulfur. The process is complicated and operates at atmospheric pressure, which is incompatible with MCFC.

Fischer Alkaline uses an aqueous solution of 20% potassium ferrocyanide and 6% potassium bicarbonate. The solution undergoes electrolysis, converting the ferrocyanide to ferricyanide, which, in turn, reacts with H_2S to form elemental sulfur. Approximately $2.1 \times 10^{-3} \text{ m}^3/\text{s}$ (2000 gal/hr) are circulated to treat feed gas of $2830 \text{ m}^3/\text{hr}$ (100,000 ft^3/hr) containing $62 \text{ g}/\text{m}^3$ (175 gr/100 scf) of H_2S , and electric consumption of 4.0 kWh/kg (1.8 kWh/lb), which is about double that theoretically required. Rather high electric consumption occurs in the process, but only limited information is available.

Ferrox uses a solution usually consisting of 3% sodium carbonate and 0.5% ferric hydroxide to oxidize H_2S to element sulfur. The sulfur product contains salt that must be continuously replenished.

Figure 9 -- Direct Liquid Phase Oxidation

Table 15

COLD GAS CLEANUP SYSTEM SUMMARY

Dwg. 5599C22

Name, Absorbent	Type of Absorption	Temp. °C (°F)	Pressure, kPa (psig)	Typical Feed and/Exit Gas Contaminants	Typical Utilities	Commercial Status	Remarks
Category One, Amines							
MEA Monoethanolamine	Chemical	27 - 43 (80-110)	0-6980 (0-1000)	In-H ₂ S 1.7%; 20 ppm HCN CO ₂ 9.7% 300 ppm COS Out-2 ppm H ₂ S CO ₂ 0.1% COS in ppm range	Steam 0.83 kg/scm (49,000 lb/10 ⁶ scf) CW 0.023 m ³ /scm (161,000 gal/10 ⁶ scf) Power 0.67 × 10 ⁴ J/scm (50 kWh/10 ⁶ scf)	Refineries; Natural gas excluding COS; commercial	COS reacts irreversibly; also O ₂ and CO ₂ degrade solution; corrosion, foaming and vaporization losses occur; redistiller required, resulting in sludge needing disposal that includes thiocyanates and thiosulfates.
DEA Diethanolamine	Chemical	38 - 54 (100-130)	0-6980 (0-1000)	In-H ₂ S 15%, 300 ppm COS, CO ₂ 10%; 600 ppm CS ₂ Out-4.5 ppm H ₂ S; 25 ppm CO ₂ COS ppm level	Steam 1.07 kg/scm (62,000 lb/10 ⁶ scf)	Natural gas containing COS; commercial	Reacts irreversibly with O ₂ and CO ₂ which can be treated with carbon absorption; slightly higher solvent costs than MEA.
SNPA-DEA Diethanolamine	Chemical	32-49 (90-120)	3538-7668 (500-1100)	In-H ₂ S 16.5% CO ₂ 8.0% Out-4 ppm H ₂ S	(5234 kg Steam/ m ³ Solvent) 44 lb. steam/ gal solvent)	Natural gas; commercial	Higher concentrations of DEA resulting in reduced recirculation rates; higher corrosion than DEA; nonfoaming utilities are the same as for MEA but actually are lower because of decreased circulation.
Fluor Econamine Diglycolamine	Chemical	32-54 (90-130)	Not pressure sensitive	In-5% H ₂ S 5% CO ₂ Out-4 ppm H ₂ S 0.01% CO ₂	Steam 0.51 kg/scm (30,000 lb/10 ⁶ scf)	Hysas; pilot plant	Vacuum distillation required, corrosive to carbon steel; need hydrocarbon flash tank; with up to 65% DGA in solution reduces circulation rate, thus permitting smaller equipment; high solvent cost.
ADIP Di-isopropanolamine	Chemical	38-60 (100-140)	0-6980 (0-1000)	In-H ₂ S-10% 2.5% CO ₂ Out-2 ppm H ₂ S 0.2% CO ₂	Steam 0.37 kg/scm (22,100 lb/10 ⁶ scf) Power 1.16 × 10 ⁴ J/scm (85 kWh/10 ⁶ scf)	Refinery gases and LPG; commercial	Usually treats refinery gases that include COS and H ₂ S/CO ₂ . The ratio of 10:1 is usually reduced to a H ₂ S level of less than 100 ppm; long residence times required for COS removal.
MOEA Methyldiethanolamine	Chemical	27-49 (80-120)	Not pressure sensitive	In-0.6% H ₂ S 10% CO ₂ Out-50 ppm H ₂ S 3.3% CO ₂	Steam 0.18 kg/scm (10,700 lb/10 ⁶ scf) Power 2.05 × 10 ³ J/scm (15 kWh/10 ⁶ scf) from DEA/MEA	Limited commercial applications; usually changed	Reacts irreversibly with HCN; corrosion & foaming occur; much higher solvent cost than MEA; low vapor pressure; requires redistiller with sludge disposal consisting of thiocyanates and thiosulfates.
Category Two, Alkali Salts							
Alkazid "DIK" Potassium Salt of Dimethylamino acetic acid Alkazid "M" Potassium Salt of methylaminopropionic acid	Chemical	21-38 (70-100)	0-6980 (0-1000)	In-0.7% H ₂ S 30% CO ₂ Out-5 ppm H ₂ S	Steam 0.26 kg/scm (15,300 lb/10 ⁶ scf) CW 0.013 m ³ /scm (93,500 gal/10 ⁶ scf) Power 3.14 × 10 ⁴ J/scm (230 kWh/10 ⁶ scf)	Commercial Overseas used in Coal Gasification	Very low vapor pressure, low pressure absorption yields H ₂ S 5 ppm, reported noncorrosive; if O ₂ or HCN present, waste sludge will be generated.

Table 15 (Cont'd)

Dwg. 5599C23

Name Absorbent	Type of Absorption	Temp. °C (°F)	Pressure kPa (psig)	Typical Feed and/Exit Gas Contaminants	Typical Utilities	Commercial Status	Remarks
Hot Pot Potassium Carbonate	Chemical	Up to 116 (240)	698-6980 (100-1000)			Obsolete Natural Gas Sweetening now uses Benfield	For bulk CO ₂ removal; acid gas concentration must be 5-8%; if H ₂ S to be low concentration, another absorber using MEA must be employed; H ₂ S/CO ₂ must be low; not good if Claus plant quality off-gas required
Benfield Hi Pure Potassium Carbonate, Amines & Activators	Chemical	Normal-110 (230) Max.-138 (280)	698-13,800 (100-2000)	In-1.5% H ₂ S 5.4% CO ₂ Out-2 ppm H ₂ S 0.01% CO ₂	Steam 0.66 kg/scm (38,200 lb/10 ⁶ scf) C.W. 0.004 m ³ /scm (30,000 gal/10 ⁶ scf) Power 1.00 × 10 ³ J/scm (735 kWh/10 ⁶ scf)	Synthane pilot plant Bureau of Mines Lurgi Scotland	No degradation of solvent by acid gases corrosion occurs; complex operation, two stage; COS shifted to H ₂ S in absorber
Catacarb Potassium Carbonate plus Amines & Activators <u>Category Three, Physical</u>	Chemical	Normal-110 (230) Max.-138 (280)	698-6980 (100-1000)	Proprietary	Proprietary	Over 80 plants installed; Commercial	Solution capacity increased by additives two stage absorber and cooling required for high purity
Estasolvon Tri-n-butylphosphate (TBP)	Physical	Ambient	6980 (1000)	In-10% H ₂ S; 150 ppm COS 7% CO ₂ Out-3 ppm H ₂ S; 2 ppm COS 6.4% CO ₂	Steam 0.036 kg/scm (2,100 lb/10 ⁶ scf) Power 6.0 × 10 ⁴ J/scm (440 kWh/10 ⁶ scf) C.W. 0.002 m ³ /scm (15,000 gal/10 ⁶ scf)	Pilot Plant	Low vapor pressure; no tendency to foam; COS has same solubility as H ₂ S; absorbs hydrocarbons; produces feed for Claus plant
Fluor Solvent Propylene Carbonate	Physical	-7-27 (20-80)	2800-13,800 (400-2000)	In-5-15% H ₂ S 10-30% CO ₂ Out-13 ppm H ₂ S 0.1% CO ₂		10 Commercial Plants; 7-N.G. 1-Ammonia 2-Hydrogen production	Absorbs hydrocarbons and water; becomes complex for high purity; feed gas must be dry; requires regeneration but only flash regeneration with bulk removal
Purisol M-Pyrol	Physical	29-41 (85-105)	6980 (1000)	In-6% H ₂ S 15% CO ₂ Out-2 ppm H ₂ S 13.6% CO ₂	Steam 0.053 kg/scm (3,125 lb/10 ⁶ scf) C.W. 0.002 m ³ /scm (13,300 gal/10 ⁶ scf) Power 3.60 × 10 ⁴ J/scm (264 kWh/10 ⁶ scf)	4 Commercial plants overseas	Low solvent vapor pressure; can use air for regeneration but requires heat for high removal efficiency; hydrocarbons are dissolved in solution; noncorrosive; nonfoaming
Rectisol Methanol	Physical	-73-18 (-100-0)	2100-13,800 (300-2000)	In-1% H ₂ S + COS 35% CO ₂ Out-0.1 ppm H ₂ S + COS; 0.1% CO ₂	Steam 0.043 kg/scm (2,550 lb/10 ⁶ scf) C.W. 0.017 m ³ /scm (121,600 gal/10 ⁶ scf) Power 7.5 × 10 ⁴ J/scm (550 kWh/10 ⁶ scf)	37 commercial operating plants; SASOL plant, S. Africa	More expensive for low-Btu gas; absorbs some H ₂ + CO and hydrocarbons; used when large amounts of impurities are present; removes NH ₃ and gum formers from coal gasification

Table 15 (Cont'd)

Dwg. 5599C24

Name Absorbent	Type of Absorption	Temp. °C (°F)	Pressure kPa (psig)	Typical Feed and/Exit Gas Contaminants	Typical Utilities	Commercial Status	Remarks
Selazol Dimethylether of Polyethylene glycol	Physical	-7 - 38 (20-100)	3500-6980 (500-1000)	In-0.9% H ₂ S 39% CO ₂ Out-0.1 ppm H ₂ S 11% CO ₂	Steam 0.051 kg/scm (3,000 lb/10 ⁶ scf); CW 0.005 m ³ /scm (35,000 gal/10 ⁶ scf); Power 1.23 x 10 ¹⁵ J/scm (900 kWh/10 ⁶ scf)	BIGas Pilot Plant Texaco Pilot Plant TVA Pilot Plant N.C. Sweetening Bulk CO ₂ Removal Commercial	Noncorrosive; low solvent loss; needs multiple flashes to minimize fuel losses; absorbs H ₂ + CO heavy hydrocarbons NH ₃ , HCN, and water; can use air for stripping
Category Four. Physical & Amine							
Amisol Methanol + DEA or MEA	Physical and Chemical	35°C (95)	Higher pressures favored; operation reported at 3000 (440 psig)	In-4.4% H ₂ S; 15 ppm COS 90.7% CO ₂ Out-3 ppm H ₂ S; 0.1 ppm COS 10 ppm CO ₂	Unusually low steam consumption	Ammonia plant; Commercial (25 10 ⁶ scfd)	Generally used for applications for low CO ₂ content; high solubility for hydrocarbons; degradation of solvent requires redistiller
Sulfinol Tetrahydrothiophene dioxide + di-isopro- panolamine	Physical and Chemical	38-52 (100-125)	0-6980 (0-1000)	In-1.6% H ₂ S; 7 ppm COS 6.9% CO ₂ Out-2.0 ppm H ₂ S Unknown % CO ₂	Steam 1.1 kg/kg (1.1 lb/lb) acid gas	Natural Gas; Commercial	Absorbs some hydrocarbons and H ₂ + CO; uses cartridge filter on lean solution, but on converted MEA plant a reclaimer is used on 10% of the solution circulated
Category Five. Direct Oxidation							
Stretford Sodium Carbonate Vanadium Salt ADA	Direct liquid phase oxidation	21-43 (70-110)	0-2100 (0-300) (6.9)	In-1% H ₂ S 0.2% HCN Out-1 ppm H ₂ S	Steam 0.012 kg/scm (730 lb/10 ⁶ scf) CW 23 x 10 ⁻⁶ m ³ /scm (160 gal/10 ⁶ scf); Power 0.26 x 10 ⁶ J/ scm (19 kWh/10 ⁶ scf)	Coke Gas Coal Liquelaction Off-gas 7 Coal Gas Commercial	Only sulfur compounds absorbed; plugging may occur for large acid gas loading. Inlet H ₂ S concentration to as low as 0.03% to 95%. 500 to 2000 ppm HCN; plants range from 0.5 to 76 ml/day; needs pollution control devices
Glammarco- Vetrocoke Potassium Carbonate and Arsenic Trioxide	Direct liquid phase oxidation	49-104 (120-220) 166 Max. (330° Max.)	698-6980 (100-1000)			Commercial coke oven gas Natural gas	Requires digester to convert sulfur; can operate with large amounts of CO ₂ ; Arsenic Control is Difficult
Perox Ammonia and Hydroquinone as Catalyst	Direct liquid phase oxidation	21 (70)	Low	In-0.6% H ₂ S 385 ppm HCN Out-1 ppm H ₂ S 30 ppm HCN		3 coal gasification plants operating in 1956	Needs periodic addition of solution and catalyst; feed gas requires cooling; sulfur recovered by froth flotation
Konox Na ₂ FeV10 ₄	Direct liquid phase oxidation	Ambient	0 (Atm)	In-0.43% H ₂ S Out-3 ppm H ₂ S	Power 18 J/kg-H ₂ S (0.3 kWh/lb-H ₂ S)	Commercially available	Sulfur separation by filtration instead of froth flotation; solution nontoxic; no environmental problems reported
Takahax 1,4-naphthoquinone 2-sulfonic acid	Direct liquid phase oxidation	Ambient	0 (Atm)	In-0.4% H ₂ S 5-10% CO ₂ Out-<5 ppm		Several Commercial plants operating in Japan	Less residence time required than Stretford; filters continuously instead of froth flotation for sulfur separation; noncorrosive; no environmental problems reported

The solution is corrosive to carbon steel, and there is no market in the United States for the salt-contaminated sulfur produced from the process. Although used extensively when first developed, most of these cleanup systems have been replaced by Benfield-type systems.

Thylox uses a slightly alkaline or neutral solution and contains sodium and ammonium thioarsenate that converts H_2S to elemental sulfur. The sulfur extracted, however, contains up to 0.5% arsenic, an undesirable contaminant. A nonregenerative process has been developed for producing high-purity gas and removing small quantities of sulfur. The Thylox process tends to be less efficient than the Benfield for treating natural gas and synthesis gases because two absorbers are required to obtain high-purity feed gas.

The Seabord process absorbs H_2S with a dilute Na_2CO_3 solution regenerated by air. This was the first regenerative liquid absorption process. The efficiency ranges between 85 and 95% in single-stage plants and, because the acid gases are driven off by air, uneconomical sulfur production results. The acid gas stream is usually vented or, preferably, as at the time of its development (1920), burned, with the resultant SO_2 vented.

Vacuum Carbonate, similar to the Seabord process, uses a Na_2CO_3 solution, which is regenerated by a vacuum distillation. The efficiency for H_2S is limited to about 90%, at which level CO_2 is also removed.

Tripotassium Phosphate has been replaced over the years by ethanolamine solutions. This complex process can be more economical than MEA if the CO_2/H_2S ratio is greater than 4:1. A high degree of H_2S removal has not been demonstrated.

Sodium Phenolate employs a relatively concentrated solution that contains about 3 moles $NaOH$ and 2 moles phenol per liter. This process has been largely supplanted by others. The main difficulty is the relatively low H_2S recovery, but high steam consumption phenolate plants have also reported corrosion difficulties.

Claus Tail-Gas Systems. Information on Claus tail-gas cleanup systems also was obtained during preparation of this study. This information is categorized in Table 16 according to dry bed or wet-scrubbing processes.

2.4.2 Hot Gas Cleanup Systems

2.4.2.1 Background

As for cold gas cleanup systems the goal is to achieve desulfurization to 0.1 ppm in the fuel gas to the MCFC. Also as for cold gas cleanup, ancillary equipment for control of particulates and of trace elements such as chlorine and heavy metals will be used as required. Ceramic filters for particulate removal, plus consideration of dechlorination guard beds and the use of zinc oxide final polishing units for desulfurization, will be specified. Ammonia will not be removed because of the anode-side tolerance for ammonia discussed in subsection 2.3 of this report and because of the ability of the platinum-catalyzed spent fuel combustor to consume NH_3 without production of NO_x . As mentioned in the Introduction of this report, we will explore analytically the effects of some chemical and heavy metal contaminants on MCFC performance. This work, to be found in subsection 3.3, was added to the scope of the contract by DOE. It investigates a few of the elements listed in Table 12 of this section.

2.4.2.2 Approach

Hot gas cleanup technology is developmental and, therefore, continues to be the subject of many investigations. There are currently no hot purification commercial processes available. Four types of hot purification processes for removal of H_2S from coal gas that fairly well cover the scope of potentially commercial technology have been considered in this portion of the study. These are:

1. Iron-oxide-based processes
2. Calcium-based processes

Table 16
CLAUS TAIL GAS CLEANUP SYSTEMS

1. Dry Bed Processes

- A. Oxidize to SO_2 and absorb or react
 - a. SFGD
 - b. Westvaco
 - c. SNPA/Topsoe
- B. Extend Claus reaction on solid bed
 - a. Sulfreen
 - b. Amoco CBA

2. Wet-scrubbing Processes

- A. Extend Claus reaction in liquid phase with catalyst
 - a. IFP
 - b. Aquaclaus
 - c. ASR Sulfoxide
 - d. Townsend
- B. Oxidize to SO_2 and Absorb or React
 - a. Chryoda 101
 - b. USBM Citrate
 - c. Wellman-Lord
- C. Reduce to H_2S and Absorb or React
 - a. Beavon
 - b. Cleanair
 - c. SCOT
 - d. Trencor-M

3. Zinc-oxide-based processes
4. Molten-salt-based processes.

Each iron-oxide- and calcium-based process was surveyed in both the fixed-bed and fluidized-bed versions. Calcium-based processes appear to be less efficient for removing H_2S than iron-oxide-based processes. The zinc oxide processes appear to have their most useful application in desulfurization polishing services. Other metal-oxide-based sorbents, such as copper oxide or manganese oxide, have been investigated for hot desulfurization of reducing gases. The iron-, calcium-, and zinc-oxide-based systems, however, use either lower cost or more readily regenerable sorbents. This survey, therefore, will review further only those hot desulfurization systems listed above.

The commercial use of molten-salt-based processes remains open to speculation because of several problems that plagued the experimental work of Battelle Northwest in their investigations. They experienced:

- Excessive solids and alkali carry-over to downstream facilities
- Buildup of soluble and insoluble ash in the molten salt
- Requirement of a large quantity of CO_2 and steam for regeneration
- Corrosion of equipment in contact with the molten salt
- Concentrations of H_2S in the H_2S - CO_2 mixture obtained during regeneration possibly too low to supply a suitable feed gas to a Claus unit.

In the on-site review of the Rockwell molten carbonate coal gasification system performed by Westinghouse and Davy McKee for this report, however, it became evident that Rockwell had solved some of those problems (ash buildup, CO_2 for generation, alkali carry-over). This report, therefore, includes a molten carbonate hot gas cleanup system that performs the function of the Battelle Northwest technology, using some of the features of Rockwell's DOE-funded molten carbonate system.

Data, where available, have been provided for hot gas cleanup processes in Table 17. A detailed compilation is in Appendix B of

Reference 2 in the same format used for listing cold gas cleanup processes.

2.5 DESIGN CONSTRAINTS ON HEAT RECOVERY EQUIPMENT

The energy-efficient use of a hot gas stream for MCFC applications requires that the sensible heat content of the gas, produced at 700°C (1300°F) or higher, not be discarded. Heat conservation via raw gas/pure gas heat exchange and/or steam generation must be considered in any economically attractive coal-gasification, fuel-cell-based application.

Design constraints on heat recovery equipment have been formulated to provide a design basis for a cost-effective, reliable, heat recovery system for use in cooling the raw fuel gas down to the temperature level required for low-temperature fuel gas cleanup processes. When high-temperature fuel gas cleanup processes are employed, the heat recovery equipment must satisfy the MCFC operating temperature requirements. Design considerations have been given for corrosion, erosion, and deposition problems associated with heat recovery equipment. Heat recovery equipment shutdowns are most often caused by fouling, corrosion, and erosion. Those problems involved in effecting heat recovery from coal gas are discussed below.

2.5.1 Heat Recovery Design Constraints

2.5.1.1 Summary

1. Each design is to be composed of commercially available units.
2. Each unit is to be built using standard fabrication techniques.
3. Probability of failure must be low.
4. Each unit is to have the lowest possible requirements for expensive materials. At the same time, the major properties considered in selecting steels for high-temperature application in heat recovery equipment design are not to be compromised: strength, thermal conductivity, corrosion resistance, and thermal expansion. (Note: In general, carbon steel should be specified for applications up to 510°C [950°F]. Chromium-molybdenum steels should be used at temperatures between 427°C

Table 17
SUMMARY OF HOT-GAS CLEANUP SYSTEMS^a

Dwg. 5599C25

Name Absorbent	Type of Reactor	Operating Range		Typical Removal of H ₂ S	Remarks
		Temp., °C (°F)	Pressure kPa (psig)		
<u>Category One, Iron Oxides</u>					
Iron Oxide - Silica/Fly Ash	Fixed Bed	400-750 (750-1380)	101-1013 (14.7-150)	To 200/ 800 ppmv. Depending on H ₂ O/H ₂ Content In Gas	METC Iron Oxide Process Presently Superseded by Zinc Ferrite Development (See below)
Iron Oxide - Zinc Oxide	Fixed Bed	Up to 650 (1200)	101-1013 (14.7-150)	To < 10 ppmv. Depending on H ₂ O Content In Gas	METC Zinc Ferrite/ Zinc Oxide Process
Iron Oxide Granules	Fluidized Bed	335-420 (635-790)	101-203 (14.7-29.4)	To ~ <150 ppmv. In Coke Oven Gas	Appleby - Frodingham Process Iron Oxide Pellet Attrition Not Solved
<u>Category Two, Calcium - Based Processes</u>					
Calcined Dolomite	Fixed Bed	870-927 (1600-1700)	101-1124 (14.7-163)	To ~ 600 ppmv	Air Products Dolomite Process Carbon Deposition Problems Not Solved
Half-Calcined Dolomite	Fluidized Bed	900 (1650)	1620 (235)	To 200/ 300 ppmv	Conoco Process Sorbent Regeneration Complex and Expensive
Dolomite	Fluidized Bed	815-925 (1500-1700)	1520 (220)	To < 600 ppmv	Westinghouse Process Once-through Dolomite
Dolomite	Gravitating Bed	1000 (1830)	101 (14.7)	To < 65 ppmv	U. S. Steel Process with Dolomite Hydration (Proprietary) for Disposal of Spent Dolomite
<u>Category Three, Zinc Oxide Processes</u>					
Zinc Oxide Pellets from United Catalysts, Haldor Topsoe, etc.	Fixed Bed	400-600 (750-1110)	Not Specified	To < 10 ppmv	Experimental Work by Institut Français Du Pétrole (I. F. P.) Has Been Performed to Extend Commercial Zinc Oxide Desulfurization to Higher Temperatures and to Include Sorbent Regeneration
<u>Category Four, Molten Salt</u>					
Sodium Carbonate	Scrubbing Tower	850-1000 (1560-1830)	1013 (147)	To < 40 ppmv	Battelle Northwest and Rockwell International Have Both Provided Experimental Data on Coal Gas Desulfurization with Molten Na ₂ CO ₃

^aNone of the Processes Listed is Commercially Available;
All of the Processes Use Chemical Sorption for Gas Desulfurization.

[800°F] and 650°C [1200°F]. Above 538°C [1000°F], austenitic and ferritic steels should be considered.)

5. Each unit is to employ an economical (optimum) pressure drop. (Note: Higher pressure drops usually result in smaller exchanges but consume more energy.)
6. Each unit is to be transportable and must meet the required delivery time.
7. Units are to provide an economical temperature approach. The effect of mean temperature difference on heat exchanger investment due to the temperature level of the heat transfer medium greatly affects the heat transfer area required.
8. Design tube-side velocity up to 12.2 m/s (40 ft/sec) increases the differential pressure but can reduce fouling and eventual downtime.
9. Entrained particles entering the waste heat recovery unit must be below their fusion temperature. Otherwise, it would be necessary to quench the hot gas with water to freeze the particles to prevent sintering on refractory walls and deposition of molten particles within the exit ducts and waste heat recovery units.
10. Waste heat recovery unit designs must comply with all required construction codes and with Section VIII of the ASME Boiler and Pressure Vessel Code. The unit must also meet ANSI standards.
11. Waste heat recovery units are generally designed for corrosion rates of 0.005 in/yr (5 mils/hr) or less. Permissible corrosion rates are an important factor and will differ with material and environment.
12. Convenience of maintenance should be considered in the unit design (i.e., heat transfer area can be added or removed without completely dismantling the equipment). Tube bundles (heat transfer area must be removable and must be available for chemical and/or physical cleaning both inside and out.
13. Operation must be safe.
14. The unit will be designed for maximum energy recovery. Fouling considerations, therefore, will be incorporated into the design.
15. The insulation design criteria will be to maintain the shell temperature at 93°C (200°F) in 27.6°C (80°F) ambient still air.
16. For steam generation service the waste heat recovery equipment will produce steam at the required pressure, temperature, and quality.

2.5.1.2 Discussion

The determination of heat recovery design constraints includes a survey of the shell/tube-side fluid possibilities. This survey considers the following factors:

- Corrosion - Fewer costly alloys or cladding components are needed if the corrosive fluid (i.e., raw gas) is inside the tubes.
- Fouling - Fouling can be minimized by placing the fouling fluid (i.e., raw gas) in the tube to allow better velocity control; increased velocities tend to reduce the fouling.
- Temperature - For high-temperature service requiring expensive alloy materials, fewer alloy components are needed when the hot fluid (i.e., raw gas) is placed on the tube side.
- Pressure - Placing a high-pressure stream in the tubes will require fewer (less costly) high-pressure components.
- Pressure Drop - For the same pressure drop, higher heat transfer coefficients are obtained on the tube side. A fluid with a low allowable pressure (i.e., raw gas) should generally be placed on the tube side.
- Viscosity - Higher heat transfer rates are generally obtained by placing a viscous fluid (i.e., BFW) on the shell side.
- Toxic and Lethal Fluids - Generally, the toxic fluid (i.e., raw gas) should be placed on the tube side to minimize the possibility of leakage to the atmosphere. ASME code requirements for lethal service must be followed.
- Flowrate - Placing the fluid with the lower flowrate on the shell side usually results in a more economical design. Turbulence exists on the shell side at much lower velocities than on the tube side.

Analysis of the aforementioned shell/tube-side fluid considerations leads to the summary in Table 18. The above summary indicates that for general service the hot raw product gas is more suitable for flow through the tube side of waste heat recovery equipment.

Corrosion and Erosion. The major areas of expected material degradation in waste heat recovery and associated equipment are summarized in Table 19, along with some of the environments. The severest conditions exist, of course, in the gasifier and the transfer lines, which experience high temperatures, high pressures, corrosive

Table 18
ANALYSIS OF MOST SUITABLE FLUID FOR SHELL/TUBE-SIDE SERVICE

Location of Fluid	Corrosion	Fouling	Temp.	Pressure	Pressure Drop	Viscosity	Toxic	Flowrate
Tube Side	G ^a	G	G	Both	G	G	G	G
Shell Side	BFW ^b	BFW	BFW	Both	BFW	BFW	BFW	BFW

^aG = Hot product gas (hot fluid)

^bBFW = Boiler feedwater (cold fluid)

gases, and high-velocity char and ash particles, all of which cause severe erosion. The hot raw fuel gas entering waste heat recovery equipment at temperatures as high as 1038°C (1900°F) is expected to contain fine particulate matter, H₂S, COS, HCN, alkali chlorides, and trace elements like Pb and Hg in addition to the basic gas constituents CO, CO₂, CH₄, and water vapor. A whole spectrum of environments will be created that are very damaging to the metals used in waste heat recovery units and to associated equipment. Other problem areas specific to the actual environment include severe corrosion of alloys in the quench systems, weld corrosion, refractory deterioration, long-term mechanical properties, and the effect of exposure on the structure and mechanical properties of alloys and refractories.

General corrosion, usually confined to the metal surface, sometimes occurs along grain boundaries or other lines of weakness because of a difference in resistance to chemical attack or local electrolytic action. Metals exposed to raw, low-Btu fuel gas at high pressure and temperature are subject to attack by hydrogen, nitrogen, carbon dioxide, and hydrogen sulfide.²¹ High-pressure hydrogen causes decarburization and intergranular cracking, commonly called hydrogen embrittlement. Hydrogen sulfide corrosion is a scaling process, and

Table 19

CORROSION/EROSION AREAS IN COAL GASIFICATION EQUIPMENT

Area	Coal Feed	Gasification	Raw Gas Cleanup
Equipment	Pumps, valves hoppers, pipes	Waste heat recovery, cyclones, transfer lines, valves, other vessel internals	Scrubber, valves, transfer lines, other vessel internals
Environment	38 to 315°C (100 to 600°F) 101 to 8336 kPa (amt. to 1200 psig), coal particles, low velocity	425 to 1483°C (800 to 2700°F) 8356 kPa (amt. to 1200 psig), coal char, and ash particles, high velocity, 30.5 m/s (100 ft/s)	38 to 260°C (100 to 500°F) 101 to 101325 kPa (amt. to 1000) psig
Equipment Degradation	Corrosion, erosion	Corrosion/erosion sensitization, metal dusting, deposition, weld cracking, hydrogen embrittlement, refractory corrosion	Pitting, stress corrosion, weld cracking, hydrogen embrittlement

the ultimate reaction product is a layer of sulfide. Nitrogen in combination with hydrogen at high pressure and at temperatures greater than 445°C (850°F) causes nitriding of any metal containing more than 2% chromium. Carbon monoxide in combination with hydrogen has also been found to be corrosive at high pressures and moderate temperatures.

Hydrogen attack is prevented by the addition of any of the carbide-stabilizing elements. The austenitic steels are resistant because of their high chromium content. Nickel and silicon have no effect upon hydrogen attack. The hydrogen partial pressure in the low-Btu fuel gasification process is well below the threshold level for accelerated hydrogen attack on carbon and low-alloy steels.

Nitriding results in a thin, hard, brittle layer that is usually limited to depths of 0.793 mm (1/32 in) or less. Nitriding is a problem, therefore, only in thin-walled equipment such as expansion bellows. Nickel is effective in resisting nitrogen attack of metals. The pressure used in low-Btu gasification is indicated to be below the level where nitriding would be significant.

Carbon monoxide is inert to most materials at low pressures, even up to very high temperatures. At very high pressures, 25,331 kPa (250 atm), however, severe corrosion occurs, particularly in the temperature range of $260 \pm 65^{\circ}\text{C}$ ($500 \pm 117^{\circ}\text{F}$). Chromium is effective in resisting carbon monoxide attack on metals. The operating pressure for low-Btu gasifiers is probably well below the level at which accelerated carbon monoxide attack occurs.

Tests conducted at the Westinghouse Research Laboratories under OCR Contract 14-01-0001-303²² evaluated the high-temperature H_2S corrosion resistance of a group of candidate materials for application to heat exchangers. The materials found to have the best H_2S corrosion resistance at a temperature of 1000°C (1832°F) were Incoloy 825, Incoloy 800 with aluminized surface and L605 (a cobalt-based superalloy). At a hydrogen sulfide concentration of 0.3 mol %, the cobalt-based alloy was found to be superior to the nickel-based alloys. None of the materials was found to be satisfactory at a H_2S concentration of 0.5% at this temperature level.

Erosion in a gasifier is the destruction of a metal by the combined action of corrosion and abrasion caused by the flow of a gas containing suspended solids. In coal gasification environments, high-temperature, high-pressure corrosive gases and high-velocity particles of char, ash, or dolomite may result in severe degradation of materials. The quality of metal removed by erosive wear generally depends on the particle size, particle velocity, angle of impingement, the particle concentration in the gas stream, and the plastic flow stress of the ductile metal being eroded. A typical curve of the effect of angle of

impingement on wear rate for SAE 1020 steel shows that maximum wear occurs at an angle of impingement of about 20 degrees. For more brittle metals this angle has been found to be about 90 degrees. These results are based on modeled experiments performed at ambient temperatures. The combined effect of corrosion and erosion will probably depend on the nature of the corrosion scale and its resistance to erosion by high-velocity particles. If the scale contains liquid sulfides, removal of this sulfide by erosion would be beneficial to the metal surface. If the scale contains solid CrS_x , which is an excellent barrier against diffusion, removal of this scale would adversely affect the rate at which it corrodes the underlying metal. Corrosion due to solid salts at elevated temperature, while less severe than those from liquid deposits, are severe on certain materials and significant on all materials. Iron-based alloys will experience accelerated attack when exposed to solid salts at temperatures above about 482°C (900°F); nickel-based alloys may be satisfactory at temperatures up to about 650°C (1200°F). At higher temperatures, and with H_2S present to 0.5 vol % or more, nickel sulfide formation can be damaging. Coatings could be effective in prolonging the life of boiler tubes, at some cost to their ability to transfer heat. Chromium is an essential constituent in alloys to be used above 538°C (1000°F). It diffuses rapidly and accumulates at the surface of the alloy, providing a tightly adherent oxide film that materially retards the oxidation process. Such an oxide film will form, even in coal gas, because the CO_2 and H_2O present produce an oxygen partial pressure greater than about 10^{-15} atm.

No data are available on high-temperature, high-pressure, erosion/corrosion phenomena. Because of the lack of information on erosion/corrosion problems for coal gasification process conditions, the selection of materials for waste heat recovery equipment should preferably be based on experience with materials under similar conditions (i.e., waste heat boilers in ethylene or secondary reformer systems). In addition, it is often desirable to obtain advice and assistance from specialists in corrosion/erosion engineering work who are familiar with

the chemical resistance characteristics and limitations of construction materials.

Deposition. Ash, tar, and char deposition in various heat transfer zones is an important constraint to be considered in waste heat recovery designs. Entrained-flow, molten-salt, and fluidized-bed gasifiers operate at high temperatures [815°C (1500°F) or higher], so significant quantities of tarry compounds are not present in the raw gas. This condition eliminates or reduces fouling by tar deposition. For high-tar gasification systems like the Lurgi process, those tarry materials must be condensed out of the gas by cooling the gas to 205°C (400°F) before waste heat can be recovered. Ash and char deposits on unit walls initially act as insulation, thereby delaying cooling of the hot gases. This delay can cause an increase in steam temperature and is one factor that can cause the deposits to advance into normally cooler parts of the unit.

If the deposits are not removed during operation, accumulations forming on unit walls may cause excessive gas temperatures downstream or, in some cases, may fall and damage internal components. Accumulations in tube banks may block gas passages and require a unit outage for manual cleaning. The occurrence and severity of char and ash deposition depend largely on the coal-ash composition and on the quantity of ash, but can be strongly influenced by the design of the equipment and the operating conditions. In practice, the design parameters and operating conditions are determined by the characteristics of the ash. For example, if the ash and char produce hard, massive deposits, the superheater and reheater tube banks are designed to permit ease of deposit removal. This design may incorporate increased lateral tube spacing, decreased tube bank depth, integral tube cleaning devices, and tube banks located in cooler gas-temperature zones. Another result of solids deposition on heat transfer area is that the difference between calculated and actual heat transfer rates can be significant. Ratios between calculated (clean surface) and measured overall heat transfer coefficients have varied from 1.1 to 4.1.²³ The deviations

were attributed primarily to surface fouling (solids depostion) and secondarily to flow maldistribution between parallel tubes.

Under certain conditions, carbon laydown may occur on metal surfaces exposed to low-Btu fuel gases, most likely in the temperature range of 425 to 704°C (800 to 1300°F). Since the presence of significant quantities of H₂S will tend to prevent carbon laydown, it can be a problem with clean fuel gas, but not with raw. Typical overall heat transfer coefficients for heat exchangers in coal conversion plants have varied over the following ranges:

Exchanger Function	Heat-transfer coefficient, W/m ² -°C (Btu/hr-ft ² -°F)	
	Dirty	Clean
Fired Coal Slurry Preheater	5.7 (1)	17 (3)
Recycle Gas Cooler	170 (30)	568 (100)
Heavy Vapor Condenser	227 (40)	454 (80)
Reactor Effluent Cooler, preheating coal-paste feed	57 (10)	284 (50)

A brief examination of the fouling potential on trace hydrocarbons in coal gas is in order. A gas-to-gas exchanger, using bare tubes, could expect to be completely plugged after 7000 hours of operation if only 1/20,000 part of the coal fed in that time were deposited in the exchanger. Actually, only 10% or less of the deposit required to plug the exchanger would be sufficient to seriously reduce its heat transfer effectiveness. Obviously, no significant part of the coal volatiles (less than 0.01 wt %) can be tolerated as fouling material on a heat recovery exchanger.

It is essential, therefore, to identify the factors responsible for the fouling characteristics of various coals so that the optimum design of a waste heat recovery unit can be achieved. Tables 20 and 21 summarize fuel characteristics and design and oerating constraints important for heat recovery system design.

Table 20

WASTE HEAT RECOVERY DESIGN PARAMETERS, DEPOSITION CONSIDERATIONS

FUEL CHARACTERISTICS

1. Properties of coal substance
 - A. Physical, including density, hardness, specific heat, thermal expansion, and thermal conductivity
 - B. Chemical behavior during gasification

Technological properties

1. Proximate analysis
2. Ultimate analysis
3. Free-swelling index
4. Differential thermal analysis
5. Thermogravimetric analysis
6. Effluent gas analysis
7. Grindability
8. Calorific value
9. Sieve analysis
10. Abrasiveness

2. Properties of coal ash determined by the concentration and type of minerals in the coal containing the following elements:

a. Alkalines	e. Calcium-Magnesium
b. Sulfur	f. Iron
c. Chlorine	g. Silica
d. Phosphorus	h. Alumina

Technological properties

1. Fusion temperatures
2. Viscosity of slag
3. Surface tension of slag
4. Volatility of constituents in slag
5. Sintering temperature and strength of ash

Table 21

WASTE HEAT RECOVERY DESIGN AND OPERATING CONSTRAINTS

1. Heat transfer unit design
 - a. Rating
 - b. Wall construction
 - c. Type, number, and arrangement of heat transfer zones
 - d. Geometry
 - e. Exit-gas temperature
2. Tube bank design
 - a. Horizontal or verticle tubes
 - b. Spacing side and back
 - c. Depth of bank
 - d. Alignment
 - e. Freedom of tube movement
3. Properties of gases
 - a. Temperature
 - b. Flow patterns
 - c. Composition
 - d. Impurities
 - e. Density
4. Properties of entrained ash
 - a. Dust loading
 - b. Size consist
 - c. Composition
 - d. Microstructure
 - e. Particle size distribution

Section 3

PREPARATION OF THE ANALYTICAL MODELS

3.1 INTRODUCTION

Because the electrochemical processes by which fuel cells generate power do not involve fuel combustion and associated Carnot cycle efficiency limitations, future power plants operating with fuel cells may be substantially more efficient than current fossil fuel power plants. Although the coal gas being considered for use with molten carbonate fuel cells will be cleaned with highly efficient scrubbers or filters, limited quantities of chemical contaminants and of particulates will be contained in the gases entering the fuel cells.

The first intent of this section is to provide an initial theoretical treatment of fuel cell deposition that will serve as a foundation for more detailed theoretical efforts in the future. Possible blockage of fuel cell anode pores by particles has been perceived to be a significant potential problem, and it has been suggested²⁴ that a safe particle concentration for fuel cell applications should be "essentially zero." Since no theoretical or experimental results appear in the open literature concerning particulate effects on fuel cells, however, their tolerances to particles are unknown, and there is little basis for specifying acceptable particle concentrations.

Dominant mechanisms and factors controlling MCFC deposition are identified here. Existing electrochemical/theoretical models for determining limiting currents generated in individual anode pores are extended to provide relations for flow rates from anode pores that have a major effect on particle transport to anode surfaces and entry into pores, and areas are suggested for future theoretical efforts related to

fuel cell deposition. Using the model, we made a preliminary assessment of the effects of particulate deposition on fuel cell performance. The assessment is based on the coal gas cleanliness expected from typical gas cleaning systems.

The second intent of this section is to provide an initial theoretical treatment of fuel cell chemical contamination that will serve as a foundation for more rigorous theoretical efforts in the future. Many of the elements in the periodic chart and their compounds are present in coal and, hence, also in the coal-derived gases. Many of these elements and compounds may damage the cell, causing loss of power output or mechanical failure within the cell itself.

The contaminants significant to fuel cell performance are those introduced by the coal and not removed in the gas cleanup system, plus those contaminants that come from the cleanup system itself. This initial theoretical treatment of the effects of those contaminants on a molten carbonate fuel cell has been divided into four subtasks. These include:

- Review of fuel cell technology, defining electrode and electrolyte compositions and their responses to various elemental and/or phase contaminants
- Selection of eight typical gasifier/gas cleaning systems and definition of the entering equilibrium anode fuel gas compositions
- Assessment of the proposed fuel cell equilibrium model and necessary revisions to provide a functional computer model
- Utilization of the computer model for assessing fuel cell performance.

3.2 PERFORMANCE DEGRADATION DUE TO PARTICULATES

3.2.1 Assessment of Particulate Deposit Mechanisms

A MCFC bank consists of stacks of individual cells electrically interconnected to produce the desired power output at the required voltage. A section of a single molten carbonate cell is illustrated in Figure 10. The cell consists of two porous electrodes separated by a

Figure 10 -- Section of Molten Carbonate Fuel Cell

porous tile containing a liquid electrolyte composed of a mixture of alkali carbonates, all of which are sandwiched between separator plates. The separator plates function as current collectors and provide channels for the fuel gas to flow over the anode and for the oxidant gas to flow over the cathode.

Fuel gas flows through the anode flow channels and penetrates the anode pores, and fuel reactants H_2 and CO in the gas react with carbonate ions in the electrolyte that occupies the pores to produce electrons according to the following reactions:

The $CO_3^{=}$ ions used in the above reactions have migrated to the anode through the electrolyte after being produced in the cathode. The

electrons generated in the anode travel through an external circuit to the fuel cell cathode to participate in the cathode reactions that produce the carbonate ions. The continuous generation and utilization of electrons according to the above reactions and their flow from the anode to the cathode through an external circuit results in the fuel cell current output.

The conceptual molten carbonate fuel cell evaluated in this study has operating characteristics that are the objectives of current development work²⁵ for future power plants. The cell area is about 15,000 cm² (16 ft²) and produces an average power density of 0.135 W/cm² (125 W/ft²) of cell area at an 0.8 V/cell potential. For operation with future power plants, the anode inlet gas pressure is assumed to be 10 atm (1013 kPa), the temperature, 650°C (1202°F), and the H₂ and CO fuel utilization in anode channels, 85%.

The theoretical models used to represent fuel cell anodes are similar to models that have been used successfully for fuel cell electrochemical analyses.^{26,27} Figure 11 represents the MCFC anode. Fuel gas flows parallel to the anode surface. Reactant species H₂ and CO from the gas enter the anode pores and diffuse through the electrolyte in the pores to the pore walls, where reactions given by equations (38) and (39) occur. Reaction products H₂O and CO₂ diffuse back through the electrolyte and out of the pores into the fuel gas flow.

The distribution of electrolyte in the anode pores is thought to be governed only by capillary absorption that progresses from smaller to larger pore sizes.⁴ All pores smaller than an equilibrium pore diameter (associated with a balance of capillary and pressure forces) are assumed to be flooded, and all pores larger than the equilibrium diameter are assumed to be virtually empty except for a thin film of electrolyte on the pore walls. Different pore models and mathematical formulations describe the diffusion of reactant gas species for the flooded pores and thin film pores.²⁷ Although an initial analysis²⁷ suggested that thin film pores produce a substantial fraction of the

Figure 11 -- Anode Pore Representation

electrons generated in MCFC anodes, later experimental work has shown that most of the current is generated in the anode flooded pores.²⁷ Fuel cell electrode performance measurements and posttest mercury porosimetry data associated with this later work have provided evidence for the validity of the above-described electrolyte distribution and electrochemical performance models.

Particles entrained in the anode fuel gas can degrade fuel cell performance by being deposited on the anode flow channel surfaces and restricting anode channel gas flow or by entering into and blocking anode pores and inhibiting H_2 - and CO -reactant migration into the pores and H_2O and CO_2 reaction product migration out of the pores, driving reactions of equations (38) and (39) to the left (opposite from the desired direction). Pore blockage is of particular concern because

anode pore diameters (a typical average anode pore diameter is 5 μm) might be expected to be prone to blockage by particles of diameters in the 0.1 to 3 μm range. Different types of gas cleanup devices, such as scrubbers and filters, are least effective in these ranges.

Mechanisms of particle transport in fuel cells are:

- Brownian diffusion
- Electrostatic migration
- Gravitational settling
- Thermophoresis
- Convection.

Because of the small dimensions [typical height = 0.25 cm (0.1 in)] and low flow velocities [typical velocity less than 30 cm/s (1 ft/sec)] for flow in anode flow channels, flow is laminar, and turbulent diffusion particle transport is not in effect. Particle deposition velocities (normalized particle arrival rates) have been determined independently for each of the above-listed mechanisms in order to learn which dominate particle transport to anode flow-channel surfaces and entrances to anode pores.

For Brownian diffusion, particle deposition velocities have been obtained at a location near the anode channel inlet (where particle arrival rates are higher than they are downstream), just beyond the region where the laminar flow velocity profile becomes approximately fully developed. Electrostatic migration velocities associated with diffusion charging of particles were determined for the 0.1 to 3 μm particle diameter range, since diffusion charge levels are much higher than for bombardment (field) charging in the low intensity (typically a few V/cm) anode-cathode electrostatic force field. To determine thermophoretic deposition velocities, a thermal gradient associated with a 2°C (3.6°F) difference between bulk gas stream temperature and anode surface temperature was used, based on results from thermal flux modeling of fuel cell channels.

While Brownian diffusion, electrostatic migration, and gravitational settling tend to deliver particles to the anode surface, thermophoresis tends to transport particles away from that surface because of the direction of the thermal gradient. Anode reactions of equations (38) and (39) release heat at the walls of the anode pores. This heat is primarily absorbed by the metal anode, thus making the anode temperature higher than the flow channel gas temperature.

Convection effects also tend to transport particles away from the anode surface and affect particle entry into anode pores. As indicated earlier, the reactions of equations (38) and (39) are accomplished by migration of H_2 and CO from the anode flow channels into the pores, reaction of these species with $CO_3^{=}$ ions from the electrolyte, and diffusion of reaction products H_2O and CO_2 out of the anode through the pores into the anode fuel channels. The lower molecular weights of H_2 and CO entering the pores than of H_2O and CO_2 leaving the pores results in a net mass flow out of the anode pores. This tends to inhibit particles delivered to the anode surface by other mechanisms from entering into the pores. Whether particles can enter into the pores and, if they can, their rates of entry depend on the magnitude of forces delivering particles to the pores relative to the forces on particles due to the flow out of the pores.

Theoretical relations for flow rates out of pores will be derived in subsequent considerations of pore blockage by particles. The net flow rate from pores, however, continually decreases in progressing from the anode channel inlet to the exit. As H_2 and CO are used as fuel along the channel length, their decreasing concentrations result in lower production (and flows) of reaction products H_2O and CO_2 from the pores.

The flow from the pores not only inhibits particle entry into the pores but also inhibits arrival on the anode surface. As particles near the anode surface are carried by the anode channel flow and slowly descend toward that surface through the various particle transport mechanisms described above, they periodically pass through "jets"

issuing from the pores. Each "jet" tends to slow, or even reverse, particle descent until it is traversed. The theoretical modeling and analysis of this complex flow and particle transport situation is beyond the intent of this initial assessment of fuel cell deposition. The net effect on particle delivery, however, has been represented roughly by using the total local mass flow per unit anode area to obtain an average local flow velocity from the anode which is assumed normal to the anode surface. By regarding the deposition velocity as relative to the fluid flow, from first-order considerations we can regard arrival on the anode surface as either substantially inhibited or eliminated if the local average pore velocity component leading from the anode surface exceeds the particle deposition velocity component in the direction of the anode surface.

3.2.2 Particle Transport to Anode Surfaces

Deposition associated with the transport of particles to the anode surfaces will be considered first, followed by particle transport into pores as affected by flow convection from pores. Figure 12 gives deposition velocities (mass arrival rates divided by gas stream particle concentrations) versus particle diameter for the various transport mechanisms affecting particle delivery to anode surfaces. The range of particle sizes given represents expected limits entering fuel cells from coal conversion processes after particle removal by scrubbers or filter cleanup devices.

Also shown in Figure 12 are average anode flow velocities at both the anode channel inlet and exit. At the channel inlet the average anode flow velocity exceeds deposition velocities for all mechanisms of transport to the anode surface. Particle delivery to the anode surface, therefore, is either substantially reduced or eliminated. At the channel exit the average anode flow velocity is of the same order of magnitude as the particle deposition velocities for particle diameters below 1 μm . It is consequently expected either to substantially reduce or to prevent particles in this size range from arriving at the anode surface.

Figure 12 -- Deposition Velocities for Molten Carbonate Fuel Cells

For regions near the channel exit and particles larger than approximately $1\text{ }\mu\text{m}$ in diameter, gravitational settling dominates the other mechanisms of particle transport, and the net movement of particles is to the anode surface. For particle diameters smaller than $1\text{ }\mu\text{m}$, thermophoretic transport of particles away from the anode surface is of the same order of magnitude as the other mechanisms that transport particles to the anode surface. Consequently, thermophoresis, in addition to the average flow from pores, can prevent or at least greatly reduce deposition on flow channel anode surfaces for particle diameters below about $1\text{ }\mu\text{m}$.

3.2.3 Particle Transport into Pores

Figure 13 represents a particle that has been delivered to the vicinity of a pore entrance by one of the mechanisms described above, with a deposition velocity, V_d , relative to the local gas. The local flow velocity of gas leaving the pore through reactions of equations (38) and (39) at the pore walls is designated U_p . If the local flow

Figure 13 -- Particle Transport near Pores

velocity, U_p , exceeds the particle deposition velocity, V_d , relative to the flow, then the particle does not enter the pore. If V_d is greater than U_p , then the net particle movement is into the pore, where it can be deposited. For the purposes of this initial analysis, detailed characteristics of pore flow, such as pore velocity profiles, will not be considered; particle penetration of the pore will be attributed to the particle deposition velocity's exceeding the average flow velocity from the pore for pore diameters significantly larger than particle diameters. Relations for average pore flow velocity versus pore diameter are derived below.

The mass flow rate, Q , from a pore with cross-sectional area, A_p , is related to average pore velocity, U_p , and gas density, ρ_g , by:

$$Q = \rho_g U_p A_p.$$

Solving for U_p , we find:

$$U_p = Q / \rho_g A_p. \quad (40)$$

For N_α , designating the net mole flow rate of species, α , out of the pore, and, μ_α , designating the mass per mole of species α ,

$$Q = \sum_{\alpha} \dot{N}_{\alpha} \mu_{\alpha} \quad (41)$$

The reaction of equation (38) indicates that the net flow of 1 mole of H_2 into the anode pore produces a net flow of 1 mole of H_2O and 1 mole of CO_2 from the pore. Similarly, the reaction of equation (39) indicates that the net flow of 1 mole of CO into the anode pore produces a net flow of 2 moles of CO_2 from the pore. Consequently,

$$\dot{N}_{CO_2} = \dot{N}_{H_2} - 2\dot{N}_{CO}, \text{ and } \dot{N}_{H_2O} = -\dot{N}_{H_2}.$$

Substitution of these relations into equation (41) gives:

$$Q = \dot{N}_{H_2} [-\mu_{H_2} + \mu_{H_2O} + \mu_{CO_2}] + \dot{N}_{CO} [-\mu_{CO} + 2\mu_{CO_2}]. \quad (42)$$

The positive direction of Q is out of the pore.

The gas density, ρ_g , is related to the universal gas constant, R_o , the absolute gas temperature, T_g , the gas pressure, P , and the summation of products ($f_{\alpha}\mu_{\alpha}$), of mole fraction times the mass per mole for each of the gas species:

$$\rho_g = \frac{P}{R_o T_g} \sum_{\alpha} f_{\alpha} \mu_{\alpha}. \quad (43)$$

Substitution of equations (43) and (42) into equation (40), after expressing pore area in terms of an equivalent circular area of radius r , gives:

$$U_P = \frac{R_o T_g}{P \pi r^2} \cdot \left\{ \frac{\dot{N}_{H_2} [-\mu_{H_2} + \mu_{H_2O} + \mu_{CO_2}] + \dot{N}_{CO} [-\mu_{CO} + 2\mu_{CO_2}]}{\sum_{\alpha} f_{\alpha} \mu_{\alpha}} \right\}. \quad (44)$$

Determination of pore flow velocity, U_p , from equation (44) requires evaluations of mole flow rates $\dot{N}_{H_2}$ and $\dot{N}_{CO}$ and of fuel reactants into the pores, which are obtained as follows.

As indicated earlier, most of the anode current generated is in flooded pores,²⁷ and the flooded pore current model²⁸ of Wasan, Schmidt, and Baker will be extended to obtain net flow rates $\dot{N}_{H_2}$ and $\dot{N}_{CO}$ of fuel reactants into pores. The result from that model is:

$$i_j^\alpha = 4\pi m F D_\alpha C_\alpha \sum_{k=1}^{\infty} \frac{\tanh \lambda_k L_j}{\lambda_k}, \quad (45)$$

where* $i_j^\alpha \triangleq$ limiting current drawn from pore j due to fuel reactant α
 $m \triangleq$ number of electrons given up per molecule of reactant α utilized.

$F \triangleq$ Faraday's constant

$D_\alpha \triangleq$ coefficient for diffusion of fuel gas reactant α in the electrolyte.

$C_\alpha \triangleq$ concentration of reactant α in the gas stream

$L_j \triangleq$ length of pore j

and λ_k are given by the roots of the equation $J_0(\lambda_k r_j) = 0$, where
 J_0 is the zero order Bessel function of the first kind and
 r_j is the radius of pore j .

For the Bessel function roots designated by $\eta_k = \lambda_k r_j$,

$$i_j^\alpha = 4\pi m F D_\alpha C_\alpha r_j \sum_{k=1}^{\infty} \frac{\tanh [\eta_k (L_j / r_j)]}{\eta_k}, \quad (46)$$

and the pore length considered longer than its radius, we can show that

$$\tanh [\eta_k (L_j / r_j)] \simeq 1, \quad k=1 \text{ to } \infty.$$

*The symbol $\triangleq$, as used here, indicates that the designated term defines the description which follows.

Thus, writing equation (46) for both fuel reactants H_2 and CO yields

$$\begin{aligned} i_j^{H_2} &= 4\pi m F D_{H_2} C_{H_2} r_j \sum_{k=1}^{\infty} \left(\frac{1}{\eta_k} \right) \\ i_j^{CO} &= 4\pi m F D_{CO} C_{CO} r_j \sum_{k=1}^{\infty} \left(\frac{1}{\eta_k} \right). \end{aligned} \quad (47)$$

The total current i_j drawn from pore j is

$$i_j = i_j^{H_2} + i_j^{CO}, \quad (48)$$

and the current, i , drawn from a local area, A , is the summation of all the n_p pores that are producing current in that area:

$$i = \sum_{j=1}^{n_p} i_j = 4\pi m F (D_{H_2} C_{H_2} + D_{CO} C_{CO}) \left(\sum_{j=1}^{n_p} r_j \right) \left(\sum_{k=1}^{\infty} \frac{1}{\eta_k} \right). \quad (49)$$

Since the local current density I per unit area is obtained by dividing the total current produced in area A by that area:

$$I = i/A, \quad (50)$$

then from equations (49) and (50),

$$I = K (D_{H_2} C_{H_2} + D_{CO} C_{CO}) \quad (51)$$

where

$$\begin{aligned} K &\triangleq 4\pi m F \left(\sum_{k=1}^{\infty} \frac{1}{\eta_k} \right) M \\ M &\triangleq \sum_{j=1}^{n_p} r_j / A \end{aligned} \quad (52)$$

Now the average cell current density, $\bar{I}$, will be computed by integrating the local current density, I , over the area, A_c , of the cell:

$$\bar{I} = \frac{1}{A_c} \int_{A_c} I \, dA .$$

For parallel fuel flow channels, the local concentration of fuel reactants and, consequently, the local current density are a function of distance x along the channel from the inlet. Integration of the above equation yields:

$$\bar{I} = p_c K (D_{H_2} \bar{C}_{H_2} + D_{CO} \bar{C}_{CO}) , \quad (53)$$

where

$$\bar{C}_\alpha = \frac{1}{L} \int_0^L C_\alpha(x) dx .$$

For various gas channel/current collector arrangements, not all of the anode surface can be directly exposed to the fuel gas stream, and, accordingly, the term p_c is the ratio of the anode area that produces current to the total anode area. Equation (53) can be solved for K :

$$K = \bar{I} / p_c (D_{H_2} \bar{C}_{H_2} + D_{CO} \bar{C}_{CO}) . \quad (54)$$

The above relation for K will be used later in the evaluation of net mole flow rates, $\dot{N}_{H_2}$ and $\dot{N}_{CO}$, of fuel reactants into representative pore j . The current generated in a pore for each reactant given by equation (47) is also related to the net mole flow rates of fuel reactants by:

$$\begin{aligned} i_j^{H_2} &= mF \dot{N}_{H_2} \\ i_j^{CO} &= mF \dot{N}_{CO} . \end{aligned} \quad (55)$$

Equating equations (47) through (55) and using equations (52) and (54) gives:

$$\dot{N}_{H_2 j} = \frac{\bar{I}}{mFMP_c} (r_j) \frac{D_{H_2} C_{H_2}}{(D_{H_2} \bar{C}_{H_2} + D_{CO} \bar{C}_{CO})} \quad (56)$$

$$\dot{N}_{CO j} = \frac{\bar{I}}{mFMP_c} (r_j) \frac{D_{CO} C_{CO}}{(D_{H_2} \bar{C}_{H_2} + D_{CO} \bar{C}_{CO})} \quad (57)$$

Since the diffusion coefficient of a gas in a liquid has been shown²⁸ to be roughly inversely proportional to the square root of the molecular weight of the gas,

$$\frac{D_{CO}}{D_{H_2}} \approx \sqrt{\frac{\mu_{H_2}}{\mu_{CO}}} = a \quad (58)$$

Substituting equation (58) into equations (56) and (57) and defining

$$G \triangleq \frac{\bar{I}}{mFMP_c} \cdot \frac{1}{(\bar{C}_{H_2} + a \bar{C}_{CO})} \quad (59)$$

gives

$$\dot{N}_{H_2 j} = r_j G C_{H_2} \quad (60)$$

$$\dot{N}_{CO j} = a r_j G C_{CO} \quad (61)$$

The local concentration C_{CO} will be related to the local concentration C_{H_2} . Summation of $\dot{N}_{H_2 j}$, $\dot{N}_{CO j}$ over all the pores at a distance x from the flow channel inlet^j gives $\dot{C}_{H_2}(x)$ and $\dot{C}_{CO}(x)$, the rates of concentration changes of H_2 and CO at location x :

$$\sum_{j=1}^{n_p} \dot{N}_{H_2 j} = \frac{d C_{H_2}(x)}{dt} = \sum_{j=1}^{n_p} r_j G C_{H_2} = M A G C_{H_2}(x) . \quad (62)$$

Similarly,

$$\frac{d C_{CO}(x)}{dt} = a M A G C_{CO}(x) . \quad (63)$$

Equations (62) and (63) can be used to show that:

$$\frac{d C_{CO}(x)}{C_{CO}(x)} = a \frac{d C_{H_2}}{C_{H_2}(x)} . \quad (64)$$

Integration of equation (64) using the boundary condition

$$C_{CO}(0) = C_{CO}^{in} ,$$

$$C_{H_2}(0) = C_{H_2}^{in} ,$$

where C_{CO}^{in} , $C_{H_2}^{in}$ are fuel gas inlet concentrations of H_2 and CO , gives

$$C_{CO}(x) = C_{CO}^{in} \left(\frac{C_{H_2}(x)}{C_{H_2}^{in}} \right)^a \quad (65)$$

Equation (65) permits the evaluation of cell outlet concentrations of fuel reactants H_2 and CO when either the overall cell fuel utilization or the utilization of one of these fuel reactants is prescribed.

For a prescribed value of fuel utilization, the relations developed above permit the computation [by using equation (44)] of flow velocity, U_p , exiting from a pore of given radius, r , at cell locations just within the inlet and just before the outlet of the fuel flow channel. Since the concentrations of C_{H_2} and C_{CO} and of H_2 and CO continually decrease in progressing from the cell fuel channel inlet to the exit as the fuel is utilized, equations (44), (60), and (61) show

that the flow velocity, U_p , from pores continually decreases from inlet to exit. Consequently, evaluation of equation (44) for inlet and exit anode regions bounds the range of pore flow velocities throughout the anode channel length.

The average flow velocity, $\bar{U}(x)$, from the anode, which was discussed earlier, is derived in a manner similar to that described above:

$$\bar{U}(x) = \mu GM [C_{H_2}(x) + aC_{CO}(x)] / \rho_g, \quad (66)$$

$$\begin{aligned} \text{where } \mu &= -\mu_{H_2} + \mu_{H_2O} + \mu_{CO_2} \\ &= -\mu_{CO} + 2\mu_{CO_2}. \end{aligned} \quad (67)$$

The evaluation of pore flow velocities requires the quantification of M defined by equation (52). Since this equation does not express M in terms of readily measurable quantities, the following evaluates M in terms of porosity data commonly available for fuel cell electrodes.

An approach for roughly determining M utilizes the pore size weighting distribution that gives the number, $N(r)$, of pores in a size range dr . Then the summation of equation (52) can be expressed as:

$$M = \sum_{j=1}^{n_p} r_j / A = \frac{1}{A} \int_0^r N(r) dr. \quad (68)$$

The distribution, $N(r)$, can be obtained from the fraction, $Ra(r)$, of cumulative volume, $V(< r)$, of pores with radii less than r divided by the total pore volume, which is frequently measured for fuel cell electrodes using Hg-porosimetry:

$$Ra(r) = \frac{V(< r)}{\gamma AT} = \frac{\int_0^r N(y) dV(y)}{\gamma AT}, \quad (69)$$

where AT is the anode volume (area A times thickness T), γ is anode porosity, and $dV(y)$ is the differential volume of a pore of radius y given for a constant average pore length $\bar{\ell}$ by:

$$V(y) = \pi y^2 \bar{\ell} \quad (70)$$

$$dV(y) = 2\pi \bar{\ell} y dy .$$

Then, substituting of equation (70) into (69) gives:

$$Ra(r) = \frac{2\pi \bar{\ell}}{\gamma AT} \int_0^r N(y) y dy . \quad (71)$$

Differentiating both sides and solving for $N(r)$ yields:

$$N(r) = \frac{\gamma AT}{2\pi \bar{\ell}} \frac{Ra'(r)}{r} dr . \quad (72)$$

so that substituting this result into equation (68) gives:

$$M = \frac{\gamma T}{2\pi \bar{\ell}} \int_0^r \frac{Ra'(r)}{r} dr . \quad (73)$$

In pore model analyses reasonable approximations have been obtained by assuming the pore lengths to be equal to the electrode thickness (i.e., $\bar{\ell} = T$). Using this approximation in equation (73) gives M in terms of commonly measured data for γ , anode porosity, and $Ra(r)$, cumulative pore volume up to radius r over total pore volume.

Experimental and analytical results²⁹ indicate that for efficient MCFC performance, anodes should have only about 5% of their total pore volume filled with the electrolyte. The electrolyte should occupy only the smallest pores, and these should be flooded. Using a cumulative anode pore size distribution,²⁴ $Ra(r)$, (approximated by

straight line segments on a log r scale), which has provided excellent MCFC performance, and a value for r of 1.5 μm , which results in 5% of the total pore volume filled by electrolyte, we have obtained the following value for M:

$$M = 1.45 \times 10^2 / \text{cm}. \quad (74)$$

Although the above determination of M depends on the assumption that all pore lengths are equal to the electrode thickness (a questionable assumption that nevertheless has yielded theoretical results in agreement with fuel cell measurements), the value of M given by equation (74) appears reasonable when compared to an upper bound M_u given by:

$$M_u = \sum_{j=1}^n r_j / A. \quad (75)$$

Here the summation of pore radii is over all n pores in local area A rather than only the flooded pores. Also, the following relation for M_u obtained makes no assumption about the anode pore lengths but does assume a constant ratio of anode pore area to total anode area at each cross section throughout the depth of the anode:

$$M_u = \gamma \bar{r} / (\bar{r}^2 + s^2). \quad (76)$$

Here γ is the anode porosity, while $\bar{r}$ and s are the mean particle radius and standard deviation of the pore size distribution. For the sharply peaked pore size distributions typical of MCFC electrodes, the standard deviation, s, can be neglected without substantial error. Using typical values of 70% anode porosity ($\gamma = 0.7$) and a 5 μm average pore radius ($\bar{r} = 2.5 \times 10^{-4} \text{ cm}$) yields:

$$M_u = 8.9 \times 10^2 / \text{cm}. \quad (77)$$

This value is nearly an order of magnitude higher than the previously calculated value of M, as might be expected, since the summation of

equation (75) for μ is over all pore sizes, while the summation of equation (68) for M is only over the smallest pores, which represent 5% of the anode pore volume.

As indicated earlier, entry into a pore and potential blockage by particles significantly smaller than the pore diameter will be addressed by comparing the particle deposition velocities relative to the average gas flow velocity leaving the pore. Figure 14 shows particle gravitational settling velocities versus particle diameter and average pore flow velocities versus pore diameter for anode regions at the channel exit, where pore flow velocities are lowest. Particle deposition velocities associated with the remaining particle transport mechanisms are considerably lower and are not shown. In all cases these values are more than an order of magnitude lower than pore flow velocities, barely extending past the lower limit of the scale and only for particle diameters smaller than $\sim 1 \mu\text{m}$. Furthermore, for these

Figure 14 -- Pore Flow Velocity vs Particle Settling Velocity

particle diameters thermophoresis and effects of the average flow velocity from the anode described earlier are expected to greatly reduce the number of particles and probably prevent them from approaching the vicinity of pore entrances.

Figure 14 shows that for all particle diameters smaller than pore diameters, flow velocities from pores greatly exceed particle gravitational settling velocities except for those particles with diameters approaching a few microns. At these particle diameters, the settling velocities approach flow velocities from pores of comparable diameters. The results given in Figure 14 indicate that the blockage of flooded pores can be prevented by the gas flowing from those pores, preventing particle entry. Because the maximum flooded pore diameter for the fuel cell evaluated was 3 μm , the flooded pore analytical results cannot be extended to the larger thin film pores. Because of their larger diameters, however, and the lower rates of anode current production, flow velocities from the thin film pores are likely to be much lower than for the flooded pores, so they may be prone to particle entry and blockage. On the other hand, since these larger thin film pores are not the major contributors to MCFC anode current, it is not clear whether the extent of blockage that may occur would result in unacceptable cell performance.

While previous discussions indicated that thermophoresis and the average flow velocity from the anode will greatly inhibit and probably eliminate arrival on the anode of particles smaller than about 1 μm , pore blockage caused by particles larger than 1 μm alighting on the entrances of pores of smaller diameter has not been considered. Determination of particle movement approaching and within a higher velocity "jet" from a pore of comparable or smaller diameter requires a complex modeling and an analytic effort beyond the intent of this initial assesement of fuel cell deposition.

In summary, an initial theoretical treatment of MCFC anode deposition has been provided for anode channel regions beyond the point

at which flow channel entry effects are significant. Dominant particle transport mechanisms have been identified, and relations have been derived for flow velocities from flooded pores that greatly affect anode arrival rates.

Flow velocities from pores decrease in progressing from anode inlet to exit because of the depletion of fuel gas reactants. Since flow from anode pores tends to restrict particle arrival on anode surfaces and entry into pores, the potential for deposition continually increases in progressing from channel inlet to exit. At near-exit regions of highest potential for deposition, flow from anode pores, together with thermophoretic effects, may prevent both particle arrival on anode surfaces and particle entry into pores for particle diameters smaller than about 1 μm . Particles with diameters larger than 1 μm are unlikely to enter flooded pores of somewhat larger diameters but may possibly alight on and block the entrances of pores of significantly smaller diameters. Further theoretical efforts are suggested to determine the pore and particle diameters at which a particle descending toward a relatively smaller pore at a low deposition velocity is repelled by the smaller but relatively higher velocity jet issuing from the pore. Other areas for additional theoretical work include analysis of the average descent velocity for particles larger than 1 μm traversing a field of jets issuing from anode pores of a specified size distribution.

3.2.4 Assessment of Particulate Effects

This section will use the relations derived in Section 3.2.3 to assess particulate effects on MCFC. Figure 15 is a simplified schematic representing a coal gasification/molten carbonate fuel cell power plant. For this plant a coal gasifier produces a fuel gas that passes through a cleanup system to remove most of the entrained particulate and chemical contaminants. The cleaned gases enter the anode sections of the MCFC bank. Figure 10, Section 3.2.1, illustrates one cell of a fuel cell bank. Fuel gas flows through the anode flow

Figure 15 -- Coal gasifier/molten carbonate fuel cell power plant schematic

channels and penetrates the anode pores. Typically, 80 to 90% of the fuel reactants H_2 and CO in the gas react with carbonate ions in the electrolyte that occupies the pores, producing electrons according to the following reactions:

The $CO_3^{=}$ ions utilized in these reactions have migrated to the anode through the electrolyte after being produced in the cathode. Product H_2O and CO_2 of the anode reactions leave the anode pores and enter the fuel channel gas stream.

After leaving the anode sections, the gas enters a catalytic burner, where unreacted fuel is catalytically burned in air. The exhaust from the catalytic burner contains a significant amount of CO_2 . This CO_2 combines with a recycled cathode gas stream and an oxidant gas stream, which contains a significant amount of O_2 . This combined gas stream enters the fuel cell cathode sections. Here the CO_2 and O_2 react to form carbonate ions, using electrons that have been produced in the anodes and have traveled by way of an external circuit to the cathodes. The continuous flow of electrons from anodes to cathodes results in a DC current that is sent through inverters to produce AC power. Heat energy is extracted from the cathode section exhaust gases to produce electric power in the bottoming cycle. The bottoming cycle uses a heat recovery steam generator and turbines driving electric generators. The major portion of gas from the bottoming cycle is recycled to the cathode section inlet, and the remainder is exhausted to the atmosphere.

Several types of coal gasifier processes are candidates for operation with future MCFC power plants. These include fluidized-bed, gravitating-bed, entrained-flow, and molten-salt gasifiers, each of which can produce different fuel gas compositions. Estimated representative gas compositions for these processes are shown in Table 22. These compositions are for gases entering the fuel cells at 10 atm and 650°C (1201°F) after humidification to eliminate carbon particle formation. Cleaning the coal gasifier product gases before they enter the fuel cell banks will probably be accomplished either by cold gas cleaning with wet scrubbers or by hot gas cleaning with ceramic filters for final-stage particulate removal. Gas cleanup with cold gas scrubbers is commercially proved, while hot gas cleaning with ceramic filters is in the initial stages of testing²⁹ and consequently has not been commercially demonstrated. If successfully commercialized, however, hot gas filtration would offer some significant advantages over cold gas wet scrubbing, since thermodynamic losses due to cooling, cleaning, and reheating the gasifier product gases would not be incurred.

Table 22

REPRESENTATIVE MOLE FRACTIONS FOR GASES ENTERING FUEL CELLS^a

	Gasifier A Fluidized Bed (oxygen blown)	Gasifier B Gravitating Bed (air blown)	Gasifier C Entrained (oxygen blown)	Gasifier D Molten Salt (air blown)
H ₂	0.2062	0.1477	0.2048	0.1427
CO	0.0926	0.0664	0.0946	0.0675
CH ₄	0.0918	0.0488	0.0941	0.0434
CO ₂	0.2937	0.1456	0.2948	0.1578
NH ₃	0.0001	0.0004	0.0001	0.0003
H ₂ O	0.3124	0.1548	0.3050	0.1595
N ₂	0.0033	0.4363	0.0066	0.4287

^aData given in this table were derived using as source configurations the Westinghouse fluidized bed, the METC gravitating bed, the Texaco entrained, and the Rockwell molten carbonate gasification systems.

Figure 16 -- Range of Particle Penetration for Scrubber Gas Cleanup Devices

Figure 16 shows penetration fractions (mass of particles passing through divided by mass of particles entering) versus particle diameter for scrubber particulate removal systems. Two curves are given, bounding the performance data measured³⁰ for eight types of scrubbers operating at various commercial plants, including two coal-fired boiler plants. Figure 16 also indicates very low penetration fractions for particles with diameters larger than 1 to 3 μm , so virtually all particles above this size range can be removed from gases by scrubbers. Scrubber performance decreases very rapidly below this size range, however, so only a relatively small fraction of particles can be removed for diameters of a few tenths of a micron up to, depending on the scrubber device, a few microns.

Experimental ceramic fiber hot gas filters have also demonstrated very low particle penetration fractions (less than 0.01) for particle diameters above approximately 1 μm ,²⁹ but like scrubbers, their particle removal performance starts to decrease very rapidly for smaller diameters. The particle carry-over from coal conversion processes ranges in diameter down to about 0.1 μm .^{30,31} Scrubber and hot gas filters are expected to remove virtually all particles with diameters larger than 1 to 3 μm . The following fuel cell evaluations were conducted, therefore, for particle diameters in the 0.1 to 3 μm range. It is in this particle size range that cleanup devices are the least effective; it is also a range in which electrode pores (a typical average anode pore diameter is 5 μm) might be expected to be susceptible to particle blockage.

The conceptual molten carbonate fuel cell (Figure 10) evaluated in this work has operating characteristics that are the objectives of current development work²⁵ for future power plants. The cell produces an average power density of 0.135 W/cm^2 (125 W/ft^2) of cell area at an 0.8 V/cell potential. In future power plants the fuel cell anode inlet gas pressure is assumed to be 1013 kPa (10 atm) and the temperature 650°C (1201°F).

As indicated by Figure 15, the gas leaving the fuel cell anodes is diluted prior to entering the fuel cell cathodes. Since this dilution results in substantially lower particle concentrations in the cathode flow channels than in the anode flow channels, only anode deposition is addressed here.

The low flow velocities [typically less than 30 cm/s (1 ft/sec)] in fuel cell channels is expected to cause negligible erosion. Particles entrained in the gases flowing through electrode channels, however, can degrade fuel cell performance by being deposited on channel surfaces to restrict flow or by entering and blocking pores. Pore blockage could reduce cell output by inhibiting H_2 and CO fuel reactant migration into anode pores and H_2O and CO_2 reaction product migration out of the pores. This would drive reactions given by equations (78) and (79) to the left (opposite from the desired direction).

Particle delivery to anode surfaces and into pores have been evaluated for each of the transport mechanisms listed in Section 3.2.1 above. Brownian diffusion, which transports particles by random impacts with thermally agitated gas molecules, was analyzed using results³² for particle transport in laminar pipe flow. Electrostatic migration due to particles accumulating charges and being driven by the anode-cathode electrostatic force field was evaluated using relations³³ for levels of charges accumulated by particles. Gravitational settling rates were obtained by balancing gravitational and fluid friction forces on the particles. Thermophoretic delivery is associated with particles in a thermal gradient that experiences a net force in the direction from higher to lower temperature caused by the higher intensity of bombardment by the thermally agitated gas molecules on the hotter side than on the cooler side. This effect was analyzed using results³⁴ for thermophoretic forces on particles. Since the fuel gas reactants H_2 and CO entering a pore have lower molecular weights than reaction products [produced according to equations (78) and (79)] leaving the pore, there results a net mass flow rate from anode pores. Convection effects associated with the flow from anode pores influence the delivery of

particles to anode surfaces and their entry into pores. As will be described in more detail in the next section, flow rates from pores have been obtained by extending electrochemical models^{26,27} that have been developed to determine currents generated by individual pores.

Because the reactions of equations (78) and (79) release heat in anode pores, which is predominantly absorbed by the metal (Ni) anode, the anode surface is at a higher temperature than the anode channel gas. As a result, thermophoresis, in addition to providing flow from anode pores, acts in opposition to the other particle transport mechanisms, which tend to deliver particles to the anode surface and pore entrances. Consequently, the intrinsic characteristics of MCFC anodes tend to counter deposition. The extent to which deposition is alleviated will be addressed in the following sections. The results obtained for anode pore flow velocities necessary for these deposition assessments will be described first.

As particles are carried parallel to the anode surface by anode channel flow and slowly descend toward that surface because of the transport mechanisms described earlier, they periodically pass through jets issuing from the anode pores. Each jet tends to slow, or even reverse, particle descent until it is traversed. Whether or not particles can reach the anode surface can be approximately assessed by comparing the near-surface deposition velocities (relative to the flow) for the various particle transport mechanisms to the average flow velocity from the anode, assumed normal to the surface. If the average local flow velocity from the anode exceeds the local deposition velocity, then, based on first-order effects, particles will be unable to reach the anode surface.

If the deposition velocity for a particle is high enough to experience a net descent to the anode surface, it can be deposited at locations between pore entrances or can potentially enter those pores with low exit flow velocities. However, the particle will still be repelled from the entrances of those pores with sufficiently high exit

gas velocities. Neglecting the fluid velocity distribution across the pore diameter, we shall address particle entry into a pore of significantly larger diameter than the particle by comparing the near-surface deposition velocities to the cross-section average flow velocity leaving the pore. If the average pore velocity exceeds the particle local deposition velocity relative to the flow, then, on the basis of first-order effects, the particle will not enter the pore.

Determination of average flow velocities from individual pores and the local average anode flow velocity requires use of detailed information concerning anode characteristics, which we will only summarize here. Electrochemical models for currents generated from individual pores and experiments on bench-scale molten carbonate fuel cells have indicated⁴ that electrodes are permeated with the electrolyte by capillary absorption. The smallest pores, therefore, are filled with electrolyte (flooded pores) up to a diameter above which pores are virtually empty except for a thin electrolyte film on their walls (thin film pores). For efficient operation of molten carbonate fuel cells, only a small fraction (typically about 5%) of anode pore volume is filled and most of the anode current generated is by flooded pores.²⁶ Consequently, a model^{26,27} that has successfully described electrochemical characteristics for flooded pores has been extended to determine flow velocities from pores. The model considers that the smallest pores are flooded up to a diameter (3 μm for the cell analyzed) associated with 5% of the total pore volume occupied by the electrolyte.

On the basis of the above considerations, the average velocity, U_p , of flow from a pore of radius r has been found to depend on the local concentrations, $C_{H_2}(x)$ and $C_{CO}(x)$, of fuel reactants H_2 and CO , the local gas density $\rho(x)$ at distance x along the anode flow channel from the inlet, the average values, $\bar{C}_{H_2}$ and $\bar{C}_{CO}$, of concentrations from the anode channel inlet to exit, the average current density $\bar{I}$ over the total fuel cell area, and the constants H and a , involving anode characteristics and gas species molecular weights, as given by:

$$U_p(x) = \frac{H}{r} \frac{\bar{I}}{\rho(x)} \frac{C_{H_2}(x) + a C_{CO}(x)}{\bar{C}_{H_2} + a \bar{C}_{CO}} \quad (80)$$

This equation shows that the average velocity of gas leaving flooded pores decreases with increasing pore diameter, so the potential for particle entry and blockage increases for larger anode pores. Flow rates from pores increase with increasing average current per cell area, so higher average cell current densities decrease the tendency for particles to enter and block pores. Because H_2 and CO concentrations vary for the output gases of the coal gasifier systems shown in Table 22, the potential for bore blockage is affected by the gasifier type and operating mode (e.g., air blown or oxygen blown). Since the concentrations of the fuel reactants H_2 and CO decrease in progressing from the anode channel inlet to the exit as the fuel is utilized, flow velocities from pores decrease along the channel length. Consequently, beyond upstream channel areas that have inlet flow disturbances (which may enhance local deposition), the tendency is for pore blockage to increase continually from regions just beyond the disturbances to regions at the exit. The potential for pore blockage at downstream channel regions increases with increasing cell fuel utilization and correspondingly decreasing exit concentrations, C_{H_2} and C_{CO} .

The average local flow velocity from the anode has been obtained by dividing the mass flow rate from a local area by the product of that area times the local gas density. A relation similar to equation (80) results, except that the first H/r term is replaced by another coefficient, H_a , involving gas species molecular weights. Because of this similarity, effects on average anode flow velocity and the resulting inhibition of particle arrival on the anode surface are related in the same way as described above — namely, to average cell current density, gasifier type and operating mode, location x from anode channel inlet to exit, and fuel utilization. Effects of these various MCFC power plant system parameters on both particle delivery to anode surfaces and into anode pores are quantified in the following sections.

Figure 17 gives particle deposition velocities (mass arrival rates divided by gas stream particle concentrations) at the anode surface versus particle diameter for the various particle delivery mechanisms described above. The particle size range that is likely to pass a power plant scrubber or filter gas cleanup system is that given in Figure 16. Also indicated in Figure 17 are average flow velocities from the anode surface, at locations near the inlet and near the exit of anode flow channels for the gasifier coal gas compositions given in Table 22 and for 85% fuel utilization in the anode channels. These values bound the decreasing average anode flow velocities over the channel length. As indicated earlier, as a result of first-order effects, if this average flow velocity from the anode surface is greater than the particle deposition velocities toward that surface, the net particle movement is away from the anode so that the particle arrival is prevented.

For anode channel inlet regions, Figure 17 shows that the average anode flow velocity exceeds the particle deposition velocities for all delivery mechanisms and particle diameters of concern. Consequently, particle arrival to anode surfaces near the inlet is expected to be eliminated, or at least substantially reduced. At regions near the anode channel exit and for particle diameters smaller than about $1\text{ }\mu\text{m}$, both the average anode flow and thermophoretic effects that tend to drive particles away from the anode surface are either about the same magnitude or greater than the other mechanisms that tend to deliver particles to that surface. Accordingly, delivery of particles with diameters smaller than about $1\text{ }\mu\text{m}$ to all anode surface locations will probably be either prevented or at least greatly reduced.

As indicated by Figure 17, the above results are not very sensitive to gasifier type, provided that for each system the fuel cell is operated at the same average current density (in this case 0.169 A/cm^2). Utilization significantly affects the average anode flow velocities, however, and the potential for particle arrival at downstream anode regions. Table 23 gives average anode flow velocities for the four gasifier types in Table 22 with the fuel cells operated at

Figure 17 -- Deposition Velocities for Molten Carbonate Fuel Cells

80 and 90% combined H_2 and CO utilization. For all gasifiers the average anode flow velocity near the channel exit at 90% utilization is a factor of about 2.7 lower than that for 80% utilization. The average anode flow near the channel inlet is not greatly affected by either gasifier type or utilization, as shown in Table 23.

Figure 17 indicates that gravitational settling dominates all other particle transport mechanisms at locations near the channel exit for particle diameters larger than about $1\text{ }\mu\text{m}$. Consequently, these larger particles can be delivered to the downstream anode surfaces. Figure 16 shows, however, that the highest efficiency scrubber systems can eliminate virtually all particles with diameters larger than $1\text{ }\mu\text{m}$ from a gas stream. For less efficient scrubbers, which pass particles with diameters from 1 to $3\text{ }\mu\text{m}$, the rates of particle delivery are so low as to restrict anode channel flow only over long durations. Even if we assume that the gas stream particle concentration is 5 ppm in the 1 to

Table 23
AVERAGE ANODE FLOW VELOCITIES

<u>Gasifier</u>	<u>Utilization</u>	<u>Average Anode Flow Velocity at Inlet, cm/s</u>	<u>Average Anode Flow Velocity at Exit, cm/s</u>
A	80%	3.07×10^{-2}	2.17×10^{-3}
	90%	3.30×10^{-2}	8.07×10^{-4}
B	80%	2.92×10^{-2}	2.35×10^{-3}
	90%	3.12×10^{-2}	8.82×10^{-4}
C	80%	3.06×10^{-2}	2.15×10^{-3}
	90%	3.27×10^{-2}	8.00×10^{-4}
D	80%	2.88×10^{-2}	2.31×10^{-3}
	90%	3.08×10^{-2}	8.72×10^{-4}

3 μm range and that all arriving particles stay on the anode surface, the time required to block 10% of an anode channel [0.25 cm (0.1 in) in height] is projected to exceed three years.

Prospects for particle arrival at anode surfaces have been discussed; we shall now consider the ability of arriving particles to enter anode pores. As described earlier, particle entry into pores can be addressed by determining whether the particle deposition velocity (relative to the flow) exceeds the flow velocity leaving a pore for pores significantly larger than the approaching particle. Figure 18 shows the gravitational settling velocity compared to the particle diameter and the pore flow velocity compared to the pore diameter, at regions near the anode channel exit, where pore flow velocities are lowest. Deposition velocities associated with other mechanisms for particle delivery into pores are not shown because they are much lower (by more than an order of magnitude) than pore flow velocities. Furthermore, as described earlier for the particle diameter range below 1 μm , where these other mechanisms are relatively more important than gravitational settling, thermophoresis and the average anode flow are expected to prevent or at least to greatly reduce the arrival of particles at the vicinity of pore entrances.

Figure 18 -- Comparison of Pore Flow Velocities and Gravitational Settling Velocities

Figure 18 indicates that flow velocities from pores greatly exceed particle deposition velocities for all particle diameters smaller than 1 μm . Gravitational settling velocities generally approach and can on special occasions be even greater than pore flow velocities for high fuel utilizations and particle diameters nearing 3 μm . Consequently, the blockage of flooded anode pores by particles of diameter smaller than the pores is in most cases prevented by the gas flow leaving the pores. Particle entry into flooded pores appears possible only for a worst case combination of particle diameters approaching 3 μm , high fuel utilizations, and regions near the anode flow channel exit where pore velocities are lowest. Although the pore flow velocity curves in Figure 18 are for the gas composition of gasifier A, the above conclusions are applicable to all gasifier types in Table 22 since, as indicated earlier, results are not very sensitive to gasifier type.

The above results apply to flooded pores, which have been shown to produce the greatest contribution to anode current. Because of larger diameters and apparently lower rates of fuel reactions, flow rates from thin film pores may be significantly lower than determined above for flooded pores. Accordingly, thin film anode pores may be prone to blockage by particles. The degree of fuel cell performance degradation due to whatever blockage may occur, however, is uncertain, since the thin film pores are not the major contributors to anode current.

Although the above results indicate that particles smaller than $1\text{ }\mu\text{m}$ will probably not arrive on anode surfaces to block channel flow or approach pore entrances and that particles larger than $1\text{ }\mu\text{m}$ in diameter will probably not enter flooded pores of larger diameters, the possibility of particles larger than $1\text{ }\mu\text{m}$ alighting on and blocking the entrances of smaller pores has not yet been addressed. Whether the relatively high velocity but smaller jets issuing from the smaller flooded pores can reverse the relatively slow descent of larger particles requires a detailed theoretical analysis beyond the intent of this initial assessment of MCFC deposition.

3.2.5 Conclusions-Particulate Effects

For future coal gasifier/MCFC power plants, the effects of particulate on fuel cell anode performance may not be as detrimental as perhaps perceived in the past. Inherent characteristics of MCFC anode operation tend to counter deposition. The most productive current generation areas of the anode are also the least prone to deposition.

Increasing average cell current density decreases the potential for fuel cell deposition. The potential for deposition is rather insensitive to variations in gas composition for a range of coal gasifier types and to air-blown versus oxygen-blown gasifier operation, provided the cells are operated at the same average current density in each case. The possibility of channel flow restriction by deposition or pore blockage by particles increases for particle diameters larger than

1 μm , for increasing fuel utilization, and in progressing from the anode flow channel inlet to exit.

Because of gas flow from anode pores and thermophoretic effects, molten carbonate anodes appear capable of absorbing significant concentrations of particles with diameters in the range of from one micron down to a few tenths of a micron. Particles in this diameter range are the most difficult to remove from gases using scrubbers, filters, and other gas cleanup devices. Operation of future MCFC power plant with highly efficient scrubbers or hot gas ceramic filters, capable of removing from the coal gas virtually all particles with diameters larger than 1 μm is expected to result in very little, if any, blockage of anode flow channels or anode pores. (A possible exception may be at regions just inside anode channel inlets, where flow entry effects could cause local deposition.) For less efficient particulate removal, allowing particles up to 3 μm in diameter to enter anode flow channels, slow rates of channel flow restriction due to deposition may occur at downstream anode locations. Particles with diameters larger than 1 μm but somewhat smaller than 3 μm may alight on entrances of smaller pores but do not appear capable of entering flooded pores. Particles in this size range, however, may be capable of entering larger thin film pores. Since these thin film pores are not the major contributors to anode current, the resulting extent of anode performance degradation is uncertain.

Molten carbonate fuel cell cathode deposition has not been considered in this work. Because of net flow of gases into cathode pores, MCFC cathodes may be more susceptible to deposition than anodes. This is true even though particle concentrations are much lower in cathode flow channels. Cathode deposition, however, could be reduced by judicious choices of cathode pore size distributions and cell operating characteristics.

3.3 PERFORMANCE DEGRADATION DUE TO CHEMICAL CONTAMINANTS

3.3.1 Review of Fuel Cell Technology

The molten carbonate fuel cell converts the chemical energy of gasifier fuel gases directly into electricity without an intermediate conversion either to heat or to mechanical energy, as in conventional power systems. The electrochemical fuel cell consists of two porous electrodes separated by an electrolyte contained within a porous matrix (Figure 19). Up to several hundred of these single-cell units can be assembled using sheet metal bipolar plates to form any size cell desired.

Fuel gases from the various gasification systems enter the anode chamber and react electrochemically with the electrolyte in the porous nickel-, cobalt-, or chromium-containing electrode, releasing electrons. Although the fuel gases consist of a mixture of CO, H₂, CH₄, CO₂, H₂O, N₂, H₂S, NH₃, and other trace materials, only H₂ and/or CO are essential constituents in the electrochemical half-cell reaction. At the anode/electrolyte interface, H₂ and CO are converted to H₂O and CO₂, respectively, releasing electrons that are transferred through an external circuit to the cathode. At the porous lithiated nickel oxide cathode, oxidant gases consisting of CO₂ and O₂ combine with the anodically produced electrons and form the carbonate ion CO₃²⁻. The ion is then transferred from the cathode through the 63 wt % (62% Li₂CO₃/38% K₂CO₃)/LiAlO₂ electrolyte to the anode, completing the reaction circuit, at which point the carbonate ion is available to react with fuel gas H₂ and/or CO. This sequence of chemical reactions can be written as:

Overall cell
reaction:

Figure 19 -- Schematic Section of a Carbonate Cell Stack²⁵

The oxidation of the fuel gas CO at the anode/electrolyte interface competes with the more favorable reaction in the bulk gas that converts CO to CO₂ by the water gas shift reaction:

In the fuel gas several additional reactions occur simultaneously. These include:

From these reactions carbon can form within the cell [reaction (86)] unless adequate water is supplied to reduce the local CO concentration and form CO_2 and H_2 [reaction (84)]. This can be achieved either through humidification of the fuel gas entering the anode or through the production of water from the electrochemical half-cell reaction shown in reaction (81a). Carbon, if formed and deposited within the anode gas passage, can restrict the flow of fuel gases through the passage, simultaneously blocking catalytic sites along the nickel anode that are essential to the electrochemical conversion of H_2 to H_2O and CO to CO_2 .

Carbon dioxide, present in the fuel gas and formed at the anode, acts as a diluent, reducing the total partial pressure of hydrogen within the system. Carbon dioxide must be present in the cell to maintain the stability of the $\text{Li}_2\text{CO}_3/\text{K}_2\text{CO}_3$ electrolyte composition at the 923 K (1202°F) operational temperatures considered in this study. The CH_4 concentration at the anode must be reformed through the reaction with water; otherwise, the overall cell efficiency would decrease.

The electrodes generally used in the MCFC have sintered porous structures of nickel or nickel-containing alloy powders. The anode typically is a 0.5 mm thick, 60 to 70 percent porous, nickel material, with a mean pore size of approximately 5 μm , and has been stabilized with additives (C, Cr, Mo, ceramic oxides) against further sintering at fuel cell conditions. The 0.3 mm thick, porous, nickel oxide cathode can be constructed in situ through the oxidation of sintered nickel, resulting in a 70 to 80 percent porous structure with a mean pore size of approximately 10 μm . The cathode is formed in situ by applying a thin layer of loose metal powder to the faces of the electrolyte disc at room temperature. The metal particles become sintered together at operating temperatures. The driving force for sintering in a single phase powder is the reduction of the free energy of the system caused by a reduction in the solid/vapor (or solid/liquid) surface area and, thus, the total surface free energy. Three stages have been distinguished in the course of sintering a powder agglomerate to dense material.^{35,36}

Although they merge continuously into each other, three features are readily identified in each stage. These are:

- Neck Growth. During the first stage in the sintering of loose powder masses, the particles, to a large extent, preserve their original shape but form necks between contacting particles, and any voids that are produced are interconnected.
- Densification and Grain Growth. When the ratio of the neck radius to the particle radius exceeds a certain value, the separate particles begin to lose their identity. Most of the shrinkage takes place at this stage. A coherent network of pores is formed and grain growth continues. When ~ 90% of theoretical density is exceeded, the relative proportion of closed pore spaces increases rapidly.
- Pore Closure. The isolated pores become increasingly spheroidized. Further densification proceeds slowly, and it is often impossible to decide whether this densification has ended.

For cathodes sintered prior to assembling the fuel cell, the loose metal powder is usually heated in a mold at 899 to 1199 K (1160 to 1700°F), forming a consolidated porous structure.

Bacon³⁷ found that the corrosion resistance of the nickel electrode in alkaline fuel cells could be improved by soaking the electrode in a lithium hydroxide solution, then heating it in air at 973 K (1292°F), thus producing a thin surface layer of lithiated-NiO with a much lower concentration of cation vacancies than pure NiO. Nickel oxide is a p-type semiconductor that must be conducting in order to serve as a useful cathode material. The conductivity can alternatively be enhanced by doping with lithium from lithium carbonate (Li₂CO₃) in the molten carbonate electrolyte.³⁸ The incorporation of lithium oxide (Li₂O) into NiO involves the oxidation of Ni²⁺ to Ni³⁺ by

Posttest analysis of NiO cathodes after 7000 hours showed evidence of a NiO diffusion layer in the electrolyte structure on the cathode side. The thickness of the diffusion layer did not show any relation to the number of cell operating hours. Nickel oxide dissolution after long-term exposure, however, may conceivably affect cell performance.

To date, fuel cell components have shown good electrochemical performance and corrosion stability under cell operating conditions over several thousands of hours in the absence of sulfur-containing species in the fuel and oxidant gases. As the nickel electrodes sinter with time, cell performance may be marginally affected. The catalytic activity of the nickel electrode to convert H_2 to H_2O [reactions (88) through (90)] and CO to CO_2 may be poisoned by the chemisorption of H_2S , which is present as a minor constituent in the fuel gases:

Smith³⁹ showed that these reactions were unaffected at H_2S concentrations below 50 ppm and were only moderately affected at higher concentrations. The uptake of sulfur may result in the formation of nickel sulfides at the porous nickel anode, possibly leading to a loss of both structural integrity and electrolytic activity. Under the oxidizing conditions at the cathode, SO_2 can be expected to be readily absorbed into the molten carbonate electrolyte present within the nickel oxide pores.

Sulfur concentrations in the fuel gas, even at low concentrations, can damage the metallic anode components, stainless steel current collector, cell housing, cathode components, electrolyte matrix, and overall fuel cell performance. Several investigations that demonstrate the deleterious effect of sulfur on the various structures are cited in the following discussion.

In a 3 cm² laboratory-scale fuel cell, Claar⁴⁰ demonstrated that the most sulfur-sensitive cell component was the porous, stabilized, nickel anode. An unacceptable initial cell performance loss was observed with sulfur concentrations as low as 10 ppm in either the fuel or the oxidant streams. With the oxidant containing 50 ppm SO_2 and a

low-Btu fuel gas, cell performance decreased because of a lower open-circuit potential (OCP), and a higher electrode polarization, particularly at the anode. In a high-Btu gas, the initial 20 hours of cell operation promoted all of the SO_2 present in the oxidant to be absorbed by the electrolyte and cell components. After 20 hours of operation the amount of sulfur, mainly as H_2S and COS in the fuel outlet, rapidly increased, and after 50 hours practically all of the SO_2 fed into the cathode (32.5 ppm SO_2) emerged as sulfur species (28.5 ppm) in the fuel outlet. When the fuel gas was changed to a low-Btu gas, the concentration of sulfur species coming out in the fuel outlet stream decreased rapidly. From the 39 ppm SO_2 in the oxidant feed, 16 ppm of sulfur was detected in the fuel and 2.5 ppm of sulfur in the oxidant. Anodic losses (i.e., polarization) become increasingly severe when sulfur was present in the fuel gas and, in particular, when a low-Btu fuel gas was used instead of a high-Btu gas. No significant losses were observed to occur at the cathode. Claar also demonstrated that under sulfur-free conditions with a high-Btu fuel gas, the surface area of the electrolyte decreased by 15 percent, but phase stability was maintained within the electrolyte matrix. When the cell was operated with low-Btu fuel gas, significant transformation of $\beta\text{-LiAlO}_2$ to $\alpha\text{-LiAlO}_2$ resulted in the sulfur-free environment.

In the UTC studies⁴¹ a significant increase of approximately 50 mV in the anode polarization at 172 mA/cm^2 could be obtained when the 51.0% H_2 , 10.5% CO_2 , 9.85% CO , and 28.6% H_2O fuel gas contained 6 ppm H_2S . Removal of H_2S from the fuel gas resulted in complete performance recovery.

IGT⁴² demonstrated that the portion of oxidized gas from the anode that was recycled to the cathode could contain 35 to 43 ppm of SO_2 in the 29.1% CO_2 , 14.3% O_2 , 3% H_2O , and 53.6% N_2 oxidant gas. This content had very little effect on the polarization of the NiO cathode in the cell tests after 500 hours at 923 K (1202°F). Cell performance decreased, however, by 158 mV, and anode polarization increased by 95 mV because of the transport of sulfur through the electrolyte and subsequent

reactions with the nickel anode. The transport sulfur reactions through the electrolyte include:

The H_2S reaction with the carbonate fraction of the electrolyte matrix may form sulfites and sulfates at the anode, in addition to the sulfides:

At these sulfur concentrations within the oxidant gas, a significant fraction of the electrolyte is converted to the sulfate, particularly at the cell exit. The presence of sulfate causes a loss in the OCP, consistent with the Nernst equation (see later discussion), as well as with an increase in the slope of the polarization curve. The presence of a large concentration of SO_4^{2-} in the electrolyte apparently has a deleterious effect on the anode performance as well as on the concentration polarization because of loss of the CO_3^{2-} and buffer capacity. Sulfation is not the only mechanism that causes loss of performance. Alternative possibilities may be that adsorbed sulfur compounds concurrently form thionates, thionites, thiosulfates, and thiocarbonates - all contributing to the problem - or that CO and H_2 shift to CO_2 and H_2O may be inhibited.

Samuels⁴³ introduced H_2S into the fuel gas at concentrations of 50 and 1000 ppm. At the higher sulfur concentration, using a low-Btu fuel gas, both nickel and cobalt underwent a negative shift in their

OCP, and he observed higher anodic and cathodic currents than with clean fuels. Exchange currents were unaffected by 50 ppm H_2S in the fuel gas. At higher sulfur concentrations, Samuels observed higher apparent exchange currents, indicating that sulfidation had occurred.

Sulfidation reactions of the electrode surface generally result in the formation of corrosive products. The corrosion rate of nickel either in pure SO_2 or in SO_2/O_2 mixtures has been shown to obey parabolic kinetics,⁴³ which can result in the growth of external NiO and Ni_3S_2 scales. At temperatures above $>918 \text{ K}$ ($>1193^\circ\text{F}$) the eutectic sulfide in contact with the nickel electrode becomes a liquid. Even at 876 K (1117°F) an inner layer of Ni_3S_2 is formed on nickel via diffusion of SO_2 through open channels or crevices in the initial NiO layer. The overall rate is controlled by diffusion of nickel through the continuous Ni_3S_2 phase in the NiO matrix. Extensive sulfidation of both nickel and cobalt is observed when fuel cells are operated with a low-Btu fuel gas containing 1000 ppm H_2S . Under these conditions the OCP is shifted to a more negative value, indicating a mixed potential effect resulting from the oxidation of the fuel gas and the presence of nickel sulfides on the anode surface. At 50 ppm H_2S in the fuel gas, the anode and cathode reaction kinetics do not appear to be drastically affected, although a small lowering in the electrode activity does become apparent at higher applied overpotentials, possibly as a result of changes within the electrolyte or structural changes of the electrode. From the above discussion, sulfur in the gasifier effluents appears to enter the anodic chamber of the fuel cell and has the capability of

- Being adsorbed as a sulfur species on the anode surface
- Sulfiding and subsequently corroding the nickel anode in the reducing environment
- Being released in the anode exhaust and transferred to the cathode primarily as SO_2
- Reacting with the carbonate fraction of the electrolyte matrix, producing sulfate ions.

All of these may lead to an overall loss in cell performance. A minimum tolerance of 1 ppm H_2S on a continuous basis, and up to 10 ppm during surges, should be achieved for functional cell operation.⁶

Sulfur is not the only element in fuel gases that has been shown to affect cell performance. After 22 days of operation at 925 K (1206°F) with a low-Btu fuel gas containing 10 ppm HCl, GE⁴⁴ demonstrated a gradual decay in performance of 200 mV. Posttest analysis of the cell components showed no evidence that related the decline in performance to the presence of HCl in the fuel gas stream. Additional data at GE¹³ indicated that the anode performance was slightly affected after 400 hours when the fuel gas contained 100 ppm HCl, while cathode performance was catastrophically affected when the oxidant gas contained 100 ppm HCl. With 10 ppm HCl in the oxidant gas, stable cathode performance was observed for 120 hours. The evidence indicates that performance decay resulted from both corrosion and chlorination of the electrolyte.

Nitrogen within the fuel and oxidant gases exists predominantly as N_2 , with trace or minor concentrations of NH_3 or nitrogen oxides (NO_x). Although nitrogen is generally considered to act as a diluent within the fuel and oxidant gases, data on the effect of NH_3 or NO_x on cell performance are unavailable. Investigation has shown, however, that NO is absorbed by the $\text{K}_2\text{CO}_3/\text{Li}_2\text{CO}_3/\text{Na}_2\text{CO}_3$ eutectic,¹⁵ while investigations of its absorption within the molten carbonate electrolyte [$\text{LiAlO}_2/(\text{Li}_2\text{CO}_3/\text{K}_2\text{CO}_3)$] have not been undertaken.

IGT⁴⁵ summarizes the maximum allowable impurity levels in the molten carbonate cell. As Table 24 shows, specifications are given only for the major fuel gas constituents and chlorides. Numerous trace and minor constituents, however, are also present in the gasifier effluents as either volatiles or condensates,* the concentrations of which depend on the feedstock composition, the temperature and pressure of the

* Condensate - solids and/or liquids.

Table 24
ESTIMATED MAXIMUM ALLOWABLE IMPURITY LEVELS IN MOLTEN
CARBONATE FUEL CELLS⁴⁵

<u>Impurity</u>	<u>Maximum Limit</u>
CO ₂	Diluent
CH ₄	Diluent/fuel
CO	Fuel
N ₂	Diluent
H ₂ S, SO ₂ , COS	< 1 ppm
C ₂ ⁺	Unknown
HCl (anode)	100 ppm
HCl (cathode)	10 ppm
NH ₃ , NO _x	Unknown
Metal ions (Fe, Cu, etc.)	Unknown

system, and the gas and particulate cleaning systems. Tables 25 through 28 briefly review the various minerals identified in coal,⁴⁶ the general classification^{*} of the various trace and minor elements in the feedstock,⁴⁷ and the concentration of these constituents within coals sampled throughout the United States.^{47,48} Note the variation of the elemental concentrations and phases. Tables 29⁴⁹ and 30⁵⁰ illustrate the partitioning of the trace and minor constituents in resulting ash, char, or tar formations when various feedstocks are gasified in either the Synthane PDU or Lurgi system. The variation of the elemental concentrations within the resulting fractions should again be noted. Very little information is available concerning the fate of trace and minor elements during coal gasification with respect to either their release mechanism from the feedstock or the nature or concentration of the specific chemical complexes. To date, there are essentially no

^{*}Lithophilic - associated with aluminosilicate minerals; chalcophilic - associated with sulfide minerals.

Table 25
MINERALS IDENTIFIED IN COALS⁴⁶

Dwg. 5592C.27

Mineral	Chemical Formula
Clay Minerals	
Montmorillonite	$\text{Al}_2\text{Si}_4\text{O}_{10}(\text{OH})_2 \cdot x \text{H}_2\text{O}$
Illite-sericite	$\text{KAl}_2(\text{AlSi}_3\text{O}_{10})(\text{OH})_2$
Kaolinite	$\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4$
Halloysite	$\text{Al}_4\text{Si}_4\text{O}_{10}(\text{OH})_8$
Chlorite (Prochlorite, Penninite)	$\text{Mg}_5\text{Al}(\text{AlSi}_3\text{O}_{10})(\text{OH})_8$
Mixed-Layer Clay Minerals	
Sulfide Minerals	
Pyrite	FeS_2
Marcasite	FeS_2
Sphalerite	ZnS
Galena	PbS
Chalcopyrite	CuFeS_2
Pyrrhotite	Fe_{1-x}S
Arsenopyrite	FeAsS
Millerite	NiS
Carbonate Minerals	
Calcite	CaCO_3
Dolomite	$(\text{Ca}, \text{Mg})\text{CO}_3$
Siderite	FeCO_3
Ankerite (Ferroan Dolomite)	$(\text{Ca}, \text{Fe}, \text{Mg})\text{CO}_3$
Witherite	BaCO_3
Sulfate Minerals	
Barite	BaSO_4
Gypsum	$\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$
Anhydrite	CaSO_4
Bassanite	$\text{CaSO}_4 \cdot 1/2\text{H}_2\text{O}$
Jarosite	$(\text{Na}, \text{K})\text{Fe}_3(\text{SO}_4)_2(\text{OH})_6$
Szomolnokite	$\text{FeSO}_4 \cdot \text{H}_2\text{O}$
Rozenite	$\text{FeSO}_4 \cdot 4\text{H}_2\text{O}$
Melanterite	$\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$
Coquimbite	$\text{Fe}_2(\text{SO}_4)_3 \cdot 9\text{H}_2\text{O}$
Roemerite	$\text{FeSO}_4 \cdot \text{Fe}_2(\text{SO}_4)_3 \cdot 12\text{H}_2\text{O}$
Mirabilite	$\text{Na}_2\text{SO}_4 \cdot 10\text{H}_2\text{O}$

Table 25 (Continued)

Dwg. 5592C88

Minerals	Chemical Formula
Kieserite	$\text{MgSO}_4 \cdot \text{H}_2\text{O}$
Sideronatrite	$2\text{Na}_2\text{O} \cdot \text{Fe}_2\text{O}_3 \cdot 4\text{SO}_3 \cdot 7\text{H}_2\text{O}$
Chloride Minerals	
Halite	NaCl
Sylvite	KCl
Bischofite	$\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$
Silicate Minerals	
Quartz	SiO_2
Biotite	$\text{K}(\text{Mg}, \text{Fe})_3(\text{AlSi}_3\text{O}_{10})(\text{OH})_2$
Zircon	ZrSiO_4
Tourmaline	$\text{Na}(\text{Mg}, \text{Fe})_3\text{Al}_6(\text{BO}_3)_3(\text{Si}_6\text{O}_{18})(\text{OH})_4$
Garnet	$(\text{Fe}, \text{Ca}, \text{Mg})_3(\text{Al}, \text{Fe})_2(\text{SiO}_4)_3$
Kyanite	Al_2SiO_5
Staurolite	$\text{Al}_4\text{FeSi}_2\text{O}_{10}(\text{OH})_2$
Epidote	$\text{Ca}_2(\text{Al}, \text{Fe})_3\text{Si}_3\text{O}_{12}(\text{OH})$
Albite	$\text{NaAlSi}_3\text{O}_8$
Sanidine	KAlSi_3O_8
Orthoclase	KAlSi_3O_8
Augite	$\text{Ca}(\text{Mg}, \text{Fe}, \text{Al})\text{Si}_2\text{O}_6$
Hornblende	$\text{NaCa}_2(\text{Mg}, \text{Fe}, \text{Al})_5(\text{SiAl})_8\text{O}_{22}(\text{OH})_2$
Topaz	$\text{Al}_2\text{SiO}_4(\text{OH}, \text{F})_2$
Oxide and Hydroxide Minerals	
Hematite	Fe_2O_3
Magnetite	Fe_3O_4
Rutile	TiO_2
Limonite	$\text{FeO} \cdot \text{OH} \cdot n\text{H}_2\text{O}$
Goethite	$\text{FeO} \cdot \text{OH}$
Lepidocrocite	$\text{FeO} \cdot \text{OH}$
Diaspore	$\text{AlO} \cdot \text{OH}$
Phosphate Minerals	
Apatite (Fluorapatite)	$\text{Ca}_5(\text{PO}_4)_3 (\text{F}, \text{Cl}, \text{OH})$

Table 26
CLASSIFICATION OF TRACE AND MINOR ELEMENTS IN COAL⁴⁷

Dwg. 1712890

Element	Classification
Be	Organic Affinity
F	Occurs in Apatite ($\text{Ca}_5(\text{PO}_4)_3(\text{F}, \text{CO}_3)$)
Hg	Inorganic Affinity, Sulfide Minerals
Pb	Chalcophilic; Occurs as Galena (PbS); Inorganic Affinity
Co	Sulfide Minerals/Organometallic Compounds/Chelated Species/Adsorbed Cations
Cr	Sulfide Minerals/Organometallic Compounds/Chelated Species/Adsorbed Cations
Fe	Inorganic Affinity; Sulfide Minerals
Mo	Inorganic Affinity; Sulfide Minerals
Mn	Inorganic Affinity as Carbonates; Mineral Matter
Ni	Sulfide Minerals/Organometallic Compounds/Chelated Species/Adsorbed Cations
Ti	Lithophilic; Organic/Inorganic Affinity
Na	Association with Chlorine; Possible Lithophilic Association
K	Lithophilic; Association with Chlorine
Al	Lithophilic
Si	Lithophilic
Br	Organic Affinity
B	Organic/Inorganic Affinity
P	Organic/Inorganic Affinity; Occurs in Apatite ($\text{Ca}_5(\text{PO}_4)_3(\text{F}, \text{CO}_3)$)
Cu	Sulfide Minerals/Organometallic Compounds/Chelated Species/Adsorbed Cations
V	Organic Affinity with Silicate Minerals; Partial Inorganic Affinity
Zn	Inorganic Affinity; Occurs as Sphalerite (ZnS)
Sb	Organic Affinity; Chalcophilic; Partial Inorganic Affinity
Sn	Possible Inorganic Affinity
Zr	Inorganic Affinity; Mineral Matter
As	Inorganic Affinity; Chalcophilic; Mineral Matter
Cd	Inorganic Affinity; Occurs as Solid Solution with Sphalerite
Se	Sulfide Minerals/Organometallic Compounds/Chelated Species/Adsorbed Cations
Ga	Organic/Inorganic Affinity
Ge	Organic Affinity; Chalcophilic; Inorganic Affinity is Possible

Table 27

CONCENTRATION OF TRACE AND MINOR ELEMENTS IN COALS THROUGHOUT
THE UNITED STATES (ARITHMETIC MEAN VALUES)⁴⁷

Orig. 1/12888

Element	U. S. Mean Coal	Eastern United States	Illinois Basin	Western United States
Be	1.61 ppm	1.3 ppm	1.7 ppm	0.46 ppm
F	60.94 ppm	89 ppm	67 ppm	62 ppm
Hg	0.20 ppm	0.20 ppm	0.2 ppm	0.09 ppm
Pb	34.78 ppm	5.9 ppm	32 ppm	3.4 ppm
Co	9.57 ppm	9.8 ppm	7.3 ppm	1.8 ppm
Cr	13.75 ppm	20 ppm	18 ppm	9.0 ppm
Fe	1.92 %	1.5 %	2.0 %	0.53 %
Mo	7.54 ppm	4.6 ppm	8.1 ppm	2.1 ppm
Mn	49.40 ppm	18 ppm	53 ppm	49 ppm
Ni	21.07 ppm	15 ppm	21 ppm	5.0 ppm
Ti	0.07 %	0.09 %	0.06 %	0.05 %
Na	0.05 %	0.04 %	0.05 %	0.14 %
K	0.16 %	0.25 %	0.17 %	0.05 %
Al	1.29 %	1.7 %	1.2 %	1.0 %
Si	2.49 %	2.8 %	2.4 %	1.7 %
Br	15.42 ppm	12 ppm	13 ppm	4.7 ppm
B	102.21 ppm	42 ppm	110 ppm	56 ppm
P	71.10 ppm	150 ppm	64 ppm	130 ppm
Cu	15.16 ppm	18 ppm	14 ppm	10 ppm
V	32.71 ppm	38 ppm	32 ppm	14 ppm
Zn	272.29 ppm	25 ppm	250 ppm	7.0 ppm
Sb	1.26 ppm	1.6 ppm	1.3 ppm	0.58 ppm
Sn	4.79 ppm	2.0 ppm	3.8 ppm	1.9 ppm
Zr	72.46 ppm	45 ppm	47 ppm	33 ppm
As	14.02 ppm	25 ppm	0.03 ppm	2.3 ppm
Cd	2.52 ppm	0.24 ppm	2.2 ppm	0.18 ppm
Se	2.08 ppm	4.0 ppm	2.2 ppm	1.4 ppm
Ga	3.12 ppm	5.7 ppm	3.2 ppm	2.5 ppm
Ge	6.59 ppm	1.6 ppm	6.9 ppm	0.91 ppm

Table 28

Dwg. 5592C 90

AVERAGE TRACE ELEMENT CONCENTRATION OF ASH FROM U.S. COALS
OF VARIOUS RANK, ppm⁴⁸

Element	Rank	Anthracite Coal	Bituminous Coals			Lignite
			Low Volatility	Medium Volatility	High Volatility	
Be		9	16	13	17	6
F						
Hg						
Pb		81	89	96	183	60
Co		81	172	105	64	45
Cr		304	221	169	193	54
Fe						
Mo						
Mn		270	280	1432	170	688
Ni		220	141	263	154	129
Ti						
Na						
K						
Al						
Si						
Br						
B		90	123	218	770	1020
P						
Cu		405	379	313	293	655
V		248	278	390	249	125
Zn			231	195	310	
Sb						
Sn		962	92	75	171	156
Zr		688	458	326	411	245
As						
Cd						
Se						
Ga		42	41		40	23
Ge						
Representative Partial Structures						

published data on the fate of trace elements in entrained-bed and molten-salt coal gasifiers.

From the TRW⁵¹ survey of the available literature, seven sets of experimental data were compiled pertaining to the fate of trace elements during coal gasification (Table 31). The quantity of trace elements in the product raw gas, designated "emission," was calculated by multiplying the fraction volatilized by either the ppm of the trace element in the coal feed or the total ppm, relative to the coal feed, in all of the effluent streams analyzed. TRW⁵¹ developed Table 32 to identify those elements consistently appearing in the gasifier raw gas. Using the above rationale, they defined trace elements for which 10 percent or more of either the concentration in the coal feed or the total concentration was recovered in the product raw gas in more than 50 percent of the cases analyzed. These were As, B, Be, Bi, Cd, Ce, Cl, F, Ge, Hg, Mo, Pb, S, Sb, Se, Te, Ti, V, Zn, and Zr. In addition, Al, B, Ca, Cl, F, Fe, K, Mg, Na, S, Si, and Ti appear in the product raw gases at concentrations equal to or greater than 50 ppm.

Attari⁵² determined the thermodynamic stability of various trace element compounds in the chemical and physical environment of the hydrogasifier in the Hygas process (Table 33). He also demonstrated that variation in gasifier operating conditions (i.e., $\pm 20\%$ change in temperature or pressure from normal levels) does not ultimately affect the formation of trace element phases. Many of the trace constituents are expected to be present as sulfides and hydrides, as well as in elemental forms, in the gasifier effluent.

We have projected the potential formation of stable phases in equilibrium with gaseous CO, CO₂, CH₄, H₂, H₂O, NH₃, and H₂S in the resulting gasifier solids for the single-staged Westinghouse gasifier operated at 1300 K (1880°F) at 15 atm total pressure with Illinois No. 6, Pittsburgh seam, or Wyoming subbituminous coal under oxygen- or air-blown conditions. These results, presented in Tables 34 through 44 and Figures 20 through 22, indicate that calcium aluminosilicate (CaO·Al₂O₃·2SiO₂),

Table 29
TRACE ELEMENT ANALYSIS AROUND THE SYNTHANE PDU GASIFIER⁴⁹

Stream Element	Feed Coal (ppm)		Filter Fines (ppm)		Char, (ppm)		Tar, (ppm)	
	Run 162	Run 163	Run 162	Run 163	Run 162	Run 163	Run 162	Run 163
Ag	0.01	<0.009	<0.01	<0.054	<0.05	<0.054	-	-
Al	>0.5%	2400	540	1000	1800	790	29	30
As	0.87	1.3	3.7	6.5	6.5	3.3	0.71	1.6
B	86	86	64	32	380	300	12	52
Ba	170	190	130	80	98	98	3.6	6.0
Be	1.5	1.3	7.2	4.6	4.6	2.1	0.03	0.07
Bi	<0.10	<0.10	<1.7	3.1	<0.44	1.2	0.20	0.17
Br	0.23	0.13	0.65	3.2	1.6	1.6	0.02	0.08
Ca	>1%	>1%	>0.5%	>0.5%	>1%	>1%	450	2000
Cd	0.097	0.097	0.88	1.6	1.6	0.77	-	0.15
Ce	47	22	25	22	54	89	0.29	1.5
Cl	93	220	11	33	33	14	1.5	1.2
Co	14	6	17	4.1	95	9.5	0.09	0.35
Cr	170	100	47	120	240	120	7.1	10
Cs	0.26	0.13	1.2	0.33	0.65	0.65	-	0.04
Cu	39	27	70	18	40	40	0.74	6.4
Dy	1.4	0.7	3.9	1.21	1.6	3.4	-	0.10
Er	2.1	1.6	0.41	0.40	0.80	0.54	-	-
Eu	0.55	<0.22	0.39	0.65	0.65	1.3	-	0.02
F	490	420	610	740	150	320	0.97	12
Fe	>1%	>0.5%	>0.5%	>1%	>1%	>1%	240	530
Ga	8.3	5.8	3.6	2.1	4.5	2.1	0.08	0.17
Gd	1.9	0.081	1.2	0.48	0.48	0.95	-	0.01
Ge	1.1	2.1	1.3	2.5	5.4	2.5	0.08	0.08
Hf	0.83	0.73	3.5	2.2	11	1.1	-	0.04
Hg	0.10	0.14	0.20	0.07			1.2	0.47
Ho	0.43	0.19	0.16	0.30	0.45	0.30	-	-
I	0.4	0.23	1.9	2.7	0.27	0.23	0.02	0.08

Table 29 (Continued)

Stream Element	Feed Coal (ppm)		Filter Fines (ppm)		Char, (ppm)		Tar, (ppm)	
	Run 162	Run 163	Run 162	Run 163	Run 162	Run 163	Run 162	Run 163
K	>1%	>0.5%	190	2300	5400	2300	14	130
La	22	11	6.7	7.7	17	7.7	0.03	0.16
Li	0.8	0.8	34	38	67	38	0.51	0.48
Lu	0.085	<0.081	<0.18	0.35	0.40	0.40	-	-
Mg	2800	1600	4600	3500	3500	3500	240	820
Mn	160	220	48	140	240	500	2.2	4.7
Mo	15	11	21	14	14	28	0.31	0.32
Na	1900	1900	>1%	>0.5%	4700	>1%	360	780
Nb	4.7	4.7	7	13	13	6.5	0.08	0.18
Nd	23	23	19	4.6	11	11	0.06	0.31
Ni	43	10	12	11	25	25	1.2	1.6
P	130	63	460	1100	460	2100	14	31
Pb	0.55	1.1	2.2	8.9	21	21	0.22	0.48
Pr	7.3	7.3	7.5	1.8	4.2	4.2	0.02	0.12
Rb	180	67	36	23	27	27	0.10	1.1
S	>1%	>1%	7700	4300	2100	2100	120	1000
Sb	0.18	0.10	0.04	0.95	1.9	0.95	-	-
Sc	5.3	7	6.4	8.3	17	8.3	0.02	0.10
Se	2.2	1.2	15	4.7	4.7	4.7	0.23	0.24
Si	>1%	>1%	>1%	>1%	>1%	>1%	500	4000
Sm	2.7	1.1	0.30	0.86	0.86	1.7	0.01	0.04
Sn	0.6	1.0	0.75	1.4	1.9	1.9	0.03	0.07
Sr	3.3	2.3	44	33	70	70	4.5	9.8
Ta	0.73	0.31	0.64	1.2	1.2	1.2	-	0.02
Tb	0.2	0.086	0.20	0.11	0.89	0.22	-	-
Te	<0.29	<0.29	<0.19	<0.11	0.15	<0.11	-	-
Th	3	6.4	5.8	4.3	4.3	9.2	0.06	0.21
Ti	880	800	1800	590	3300	1700	8.4	67
Tl	<0.12	<0.12	<0.19	0.25	<0.25	<0.25	0.11	0.24

Table 29 (Continued)

Stream Element	Feed Coal (ppm)		Filter Fines (ppm)		Char, (ppm)		Tar, (ppm)	
	Run 162	Run 163	Run 162	Run 163	Run 162	Run 163	Run 162	Run 163
Tm	0.24	0.24	0.10	0.12	0.20	0.13	-	-
U	1.4	3	5.6	2.7	5.4	14	0.01	0.06
V	100	43	44	41	190	95	0.21	2.6
W	0.08	<0.024	2.2	4.8	4.8	9.6	0.09	0.21
Y	21	10	37	9.5	48	20	0.10	0.37
Yb	0.35	0.4	2.7	0.96	2.2	0.96	-	0.03
Zn	25	49	11	48	100	100	0.48	3.3
Zr	10	4.8	22	9.3	28	28	0.26	0.57

Table 30

TRACE ELEMENT ANALYSIS IN LURGI ASHES⁵⁰

Element/Process	Lurgi Ash - Illinois No. 5 Coal, (ppm)	Lurgi Ash - Illinois No.6 Coal, (ppm)	Lurgi Ash - Rosebud Coal, (ppm)
Ag	<0.4	<0.4	< 0.4
Al	95,506	108,121	101,188
Au	<0.001	<0.001	0.007
As	11	3	22
B	465	355	810
Ba	760	950	3,900
Be	15	12	4.3
Br	<1.0	<1.0	<1.0
Ca	22,571	16,652	60,106
Cd	<1.6	<1.6	<1.6
Ce	107	140	105
Cl	80	100	205
Cr	171	212	55
Co	36	34	5.0
Cu	50	57	4 ^a
Cs	10	11	3
Eu	1.7	1.9	1.0
F	<10	<10	300
Fe (total)	151,016	143,780	60,059
Ga	23	26	24
Ge	13	7.0	8.2
Hf	64	6.1	12
Hg	0.05	0.05	0.03
K	12,867	14,611	5,230
La	49	47	47
Li	31	42	65
Lu	1.1	1.5	0.5
Mg	3,618	3,739	21,531
Mn	2,014	1,859	929
Mo	61	30	29
Na	2,152	1,929	74
Ni	195	89	5
Pb	182	45	38
P	218	87	2,095
Rb	180	162	46
S (Total)	5,400	6,100	5,400
Sb	2.8	4.2	12
Sc	23	29	15
Se	<2	<1	<3
Si	245,653	229,946	225,739
Sm	8.2	8.21	66
Sn	-	-	-
Sr	275	370	1,500
Ta	0.9	1.1	1.7
Te	-	-	-
Th	19	21	26
Ti	6,415	6,295	6,475
Tl	4.2	4.6	2.0
U	13	17	8.0
V	172	184	30.8
W	2.2	1.5	5.4
Yb	3.0	2.9	1.8
Zn	1,500	400	31
Zr	185	170	251

Table 31
VOLATILITY AND EMISSION OF COAL TRACE AND MINOR ELEMENTS
DURING GASIFICATION⁵¹⁻⁵⁹

Coal Gasifier Type	North Dakota Lignite Lurgi	Montana Lignite Fluid bed	Illinois No. 5 Lurgi	Illinois No. 6 Lurgi	Illinois No. 6 Fluid bed	Illinois No. 6 Fluid bed
Ag	0	0.011	—	—	0.063	0
Al	92.1	—	—	—	—	0.892
As	0.83	9.33	1.97	0.991	8.25	0.0386
Au	—	—	—	—	—	—
B	1.31	24.2	248	76.0	22.2	69.0
Ba	31.2	0	—	—	0	0.22
Be	6.03×10^{-3}	0.23	0.26	0.34	0.231	1.62×10^{-3}
Bi	0.19	0.315	—	—	0.572	$< 8.27 \times 10^{-3}$
Br	9.52×10^{-3}	—	—	—	—	1.92×10^{-3}
Ca	161.7	0	—	—	1191	—
Cd	< 0.055	0.387	$\sim 3.9 \times 10^{-3}$	0.003	0.682	1.15×10^{-3}
Ce	0.255	—	—	—	—	0.0185
Cl	2.26	85.5	—	—	1706	304
Co	0.041	0	3.96	3.96	0	8.65×10^{-3}
Cr	0.366	3.36	0	0	0	0.22
Cs	0.01	—	—	—	—	3.1×10^{-4}
Cu	0.207	2.75	0	0	0	0.084
Dy	0	—	—	—	—	7.44×10^{-4}
Er	0	—	—	—	—	0
Eu	5.85×10^{-3}	—	—	—	—	1.47×10^{-4}
F	10.49	25.9	56.6	78.5	15.8	49.7
Fe	87.8	0	—	—	1048	—
Ga	0.0354	—	—	—	—	2.5×10^{-3}
Gd	0	—	—	—	—	6.8×10^{-5}
Ge	5.75×10^{-3}	0.619	—	—	0.377	2.34×10^{-3}
Hf	0	—	—	—	—	3.5×10^{-3}
Hg	0.424	0.723	0.198	1.09	0.116	0.057
Ho	0	—	—	—	—	0
I	5.7×10^{-3}	—	—	—	—	1.31×10^{-3}
Ir	—	—	—	—	—	—
K	11.4	10.1	—	—	0	—
La	0.125	—	—	—	—	0.24
Li	0.0485	0	—	—	0	0.016
Lu	0	—	—	—	—	0
Mg	42.2	112	—	—	0	15.4

Table 31 (Continued)

Coal	North Dakota Lignite	Montana Lignite	Illinois No. 5	Illinois No. 6	Illinois No. 6	Illinois No. 6
Gasifier Type	Lurgi	Fluid bed	Lurgi	Lurgi	Fluid bed	Fluid bed
Mn	0.676	0.556	0	2	9.0	0.18
Mo	0.248	0.227	6.3	6.46	0.203	7.9×10^{-3}
Na	165	10.1	-	-	0	27.0
Nb	0.0246	-	-	-	-	2.7×10^{-3}
Nd	0.05	-	-	-	-	4.46×10^{-3}
NI	0.201	2.25	0	0	0.75	0.0497
Os	-	-	-	-	-	-
P	13.8	-	-	-	-	0.58
Pb	0.842	0.894	10.6	1.36	5.35	0.011
Pd	-	-	-	-	-	-
Pr	0.0218	-	-	-	-	1.86×10^{-3}
Pt	-	-	-	-	-	-
Rb	0.12	-	-	-	-	1.2×10^{-3}
Re	-	-	-	-	-	-
Rh	-	-	-	-	-	-
Ru	-	-	-	-	-	-
S	10600	659	-	-	30250	10.8
Sb	0	0.266	0	0.082	0.396	0
Sc	0.074	-	-	-	-	1.1×10^{-3}
Se	0.345	1.13	-	-	5.35	0.16
Si	417	989	-	-	0	-
Sm	0.011	7.34×10^{-3}	-	-	0	2×10^{-3}
Sn	0	0.111	-	-	1.03	1.17×10^{-3}
Sr	4.28	120	-	-	0	0.257
Ta	0	-	-	-	-	1.52×10^{-4}
Tb	0	-	-	-	-	0
Te	0.24	0.182	-	-	3.3	0
Th	0.055	-	-	-	-	2.9×10^{-3}
Tl	5.29	0	-	-	22.4	0.767
Tl	0	-	-	-	-	5.57×10^{-3}
Tm	0	-	-	-	-	0
U	0.0515	-	-	-	-	9.08×10^{-4}
V	0.167	13.4	5.25	1.91	2.96	-
W	0	-	-	-	-	2.77×10^{-3}
Y	0.178	-	-	-	-	-
Yb	0	0.0394	-	-	0.0448	-
Zn	0.38	3.39	60.8	0.79	12.8	15.6
Zr	0.58	2.84	-	-	0	1.82

Table 32

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FREQUENCY OF APPEARANCE OF TRACE ELEMENTS IN COAL GASIFIER
PRODUCT RAW GAS⁵¹

Coal Gasifier	North Dakota Lignite Lurgi	Illinois No. 5 Lurgi	Illinois No. 6 Lurgi	Illinois No. 6 HYGAS	Illinois No. 6 Synthane
Elements More Than 10 % Volatilized during Gasification Based on Both Feed Coal and/or Total Recovered	As	As	As	Ag	Al
	Bi	B	B	As	B
	Cd	Be	Be	B	Ba
	Ce	Cd	Cd	Be	Ce
	Cl	Co	Co	Bi	Cl
	Cs	F	F	Ca	Cr
	Cu	Hg	Hg	Cd	Cu
	F	Mo	Mn	Cl	Dy
	Gd	Pb	Mo	F	Er
	Ge	V	Pb	Ge	F
	Hg	Zn	Sb	Hg	Ga
	La		V	Mn	Gd
	Mo		Zn	Pb	Hg
	Nd			S	Ho
	Ni			Sb	I
	Pb			Se	La
	Pr			Sn	Mg
	Rb			Te	Mn
	S			Ti	Mo
	Sc			V	Nb
	Se			Zn	Nd
	Sr				Ni
	Tb				Pr
	Te				Rb
	Ti				S
	U				Sc
	V				Se
	Zn				Sm
	Zr				Sn
					Ta
					Te
					Th
					Ti
					Tl
					Tm
					V
					Y
					Zn
					Zr

Table 33

THERMODYNAMICALLY STABLE FORMS OF ELEMENTS IN THE HYGAS GASIFIER^{51,58}

<u>Elemental</u>	<u>Sulfide</u>
As	Sb
Bi	Bi
Hg	Cd
Ag	Ca
Sn	Cr
	Co
<u>Oxide</u>	Cu
Be	Fe
Sm	Pb
Si	Mg
Ti	Mn
V	Hg
Yb	Mo
Zr	Ni
	Ag
<u>Hydride</u>	Zn
As	
Cl	<u>Carbonate</u>
F	Ba
Ge	Li
N	K
S	Na
Te	Sr
Se	

Table 34

FEEDSTOCK COMPOSITION AND FEED RATES INTO THE SINGLE-STAGE WESTINGHOUSE GASIFIER

Element, wt %	Illinois No. 6 ⁴⁷		Pittsburgh Seam ^{60,61 *}		Wyoming Sub- ^{47,60,62**} bituminous	
C	70		75.21		51.28	
H	5		5.20		6.44	
N	1.3		1.53		0.75	
O	8.2		8.19		34.83	
S	3.6		2.17		0.51	
Cl	0.14		0.113		0.03	
Si	2.4		1.65		0.75	
Al	1.2		1.06		0.18	
K	0.17		0.062		0.013	
Na	0.05		0.078		0.03	
Fe	2.0		0.72		0.08	
Ca	0.67		0.16		1.06	
Mg	0.05		0.012		0.26	
Ti	0.06		0.056		0.05	
Feed Rate, lb/hr	Oxygen Blown	Air Blown	Oxygen Blown	Air Blown	Oxygen Blown	Air Blown
Coal	100,000	100,000	100,000	100,000	100,000	100,000
Oxidant	58,420	294,650	62,970	324,910	55,040	267,960
Steam	50,000	25,000	50,000	25,000	50,000	25,000

*Pittsburgh Seam: C, H, N, O, S from 60; Cl, Si, Al, K, Na, Fe, Ca, Mg, Ti from 61

**Wyoming Subbituminous: C, H, N, O, S from 60; Cl, Ti from 47; Si, Al, K, Na, Fe, Ca, Mg from 62

Table 35

INFLUENCE OF TOTAL SYSTEM PRESSURE ON EQUILIBRIUM RAW GAS PRODUCTS
AND ASH COMPOSITION

Illinois No. 6 Coal

Oxygen Blown

15 Atmospheres, 1300 K

Raw Gas Composition (mole %)	Moles x 10 ⁶ (lb/hr) Solids	
48.86% CO	0.1951-2 KAlSi_3O_8	(1197.2)
40.25% H_2	0.8900-3 $\text{NaAlSi}_3\text{O}_8$	(514.5)
4.98% H_2O	0.7583-2 $\text{CaO} \cdot \text{Al}_2\text{O}_3 \cdot 2\text{SiO}_2$	(4651.0)
3.49% CO_2	0.1511-3 $\text{Al}_2\text{O}_3 \cdot \text{TiO}_2$	(60.6)
0.95% CH_4	0.4171-3 $\text{FeO} \cdot \text{TiO}_2$	(139.5)
0.72% N_2	0.1507-1 SiO_2	(1996.2)
0.68% H_2S	0.9329-3 MgAl_2O_4	(292.6)
0.03% HCl	0.1583-1 FeS	(3068.0)
0.03% COS		(11919.6 lb/hr)

35 Atmospheres, 1300K

Raw Gas Composition (mole %)	Moles x 10 ⁶ (lb/hr) Solids	
47.77% CO	0.1961-2 KAlSi_3O_8	(1203.3)
36.71% H_2	0.9334-3 $\text{NaAlSi}_3\text{O}_8$	(539.6)
6.23% H_2O	0.7583-2 $\text{CaO} \cdot \text{Al}_2\text{O}_3 \cdot 2\text{SiO}_2$	(4651.0)
4.68% CO_2	0.1246-3 $\text{Al}_2\text{O}_3 \cdot \text{TiO}_2$	(49.9)
3.07% CH_4	0.4436-3 $\text{FeO} \cdot \text{TiO}_2$	(148.4)
0.75% N_2	0.1491-1 SiO_2	(1975.0)
0.70% H_2S	0.9328-3 MgAl_2O_4	(292.6)
0.40% HCl	0.1580-1 FeS	(3062.2)
0.03% COS		(11922.0 lb/hr)

Table 36

PROJECTED RAW GAS COMPOSITION AND SOLIDS FORMED DURING THE
AIR-BLOWN GASIFICATION OF ILLINOIS NO. 6 COAL AT
1300 K (1880°F) AND 15 atm

Raw Gas Composition (mole %)	Moles x 10 ⁶ (lb/hr) Solids		
29.49% CO	0.2407	C	(6373.0)
20.05% H ₂	0.1877-2	KAlSi ₃ O ₈	(1151.8)
0.80% H ₂ O	0.7583-2	CaO·Al ₂ O ₃ ·2SiO ₂	(4651.0)
0.68% CO ₂	0.5682-3	Al ₂ O ₃ ·TiO ₂	(227.8)
0.44% CH ₄	0.5963-3	MgAl ₂ O ₄	(187.0)
48.06% N ₂	0.3365-3	MgSiO ₃	(74.5)
0.42% H ₂ S	0.1522-1	SiO ₂	(2016.1)
0.02% HCl	0.8026-3	NaAlSi ₃ O ₈	(463.9)
0.02% COS	0.1624-1	FeS	<u>(3147.4)</u>
			(18292.5 lb/hr)

Table 37

PROJECTED RAW GAS COMPOSITION AND SOLIDS FORMED DURING THE
OXYGEN-BLOWN GASIFICATION OF PITTSBURGH SEAM COAL AT
1300 K (1880°F) AND 15 atm

Raw Gas Composition (mole %)	Moles x 10 ⁶ (lb/hr) Solids		
50.47% CO	0.6973-3	KAlSi ₃ O ₈	(427.9)
39.74% H ₂	0.1808-2	CaO·Al ₂ O ₃ ·2SiO ₂	(1108.9)
4.02% H ₂ O	0.5296-3	Al ₂ O ₃ ·TiO ₂	(212.3)
3.08% CO ₂	0.5237-2	FeO·Al ₂ O ₃	(2006.7)
1.12% CH ₄	0.2236-3	MgAl ₂ O ₄	(70.1)
0.78% N ₂	0.1641-1	SiO ₂	(2173.7)
0.56% H ₂ S	0.1496-2	NaAlSi ₃ O ₈	(864.8)
0.03% HCl	0.6029-3	FeS	<u>(116.8)</u>
0.02% COS			(6981.2 lb/hr)

Table 38

SOLIDS FORMED AS A FUNCTION OF TEMPERATURE AT 15 atm DURING THE
GASIFICATION OF PITTSBURGH SEAM COAL (OXYGEN-BLOWN)

15 Atm

TEMP. (K)	300	400	500	600	700	800	900	1000	1100	1200	1300
MgCO ₃	✓	✓									
C	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
CaSO ₄ ·2H ₂ O	✓										
H ₂ O	✓										
KAlSi ₃ O ₈	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Al ₂ SiO ₅	✓	✓	✓	✓							
Al ₂ O ₃ ·TiO ₂	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Na ₂ SO ₄	✓										
SiO ₂	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
FeS ₂	✓	✓	✓								
S	✓										
NaCl	✓	✓	✓	✓	✓						
CaCO ₃		✓	✓								
NaAlSi ₃ O ₈		✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CaO·MgO·2SiO ₂			✓		✓	✓	✓				
CaO·Al ₂ O ₃ ·2SiO ₂				✓	✓	✓	✓	✓	✓	✓	✓
FeO·Al ₂ O ₃				✓	✓	✓	✓	✓	✓	✓	✓
MgAl ₂ O ₄				✓				✓	✓	✓	✓
FeO·TiO ₂						✓	✓	✓			
FeS										✓	✓

Heat Exchanger Range

Table 39

PROJECTED RAW GAS COMPOSITION AND SOLIDS FORMED DURING THE
AIR-BLOWN GASIFICATION OF PITTSBURGH SEAM COAL AT
1300 K (1880°F) AND 15 atm

Raw Gas Composition (mole %)	Moles x 10 ⁶ (lb/hr) Solids		
29.63% CO	0.2161	C	(5722.2)
19.19% H ₂	0.6715-3	KAlSi ₃ O ₈	(412.0)
0.77% H ₂ O	0.1808-2	CaO·Al ₂ O ₃ ·2SiO ₂	(1108.9)
0.69% CO ₂	0.5275-2	Al ₂ SiO ₅	(1884.5)
0.41% CH ₄	0.5296-3	Al ₂ O ₃ ·TiO ₂	(212.3)
48.99% N ₂	0.2236-3	MgAl ₂ O ₄	(70.1)
0.28% H ₂ S	0.1137-1	SiO ₂	(1506.1)
0.02% HCl	0.1446-2	NaAlSi ₃ O ₈	(835.9)
0.02% COS	0.5840-2	FeS	(1131.8)
			(12883.9 lb/hr)

Table 40

SOLIDS FORMED AS A FUNCTION OF TEMPERATURE AT 15 atm DURING
THE GASIFICATION OF PITTSBURGH SEAM COAL (AIR-BLOWN)

Pittsburgh Seam Coal: 100,000 lb/hr

Oxidant: 324,910 lb/hr

Steam: 25,000 lb/hr

15 Atm

TEMP. (K)	300	400	500	600	700	800	900	1000	1200	1300
CaCO_3	✓	✓								
MgCO_3	✓	✓								
C	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
H_2O	✓									
KAlSi_3O_8	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Al_2SiO_5	✓	✓	✓	✓					✓	✓
$\text{Al}_2\text{O}_3 \cdot \text{TiO}_2$	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Na_2SO_4	✓									
SiO_2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
FeS_2	✓	✓	✓							
NaCl	✓	✓	✓	✓	✓					
$\text{NaAlSi}_3\text{O}_8$		✓	✓	✓	✓	✓	✓	✓	✓	✓
$\text{CaO} \cdot \text{Al}_2\text{O}_3 \cdot 2\text{SiO}_2$			✓	✓	✓	✓	✓	✓	✓	✓
$\text{CaO} \cdot \text{MgO} \cdot 2\text{SiO}_2$			✓		✓	✓	✓			
$\text{FeO} \cdot \text{Al}_2\text{O}_3$				✓	✓	✓	✓	✓		
MgAl_2O_4				✓				✓	✓	✓
$\text{FeO} \cdot \text{TiO}_2$						✓	✓	✓		
FeS									✓	✓

Heat Exchanger Range

Table 41

PROJECTED RAW GAS COMPOSITION AND SOLIDS FORMED DURING THE
OXYGEN-BLOWN GASIFICATION OF WYOMING SUBBITUMINOUS COAL
AT 1300 K (1880°F) AND 15 atm

Raw Gas Composition (mole %)	Moles x 10 ⁶ (lb/hr) Solids		
27.9% CO	0.1511-2	MgAl ₂ O ₄	(473.9)
31.4% H ₂	0.1576-3	4CaO·3TiO ₂	(161.2)
26.4% H ₂ O	0.1096-2	Ca ₂ SiO ₄	(416.2)
13.5% CO ₂	0.1667-2	Mg ₂ SiO ₄	(517.1)
0.05% CH ₄	0.1759-3	Na ₂ SiO ₃	(47.3)
0.56% N ₂	0.9157-2	CaSiO ₃	(2026.7)
0.15% H ₂ S	0.6489-3	FeO	(204.4)
0.001% HCl			(3846.8 lb/hr)
0.005% COS			

Table 42

SOLIDS FORMED AS A FUNCTION OF TEMPERATURE AT 15 atm DURING
THE GASIFICATION OF WYOMING SUBBITUMINOUS COAL (OXYGEN-BLOWN)

Wyoming Subbituminous Coal: 100,000 lb/hr

Oxidant: 55,040 lb/hr

Steam: 50,000 lb/hr

15 Atm

TEMP. (K)	300	400	500	600	700	800	900	1000	1100	1200	1300
CaCO_3	✓	✓	✓	✓	✓	✓					
MgCO_3	✓	✓									
C	✓	✓	✓	✓	✓	✓	✓	✓			
H_2O	✓										
KAlSi_3O_8	✓	✓	✓	✓	✓						
Al_2SiO_5	✓	✓	✓								
$\text{Al}_2\text{O}_3 \cdot \text{TiO}_2$	✓	✓	✓	✓							
Na_2SO_4	✓										
SiO_2	✓	✓	✓								
FeS_2	✓	✓	✓								
NaCl	✓	✓	✓	✓	✓	✓	✓	✓			
$\text{NaAlSi}_3\text{O}_8$		✓	✓	✓							
$\text{CaO} \cdot \text{MgO} \cdot 2\text{SiO}_2$			✓	✓	✓	✓					
$\text{CaO} \cdot \text{Al}_2\text{O}_3 \cdot 2\text{SiO}_2$				✓							
$\text{FeO} \cdot \text{Al}_2\text{O}_3$				✓	✓	✓					
CaSiO_3				✓	✓	✓	✓	✓	✓	✓	
MgAl_2O_4					✓	✓	✓	✓	✓	✓	✓
NaAlSiO_4					✓						
$\text{CaO} \cdot \text{TiO}_2$					✓	✓					
KCl						✓	✓	✓			
Na_2CO_3						✓	✓	✓	✓		
FeS							✓				
$4\text{CaO} \cdot 3\text{TiO}_2$							✓	✓	✓	✓	✓
Ca_2SiO_4							✓	✓	✓	✓	✓
Mg_2SiO_4							✓	✓	✓	✓	✓
FeO								✓	✓	✓	✓
Na_2SiO_3										✓	✓
Heat Exchanger Range											

Table 43

PROJECTED RAW GAS COMPOSITION AND SOLIDS FORMED DURING THE
AIR-BLOWN GASIFICATION OF WYOMING SUBBITUMINOUS COAL
AT 1300 K (1880°F) AND 15 atm

Raw Gas Composition (mole %)	Moles x 10 ⁶ (lb/hr) Solids		
19.2% CO	0.1511-2	MgAl ₂ O ₄	(473.9)
17.2% H ₂	0.1576-3	4CaO·3TiO ₂	(161.2)
10.5% H ₂ O	0.1089-2	Ca ₂ SiO ₄	(413.5)
6.8% CO ₂	0.1667-2	Mg ₂ SiO ₄	(517.1)
0.01%CH ₄	0.1686-3	Na ₂ SiO ₃	(45.4)
46.2% N ₂	0.9171-2	CaSiO ₃	(2029.8)
0.09%H ₂ S	0.6489-3	FeO	(204.4)
			(3845.4 lb/hr)

Table 44

SOLIDS FORMED AS A FUNCTION OF TEMPERATURE AT 15 atm DURING
THE GASIFICATION OF WYOMING SUBBITUMINOUS COAL (AIR-BLOWN)

Wyoming Subbituminous Coal: 100,000 lb/hr
Oxidant: 267,960 lb/hr
Steam: 25,000 lb/hr

15 Atm

Temp. (K)	300	400	500	600	700	800	900	1000	1100	1200	1300
CaCO ₃	✓	✓	✓	✓	✓	✓					
MgCO ₃	✓	✓									
C	✓	✓	✓	✓	✓	✓	✓				
H ₂ O	✓										
KAlSi ₃ O ₈	✓	✓	✓	✓							
Al ₂ SiO ₅	✓	✓	✓								
Al ₂ O ₃ ·TiO ₂	✓	✓	✓	✓							
Na ₂ SO ₄	✓										
SiO ₂	✓	✓									
FeS ₂	✓	✓	✓								
NaCl	✓	✓	✓	✓	✓	✓	✓	✓			
NaAlSi ₃ O ₈		✓	✓	✓							
CaO·Al ₂ O ₃ ·2SiO ₂			✓	✓							
CaO·MgO·2SiO ₂			✓	✓	✓	✓					
FeO·Al ₂ O ₃				✓	✓						
CaSiO ₃				✓	✓	✓	✓	✓	✓	✓	✓
MgAl ₂ O ₄					✓	✓	✓	✓	✓	✓	✓
NaAlSiO ₄					✓						
KCl					✓	✓	✓	✓			
CaO·TiO ₂					✓						
FeS						✓	✓				
Na ₂ CO ₃						✓	✓	✓			
4CaO·3TiO ₂						✓	✓	✓	✓	✓	✓
Ca ₂ SiO ₄							✓	✓	✓	✓	✓
Mg ₂ SiO ₄							✓	✓	✓	✓	✓
FeO								✓	✓	✓	✓
Na ₂ SiO ₃									✓	✓	✓

Heat Exchanger Range

RAW GAS PRODUCTS

Gas Partial Pressure (atm) at 1300K, 15 atm			
0.7393+1	CO	0.5040-2	HCl
0.6037+1	H ₂	0.4197-2	COS
0.7477	H ₂ O	0.8637-4	HCN
0.5234	CO ₂	0.5257-5	C ₂ H ₆
0.1427	CH ₄	0.2908-3	NaCl
0.1081	N ₂	0.6398-4	KCl
0.1051	H ₂ S	0.245-5	S ₂
		0.120-15	O ₂

Steam: 50,000 lb/hr
Oxidant: 58,420 lb/hr
Coal: Illinois #6
 100,000 lb/hr
 70% C 1.2% Al
 5% H 0.17% K
 1.3% N 0.05% Na
 8.2% O 2.0% Fe
 3.6% S 0.67% Ca
 0.14% Cl 0.05% Mg
 2.4% Si 0.06% Ti

Solids Formed As A Function of Temperature at 15 Atm

TEMP (K)	300	400	500	600	700	800	900	1000	1100	1200	1300
C	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
S	✓										
H ₂ O	✓										
MgCO ₃	✓	✓									
CaSO ₄ ·2H ₂ O	✓										
CaCO ₃		✓									
Al ₂ SiO ₅	✓	✓	✓								
Al ₂ O ₃ ·TiO ₂	✓	✓	✓							✓	✓
FeO·TiO ₂						✓	✓	✓	✓		
FeO·Al ₂ O ₃						✓	✓	✓	✓		
FeS ₂	✓	✓	✓	✓							
FeS						✓	✓	✓	✓	✓	✓
K ₂ SO ₄	✓	✓									
KCl	✓	✓	✓	✓	✓	✓					
KAlSi ₃ O ₈				✓	✓	✓	✓	✓	✓	✓	✓
NaCl	✓										
NaAlSi ₃ O ₈	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
SiO ₂	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CaO·Al ₂ O ₃ ·2SiO ₂				✓	✓	✓	✓	✓	✓	✓	✓
CaO·MgO·2SiO ₂					✓	✓	✓	✓	✓		
MgSiO ₃										✓	✓
MgAl ₂ O ₄										✓	✓

 Heat Exchanger Range

Figure 20 -- Composition of Raw Gas and Ash Products Formed during the Gasification of Illinois No. 6 Coal under Oxygen-Blown Conditions

Figure 21 -- Volatile Hydrocarbon Partial Pressures Formed in the Westinghouse Single-Stage Gasifier as a Function of Temperature at 15 atm Total Pressure over Solid Carbon and Ash Deposits

RAW GAS PRODUCTS

Gas Partial Pressure (atm) at 1300K, 15 atm			
0.4424+1	CO	0.2877-2	HCl
0.3007+1	B ₂	0.3146-2	COS
0.1201	H ₂ O	0.9323-3	HCN
0.1018	CO ₂	0.2278-5	C ₂ H ₄
0.6629-1	CH ₄	0.3499-3	NaCl
0.7209+1	N ₂	0.1807-3	KCl
0.6280-1	H ₂ S	0.376-5	S ₂
		0.125-16	O ₂

Steam: 25,000 lb/hr
Oxidant: 294,650 lb/hr
 21% O₂, 79% N₂
Coal: Illinois #6 100,000 lb/hr
 7.0% C 1.2% Al
 5% H 0.17% K
 1.3% N 0.05% Na
 8.2% O 2.0% Fe
 3.6% S 0.67% Ca
 0.14% Cl 0.05% Mg
 2.4% Si 0.06% Ti

Solids Formed As A Function of Temperature at 15 Atm

TEMP (K)	300	400	500	600	700	800	900	1000	1200	1300
CaCO ₃	✓	✓								
MgCO ₃	✓	✓								
C	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
H ₂ O(l)	✓									
KAlSi ₃ O ₈	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Al ₂ Si ₂ O ₅	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
SiO ₂	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
FeS ₂	✓	✓	✓	✓						
S	✓									
KCl	✓	✓	✓	✓						
NaCl	✓	✓	✓	✓	✓					
Al ₂ O ₃ ·TiO ₂		✓	✓					✓	✓	✓
CaO·Al ₂ O ₃ ·2SiO ₂			✓	✓	✓	✓	✓	✓	✓	✓
CaO·MgO·2SiO ₂			✓	✓	✓	✓	✓			
FeO·Al ₂ O ₃				✓	✓	✓	✓			
FeO·TiO ₂				✓	✓	✓	✓	✓		
FeS				✓	✓	✓	✓	✓	✓	✓
NaAlSi ₃ O ₈					✓	✓	✓	✓	✓	✓
MgAl ₂ O ₄								✓	✓	✓
MgSiO ₃									✓	✓

 Heat Exchanger Range

Figure 22 -- Composition of Raw Gas and Ash Products Formed during the Gasification of Illinois No. 6 Coal under Air-Blown Conditions

iron sulfide (FeS), silica (SiO_2), potassium aluminosilicate (KAlSi_3O_8), and carbon are projected to form as principal solid or condensed equilibrium constituents in the 1300 K (1800°F) gasifier, and sodium silicate (Na_2SiO_3) and aluminosilicate ($\text{NaAlSi}_3\text{O}_8$), magnesium aluminate (MgAl_2O_4), and aluminum-, iron-, and calcium titanates ($\text{Al}_2\text{O}_3 \cdot \text{TiO}_2$, $\text{FeO} \cdot \text{TiO}_2$, $4\text{CaO} \cdot 3\text{TiO}_2$) will form at minor and trace concentrations. In equilibrium with the C, H, N, O, S, Cl, Si, Al, K, Na, Fe, Ca, Mg, and Ti solids are volatile alkali chlorides (NaCl , KCl) and hydroxides [NaOH , $(\text{NaOH})_2$, KOH , $(\text{KOH})_2$] (Table 45).

Projections of the partitioning of additional trace and minor elements into the gasifier solids or effluent have not been made to date.

In order to assess the probable fate of the trace elements in the gas- and particulate-cleaning systems, TRW⁵¹ assembled physical properties for the stable trace element compounds identified in Table 32. These are presented in Table 46. The boiling- and melting-point data for these complexes indicate that the less volatile species (As, Be, Bi, Cd, Hg, Mo, Pb, Sb, Ti, V, Zn, Zr, Ca, Fe, Mg, Na, and K) will condense with coal tar vapor as an aerosol or condense/adsorb on the surfaces of entrained gasified fines at temperatures below 811 K (1000°F). These particulates will be removed when cyclones and scrubbing systems are the principal means of particle removal and will be potentially released in minute quantities when electrostatic precipitators are used. From the TRW solubility data, Cl, F, Na, K, and S appear to be removed from the gasifier raw gas and accumulated in the conventional scrubbing systems.

If the trace and minor elements are released during the gasification process and become entrained in the effluent stream without further removal by the gas- or particulate-cleaning devices, these elements or phases can enter the anode as contaminants in the fuel gas. Park and O'Brien¹⁷ investigated the electrochemical reactivity of several trace constituents [mercury/mercury (II) sulfide (Hg/HgS), lead sulfide (PbS), cadmium sulfide (CdS), tin/tin (II) chloride/tin (IV)

Table 45
PROJECTED ALKALI RELEASE DURING COAL GASIFICATION
IN THE 1300 K (1880°F), 15 atm
WESTINGHOUSE SINGLE-STAGE GASIFIER

<u>Coal, Conditions</u>	<u>pNaCl,* atm</u>	<u>Percent Feedstock Na Released</u>	<u>pKCl, atm</u>	<u>Percent Feedstock K Released</u>
Illinois No. 6, Oxygen Blown	0.2908×10^{-3}	9.79	0.6398×10^{-4}	1.08
Illinois No. 6, Air Blown	0.3499×10^{-3}	18.65	0.1807×10^{-3}	4.82
Pittsburgh Seam, Oxygen Blown	0.1175×10^{-3}	2.65	0.6067×10^{-4}	2.92
Pittsburgh Seam, Air Blown	0.1592×10^{-3}	5.89	0.8223×10^{-4}	6.51
Wyoming Subbituminous, Oxygen Blown	0.6619×10^{-3}	34.82	0.4195×10^{-3}	86.61
Wyoming Subbituminous, Air Blown	0.4432×10^{-3}	37.23	0.2646×10^{-3}	87.25

*Partial pressures of NaOH and KOH and corresponding percent feedstock release are lower than those shown for the chlorides.

Table 46

PHYSICAL PROPERTIES OF TRACE ELEMENT COMPOUNDS AND THEIR POSSIBLE
FATE IN GAS CLEANUP SYSTEMS⁵¹

Compound	Melting Point, °C	Boiling Point, °C	Possible Removal Cleanup System	
			As Particulate/ Aerosol	By Solubility
As	814 (36 atm)	subl 615	Yes	No
AsH ₃	-116.3	-55	No	No
BF ₃	-56	-34	No	No
BeO	2530 ± 30	ca 3900	Yes	No
Bi	271.3	1560 ± 5 (760)	Yes	No
Bi ₂ S ₃	d 685		Yes	No
CdS	1756 (100 atm)	subl in (N ₂) 980	Yes	No
Ce (?)				
HCl	-114.8	-84.9	No	Yes
HF	-83.1	19.54	No	Yes
Ge ₂ H ₆	-109	29; d 215	No	No
Ge ₃ H ₈	-105.6	110.5; d 195	No	No
GeH ₄	-165	-88.5; d 350	No	No
Hg	-38.87	356.9	Yes/No	No
HgS	subl 583.5		Yes	No
Mo ₂ S ₃	d 1100	vol 1200	Yes	No
PbS	1114		Yes	No
H ₂ S	-85.5	-60.7	No	Yes
Sb ₂ S ₃	550	ca 1150	Yes	No
SeH ₂	-60.4	-41.5	No	Yes/No
TeH ₂	-48.9	-2.2 (160)	No	No
TiO ₂	1830-1850	2500-3000	Yes	No
V ₂ O ₃	d 480		Yes/No	?
ZnS	subl 1185		Yes	No
ZrO ₂	ca 2700	ca 5000	Yes	No
Al ₂ O ₃	2072	2980	Yes	No
3Al ₂ O ₃ ·2SiO ₂	1920		Yes	No
CuS	d 2400		Yes	No
FeS	1193-1199	d	Yes	No
FeS ₂	1171		Yes	No
K ₂ CO ₃	891	d	Yes	No
MgS	d > 2000		Yes	No
Na ₂ CO ₃	851	d	Yes	No
SiO ₂	1723 ± 5	2230	Yes	No

d - Decomposes
 Subl - Sublimes
 Vol - Volatilizes
 ca - Calcines

chloride ($\text{Sn}/\text{SnCl}_2/\text{SnCl}_4$), and titanium oxide (TiO_2)] in coal gas at the anode and cathode interface and within the electrolyte. Their calculations indicate that Sn^{2+} , HgS , H_2S , and HCl are candidate phases formed at the nickel anode; mercury could physically interact with the anode, forming an alloy; and Sn , SnCl_2 , H_2S , and HCl are likely to exist at the nickel oxide cathode. Because of the electrochemical nature of the molten carbonate fuel cell, contaminants may be transferred from the anode exhaust to the entrance of the cathode, possibly leading to phase transformations. According to Park and O'Brien the reduced forms of CdS , PbS , TiO_2 , Hg/HgS , and $\text{Sn}/\text{SnCl}_2/\text{SnCl}_4$ can be adsorbed at the electrode surface, degrading the performance of the electrodes to oxidize the fuel gases or to reduce the oxidant source.

At the cathode Sn^{4+} is predicted thermochemically to be reduced to Sn^{2+} , while the remaining elements and phases Park studied remained in their original form. Park proposed that the Sn^{2+} ion was capable of dissolving and accumulating within the electrolyte matrix, while the other contaminants (Sn , Hg , CdS , HgS , and PbS) would accumulate only in the electrolyte or would exist as a separate phase after saturation.

Park proposed that the chemical reactions of the trace species with the fuel cell materials involved either a simple transfer of electrons or the replacement of an element or species. He considered the following reactions at the nickel anode:

Based on the net negative Gibbs free energy for these reactions, only reactions (97), (100), (102), and (103) are likely to occur spontaneously. Reaction (97) will lead to deposition of metallic tin on the anode, reactions (100) and (102) will sulfide the external nickel surface, and reaction (103) will promote dissolution of the anode into a chloride-nickel complex. All these reactions are detrimental to the anode and to the overall cell performance. The deposition of tin or the sulfidation or chlorination of the nickel surface reduces the catalytic activity of the metal by blocking the available sites at which H_2 is converted to H_2O and CO to CO_2 .

Electron transfer reactions at the cathode have been considered. These include:

With the deposition of the n-type SnO_2 film on the cathode, a loss of power could result from a p-n junction of tin with the p-type nickel oxide. Exchange reactions are also likely to occur. These are:

Reactions (109) through (111) have a net negative free energy for the reactions as written and can cause dissolution or sulfidation of the cathode. The remaining species, CdS , PbS , and HgS , which on the basis of thermodynamic equilibrium are expected to remain inert at the cathode, are likely to accumulate within the electrolyte or plug the electrode pores.

In the following series of reactions, reactions (115), (116), and (118) are likely to change the physical properties of the electrolyte matrix, introduce sulfate ions (SO_4^{2-}) in exchange for the electrolyte carbonate ion (CO_3^{2-}) or form deposits of SnO_2 , all of which are potentially detrimental to cell performance:

Efforts by Bloomfield⁶³ supported Park's assessment that the trace species reactions with the nickel electrodes can reduce the active surface area of the catalyst for hydrogen oxidation, which simultaneously can decrease the electronic conductivity of the electrode. Bloomfield also proposed that the trace species reactions within the electrolyte may lead to precipitation or evaporation of the reaction products or alteration of the ionic conductivity within the melt. For 1 atm operations he considered hydrogen bromide (HBr), HCl, hydrogen iodide (HI), hydrogen fluoride (HF), lead chloride (PbCl_2), copper chloride (CuCl_2), and SO_2 to react strongly with the electrolyte melt and NH_3 and boric acid (H_3BO_3) to promote electrolyte loss. Unless high concentrations of COS, PbS, phosphine (PH_3), arsine (AsH_3), or hydrogen cyanide (HCN) were present within the electrolyte matrix, these phases were likely to have little or no effect on the melt. Bloomfield also proposed that HBr, Hg, AsH_3 , PbS, COS, and H_2S would effectively cover 50 percent of the anode when partial pressures as low as 10^{-5} atm were attained, drastically affecting fuel cell performance through this

absorptionlike mechanism.* Similarly, HCl, PH₃, and NH₃ were candidate phases that would lead to 50 percent coverage of the electrode surface for partial pressures as low as 10⁻⁴ atm. A summary of the trace reactions in the molten carbonate fuel cell that Bloomfield considered follows:

Anode or Cathode Surface Absorption Reactions

Anode/Electrolyte Reactions

where $\text{Me}_2\text{CO}_3 = \text{K}_2\text{CO}_3$ or Na_2CO_3 .

Cathode/Electrolyte Reactions

*Cell surface area = $3.5 \times 10^6 \text{ ft}^2$.

Electrolyte Reactions

where $\text{HX} = \text{HF}, \text{HCl}, \text{HBr}, \text{HI}$

The preceeding discussion has alluded to the loss of cell performance through polarization either, for example, when the fuel gas has been modified to reflect a high-Btu or a low-Btu stream or when trace and minor elements are present within the fuel or oxidant gases, promoting chemical reactions or deposition products at the electrode or within the electrolyte matrix. The following discussion reviews polarization within the fuel cell and provides a basis for the final section of this subtask, which considers the fuel cell electrochemistry.

The electrochemical reaction rate in the MCFC is limited by the physical and chemical interactions of either the fuel gas or the oxidant and the electrodes. The reaction may be polarized or retarded by these environments through either a diffusion-limited concentration polarization, or an electron-transfer-limited activation polarization. Polarization is generally defined as a displacement of the electrode potential resulting from a net current. The magnitude of polarization with respect to the equilibrium potential of the electrode⁶⁴ is frequently measured in terms of overvoltage (η). The expression in equation (142) relates the overvoltage as a reduction in voltage from the expected reversible potential (E):

$$\eta = E - V. \quad (142)$$

Hydrogen is adsorbed on the nickel anode surface. An electron transfer occurs through the reaction of the electrolyte carbonate ion and the adsorbed hydrogen, forming H_2O and CO_2 at the fuel cell operating temperatures, where they may remain in contact with the anode surface for a finite time before being released from the anode and carried along in the fuel gas stream.

The exchange current density (i_o) that results is related to the electrochemical reaction rate by:

$$i_o = nFr, \quad (143)$$

where n = number of electrons involved in the reaction

F = Faraday constant

r = reaction rate ($r_{\text{oxidation}} = r_{\text{reduction}}$).

At equilibrium the forward rate of reaction (144) is equal to its reverse reaction rate:

The rate of oxidation is effectively equal to the rate of reduction and therefore exchange current reaction rate can be expressed simply as the sum of the rates of both forward and reverse reactions.

Concentration polarization results when the electrode reaction is hindered by mass transport effects in which the controlling process is governed by slow diffusion in the gas phase through the electrode pores, solution/dissolution of reactants/products into/out of the electrolyte, or diffusion through the electrolyte to the reaction site along the catalyst. With a low hydrogen content within the fuel gas, the electrode reaction is governed by the diffusion processes or by depletion of the reactant resulting from conversion of the initial H_2

concentration into H_2O . When either of these occurs, the limiting diffusion current density, i_L , is attained, and rapid drop in the cell voltage follows. If we apply Fick's law,

$$i_L = \frac{DnFC_B}{x}, \quad (145)$$

where D is the diffusion coefficient of the reacting ions, C_B is the bulk concentration of the reacting ion, and x is the equivalent of the diffusion layer thickness, which is influenced by the geometry of the system. For a system free of activation polarization effects, the concentration overpotential (η_{conc}) becomes:

$$\eta_{conc} = \frac{RT}{nF} \left[1 - \frac{i}{i_L} \right]. \quad (146)$$

Concentration polarization does not become apparent until the net reduction in the current density approaches the limiting current density (Figure 23). When the net reducing current is equal to the limiting diffusion current, the overpotential becomes infinity. As the gas velocity, concentration, or system temperature increases, i_L also increases.

Most chemical reactions involve an energy barrier that must be overcome by the reacting species. This is the activation polarization (η_{act}), and is related to the current, i , by the Tafel equation.

$$\eta_{act} = a + b' \log(i), \quad (147)$$

or

$$i = i_0 \exp(2.3\eta_{act}/b'), \quad (148)$$

where b' is the Tafel slope.

The relation of the overvoltage for activation polarization and the reaction rate is:

Figure 23 -- Concentration Polarization Curve - Reduction Process (from Fontana)⁶⁴

$$\eta_{\text{act}} = \pm \beta \log \left[\frac{i}{i_0} \right], \quad (149)$$

where β = Tafel constant = $\frac{2.3RT}{\alpha nF}$ (150)

α = symmetry coefficient, which expresses the slope of the rate-controlling energy barrier

i = rate of oxidation or reduction in terms of current density

i_0 = exchange current density.

Activation polarization is related to the slow step in the electrochemical reaction sequence, whether that be the adsorption of the reactants onto the electrode surface, the transfer of electrons, or the desorption of the resulting product. It is effectively governed by the reaction sequence at the metal-electrolyte interface, unlike concentration polarization, which is controlled by processes within the bulk

solution rather than at the metal surface. Although the influence of activation polarization is generally evident when the resulting over-voltages are equal to or greater than 50 mV, note that as temperature increases, the activation polarization tends to decrease.

Thus, at the electrode surface a combined polarization results that is the sum of the concentration and activation polarization terms [Equation (151)]:

$$\eta_T = \eta_{act} + \eta_{conc}, \quad (151)$$

where η_T = total overpotential
 η_{act} = activation polarization
 η_{conc} = concentration polarization.

Equation (151) can be rewritten as:

$$\eta_T = \frac{RT}{nF} \log \left[\frac{i}{i_o} \right] + \frac{RT}{nF} \left[1 - \frac{i}{i_L} \right]. \quad (152)$$

If we incorporate equations (145) and (147) into the final equation, η_T becomes

$$\eta_T = [a + b' \log(i)] + \frac{RT}{nF} \ln \left[1 - \frac{i_o \exp(2.3 \eta_{act}/b')}{DnFC_B/x} \right]. \quad (153)$$

Additional losses result when the anode and cathode are connected to an external load, completing the circuit and providing a means by which current flows. Resistance to conducting the ions through the electrolyte, or electrons through the electrodes and current collectors, or contact resistance between the components causes ohmic or iR polarization. The total cell resistance, R , is related to the ohmic polarization and current, as shown in equation (154):

$$R = \frac{\eta_{ohm}}{i} . \quad (154)$$

Taking this into account, the generalized form of the total cell voltage is expressed as:

$$V_{cell} = V_{anode} + V_{cathode} - iR. \quad (155)$$

The overall cell voltage is illustrated schematically in Figure 24. The iR loss can be reduced by using thin electrolyte matrices and efficient contacts between the electrodes and leads. Concentration polarization depends on the mass transport properties of the system, while activation polarization depends on the electrochemical reaction rate, both of which are functions of system temperature and pressure and of species concentrations within the fuel and oxidant gases. An increase in the fuel cell operating temperature increases the electrochemical reaction rate, decreases cell resistance, reduces polarization, increases cell performance, and increases corrosion, recrystallization, and loss of the electrolyte through evaporation. An increase in the fuel cell operating pressure increases the reactant partial pressure, increases gas solubility in the electrolyte, may lead to leakage of the electrolyte through components (i.e., seals), and may enhance carbon deposition and CH_4 formation.

We shall now consider the laws of chemical and electrochemical reactions that must hold within the fuel cell. In the isothermal transfer at both the anode and cathode, the free energy (G) of the system decreases, with the overall reactions in (156) and (157) being thermodynamically spontaneous, as written from left to right,

When the free energy of the system reaches a maximum value, the net reaction ceases and equilibrium is attained. Throughout the remainder

Figure 24 -- Schematic Polarization Curve (from IGT Handbook)⁴⁵

of this section we shall use reaction (156) as the principal reaction to illustrate the details in the cell electrochemistry. The computer model designed for this study, however, incorporates the simultaneous CO reaction with the carbonate ion [reaction (158)]:

At the anode reaction (156) is rearranged so that the sum of the products and reactants is equal to zero:

or, more concisely,

$$\sum_Y \nu_Y M_Y + ne^- = 0, \quad (160)$$

where M_Y represents the fuel gas constituents taking part in the reaction and e^- , the electrons. At equilibrium this can be expressed in the general form

$$-\sum_Y \nu_Y \mu_Y + 23,060nE = 0 \quad (161)$$

as derived from the laws of thermodynamics.⁶⁵ The chemical potentials, μ_Y , are expressed in cal/g mol or cal/g ion, and the electrical potential or electromotive force, E , is in volts. The chemical potential for a given constituent is related to its standard chemical potential, μ'_Y , and concentration, C_Y (for solutes in ideal solutions), or partial pressure, p_Y (for perfect gases), or activity, a_Y , or fugacity, ϕ_Y (for nonideal solutions or gases) as shown below:

$$\mu_Y = \mu'_Y + RT \ln C_Y \quad (162)$$

$$\mu_Y = \mu'_Y + RT \ln p_Y \quad (163)$$

$$\mu_Y = \mu'_Y + RT \ln a_Y \quad (164)$$

$$\mu_Y = \mu'_Y + RT \ln \phi_Y \quad (165)$$

We can rewrite the net anode reaction, therefore, as:

$$[-\mu_{H_2O} - \mu_{CO_2} + \mu_{H_2} + \mu_{CO_3^{2-}}] + nFE_a = 0, \quad (166)$$

or

$$[-\mu'_{H_2O} - RT \ln C_{H_2O} - \mu'_{CO_2} - RT \ln C_{CO_2} + \mu'_{H_2} + RT \ln C_{H_2} + \mu'_{CO_3^{2-}} + RT \ln C_{CO_3^{2-}}] + 2(23,060)E_a = 0. \quad (167)$$

Collecting terms, we rewrite equation (167) as:

$$[-\mu'_{H_2O} - \mu'_{CO_2} + \mu'_{H_2} + \mu'_{CO_3^{2-}}] + RT \ln \left[\frac{C_{CO_3^{2-}} C_{H_2}}{C_{H_2O} C_{CO_2}} \right] + 2(23,060)E_a = 0, \quad (168)$$

or

$$RT \ln \left[\frac{C_{H_2O}^C C_{CO_2}}{C_{CO_3}^{2-} C_{H_2}} \right] = [-\mu_{H_2O}' - \mu_{CO_2}' + \mu_{H_2}' + \mu_{CO_3}^{2-}'] + 2(23,060)E_a. \quad (169)$$

Equation (169) expresses the relation of the concentration of the constituents and the μ_Y' of all reactants and products at the anode with the electrical potential, E_a , at a given temperature. In terms of the standard chemical potentials of the anode reactants and products, E_a^o becomes:

$$E_a^o = \frac{\sum_Y \nu_Y \mu_Y^o}{nF} \quad (170)$$

so that

$$\frac{RT}{nF} \ln \left[\frac{C_{H_2O}^C C_{CO_2}}{C_{CO_3}^{2-} C_{H_2}} \right] = -E_a^o + E_a \quad (171)$$

follows.

Once again, rearranging equation (171), we can express E_a as

$$E_a = E_a^o + \frac{RT}{nF} \ln \left[\frac{C_{H_2O}^C C_{CO_2}}{C_{CO_3}^{2-} C_{H_2}} \right] \quad (172)$$

Similarly, we can write the cathode reactions as follows:

$$\sum_Y \nu_Y \mu_Y + ne^- = 0 \quad (175)$$

$$-\sum_Y \nu_Y \mu_Y + nFE_c = 0 \quad (176)$$

$$[-\mu_{CO_2} - \frac{1}{2} \mu_{O_2} + \mu_{CO_3}^{2-}] + nFE_c = 0 \quad (177)$$

$$[-\mu'_{\text{CO}_2} - RT \ln C_{\text{CO}_2} - \frac{1}{2} \mu'_{\text{O}_2} - RT \ln C_{\text{O}_2}^{1/2} + \mu'_{\text{CO}_3^{2-}} + RT \ln C_{\text{CO}_3^{2-}}] + 2(23,060)E_c = 0 \quad (178)$$

$$[-\mu'_{\text{CO}_2} - \frac{1}{2} \mu'_{\text{O}_2} + \mu'_{\text{CO}_3^{2-}}] + RT \ln \frac{C_{\text{CO}_3^{2-}}}{C_{\text{CO}_2} C_{\text{O}_2}^{1/2}} + 2(23,060)E_c = 0 \quad (179)$$

$$RT \ln \left[\frac{C_{\text{CO}_2}^{1/2} C_{\text{O}_2}^{1/2}}{C_{\text{CO}_3^{2-}}} \right] = [-\mu'_{\text{CO}_2} - \frac{1}{2} \mu'_{\text{O}_2} + \mu'_{\text{CO}_3^{2-}}] + 2(23,060)E_c \quad (180)$$

$$\frac{RT}{nF} \ln \left[\frac{C_{\text{CO}_2}^{1/2} C_{\text{O}_2}^{1/2}}{C_{\text{CO}_3^{2-}}} \right] = -E_c^o + E_c \quad (181)$$

$$E_c = E_c^o + \frac{RT}{nF} \ln \left[\frac{C_{\text{CO}_2}^{1/2} C_{\text{O}_2}^{1/2}}{C_{\text{CO}_3^{2-}}} \right] \quad (182)$$

The overall Nernst equation is:

$$E = E_c - E_a = E_c^o + \frac{RT}{nF} \ln \left[\frac{C_{\text{CO}_2}^{1/2} C_{\text{O}_2}^{1/2}}{C_{\text{CO}_3^{2-}}} \right]_c - E_a^o - \frac{RT}{nF} \ln \left[\frac{C_{\text{H}_2\text{O}} C_{\text{CO}_2}}{C_{\text{CO}_3^{2-}} C_{\text{H}_2}} \right]_a \quad (183)$$

From the overall cell reaction

the difference of the standard emf becomes

$$E_c^o - E_a^o = a_{\text{H}_2} + \frac{1}{2} a_{\text{O}_2} - a_{\text{H}_2\text{O}} = E^o, \quad (185)$$

and equation (183) is rewritten as:

$$E = E^o + \frac{RT}{nF} \ln \left[\frac{C_{CO_2}^{1/2} C_{O_2}^{1/2}}{C_{CO_3}^{2-}} \right]_c \left[\frac{C_{CO_3}^{2-} C_{H_2}}{C_{H_2O} C_{CO_2}} \right]_a, \quad (186)$$

where $(C_{CO_3}^{2-})_c$ equals $(C_{CO_3}^{2-})_a$.

The overall cell potential balance⁶⁶ is:

$$V = -IR + E_c - E_a + \eta_c - \eta_a, \quad (187)$$

where V = terminal voltage

IR = ohm losses

E_c = Nernst potential at the cathode

E_a = Nernst potential at the anode

η_c = cathode overpotential

η_a = anode overpotential.

Making the appropriate substitutions, we can rewrite equation (187) as:

$$V = -IR + E_c^o - E_a^o + \frac{RT}{nF} \ln \left[\frac{C_{CO_2}^{1/2} C_{O_2}^{1/2}}{C_{CO_3}^{2-}} \right]_c - \frac{RT}{nF} \ln \left[\frac{C_{H_2O} C_{CO_2}}{C_{CO_3}^{2-} C_{H_2}} \right]_a + \eta_c - \eta_a, \quad (188)$$

so that T_c may differ from T_a . Linear current overpotential relations are assumed:

$$\eta_a = i_a Z_a \quad (189)$$

$$\eta_c = i_c Z_c = i_a Z_c, \quad (190)$$

where Z_a and Z_c are the effective electrode impedances. The above discussion serves as background, detailing some of the aspects involved in the electrochemical reactions in the fuel cell that are employed in the computer model used in this study.

3.3.2 Selection of Gasifier Gas Cleaning Systems and Definition of the Entering Equilibrium Anode Fuel Gas Compositions

In order to predict the material stability and overall fuel cell performance, we must estimate the composition of the fuel gas entering the anode channel. This section considers the following arbitrarily chosen gasification systems that utilize various hypothetical gas cleaning systems with either an air-blown or an oxygen-blown coal gas as their oxidant source:

1. Rockwell Molten Carbonate Gasifier - Air-Blown Coal Gas System
2. Rockwell Molten Carbonate Gasifier - Air-Blown Coal Gas System - ZnO Polished
3. METC Gasifier - Air-Blown Coal Gas System - FeO/ZnO
4. METC Gasifier - Air-Blown Coal Gas System - FeO
5. Westinghouse Gasifier - Oxygen-Blown Coal Gas System - Dolomite/ZnO
6. Westinghouse Gasifier - Oxygen-Blown Coal Gas System - Selexol/ZnO
7. Texaco Gasifier - Oxygen-Blown Coal Gas System - Benfield/ZnO
8. Texaco Gasifier - Oxygen-Blown Coal Gas System - Molten Carbonate/ZnO.

The systems chosen were intended to typify the molten-carbonate, gravitating-bed, fluidized-bed, and entrained gasification coal gas compositions with a wide variety of desulfurization options. The chemical contaminant model will be designed to accommodate these typical coal gases, although in Section 4 the METC gasifier is removed from consideration.

Hot gas leaving the gasifiers can deposit solid carbon through the decomposition of CO, as shown in the Boudouard reaction:

Temperatures ranging between 773 and 973 K (932 and 1292°F) promote carbon deposition from the CO decomposition reaction in the presence of

nickel, cobalt, or iron surfaces, enhancing the potential for plugging essential electrolyte pores at the anode surface.

Similarly, solid carbon can be formed through the reverse carbon-steam reaction:

In order to minimize carbon deposition from the bulk fuel gases, the gasifier effluent composition was humidified.

The mole fractions of the various bulk gas constituents in the fuel gases produced from the eight gasifier/gas cleaning systems were initially generated by normalizing the hydrogen/carbon ratio (h) and the oxygen content (x) in terms of the chemically active species, CH_4 , CO , CO_2 , H_2 , and H_2O , present at the anode.²⁴ The parameters h and x are defined as follows:

$$h = (2X_{\text{CH}_4} + X_{\text{H}_2} + X_{\text{H}_2\text{O}}) / (3X_{\text{CH}_4} + X_{\text{CO}} + X_{\text{CO}_2} + X_{\text{H}_2} + X_{\text{H}_2\text{O}}) \quad (193)$$

and

$$x = (X_{\text{CO}_2} + X_{\text{H}_2\text{O}} - X_{\text{CH}_4}) / (3X_{\text{CH}_4} + X_{\text{CO}} + X_{\text{CO}_2} + X_{\text{H}_2} + X_{\text{H}_2\text{O}}) . \quad (194)$$

The dewpoint of the gases leaving the gasifier and desulfurization system were adjusted to $h \sim 0.5$ and $x \sim 0.3$ in order to avoid carbon deposition at 923 K (1202°F) if 30 percent nitrogen were present in the system. The resulting humidified, unequilibrated fuel gas compositions are shown in Table 47. Their resulting equilibrium product distributions at 923 K (1202°F) and 1 atm total pressure are shown in Table 48. As adjusted, these compositions do not project the presence of solid carbon in the bulk fuel gases at the anode entrance. When these gas compositions are evaluated on the bases of projecting the resulting equilibrium product distribution at 923 K (1202°F) and 10 atm total pressure, solid carbon is present at equilibrium concentrations of 18 to 23 percent of the total fuel gas carbon content.

Table 47

FUEL GAS COMPOSITIONS

(I) Rockwell Molten Carbonate Gasifier - Air Blown

Gas Location	From 1255K (1800°F), 11.2 atm (150 psig) gasifier		To MCFC at 922K (1200°F), 10.5 atm (140 psig), humidified to 389K (240°F) dew point (25 psi)	
Mole Fractions	CO	0.287	CO	0.245
	H ₂	0.120	H ₂	0.102
	CH ₄	0.017	CH ₄	0.015
	CO ₂	0.028	CO ₂	0.024
	H ₂ O	0.018	H ₂ O	0.161
	N ₂	0.530	N ₂	0.453
Trace Contaminants	NH ₃	15 ppm	NH ₃	10 ppm
	H ₂ S	150 ppm	H ₂ S	100 ppm
	Na ₂ CO ₃	500 ppm	Na ₂ CO ₃	300 ppm
			HCl	nil
			Pb	1 ppm
			As	5 ppm

The gas leaving the gasifier is humidified, but has no other treatment to make it suitable for use in the fuel cells.

Table 47 (Continued)

(II) Rockwell Molten Carbonate Gasifier - Air Blown - Zinc Oxide Polished

Gas Location	From 1255K (1800°F), 11.2 atm (150 psig) gasifier		To MCFC at 922K (1200°F), 10.5 atm (140 psig), humidified to 389K (240°F) dew point (25 psi)	
Mole Fractions	CO	0.287	CO	0.245
	H ₂	0.120	H ₂	0.102
	CH ₄	0.017	CH ₄	0.015
	CO ₂	0.028	CO ₂	0.024
	H ₂ O	0.018	H ₂ O	0.161
	N ₂	0.530	N ₂	0.453
Trace Contaminants	NH ₃	15 ppm	NH ₃	10 ppm
	H ₂ S	150 ppm	H ₂ S	50 ppb
	Na ₂ CO ₃	500 ppm	Na ₂ CO ₃	3 ppm
			HCl	nil
			Pb	1 ppm
			As	5 ppm
			ZnO	100 ppb

The gas leaving the gasifier is humidified and given final ZnO desulfurization prior to entering the fuel cells.

Table 47 (Continued)

(III) METC Gravitating-Bed Gasifier - Air Blown - FeO Desulfurization

Gas Location	From 811K (1000°F), 11.2 atm (150 psig) gasifier			To MCFC at 922K (1200°F), 10.5 atm (140 psig), humidified to 382K (228°F) dew point at 20 psi	
Mole Fractions		<u>Dry</u>	<u>Heated</u>		
	CO	0.217	0.214	CO	0.192
	H ₂	0.158	0.153	H ₂	0.133
	CH ₄	0.303	0.030	CH ₄	0.026
	CO ₂	0.068	0.071	CO ₂	0.061
	H ₂ O	-	0.005	H ₂ O	0.129
	N ₂	0.527	0.527	N ₂	0.458
Trace Contaminants	NH ₃	4400 ppm		NH ₃	2500 ppm
	H ₂ S	5300 ppm		H ₂ S	100 ppm
	HCl	700 ppm		HCl	500 ppm
	Pb	2 ppm		Pb	1.2 ppm
	C	300 ppm		C	200 ppm
	Tar	7000 ppm		Tar	4000 ppm

The gas leaving the gasifier is desulfurized in FeO, and heated at 922 K (1200°F) by O₂ injection to superheat and to avoid tar deposition, prior to entering the fuel cells.

Table 47 (Continued)

(IV) METC Gravitating-Bed Gasifier - Air Blown - FeO/ZnO Desulfurization and Filtered.

Gas Location	From 811K (1000°F), 11.2 atm (150 psig) gasifier			To MCFC at 922K (1200°F), 10.5 atm (140 psig), humidified to 382K (228°F) dew point at 20 psi	
Mole Fractions		Dry	Heated		
	CO	0.217	0.214	CO	0.192
	H ₂	0.158	0.153	H ₂	0.133
	CH ₄	0.030	0.030	CH ₄	0.026
	CO ₂	0.068	0.071	CO ₂	0.061
	H ₂ O	-	0.005	H ₂ O	0.129
	N ₂	0.527	0.527	N ₂	0.458
Trace Contaminants	NH ₃	4400 ppm		NH ₃	2500 ppm
	H ₂ S	5300 ppm		H ₂ S	50 ppb
	HCl	700 ppm		HCl	500 ppm
	Pb	2 ppm		Pb	1.2 ppm
	C	300 ppm		C	3 ppm
	Tar	7000 ppm		Tar	4000 ppm
				ZnO	100 ppb

The gas leaving the gasifier is desulfurized in FeO/ZnO, heated to 922 K (1200°F) by O₂ injection to superheat and filter prior to entering the fuel cells.

Table 47 (Continued)

(V) Westinghouse Fluidized-Bed Gasifier - Oxygen Blown - Dolomite Desulfurization with ZnO.

Gas Location	From 1255K (1800°F), 11.2 atm (150 psig) gasifier		To MCFC at 922K (1200°F), 10.5 atm (140 psig), humidified to 404K (267°F) dew point at 40 psig	
Mole Fractions	CO	0.540	CO	0.3834
	H ₂	0.270	H ₂	0.1917
	CH ₄	0.050	CH ₄	0.0355
	CO ₂	0.135	CO ₂	0.0959
	H ₂ O	-	H ₂ O	0.2900
	N ₂	0.005	N ₂	0.0036
Trace Contaminants	NH ₃	400 ppm	NH ₃	200 ppb
	H ₂ S	5300 ppm	H ₂ S	0.05 ppm
	HCl	700 ppm	HCl	400 ppm
	Pb	2 ppm	Pb	1 ppm
	As	9 ppm	As	5 ppm
	C	3000 ppm	C	3 ppm

The gas leaving the gasifier is desulfurized in a fluidized dolomite system, plus ZnO, and filtered, prior to entering the fuel cells.

Table 47 (Continued)

(VI) Westinghouse Fluidized-Bed Gasifier - Oxygen Blown - Selexol Desulfurization with ZnO.

Gas Location	From 1255K (1800°F), 11.2 atm (150 psig) gasifier		To MCFC at 922K (1200°F), 10.5 atm (140 psig), humidified to 404K (267°F) dew point at 40 psi	
Mole Fractions	CO	0.540	CO	0.3834
	H ₂	0.270	H ₂	0.1917
	CH ₄	0.050	CH ₄	0.0355
	CO ₂	0.135	CO ₂	0.0959
	H ₂ O	-	H ₂ O	0.2900
	N ₂	0.005	N ₂	0.0036
Trace Contaminants	NH ₃	400 ppm	NH ₃	nil
	H ₂ S	5300 ppm	H ₂ S	50 ppb
	HCl	700 ppm	HCl	nil
	Pb	2 ppm	Pb	100 ppb
	As	9 ppm	As	100 ppb
	C	3000 ppm	C	18 ppm
			Polyethylene glycol in dimethyl ether	100 ppb

The gas leaving the gasifier is desulfurized prior to enter the fuel cells.

Table 47 (Continued)

(VII) Texaco Entrained Gasifier - Oxygen Blown - Benfield Desulfurizer with ZnO.

Gas Location	From the gasifier to the Benfield Desulfurizer		From the Benfield Desulfurizer to the MCFC at 922K (1200°F), 10.5 atm (140 psig), humidified to 399K (259°F) dew point at 35 psi	
Mole Fractions	CO	0.390	CO	0.410
	H ₂	0.260	H ₂	0.274
	CH ₄	0.001	CH ₄	0.001
	CO ₂	0.080	CO ₂	0.082
	H ₂ O	0.265	H ₂ O	0.226
	N ₂	0.004	N ₂	0.007
Trace Contaminants	NH ₃	1100 ppm	NH ₃	nil
	H ₂ S	1100 ppm	H ₂ S	50 ppb
	HCl	400 ppm	HCl	nil
	Pb	2 ppm	Pb	1 ppm
	As	5 ppm	As	3 ppm
	C	300 ppm	C	3 ppm
			K ₂ CO ₃	18 ppm

The gas leaving the gas cooling system is desulfurized prior to entering the fuel cells.

Table 47 (Continued)

(VIII) Texaco Entrained Gasifier - Oxygen Blown - Molten Carbonate and ZnO Desulfurization.

Gas Location	From the gasifier to the Desulfurizer		From the ZnO Desulfurizer to the MCFC at 922K (1200°F), 10.5 atm (140 psig), humidified to 399K (259°F) dew point at 35 psi	
Mole Fractions	CO	0.390	CO	0.410
	H ₂	0.260	H ₂	0.274
	CH ₄	0.001	CH ₄	0.001
	CO ₂	0.080	CO ₂	0.082
	H ₂ O	0.265	H ₂ O	0.226
	N ₂	0.004	N ₂	0.007
Trace Contaminants	NH ₃	1100 ppm	NH ₃	1100 ppm
	H ₂ S	1100 ppm	H ₂ S	50 ppb
	HCl	400 ppm	HCl	nil
	Pb	2 ppm	Pb	1 ppm
	As	5 ppm	As	5 ppm
	C	300 ppm	C	3 ppm
			Na ₂ CO ₃	300 ppm

This gas is scrubbed at high temperature and polished of H₂S by ZnO prior to entering the fuel cells.

Table 48

EQUILIBRIUM PRODUCT DISTRIBUTION IN FUEL GASES
AT 923 K, AND 1 ATMOSPHERE PRESSURE

Rockwell

CO 0.2450
H₂ 0.1020
CH₄ 0.0150
CO₂ 0.0240
H₂O 0.1610
N₂ 0.4530

CH ₄	.91669-02	.89818-02	.89818-02	.71524+17	.19046-05	.14706+00
CO ₂	.10792+00	.10574+00	.10574+00	.84202+18	.61509-04	.47494+01
CO	.17592+00	.17237+00	.17237+00	.13726+19	.63817-04	.49276+01
NH ₃	.63466-04	.62205-04	.62205-04	.49535+15	.14003-07	.10812-02
H ₂ O	.62250-01	.60994-01	.60994-01	.48571+18	.14524-04	.11214+01
N ₂	.21232+00	.20803+00	.20803+00	.16566+19	.55435-05	.42804+00
N ₂	.45297+00	.44382+00	.44382+00	.35343+19	.16433-03	.12689+02

THE TRACE VALUES ARE

HCN	.36528-06	.35791-06	.35791-06	.28501+13	.12785-09	.98722-05
CH ₃	.94372-10	.92467-10	.92467-10	.73634+09	.18376-13	.14189-08
C	.38574-32	.37796-32	.37796-32	.30098-13	.60004-36	.46332-31
NH ₂	.58215-12	.57040-12	.57040-12	.45422+07	.12080-15	.93278-11
MN ₃	.23751-23	.23271-23	.23271-23	.18532-04	.13235-26	.10220-21
MNO ₃	.00000	.00000	.00000	.00000	.00000	.00000
MNO ₂	.16889-25	.16548-25	.16548-25	.13178-06	.10283-28	.79400-24
MNO ₂	.22521-25	.22067-25	.22067-25	.17572-06	.13712-28	.10588-23
MNO	.58716-20	.57531-20	.57531-20	.45813-01	.23584-23	.16210-18
H	.10821-09	.10603-09	.10603-09	.84433+09	.14127-14	.10908-09
AO ₃	.00000	.00000	.00000	.00000	.00000	.00000
AO ₂	.21642-28	.21205-28	.21205-28	.16886-09	.12894-31	.99563-27
AO	.49400-16	.48403-16	.48403-16	.38545+05	.19197-19	.14823-14
A	.15726-23	.15409-23	.15409-23	.12270-04	.28528-27	.22028-22
C ₂	.45305-23	.44390-23	.44390-23	.35349-04	.18775-26	.14497-21
C	.25579-22	.25063-22	.25063-22	.19958-03	.53000-26	.40924-21
NH	.14759-20	.14461-20	.14461-20	.11516-01	.28701-24	.22161-19
CH	.35950-13	.35224-13	.35224-13	.28050+06	.79182-17	.61140-12
C	.00000	.91396+00	.00000	.00000	.00000	.00000

Table 48 (cont'd)

METC

CO	0.1920
H ₂	0.1330
CH ₄	0.0260
CO ₂	0.0610
H ₂ O	0.1290
N ₂	0.4580

CH4	.92779-02	.89870-02	.89870-02	.71566+17	.19057-05	.14885+00
CO2	.10462+00	.10134+00	.10134+00	.80701+18	.58952-04	.46044+01
CO	.16510+00	.15992+00	.15992+00	.12735+19	.59210-04	.46246+01
NH3	.69619-04	.67436-04	.67436-04	.53701+15	.15180-07	.11857-02
H2O	.68655-01	.66502-01	.66502-01	.52957+18	.15635-04	.12368+01
H2	.22666+00	.21958+00	.21958+00	.17485+19	.58510-05	.45700+00
N2	.45797+00	.44360+00	.44360+00	.35325+19	.16425-03	.12829+02

THE TRACE VALUES ARE

HCM	.34086-06	.33018-06	.33018-06	.26293+13	.11795-09	.92122-05
CH3	.92971-10	.90056-10	.90056-10	.71714+09	.17897-13	.13978-08
C	.35046-32	.33947-32	.33947-32	.27033-13	.53893-36	.42093-31
NH2	.62138-12	.60189-12	.60189-12	.47930+07	.12747-15	.99564-11
HN3	.24664-23	.23890-23	.23890-23	.19025-04	.13587-26	.10612-21
HNOS	.00000	.00000	.00000	.00000	.00000	.00000
HN02	.18724-25	.18137-25	.18137-25	.14443-06	.11270-28	.68029-24
HN02	.24969-25	.24186-25	.24186-25	.19260-06	.15029-28	.11739-23
HN0	.63017-20	.61041-20	.61041-20	.48608-01	.25023-23	.19544-18
H	.11246-09	.10893-09	.10893-09	.86743+09	.14513-14	.11336-09
NC3	.00000	.00000	.00000	.00000	.00000	.00000
NC2	.23354-28	.22622-28	.22622-28	.18014-09	.13756-31	.10744-26
NC	.51607-16	.49988-16	.49988-16	.39807+03	.19826-19	.15485-14
N	.15904-23	.15405-23	.15405-23	.12267-04	.28521-27	.22276-22
O2	.48902-23	.47369-23	.47369-23	.37721-04	.20035-26	.15648-21
O	.26728-22	.25890-22	.25890-22	.20617-03	.54749-26	.42762-21
NH	.15334-20	.14653-20	.14653-20	.11828-01	.29479-24	.23025-19
OH	.38593-13	.37383-13	.37383-13	.29769+06	.84033-17	.65635-12
C	.00000	.82088+00	.00000	.00000	.00000	.00000

CTS
TRANS

S

Table 48 (cont'd)

Westinghouse

CO	0.3834
H ₂	0.1917
CH ₄	0.0355
CO ₂	0.0959
H ₂ O	0.2900
N ₂	0.0036

CH ₄	.26154-01	.25671-01	.25671-01	.20443+18	.54437-05	.41958+00
CO ₂	.22856+00	.22434+00	.22434+00	.17865+19	.13050-03	.10059+02
CO	.26009+00	.25529+00	.25529+00	.20330+19	.94520-04	.72854+01
NH ₃	.12112-04	.11889-04	.11889-04	.94677+14	.26764-08	.20629-03
H ₂ O	.14800+00	.14527+00	.14527+00	.11568+19	.34591-04	.26662+01
H ₂	.35236+00	.34588+00	.34588+00	.27544+19	.92167-05	.71039+00
N ₂	.35939-02	.35277-02	.35277-02	.28092+17	.13062-05	.10068+00

THE TRACE VALUES ARE

HCN	.43340-07	.42541-07	.42541-07	.33877+12	.15197-10	.11713-05
CH ₃	.20881-09	.20496-09	.20496-09	.16322+10	.40732-13	.31395-08
C	.39815-32	.39079-32	.39079-32	.31120-13	.62041-36	.47819-31
NH ₂	.86137-13	.84550-13	.84550-13	.67329+06	.17906-16	.13802-11
HN ₃	.21063-26	.21264-26	.21264-26	.16933-07	.12093-29	.93211-25
HN ₂ O	.00000	.00000	.00000	.00000	.00000	.00000
HN ₂ O ₂	.39769-26	.39036-26	.39036-26	.31085-07	.24257-29	.18697-24
HN ₂ O	.53032-26	.52054-26	.52054-26	.41452-07	.32347-29	.24932-24
HN ₂	.96518-21	.94739-21	.94739-21	.75443-02	.38837-24	.29934-19
H	.13928-09	.13672-09	.13672-09	.10887+10	.18215-14	.14040-09
NO ₃	.00000	.00000	.00000	.00000	.00000	.00000
NO ₂	.39522-29	.38793-29	.38793-29	.30892-10	.23589-32	.18182-27
NO	.62977-17	.61816-17	.61816-17	.49226+02	.24517-20	.18897-15
N	.13995-24	.13737-24	.13737-24	.10939-05	.25433-28	.19603-23
O ₂	.92800-23	.91090-23	.91090-23	.72537-04	.38527-26	.29695-21
O	.36576-22	.35902-22	.35902-22	.28590-03	.75922-26	.58518-21
NH	.16937-21	.16624-21	.16624-21	.13239-02	.32994-25	.25430-20
OH	.66284-13	.65062-13	.65062-13	.51811+06	.14626-16	.11273-11
C	.00000	.94499+00	.00000	.00000	.00000	.00000

Table 48 (cont'd)

Texaco

CO 0.4100
H₂ 0.2740
CH₄ 0.0010
CO₂ 0.0820
H₂O 0.2260
N₂ 0.0020

CH ₄	.52024-02	.52466-02	.52466-02	.41780+17	.11125-05	.83463-01
HCN	.17738-07	.17889-07	.17889-07	.14245+12	.63903-11	.47940-06
CO ₂	.31229+00	.31494+00	.31494+00	.25079+19	.18320-03	.13744+02
CO	.17551+00	.17700+00	.17700+00	.14095+19	.65533-04	.49163+01
NH ₃	.11349-04	.11446-04	.11446-04	.91145+14	.25765-08	.19329-03
H ₂ O	.22592+00	.22783+00	.22783+00	.18143+19	.54281-04	.40699+01
H ₂	.26866+00	.26792+00	.26792+00	.21335+19	.71391-05	.53557+00
N ₂	.69943-02	.70537-02	.70537-02	.56170+17	.26117-05	.19593+00
C	S .00000	.00000	.00000	.00000	.00000	.00000

THE TRACE VALUES ARE

CH ₃	.47171-10	.47500-10	.47500-10	.37826+09	.94397-14	.70816-09
C	.13182-32	.13293-32	.13293-32	.10586-13	.21104-36	.15832-31
NH ₂	.91679-13	.92457-13	.92457-13	.73626+06	.19581-16	.14690-11
HN ₃	.52268-26	.52711-26	.52711-26	.41975-07	.29979-29	.22490-24
HN ₃	.67557-38	.68231-38	.68231-38	.54334-19	.00000	.42633-36
HN ₂	.19855-25	.20023-25	.20023-25	.15945-06	.12442-28	.93342-24
HN ₂	.26476-25	.26700-25	.26700-25	.21262-06	.16592-28	.12447-23
HN ₂	.23718-20	.23919-20	.23919-20	.19048-01	.98054-24	.73559-19
H	.11929-09	.12030-09	.12030-09	.95797+09	.16028-14	.12024-09
NO ₃	.00000	.00000	.00000	.00000	.00000	.00000
NO ₂	.22424-28	.22614-28	.22614-28	.18008-09	.13751-31	.10316-26
NO	.17588-16	.17737-16	.17737-16	.14125+03	.70347-20	.52774-15
N	.19239-24	.19402-24	.19402-24	.15450-05	.35921-28	.26948-23
O ₂	.37280-22	.37596-22	.37596-22	.29939-03	.15902-25	.11929-20
O	.72325-22	.72939-22	.72939-22	.58083-03	.15424-25	.11571-20
NH	.20485-21	.20660-21	.20660-21	.16452-02	.41003-25	.30760-20
OH	.11573-12	.11631-12	.11631-12	.92620+06	.26145-16	.19614-11

In order to satisfy the condition that solid carbon formations not result in the 10 atm fuel gases entering the anode chamber, a series of calculations were performed (Table 49) varying the fuel gas water content. The equilibrated compositions that minimized carbon formation at 923 K (1202°F) and 10 atm with the least amount of water added to the system were selected, and the initial equilibrium mole fractions of the bulk gas species are summarized in Table 50.

The trace elements and compounds chosen for inclusion in the typical coal gas compositions were those acknowledged by the principal MCFC developers to be potentially troublesome [i.e., arsenic, chlorine (as HCl), and H₂S]. Also, those compounds that would typically be added by desulfurization systems of various types, such as K₂CO₃ from Benfield desulfurization, Na₂CO₃ from molten carbonate desulfurization, and ZnO from zinc oxide polishing desulfurization, were included in the coal gases entering the anode channel.

The composition of the oxidant gas in the air-blown and oxygen-blown coal gas systems is shown in Table 51.

For the 10 atm fuel cell, the anode inlet temperature of 923 K (1202°F) and exhaust stream temperature of 977 K (1299°F) and the cathode inlet temperature of 866 K (1099°F) and exhaust stream temperature of 977 K (1299°F) are used in this study.

3.3.3 Assessment of the Fuel Cell Equilibrium Models

An existing Westinghouse computer routine minimized the free energy for a multicomponent, polyphase system at constant gas temperature and pressure while satisfying the mass balance constraints for a high-temperature, solid oxide electrolyte fuel cell system. The computer routine utilized a linear programming technique,⁶⁷ focusing on the chemical potential of the involved species, but was not able to account for the possible formation of carbon within the fuel gas. Basically, the only species property required is the molal standard Gibbs free energy function G^0/RT . For a mixture of n chemical species

Table 49
EQUILIBRIUM GAS/SOLID PRODUCT DISTRIBUTION IN 923 K,
10 atm GASIFICATION SYSTEMS

Rockwell Molten Carbonate Air-Blown Gas

CO 0.1754
H₂ 0.0733
CH₄ 0.0104
CO₂ 0.0171
H₂O 0.4000
N₂ 0.3238

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.21890-01	.22403-01	.22403+00	.17640+19	.47506-04	.35103+00
HCN	.10444-06	.10694-06	.10694-05	.65155+13	.38200-09	.28226-05
CO ₂	.14223+00	.14563+00	.14563+01	.11597+20	.84712-03	.62594+01
CO	.38793-01	.39720-01	.39720+00	.31630+19	.14706-03	.10866+01
NH ₃	.37865-03	.38769-03	.38769-02	.30873+17	.87274-06	.64487-02
H ₂ O	.28635+00	.29320+00	.29320+01	.23348+20	.69815-03	.51587+01
H ₂	.16342+00	.16732+00	.16732+01	.13324+20	.44586-04	.32945+00
N ₂	.32361+00	.33134+00	.33134+01	.26386+20	.12269-02	.90653+01
C	S .00000	.00000	.00000	.00000	.00000	.00000

THE TRACE VALUES ARE

CH ₃	.79426-10	.81324-10	.81324-09	.64761+10	.16161-12	.11942-08
C	.14233-33	.14573-33	.14573-32	.11605-13	.23136-36	.17095-32
NH ₂	.12243-11	.12535-11	.12535-10	.99822+08	.26548-14	.19616-10
NH ₃	.13144-22	.13463-22	.13463-21	.10721-02	.76567-25	.56576-21
HNO ₃	.31305-36	.32053-36	.32053-35	.25525-16	.26697-38	.19726-34
HNO ₂	.44734-24	.45603-24	.45603-23	.36474-04	.28462-26	.21031-22
HNO	.59653-24	.61078-24	.61078-23	.48638-04	.37954-26	.28044-22
H ₂ O	.26022-19	.26644-19	.26644-18	.21217+01	.10922-21	.80704-18
H ₂	.29368-10	.30070-10	.30070-09	.23945+10	.40063-14	.29603-10
H	.00000	.00000	.00000	.00000	.00000	.00000
NO ₃	.20212-27	.20695-27	.20695-26	.16480-07	.12584-29	.92987-26
NO ₂	.77197-16	.79042-16	.79042-15	.62943+04	.31349-18	.23164-14
N	.41119-24	.42102-24	.42102-23	.33527-04	.77947-27	.57595-23
O ₂	.15486-22	.15856-22	.15856-21	.12626-02	.67063-25	.49553-21
O	.14679-22	.14979-22	.14979-21	.11928-02	.31676-25	.23405-21
NH	.10945-20	.11206-20	.11206-19	.89238-01	.22240-23	.16433-19
OH	.58311-13	.59704-13	.59704-12	.47544+07	.13421-15	.99169-12

CO 0.1900
H₂ 0.0794
CH₄ 0.0112
CO₂ 0.0185
H₂O 0.3500
N₂ 0.3508

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.31486-01	.32000-01	.32000+00	.25483+19	.67857-04	.50513+00
HCN	.15298-06	.15548-06	.15548-05	.12381+14	.55541-09	.41345-05
CO ₂	.14225+00	.14457+00	.14457+01	.11513+20	.84099-03	.62603+01
CO	.45966-01	.46717-01	.46717+00	.37202+19	.17296-03	.12675+01
NH ₃	.40300-03	.40958-03	.40958-02	.32616+17	.92201-06	.68634-02
H ₂ O	.24654+00	.25057+00	.25057+01	.19953+20	.59664-03	.44414+01
H ₂	.16063+00	.16941+00	.16941+01	.13490+20	.45142-04	.33604+00
N ₂	.35060+00	.35633+00	.35633+01	.28375+20	.13194-02	.98213+01
C	S .00000	.00000	.00000	.00000	.00000	.00000

THE TRACE VALUES ARE

CH ₃	.11354-09	.11544-09	.11544-08	.91932+10	.22942-12	.17078-08
C	.19980-33	.20306-33	.20306-32	.16170-13	.32238-36	.23998-32
NH ₂	.12950-11	.13161-11	.13161-10	.10481+09	.28774-14	.20749-10
NH ₃	.14864-22	.15107-22	.15107-21	.12030-02	.85918-25	.63957-21
HNO ₃	.19790-36	.20113-36	.20113-35	.16017-16	.16752-38	.12470-34
HNO ₂	.33504-24	.34051-24	.34051-23	.27116-04	.21160-26	.15751-22
HNO	.44677-24	.45407-24	.45407-23	.36159-04	.28216-26	.21004-22
H ₂ O	.23089-19	.23467-19	.23467-18	.18687+01	.96196-22	.71609-18
H ₂	.29770-10	.30257-10	.30257-09	.24094+10	.40312-14	.30009-10
H	.00000	.00000	.00000	.00000	.00000	.00000
NO ₃	.15043-27	.15290-27	.15290-26	.12176-07	.92978-30	.69213-26
NO ₂	.68075-16	.69187-16	.69187-15	.55095+04	.27400-18	.20426-14
N	.42958-24	.43660-24	.43660-23	.34767-04	.40832-27	.60171-23
O ₂	.11113-22	.11297-22	.11297-21	.89959-03	.47780-25	.35567-21
O	.12440-22	.12643-22	.12643-21	.10068-02	.26737-25	.19903-21
NH	.11505-20	.11693-20	.11693-19	.93115-01	.23207-23	.17275-19
OH	.49893-13	.50708-13	.50708-12	.40380+07	.11399-15	.84853-12

Table 49 (cont'd)

Rockwell Molten Carbonate Air-Blown Gas

CO 0.2046
 H₂ 0.0855
 CH₄ 0.0121
 CO₂ 0.0200
 H₂O 0.3000
 N₂ 0.3778

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.34249-01	.35850-01	.35850+00	.28549+19	.76021-04	.54946+00
CO ₂	.14653+00	.15548+00	.15548+01	.12381+20	.90443-03	.65370+01
CO	.53917-01	.56437-01	.56437+00	.44942+19	.20695-03	.15103+01
NH ₃	.35693-03	.37361-03	.37361-02	.29752+17	.84104-06	.60789-02
H ₂ O	.19362+00	.20267+00	.20267+01	.16139+20	.48258-03	.34680+01
H ₂	.14705+00	.15392+00	.15392+01	.12257+20	.41016-04	.29645+00
N ₂	.37762+00	.39527+00	.39527+01	.31477+20	.14636-02	.10578+02

THE TRACE VALUES ARE

HCN	.20237-06	.21183-06	.21183-05	.16869+14	.75671-09	.54693-05
CH ₃	.12963-09	.13568-09	.13568-08	.10605+11	.26964-12	.19489-08
C	.26326-33	.27557-33	.27557-32	.21944-13	.43749-36	.31621-32
NH ₂	.12072-11	.12595-11	.12595-10	.10030+09	.26679-14	.19280-10
HN ₃	.16073-22	.16824-22	.16824-21	.13398-02	.95685-25	.69159-21
HN ₃	.13609-36	.14245-36	.14245-35	.11344-16	.00000	.85755-35
HN ₂	.25681-24	.27091-24	.27091-23	.21573-04	.16834-26	.12167-22
HN ₂	.34512-24	.36123-24	.36123-23	.28768-04	.22448-26	.16225-22
HN ₂	.20036-19	.20973-19	.20973-18	.16701+01	.85974-22	.62140-18
H	.27553-10	.28841-10	.28841-09	.22967+10	.38426-14	.27773-10
H	.00000	.00000	.00000	.00000	.00000	.00000
NO ₃	.12192-27	.12762-27	.12762-26	.10163-07	.77604-30	.56090-26
NO ₂	.61972-16	.64866-16	.64866-15	.51657+04	.25728-18	.18595-14
N	.47931-24	.45984-24	.45984-23	.36618-04	.85135-27	.61534-23
O ₂	.85525-23	.89523-23	.89523-22	.71289-03	.37864-25	.27367-21
O	.10753-22	.11255-22	.11255-21	.89627-03	.23801-25	.17203-21
NH	.11213-20	.11739-20	.11739-19	.93483-01	.23298-23	.16839-19
OH	.41107-13	.43026-13	.43026-12	.34264+07	.96724-16	.69910-12
C	.00000	.66637+00	.00000	.00000	.00000	.00000

CO 0.2192
 H₂ 0.0916
 CH₄ 0.0130
 CO₂ 0.0214
 H₂O 0.2500
 N₂ 0.4048

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.41001-01	.43444-01	.43444+00	.34596+19	.92124-04	.65779+00
CO ₂	.14890+00	.15777+00	.15777+01	.12564+20	.91778-03	.65532+01
CO	.53697-01	.57492-01	.57492+00	.33746+19	.24988-03	.17842+01
NH ₃	.32791-03	.34745-03	.34745-02	.27668+17	.78215-06	.55847-02
H ₂ O	.15050+00	.15947+00	.15947+01	.12699+20	.37972-03	.27113+01
H ₂	.13471+00	.14273+00	.14273+01	.11366+20	.38033-04	.27157+00
N ₂	.40464+00	.42674+00	.42674+01	.34142+20	.15875-02	.11335+02
C	.00000	.00000	.00000	.00000	.00000	.00000

THE TRACE VALUES ARE

HCN	.28257-06	.29941-06	.29941-05	.23843+14	.10695-08	.76368-05
CH ₃	.16115-09	.17075-09	.17075-08	.13597+11	.33933-12	.24229-08
C	.36653-33	.38837-33	.38837-32	.30927-13	.61657-36	.44024-32
NH ₂	.11479-11	.12163-11	.12163-10	.96861+08	.25761-14	.18394-10
HN ₃	.17273-22	.18302-22	.18302-21	.14574-02	.10409-24	.74321-21
HN ₃	.87380-37	.87288-37	.87288-36	.69510-17	.00000	.51910-35
HN ₂	.18463-24	.19563-24	.19563-23	.15578-04	.12156-26	.86800-23
HN ₂	.24620-24	.26087-24	.26087-23	.20774-04	.16211-26	.11575-22
HN ₂	.16844-19	.17848-19	.17848-18	.14213+01	.73164-22	.52241-18
H	.26211-10	.27772-10	.27772-09	.37002-14	.26420-10	.26420-10
H	.00000	.00000	.00000	.00000	.00000	.00000
NO ₃	.90322-28	.95704-28	.95704-27	.76211-08	.58195-30	.41553-26
NO ₂	.34104-16	.37328-16	.37328-15	.45652+04	.22737-18	.16235-14
N	.45199-24	.47891-24	.47891-23	.38137-04	.68666-27	.63310-23
O ₂	.60635-23	.64459-23	.64459-22	.51331-03	.27263-25	.19467-21
O	.90135-23	.95505-23	.95505-22	.76053-03	.20196-25	.14421-21
NH	.11111-20	.11773-20	.11773-19	.93754-01	.23366-23	.16684-19
OH	.33182-13	.35159-13	.35159-12	.27998+07	.79035-16	.56432-12

Table 49 (cont'd)

Rockwell Molten Carbonate Air-Blown Gas

CO 0.2221
H₂ 0.0929
CH₄ 0.0131
CO₂ 0.0214
H₂O 0.2400
N₂ 0.4102

SPECIESNAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.41987-01	.44628-01	.44628+00	.35539+19	.94635-04	.67359+00
CO ₂	.14833+00	.15766+00	.15766+01	.12555+20	.91710-03	.65278+01
CO	.65498-01	.69619-01	.69619+00	.55439+19	.25776-03	.18347+01
NH ₃	.32082-03	.34100-03	.34100-02	.27155+17	.76763-06	.54639-02
H ₂ O	.14275+00	.15173+00	.15173+01	.12083+20	.36130-03	.25717+01
H ₂	.13189+00	.14019+00	.14019+01	.11164+20	.37357-04	.26550+00
N ₂	.41004+00	.43583+00	.43583+01	.34707+20	.16136-02	.11486+02
C	S .78942-03	.10000+01	.00000	.00000	.00000	.94617-02

THE TRACE VALUES ARE

H ₂ CO	.29971-06	.31856-06	.31856-05	.25368+14	.11380-08	.80999-05
CH ₃	.16651-09	.17698-09	.17698-08	.14094+11	.35172-12	.25035-08
C	.38906-33	.41354-33	.41354-32	.32931-13	.65652-36	.46730-32
NH ₂	.11332-11	.12045-11	.12045-10	.95923+08	.25510-14	.18158-10
NH ₃	.17490-22	.18590-22	.18590-21	.14604-02	.10573-24	.75255-21
HNO ₃	.74509-37	.79291-37	.79291-36	.63142-17	.00000	.47007-35
HNO ₂	.17259-24	.18344-24	.18344-23	.14608-04	.11399-26	.81138-23
HNO ₂ TRANS	.23014-24	.24462-24	.24462-23	.19480-04	.15201-26	.10820-22
HNO	.16254-19	.17276-19	.17276-18	.13758+01	.70821-22	.50410-18
H	.25895-10	.27524-10	.27524-09	.21918+10	.36672-14	.26102-10
H ₂ O ₃	.00000	.00000	.00000	.00000	.00000	.00000
NO ₂	.51192-28	.50551-28	.50551-27	.72108-08	.55062-30	.39193-26
NO	.52679-16	.55593-16	.55593-15	.44588+04	.22207-18	.15807-14
N	.45426-24	.48286-24	.48286-23	.38451-04	.89366-27	.63631-23
O ₂	.56911-23	.60491-23	.60491-22	.48171-03	.26585-25	.18211-21
O	.67043-23	.92519-23	.92519-22	.73675-03	.19565-25	.13926-21
NH	.11066-20	.11764-20	.11764-19	.93681-01	.23348-23	.16618-19
OH	.21757-13	.33755-13	.33755-12	.26680+07	.75879-16	.94010-12

CO 0.2450
H₂ 0.1020
CH₄ 0.0150
CO₂ 0.0240
H₂O 0.1610
N₂ 0.4530

SPECIESNAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.31190-01	.34146-01	.34146+00	.27191+19	.72406-04	.50038+00
CO ₂	.13690+00	.14987+00	.14987+01	.11975+20	.87182-03	.60249+01
CO	.62003-01	.67878-01	.67878+00	.54053+19	.25131-03	.17368+01
NH ₃	.27178-03	.29753-03	.29753-02	.23693+17	.66978-06	.46287-02
H ₂ O	.11820+00	.12940+00	.12940+01	.10305+20	.30613-03	.21294+01
H ₂	.11201+00	.12263+00	.12263+01	.97650+19	.32676-04	.22582+00
N ₂	.45286+00	.49578+00	.49578+01	.39980+20	.18357-02	.12686+02
C	S .53909-01	.10000+01	.00000	.00000	.00000	.64750+00

THE TRACE VALUES ARE

H ₂ CO	.29026-06	.31777-06	.31777-05	.25305+14	.11351-08	.78446-05
CH ₃	.13225-09	.14479-09	.14479-08	.11530+11	.28773-12	.19884-08
C	.37774-33	.41354-33	.41354-32	.32931-13	.65652-36	.45371-32
NH ₂	.10265-11	.11237-11	.11237-10	.89486+08	.23799-14	.16447-10
NH ₃	.19268-22	.21094-22	.21094-21	.16798-02	.11997-24	.82907-21
HNO ₃	.66983-37	.73308-37	.73308-36	.58377-17	.00000	.42195-35
HNO ₂	.15889-24	.17395-24	.17395-23	.13852-04	.10809-26	.74700-23
HNO ₂ TRANS	.21188-24	.23196-24	.23196-23	.18472-04	.14414-26	.99612-23
HNO	.16348-19	.16802-19	.16802-18	.13388+01	.68878-22	.47600-18
H	.23514-10	.25742-10	.25742-09	.20409+10	.34297-14	.23702-10
H ₂ O ₃	.00000	.00000	.00000	.00000	.00000	.00000
NO ₂	.83862-28	.91809-28	.91809-27	.73110-08	.55827-30	.38581-26
NO	.53186-16	.58226-16	.58226-15	.46367+04	.23093-18	.15959-14
N	.47042-24	.51499-24	.51499-23	.41010-04	.95346-27	.65891-23
O ₂	.52527-23	.57504-23	.57504-22	.45792-03	.24322-25	.16808-21
O	.62397-23	.90206-23	.90206-22	.71833-03	.19076-25	.13183-21
NH	.10719-20	.11735-20	.11735-19	.93447-01	.23289-23	.16095-19
OH	.28116-13	.30780-13	.30780-12	.24511+07	.69192-16	.47817-12

Table 49 (cont'd)

Gravitating Bed (METC) Air-Blown Gas

CO 0.1302
 H₂ 0.0948
 CH₄ 0.0180
 CO₂ 0.0408
 H₂O 0.4000
 N₂ 0.3162

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.21600-01	.21760-01	.21760-00	.17333+19	.46155-04	.34653+00
CO ₂	.13209+00	.13310+00	.13310+01	.10599+20	.77427-03	.58133+01
CO	.35310-01	.35580-01	.35580+00	.28333+19	.13173-03	.98906+00
NH ₃	.40694-03	.41006-03	.41006-02	.32654+17	.92310-06	.69307-02
H ₂ O	.31231+00	.31470+00	.31470+01	.25061+20	.74936-03	.56263+01
H ₂	.17468+00	.17602+00	.17602+01	.14017+20	.46903-04	.35215+00
N ₂	.31600+00	.31842+00	.31842+01	.25357+20	.11790-02	.88520+01
C	S .00000	.00000	.00000	.00000	.00000	.00000

THE TRACE VALUES ARE

H ₂ CN	.93676-07	.94394-07	.94394-06	.75168+13	.33720-09	.25317-05
CH ₃	.76448-10	.77034-10	.77034-09	.61344+10	.15309-12	.11404-08
C	.12697-33	.12794-33	.12794-32	.10188-13	.20312-36	.15250-32
NH ₂	.12629-11	.12927-11	.12927-10	.10294+09	.27378-14	.20555-10
HN ₃	.12909-22	.13008-22	.13008-21	.10359-02	.73981-25	.55546-21
HNO ₃	.33974-36	.34234-36	.34234-35	.27261-16	.28513-38	.21408-34
HNO ₂	.47580-24	.47945-24	.47945-23	.38180-04	.29793-26	.22369-22
HNO ₂	.63448-24	.63934-24	.63934-23	.50912-04	.39729-26	.29829-22
HNO	.27126-19	.27334-19	.27334-18	.21767+01	.11205-21	.84128-18
H	.30607-10	.30841-10	.30841-09	.24560+10	.41091-14	.30652-10
NO ₃	.00000	.00000	.00000	.00000	.00000	.00000
NO ₂	.20960-27	.21121-27	.21121-26	.16819-07	.12843-29	.96429-26
NO	.78459-16	.79061-16	.79061-15	.62958+04	.31356-18	.23543-14
N	.40958-24	.41272-24	.41272-23	.32866-04	.76412-27	.57370-23
O ₂	.16382-22	.16507-22	.16507-21	.13145-02	.69818-25	.52420-21
O	.15167-22	.15283-22	.15283-21	.12171-02	.32320-25	.24266-21
NH	.11182-20	.11267-20	.11267-19	.89724-01	.22361-23	.16789-19
OH	.62006-13	.62481-13	.62481-12	.49755+07	.14045-15	.10545-11

CO 0.1411
 H₂ 0.1027
 CH₄ 0.0195
 CO₂ 0.0442
 H₂O 0.3500
 N₂ 0.3426

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.27583-01	.28045-01	.28045+00	.22333+19	.59471-04	.44252+00
H ₂ CN	.12908-06	.13124-06	.13124-05	.10451+14	.46880-09	.34885-05
CO ₂	.13589+00	.13616+00	.13616+01	.11002+20	.80371-03	.59804+01
CO	.41329-01	.42021-01	.42021+00	.33463+19	.15558-03	.11577+01
NH ₃	.40664-03	.41549-03	.41549-02	.33086+17	.93531-06	.69596-02
H ₂ O	.26640+00	.27086+00	.27086+01	.21569+20	.64496-03	.47991+01
H ₂	.16952+00	.17236+00	.17236+01	.13726+20	.45930-04	.34176+00
N ₂	.34240+00	.34813+00	.34813+01	.27723+20	.12890-02	.95615+01
C	S .00000	.00000	.00000	.00000	.00000	.00000

THE TRACE VALUES ARE

CH ₃	.98653-10	.10031-09	.10031-08	.79876+10	.19934-12	.14833-08
C	.16908-33	.17192-33	.17192-32	.13690-13	.27293-36	.20309-32
NH ₂	.13018-11	.13236-11	.13236-10	.10540+09	.28032-14	.20859-10
HN ₃	.14473-22	.14716-22	.14716-21	.11718-02	.86692-25	.62275-21
HNO ₃	.23654-36	.24051-36	.24051-35	.19152-16	.20311-38	.14905-34
HNO ₂	.37692-24	.38323-24	.38323-23	.30518-04	.23814-26	.17720-22
HNO ₂	.50261-24	.51103-24	.51103-23	.40695-04	.31756-26	.23629-22
HNO	.24448-19	.24858-19	.24858-18	.19795+01	.10190-21	.75824-18
H	.30017-10	.30520-10	.30520-09	.24303+10	.40662-14	.30257-10
NO ₃	.00000	.00000	.00000	.00000	.00000	.00000
NO ₂	.16779-27	.17060-27	.17060-26	.13586-07	.10374-29	.77193-26
NO	.71461-16	.72658-16	.72658-15	.57859+04	.28817-18	.21443-14
N	.42444-24	.43155-24	.43155-23	.34365-04	.79897-27	.59451-23
O ₂	.12542-22	.12752-22	.12752-21	.10155-02	.53935-25	.40133-21
O	.13212-22	.13433-22	.13433-21	.10697-02	.28407-25	.21137-21
NH	.11466-20	.11658-20	.11658-19	.92838-01	.23137-23	.17216-19
OH	.53448-13	.54343-13	.54343-12	.43275+07	.12216-15	.90898-12

Table 49 (cont'd)

Gravitating Bed (METC) Air-Blown Gas (Cont'd)

CO 0.1519
 H₂ 0.1106
 CH₄ 0.0210
 CO₂ 0.0476
 H₂O 0.3000
 N₂ 0.3689

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.34040-01	.34966-01	.34966+00	.27645+19	.74147-04	.54611+00
HCN	.17573-06	.18050-06	.18050-05	.14374+14	.64480-09	.47491-05
CO ₂	.13637+00	.14213+00	.14213+01	.11318+20	.82679-03	.60895+01
CO	.48093-01	.49401-01	.49401+00	.39339+19	.18290-03	.13471+01
NH ₃	.39889-03	.40974-03	.40974-02	.32629+17	.92238-06	.67936-02
H ₂ O	.22227+00	.22832+00	.22832+01	.18182+20	.54367-03	.40043+01
H ₂	.16165+00	.16604+00	.16604+01	.13222+20	.44245-04	.32588+00
N ₂	.36870+00	.37873+00	.37873+01	.30159+20	.14623-02	.10328+02
C	S .00000	.00000	.00000	.00000	.00000	.00000

THE TRACE VALUES ARE

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₃	.12404-09	.12742-09	.12742-08	.10147+11	.25321-12	.18650-08
C	.22485-33	.23097-33	.23097-32	.18393-13	.36668-36	.27007-32
NH ₂	.12947-11	.13299-11	.13299-10	.10590+09	.28166-14	.20745-10
NH ₃	.15955-22	.16389-22	.16389-21	.13051-02	.93207-25	.68650-21
HN03	.16059-36	.16496-36	.16496-35	.13136-16	.00000	.10120-14
HN02	.29244-24	.30039-24	.30039-23	.23921-04	.18667-26	.13749-22
HN02	.38997-24	.40057-24	.40057-23	.31899-04	.24892-26	.18333-22
HN0	.21678-19	.22268-19	.22268-18	.17732+01	.91282-22	.67232-18
H	.29162-10	.29955-10	.29955-09	.23854+10	.39910-14	.29395-10
N03	.00000	.00000	.00000	.00000	.00000	.00000
N02	.13264-27	.13625-27	.13625-26	.10850-07	.87651-30	.61022-26
N0	.64558-16	.66314-16	.66314-15	.52807+04	.26301-18	.19371-14
N	.43820-24	.45011-24	.45011-23	.35844-04	.83334-27	.61378-23
O2	.95055-23	.97640-23	.97640-22	.77753-03	.41297-25	.30417-21
O	.11443-22	.11754-22	.11754-21	.93603-03	.24857-25	.18308-21
NH	.11619-20	.11935-20	.11935-19	.95040-01	.23686-23	.17446-19
OH	.45436-13	.46672-13	.46672-12	.37166+07	.10492-15	.77273-12

CO 0.1628
 H₂ 0.1185
 CH₄ 0.0225
 CO₂ 0.0510
 H₂O 0.2500
 N₂ 0.3953

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.40900-01	.42474-01	.42474+00	.37623+19	.90068-04	.65615+00
CO ₂	.13943+00	.14480+00	.14480+01	.11531+20	.84270-03	.61363+01
CO	.55972-01	.58127-01	.58127+00	.46288+19	.21521-03	.15678+01
NH ₃	.37753-03	.39207-03	.39207-02	.31222+17	.88259-06	.64298-02
H ₂ O	.17997+00	.18690+00	.18690+01	.14883+20	.44504-03	.32422+01
H ₂	.15116+00	.15698+00	.15698+01	.12501+20	.41831-04	.30475+00
N ₂	.39511+00	.41032+00	.41032+01	.32675+20	.15193-02	.11068+02

THE TRACE VALUES ARE

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
HCN	.23906-06	.24826-06	.24826-05	.19770+14	.88685-09	.64608-05
CH ₃	.15328-09	.15918-09	.15918-08	.12676+11	.31633-12	.23045-09
C	.30224-33	.31388-33	.31388-32	.24995-13	.49831-36	.36302-32
NH ₂	.12602-11	.13088-11	.13088-10	.10422+09	.27718-14	.20193-10
NH ₃	.17304-22	.17970-22	.17970-21	.14310-02	.10220-24	.74456-21
HN03	.10435-36	.10837-36	.10837-35	.86296-17	.00000	.65754-35
HN02	.21947-24	.22792-24	.22792-23	.18150-04	.14163-26	.10318-22
HN02	.29265-24	.30392-24	.30392-23	.24202-04	.18886-26	.13759-22
HN0	.18789-19	.19513-19	.19513-18	.15539+01	.79990-22	.58274-18
H	.28046-10	.29126-10	.29126-09	.23194+10	.38806-14	.28271-10
N03	.00000	.00000	.00000	.00000	.00000	.00000
N02	.10237-27	.10632-27	.10632-26	.84662-08	.64649-30	.47097-26
N0	.57548-16	.59763-16	.59763-15	.47591+04	.23703-18	.17266-14
N	.45114-24	.46851-24	.46851-23	.37309-04	.86741-27	.63192-23
O2	.70483-23	.73197-23	.73197-22	.58289-03	.30959-25	.22554-21
O	.97999-23	.10177-22	.10177-21	.81044-03	.21522-25	.15679-21
NH	.11631-20	.12079-20	.12079-19	.96188-01	.23972-23	.17464-19
OH	.37835-13	.39292-13	.39292-12	.31289+07	.88326-16	.64347-12
C	S .00000	.75901+00	.00000	.00000	.00000	.00000

Table 49 (cont'd)

Gravitating Bed (METC) Air-Blown Gas (Cont'd)

CO 0.1714
 H₂ 0.1248
 CH₄ 0.0237
 CO₂ 0.0537
 H₂O 0.2100
 N₂ 0.4163

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.46558-01	.48811-01	.48811+00	.38870+19	.10351-03	.74693+00
CO ₂	.13890+00	.14562+00	.14562+01	.11596+20	.84709-03	.61129+01
CO	.63344-01	.66410-01	.66410+00	.52384+19	.24588-03	.17743+01
NH ₃	.35107-03	.36901-03	.36901-02	.29385+17	.81067-06	.59944-02
H ₂ O	.14766+00	.15481+00	.15481+01	.12326+20	.36862-03	.26601+01
H ₂	.14090+00	.14772+00	.14772+01	.11763+20	.39362-04	.28405+00
N ₂	.41612+00	.43627+00	.43627+01	.34741+20	.16153-02	.11657+02
C	S .00000	.00000	.00000	.00000	.00000	.00000

THE TRACE VALUES ARE

HCN	.30742-06	.32230-06	.32230-05	.25666+14	.11513-08	.83084-05
CH ₃	.17987-09	.18858-09	.18858-08	.15017+11	.37476-12	.27044-08
C	.38859-33	.40739-33	.40739-32	.32442-13	.64677-36	.46673-32
NH ₂	.12112-11	.12698-11	.12698-10	.10112+09	.26893-14	.19407-10
NH ₃	.18226-22	.19111-22	.19111-21	.15218-02	.10869-24	.78434-21
NH ₃	.70517-37	.73930-37	.73930-36	.58872-17	.00000	.44435-35
HN ₂	.16848-24	.17664-24	.17664-23	.14066-04	.10976-26	.79209-23
HN ₂	.22467-24	.23555-24	.23555-23	.18757-04	.14637-26	.10562-22
HN ₂	.16387-19	.17180-19	.17180-18	.13681+01	.70427-22	.50823-18
H	.26949-10	.28253-10	.28253-09	.22499+10	.37643-14	.27164-10
NO ₃	.00000	.00000	.00000	.00000	.00000	.00000
NO ₂	.81021-28	.84943-28	.84943-27	.67642-08	.51652-30	.37274-26
NO	.51740-16	.54244-16	.54244-15	.43196+04	.21514-18	.15525-14
N	.46079-24	.48310-24	.48310-23	.38470-04	.69441-27	.64543-23
O ₂	.54098-23	.56716-23	.56716-22	.45165-03	.23988-25	.17311-21
O	.85450-23	.89586-23	.89586-22	.71339-03	.18945-25	.13671-21
NH	.11524-20	.12082-20	.12082-19	.96210-01	.23978-23	.17303-19
OH	.32002-13	.33551-13	.33551-12	.26717+07	.75419-16	.54425-12

CO 0.1736
 H₂ 0.1264
 CH₄ 0.0240
 CO₂ 0.0544
 H₂O 0.2000
 N₂ 0.4216

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.45633-01	.48199-01	.48199+00	.38382+19	.10221-03	.73530+00
CO ₂	.13765+00	.14475+00	.14475+01	.11527+20	.84204-03	.60578+01
CO	.63434-01	.66709-01	.66709+00	.53122+19	.24698-03	.17768+01
NH ₃	.34642-03	.36431-03	.36431-02	.29011+17	.82009-06	.58998-02
H ₂ O	.14368+00	.15109+00	.15109+01	.12032+20	.35978-03	.25883+01
H ₂	.13854+00	.14569+00	.14569+01	.11602+20	.38822-04	.27929+00
N ₂	.42143+00	.44319+00	.44319+01	.35292+20	.16410-02	.11805+02
C	S .50883-02	.10000+01	.00000	.00000	.00000	.61116-01

THE TRACE VALUES ARE

HCN	.31140-06	.32748-06	.32748-05	.26078+14	.11698-08	.84159-05
CH ₃	.17830-09	.18750-09	.18750-08	.14931+11	.37262-12	.26807-08
C	.39323-33	.41354-33	.41354-32	.32931-13	.65652-36	.47231-32
NH ₂	.12003-11	.12623-11	.12623-10	.10052+09	.26734-14	.19233-10
NH ₃	.18479-22	.19433-22	.19433-21	.15475-02	.11052-24	.79510-21
NH ₃	.68191-37	.71712-37	.71712-36	.57106-17	.00000	.42969-35
HN ₂	.16464-24	.17314-24	.17314-23	.13788-04	.10759-26	.77404-23
HN ₂	.21955-24	.23089-24	.23089-23	.18386-04	.14347-26	.10322-22
HN ₂	.16182-19	.17018-19	.17018-18	.13552+01	.69761-22	.50187-18
H	.26681-10	.28059-10	.28059-09	.22344+10	.37384-14	.26895-10
NO ₃	.00000	.00000	.00000	.00000	.00000	.00000
NO ₂	.79722-28	.83839-28	.83839-27	.66763-08	.50981-30	.36676-26
NO	.51447-16	.54103-16	.54103-15	.43084+04	.21458-18	.15437-14
N	.46301-24	.48691-24	.48691-23	.38774-04	.90147-27	.64853-23
O ₂	.52813-23	.55540-23	.55540-22	.44226-03	.23491-25	.16900-21
O	.84299-23	.88652-23	.88652-22	.70596-03	.18747-25	.13487-21
NH	.11500-20	.12093-20	.12093-19	.96304-01	.24001-23	.17267-19
OH	.31354-13	.32973-13	.32973-12	.26257+07	.74120-16	.53323-12

Table 49 (cont'd)

Gravitating Bed (METC) Air-Blown Gas

CO 0.1845
 H₂ 0.1343
 CH₄ 0.0255
 CO₂ 0.0578
 H₂O 0.1500
 N₂ 0.4480

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.39258-01	.41999-01	.41999+00	.33445+19	.89060-04	.62982+00
CO ₂	.12991+00	.13898+00	.13898+01	.11067+20	.80847-03	.57173+01
CO	.61099-01	.65366-01	.65366+00	.52052+19	.24201-03	.17114+01
NH ₃	.31932-03	.34162-03	.34162-02	.27204+17	.76902-06	.54384-02
H ₂ O	.12918+00	.13820+00	.13820+01	.11005+20	.32908-03	.23272+01
H ₂	.12712+00	.13600+00	.13600+01	.10630+20	.36240-04	.25628+00
N ₂	.44784+00	.47911+00	.47911+01	.38153+20	.17740-02	.12545+02
C	S .37533-01	.10000+01	.00000	.00000	.00000	.45081+00

THE TRACE VALUES ARE

HCN	.30750-06	.32897-06	.32897-05	.26197+14	.11752-08	.83105-05
CH ₃	.15807-09	.16911-09	.16911-08	.13466+11	.33606-12	.23766-08
C	.38655-33	.41354-33	.41354-32	.32971-13	.65652-36	.46428-32
NH ₂	.11452-11	.12252-11	.12252-10	.97563+08	.25947-14	.18350-10
HN ₃	.19726-22	.21104-22	.21104-21	.16806-02	.12002-24	.84819-21
HN ₃	.63350-37	.67773-37	.67773-36	.53970-17	.00000	.39919-35
HN ₂	.15610-24	.16700-24	.16700-23	.13298-04	.10377-26	.73387-23
HN ₂	.20816-24	.22269-24	.22269-23	.17733-04	.13838-26	.97860-23
HN ₂	.15658-19	.16751-19	.16751-18	.13339+01	.68668-22	.48561-18
H	.25340-10	.27110-10	.27110-09	.21588+10	.36119-14	.25543-10
NO ₃	.00000	.00000	.00000	.00000	.00000	.00000
NO ₂	.78232-28	.83694-28	.83694-27	.66648-08	.50893-30	.35991-26
NO	.51523-16	.55120-16	.55120-15	.43694+04	.21861-18	.15460-14
N	.47322-24	.50626-24	.50626-23	.40315-04	.93730-27	.66284-23
O ₂	.49845-23	.53326-23	.53326-22	.42465-03	.22554-25	.15950-21
O	.81197-23	.86866-23	.86866-22	.69174-03	.18370-25	.12991-21
NH	.11356-20	.12149-20	.12149-19	.96742-01	.24111-23	.17051-19
OH	.29178-13	.31215-13	.31215-12	.24458+07	.70170-16	.49623-12

CO 0.1920
 H₂ 0.1330
 CH₄ 0.0260
 CO₂ 0.0610
 H₂O 0.1290
 N₂ 0.4580

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.35386-01	.38176-01	.38176+00	.30400+19	.80952-04	.56770+00
CO ₂	.12980+00	.14003+00	.14003+01	.11151+20	.81456-03	.57123+01
CO	.60617-01	.65611-01	.65611+00	.52248+19	.24292-03	.17035+01
NH ₃	.29931-03	.32290-03	.32290-02	.25714+17	.72689-06	.50975-02
H ₂ O	.12259+00	.13226+00	.13226+01	.10532+20	.31492-03	.22085+01
H ₂	.12019+00	.12966+00	.12966+01	.10325+20	.34551-04	.24230+00
N ₂	.45785+00	.49394+00	.49394+01	.39334+20	.18289-02	.12826+02
C	S .53001-01	.10000+01	.00000	.00000	.00000	.63660+00

THE TRACE VALUES ARE

HCN	.30232-06	.32615-06	.32615-05	.25972+14	.11651-08	.81704-05
CH ₃	.14592-09	.15742-09	.15742-08	.12536+11	.31285-12	.21939-08
C	.38332-33	.41354-33	.41354-32	.32931-13	.65652-36	.46041-32
NH ₂	.10993-11	.11860-11	.11860-10	.94445+08	.25118-14	.17615-10
HN ₃	.19994-22	.21571-22	.21571-21	.17177-02	.12268-24	.86031-21
HN ₃	.62987-37	.67952-37	.67952-36	.54112-17	.00000	.39690-35
HN ₂	.15462-24	.16681-24	.16681-23	.13284-04	.10366-26	.72693-23
HN ₂	.20619-24	.22244-24	.22244-23	.17714-04	.13823-26	.96935-23
HN ₂	.15452-19	.16676-19	.16676-18	.13274+01	.68334-22	.47921-18
H	.24336-10	.26470-10	.26470-09	.21079+10	.35268-14	.24732-10
NO ₃	.00000	.00000	.00000	.00000	.00000	.00000
NO ₂	.79364-28	.85620-28	.85620-27	.68182-08	.52064-30	.36511-26
NO	.52072-16	.56177-16	.56177-15	.44735-04	.22280-18	.15625-14
N	.47648-24	.51404-24	.51404-23	.40874-04	.95170-27	.66740-23
O ₂	.49801-23	.53727-23	.53727-22	.42785-03	.22724-25	.15936-21
O	.80822-23	.87193-23	.87193-22	.69434-03	.18439-25	.12991-21
NH	.11164-20	.12044-20	.12044-19	.95912-01	.23904-23	.16763-19
OH	.29358-13	.30594-13	.30594-12	.24363+07	.68773-16	.48229-12

Table 49 (cont'd)

Fluidized Bed (Westinghouse) Oxygen-Blown Gas

CO 0.3070
 H₂ 0.1530
 CH₄ 0.0280
 CO₂ 0.0770
 H₂O 0.4320
 N₂ 0.0030

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.76209-01	.84345-01	.84345+00	.67166+19	.17886-03	.12226+01
CO ₂	.25789+00	.28542+00	.28542+01	.22729+20	.16603-02	.11350+02
CO	.77901-01	.86221-01	.86221+00	.68660+19	.31922-03	.21822+01
NH ₃	.48681-04	.54107-04	.54107-03	.43087+16	.12180-06	.83260-03
H ₂ O	.29932+00	.33128+00	.33128+01	.26381+20	.78883-03	.53923+01
H ₂	.18919+00	.20939+00	.20939+01	.16674+20	.55795-04	.38140+00
N ₂	.29756-02	.32933-02	.32933-01	.26225+18	.12194-09	.83354-01
C	S .00000	.00000	.00000	.00000	.00000	.00000

THE TRACE VALUES ARE

HCN	.25906-07	.28672-07	.28672-06	.22832+13	.10242-09	.70014-06
CH ₃	.24730-09	.27370-09	.27370-08	.21795+11	.59392-12	.37181-08
C	.31056-33	.35036-33	.35036-32	.27900-13	.55622-36	.38022-32
NH ₂	.14130-12	.15639-12	.15639-11	.12453+08	.33121-15	.22641-11
NH ₃	.13483-25	.14923-25	.14923-24	.11883-05	.84870-28	.58016-24
HNO ₃	.23774-37	.26313-37	.26313-36	.20953-17	.00000	.14981-35
HNO ₂	.37626-25	.41644-25	.41644-24	.33162-05	.25877-27	.17689-23
HNO ₂	.50174-25	.55531-25	.55531-24	.44221-05	.34507-27	.23588-23
HNO	.24241-20	.26629-20	.26629-19	.21365+00	.10998-22	.75181-19
H	.30393-10	.33638-10	.33638-09	.26787+10	.44617-14	.30636-10
N ₂	.00000	.00000	.00000	.00000	.00000	.00000
N ₂	.15197-28	.16820-28	.16820-27	.13394-08	.10228-30	.69916-27
N ₂	.64286-17	.71150-17	.71150-16	.56658+03	.28219-19	.19290-15
N	.37924-25	.41973-25	.41973-24	.33424-05	.77709-28	.53120-24
O ₂	.11679-22	.12926-22	.12926-21	.10294-02	.54672-25	.37373-21
O	.12220-22	.13524-22	.13524-21	.10770-02	.28600-25	.19550-21
NH	.11292-21	.12498-21	.12498-20	.99522-02	.24803-24	.16955-20
OH	.54486-13	.60304-13	.60304-12	.48071+07	.13556-15	.92665-12

CO 0.3186
 H₂ 0.1593
 CH₄ 0.0295
 CO₂ 0.0797
 H₂O 0.4100
 N₂ 0.0030

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.82109-01	.91759-01	.91759+00	.73070+19	.19458-03	.13173+01
CO ₂	.26279+00	.29368+00	.29368+01	.23380+20	.17083-02	.11545+02
CO	.52900-01	.62042-01	.62042+00	.73773+19	.34300-03	.23221+01
NH ₃	.47542-04	.53129-04	.53129-03	.42308+16	.11963-06	.80969-03
H ₂ O	.27952+00	.31237+00	.31237+01	.24675+20	.74380-03	.50355+01
H ₂	.18449+00	.20618+00	.20618+01	.16418+20	.54939-04	.37194+00
N ₂	.29762-02	.33260-02	.33260-01	.26486+18	.12315-04	.83373-01
C	S .00000	.00000	.00000	.00000	.00000	.00000

THE TRACE VALUES ARE

HCN	.28708-07	.32082-07	.32082-06	.25548+13	.11460-09	.77586-06
CH ₃	.26651-09	.30007-09	.30007-08	.23895+11	.59632-12	.40371-08
C	.35178-33	.39312-33	.39312-32	.31305-13	.62411-36	.42252-32
NH ₂	.13848-12	.15475-12	.15475-11	.12323+08	.32775-15	.22188-11
NH ₃	.13449-25	.15029-25	.15029-24	.11968-05	.85477-28	.57868-24
HNO ₃	.20618-37	.23042-37	.23042-36	.18349-17	.00000	.12992-35
HNO ₂	.34077-25	.38081-25	.38081-24	.30325-05	.23664-27	.16020-23
HNO ₂	.45441-25	.50781-25	.50781-24	.40438-05	.31556-27	.21363-23
HNO	.22926-20	.25620-20	.25620-19	.20402+00	.10503-22	.71103-19
H	.29869-10	.33379-10	.33379-09	.26581+10	.44477-14	.30108-10
N ₂	.00000	.00000	.00000	.00000	.00000	.00000
N ₂	.13870-28	.15501-28	.15501-27	.12344-08	.94256-31	.63811-27
N ₂	.61270-17	.68471-17	.68471-16	.54525+03	.27156-19	.18385-15
N	.37745-25	.42181-25	.42181-24	.33500-05	.78095-28	.52870-24
O ₂	.10007-22	.11853-22	.11853-21	.94392-03	.50134-25	.33941-21
O	.11589-22	.12951-22	.12951-21	.10313-02	.27388-25	.18541-21
NH	.11152-21	.12463-21	.12463-20	.99245-02	.24734-24	.16745-20
OH	.51176-13	.57302-13	.57302-12	.45631+07	.12881-15	.87205-12

Table 49 (cont'd)

Fluidized Bed (Westinghouse) Oxygen-Blown Gas (Cont'd)

CO 0.3240
 H₂ 0.1620
 CH₄ 0.0300
 CO₂ 0.0810
 H₂O 0.4000
 N₂ 0.0030

SPECIESNAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.84538-01	.94920-01	.94920+00	.75587+19	.20128-03	.13562+01
CO ₂	.26503+00	.29757+00	.29757+01	.23697+20	.17310-02	.11664+02
CO	.85185-01	.95646-01	.95646+00	.76166+19	.35412-03	.23861+01
NH ₃	.46840-04	.52592-04	.52592-03	.41880+16	.11839-06	.79773-03
H ₂ O	.27076+00	.30401+00	.30401+01	.24209+20	.72390-03	.48778+01
H ₂	.18209+00	.20445+00	.20445+01	.16281+20	.54480-04	.36710+00
N ₂	.29766-02	.33421-02	.33421-01	.26614+18	.12375-04	.83383-01
C	S .24977-03	.10000+01	.00000	.00000	.00000	.29999-02

THE TRACE VALUES ARE

SPECIESNAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
HCN	.30004-07	.33689-07	.33689-06	.26827+13	.12034-09	.61089-06
CH ₃	.27762-09	.31171-09	.31171-08	.24822+11	.61945-12	.41740-08
C	.36831-33	.41354-33	.41354-32	.32931-13	.65652-36	.44238-32
NH ₂	.13701-12	.15383-12	.15383-11	.12250+08	.32579-15	.21952-11
NH ₃	.13427-25	.15075-25	.15075-24	.12005-05	.85738-28	.57772-24
HN03	.19366-37	.21744-37	.21744-36	.17315-17	.00000	.12203-35
HN02	.32611-25	.36616-25	.36616-24	.29168-05	.22753-27	.15332-23
HN02	.43487-25	.48827-25	.48827-24	.38882-05	.30341-27	.20444-23
HN0	.22355-20	.25100-20	.25100-19	.19988+00	.10289-22	.69332-19
H	.29004-10	.33239-10	.33239-09	.26469+10	.44286-14	.29841-10
NO3	.00000	.00000	.00000	.00000	.00000	.00000
NO2	.13330-28	.14967-28	.14967-27	.11918-08	.91010-31	.61324-27
NO	.59496-17	.67363-17	.67363-16	.53643+03	.26717-19	.18002-15
N	.37659-25	.42283-25	.42283-24	.33671-05	.78284-28	.52749-24
O ₂	.10169-22	.11418-22	.11418-21	.90922-03	.48291-25	.32539-21
O	.11321-22	.12711-22	.12711-21	.10122-02	.26879-25	.18112-21
NH	.11080-21	.12441-21	.12441-20	.99069-02	.24690-24	.16637-20
OH	.49878-13	.56004-13	.56004-12	.44597+07	.12589-15	.84828-12

CO 0.3510
 H₂ 0.1755
 CH₄ 0.0325
 CO₂ 0.0878
 H₂O 0.3500
 N₂ 0.0033

SPECIESNAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.78333-01	.90531-01	.90531+00	.72092+19	.19197-03	.12567+01
CO ₂	.26576+00	.30715+00	.30715+01	.24459+20	.17867-02	.11696+02
CO	.84080-01	.97173-01	.97173+00	.77381+19	.35977-03	.23552+01
NH ₃	.46749-04	.54029-04	.54029-03	.43025+16	.12163-06	.79619-03
H ₂ O	.26100+00	.30164+00	.30164+01	.24020+20	.71825-03	.47018+01
H ₂	.17277+00	.19967+00	.19967+01	.15900+20	.53206-04	.34810+00
N ₂	.32166-02	.37869-02	.37869-01	.30156+18	.14021-04	.91788-01
C	S .43125-01	.10000+01	.00000	.00000	.00000	.51797+00

THE TRACE VALUES ARE

SPECIESNAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
HCN	.30663-07	.35438-07	.35438-06	.28220+13	.12659-09	.82871-06
CH ₃	.26033-09	.30083-09	.30083-08	.23956+11	.59794-12	.39136-08
C	.35782-33	.41354-33	.41354-32	.32931-13	.65652-36	.44278-32
NH ₂	.13637-12	.15992-12	.15992-11	.12735+08	.33868-15	.22171-11
NH ₃	.15548-25	.17969-25	.17969-24	.14309-05	.10219-27	.66898-24
HN03	.20754-37	.23986-37	.23986-36	.19100-17	.00000	.13078-35
HN02	.34400-25	.39757-25	.39757-24	.31659-05	.24705-27	.16173-23
HN02	.45672-25	.53015-25	.53015-24	.42218-05	.32944-27	.21566-23
HN0	.23211-20	.26825-20	.26825-19	.21362+00	.10997-22	.71986-19
H	.28422-10	.32848-10	.32848-09	.26158+10	.43765-14	.28650-10
NO3	.00000	.00000	.00000	.00000	.00000	.00000
NO2	.14228-28	.16444-28	.16444-27	.13095-08	.99993-31	.65458-27
NO	.63034-17	.72850-17	.72850-16	.58012+03	.28893-19	.18914-15
N	.38944-25	.45009-25	.45009-24	.35842-05	.83330-28	.54550-24
O ₂	.10197-22	.11785-22	.11785-21	.93846-03	.49845-25	.32629-21
O	.11174-22	.12914-22	.12914-21	.10283-02	.27308-25	.17877-21
NH	.11324-21	.13087-21	.13087-20	.10421-01	.25973-24	.17002-20
OH	.44652-13	.56226-13	.56226-12	.44776+07	.12640-15	.82742-12

Table 49 (cont'd)

Fluidized Bed (Westinghouse) Oxygen-Blown Gas (Cont'd)

CO 0.3780
H₂ 0.1890
CH₄ 0.0350
CO₂ 0.0945
H₂O 0.3000
N₂ 0.0035

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.72242-01	.86035-01	.86035+00	.68512+19	.18244-03	.11590+01
CO ₂	.26653+00	.31741+00	.31741+01	.25276+20	.18464-02	.11730+02
CO	.62947-01	.87883-01	.87883+00	.78664+19	.36574-03	.23234+01
NH ₃	.45663-04	.54382-04	.54382-03	.43305+16	.12242-06	.77769-03
H ₂ O	.25100+00	.29893+00	.29893+01	.23804+20	.71179-03	.45218+01
H ₂	.16344+00	.19465+00	.19465+01	.15500+20	.51868-04	.32950+00
N ₂	.34772-02	.41411-02	.41411-01	.32976+18	.15333-04	.97406-01
C	S .85786-01	.10000+01	.00000	.00000	.00000	.10304+01

THE TRACE VALUES ARE

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
HCN	.30724-07	.36589-07	.36589-06	.29137+13	.13071-09	.83034-06
CH ₃	.24314-09	.28956-09	.28956-08	.23058+11	.57543-12	.36556-08
C	.34724-33	.41354-33	.41354-32	.32931-13	.65652-36	.41707-32
NH ₂	.13689-12	.16302-12	.16302-11	.12982+08	.34526-15	.21933-11
NH ₃	.17035-25	.20288-25	.20288-24	.16156-05	.11538-27	.73299-24
HNO ₃	.21846-37	.26017-37	.26017-36	.20718-17	.00000	.13766-35
HNO ₂	.35020-25	.42420-25	.42420-24	.33780-05	.26360-27	.16746-23
HNO ₂	.47498-25	.56567-25	.56567-24	.45046-05	.35151-27	.22330-23
HNO	.23642-20	.28156-20	.28156-19	.22421+00	.11542-22	.73323-19
H	.27233-10	.32433-10	.32433-09	.25627+10	.43211-14	.27451-10
N ₂	.00000	.00000	.00000	.00000	.00000	.00000
NO ₂	.14922-28	.17771-28	.17771-27	.14151-08	.10806-30	.68647-27
NO	.65028-17	.77443-17	.77443-16	.61670+03	.30715-19	.19512-15
N	.39521-25	.47067-25	.47067-24	.37480-05	.87139-28	.55357-24
O ₂	.10226-22	.12179-22	.12179-21	.96983-03	.51510-25	.32723-21
O	.11023-22	.13128-22	.13128-21	.10454-02	.27761-25	.17636-21
NH	.11346-21	.13512-21	.13512-20	.10760-01	.26816-24	.17036-20
OH	.47389-13	.56437-13	.56437-12	.44942+07	.12687-15	.80594-12

CO 0.4010
H₂ 0.1990
CH₄ 0.0370
CO₂ 0.1010
H₂O 0.2580
N₂ 0.0040

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.66793-01	.81587-01	.81587+00	.64970+19	.17301-03	.10716+01
CO ₂	.26833+00	.32776+00	.32776+01	.26101+20	.19066-02	.11809+02
CO	.82178-01	.10038+00	.10038+01	.79936+19	.37165-03	.23019+01
NH ₃	.46337-04	.56601-04	.56601-03	.45072+16	.12741-06	.78917-03
H ₂ O	.24217+00	.29580+00	.29580+01	.23556+20	.70436-03	.43626+01
H ₂	.15516+00	.18955+00	.18955+01	.15094+20	.50509-04	.31284+00
N ₂	.39768-02	.48577-02	.48577-01	.38683+18	.17986-04	.11140+00
C	S .12170+00	.10000+01	.00000	.00000	.00000	.14617+01

THE TRACE VALUES ARE

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
HCN	.32015-07	.39107-07	.39107-06	.31142+13	.13970-09	.86525-06
CH ₃	.22780-09	.27826-09	.27826-08	.22158+11	.55297-12	.34250-08
C	.33055-33	.41354-33	.41354-32	.32931-13	.65652-36	.40663-32
NH ₂	.14076-12	.17194-12	.17194-11	.13692+08	.36419-15	.22534-11
NH ₃	.20823-25	.25436-25	.25436-24	.20255-05	.14466-27	.89599-24
HNO ₃	.23687-37	.29178-37	.29178-36	.23235-17	.00000	.15052-35
HNO ₂	.38328-25	.46817-25	.46817-24	.37282-05	.29092-27	.18019-23
HNO ₂	.51110-25	.62430-25	.62430-24	.49715-05	.38794-27	.24028-23
HNO	.25035-20	.30580-20	.30580-19	.24351+00	.12536-22	.77642-19
H	.26201-10	.32005-10	.32005-09	.25486+10	.42642-14	.26411-10
N ₂	.00000	.00000	.00000	.00000	.00000	.00000
NO ₂	.16271-28	.19875-28	.19875-27	.15827-08	.12085-30	.74855-27
NO	.69778-17	.85233-17	.85233-16	.67873+03	.33804-19	.20937-15
N	.41733-25	.50977-25	.50977-24	.40594-05	.94379-28	.58456-24
O ₂	.10295-22	.12576-22	.12576-21	.10015-02	.53190-25	.32945-21
O	.10921-22	.13340-22	.13340-21	.10623-02	.28210-25	.17472-21
NH	.11823-21	.14442-21	.14442-20	.11500-01	.28661-24	.17752-20
OH	.46331-13	.56593-13	.56593-12	.45067+07	.12722-15	.78795-12

Table 49 (cont'd)

Texaco Entrained Oxygen-Blown Gas

CO 0.3179
H₂ 0.2123
CH₄ 0.0011
CO₂ 0.0634
H₂O 0.4000
N₂ 0.0053

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PARI/CC	DENSITY	MASS
CH ₄	.70236-01	.81511-01	.81511+00	.64910+19	.17285-03	.11268+01
CO ₂	.24054+00	.27915+00	.27915+01	.22230+20	.16239-02	.10586+02
CO	.71628-01	.63127-01	.63127+00	.66197+19	.30777-03	.20064+01
NH ₃	.64322-04	.74649-04	.74649-03	.59445+16	.16604-06	.10955-02
H ₂ O	.29200+00	.33888+00	.33888+01	.26986+20	.80692-03	.52604+01
H ₂	.18193+00	.21114+00	.21114+01	.16614+20	.56263-04	.36678+00
N ₂	.52678-02	.61136-02	.61136-01	.48684+18	.22637-08	.14757+00

THE TRACE VALUES ARE

HCN	.32125-07	.37283-07	.37283-06	.29689+13	.13318-09	.86822-06
CH ₃	.22696-09	.26340-09	.26340-08	.20975+11	.52345-12	.34124-08
C	.28692-33	.33298-33	.33298-32	.26516-13	.52863-36	.34462-32
NH ₂	.18514-12	.21486-12	.21486-11	.17110+08	.45805-15	.29665-11
NH	.32659-25	.37902-25	.37902-24	.30183-05	.21556-27	.14053-23
NH ₃	.32383-37	.37582-37	.37582-36	.29928-17	.00000	.20406-35
NH ₂	.30522-25	.38633-25	.38633-24	.46691-05	.36435-27	.23752-23
NH ₂ CIS	.67371-25	.78187-25	.78187-24	.62262-05	.48586-27	.31673-23
NH ₂ TRANS	.32086-20	.37237-20	.37237-19	.29653+00	.15265-22	.99536-19
H	.29106-10	.33779-10	.33779-09	.26899+10	.45005-14	.29339-10
NH ₃	.00000	.00000	.00000	.00000	.00000	.00000
NH ₂	.20321-28	.23584-28	.23584-27	.18780-08	.14341-30	.93488-27
NH	.84736-17	.98340-17	.98340-16	.78311+03	.39003-19	.25426-15
N	.49277-25	.57188-25	.57188-24	.45540-05	.10588-27	.69022-24
O ₂	.11462-22	.13302-22	.13302-21	.10593-02	.56262-25	.36677-21
O	.11822-22	.13720-22	.13720-21	.10925-02	.29013-25	.18914-21
NH	.14734-21	.17099-21	.17099-20	.13616-01	.33936-24	.22123-20
OH	.52932-13	.61430-13	.61430-12	.48918+07	.13809-15	.90021-12
C	.00000	.00000	.00000	.00000	.00000	.00000

CO 0.3391
H₂ 0.2265
CH₄ 0.0011
CO₂ 0.0676
H₂O 0.3600
N₂ 0.0056

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PARI/CC	DENSITY	MASS
CH ₄	.79347-01	.94087-01	.94087+00	.74924+19	.19951-03	.12730+01
CO ₂	.24054+00	.29484+00	.29484+01	.23479+20	.17151-02	.10943+02
CO	.79803-01	.94627-01	.94627+00	.75354+19	.35035-03	.22354+01
NH ₃	.62497-04	.74107-04	.74107-03	.59013+16	.16682-06	.10644-02
H ₂ O	.25720+00	.30497+00	.30497+01	.24286+20	.72619-03	.46334+01
H ₂	.17271+00	.20480+00	.20480+01	.16309+20	.54572-04	.34819+00
N ₂	.55688-02	.66632-02	.66632-01	.52583+18	.24449-04	.15600+00
C	.00000	.00000	.00000	.00000	.00000	.00000

THE TRACE VALUES ARE

HCN	.39484-07	.46619-07	.46619-06	.37283+13	.16725-09	.10671-05
CH ₃	.26033-09	.30871-09	.30871-08	.24583+11	.61349-12	.39143-08
C	.34463-33	.40853-33	.40853-32	.27533-13	.64858-36	.41382-32
NH ₂	.18266-12	.21659-12	.21659-11	.17247-08	.45870-15	.29267-11
NH ₃	.35337-25	.41901-25	.41901-24	.33367-05	.23830-27	.15205-23
NH ₃	.25911-37	.30724-37	.30724-36	.24467-17	.00000	.16327-35
NH ₂ CIS	.43569-25	.51663-25	.51663-24	.41140-05	.32103-27	.20483-23
NH ₂ TRANS	.58099-25	.68892-25	.68892-24	.54860-05	.42810-27	.27314-23
NH	.29823-20	.35363-20	.35363-19	.29160+00	.14496-27	.92493-19
H	.28005-10	.33267-10	.33267-09	.26401+10	.44323-14	.28280-10
NH ₃	.00000	.00000	.00000	.00000	.00000	.00000
NH ₂	.17794-28	.21099-28	.21099-27	.16802-08	.12830-30	.81862-27
NH	.79470-17	.94826-17	.94826-16	.75512+03	.37609-19	.23996-15
N	.50123-25	.59434-25	.59434-24	.47329-05	.11004-27	.70207-24
O ₂	.96574-23	.11451-22	.11451-21	.91190-03	.48434-25	.30903-21
O	.10735-22	.12729-22	.12729-21	.10137-02	.26919-25	.17175-21
NH	.14760-21	.17501-21	.17501-20	.13937-01	.34734-24	.22162-20
OH	.47340-13	.56133-13	.56133-12	.44700+07	.12618-15	.60510-12

Table 49 (cont'd)

Texaco Entrained Oxygen-Blown Gas (Cont'd)

CO 0.3444
 H₂ 0.2300
 CH₄ 0.0011
 CO₂ 0.0686
 H₂O 0.3500
 N₂ 0.0057

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.78931-01	.94194-01	.94194-00	.75009+19	.19974-03	.12663+01
CO ₂	.24697+00	.29711+00	.29711+01	.23660+20	.17283-02	.10957+02
CO	.80086-01	.95572-01	.95572+00	.76107+19	.35385-03	.22433+01
NH ₃	.62340-04	.74395-04	.74395-03	.59242+16	.16747-06	.10617-02
H ₂ O	.25354+00	.30261+00	.30261+01	.24098+20	.72057-03	.45682+01
H ₂	.17067+00	.20367+00	.20367+01	.16219+20	.54272-04	.34407+00
N ₂	.56688-02	.67650-02	.67650-01	.53872+18	.25049-04	.15880+00
C	S .61150-02	.10000+01	.00000	.00000	.00000	.73447-01

THE TRACE VALUES ARE

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
HCN	.40086-07	.47838-07	.47838-06	.38095+13	.17089-09	.10834-05
CH ₃	.25270-09	.30992-09	.30992-08	.24680+11	.61589-12	.39086-08
C	.34553-33	.41354-33	.41354-32	.32931-13	.65652-36	.41622-32
NH ₂	.18269-12	.21802-12	.21802-11	.17362+08	.46174-15	.29273-11
HN ₃	.36310-25	.43332-25	.43332-24	.34506-05	.24644-27	.15624-23
HN ₃	.25813-37	.30605-37	.30605-36	.24531-17	.00000	.16266-35
HN ₂	.43502-25	.51915-25	.51915-24	.41341-05	.32260-27	.20452-23
HN ₂	.58010-25	.69228-25	.69228-24	.55128-05	.43018-27	.27272-23
HN ₂	.29844-20	.35615-20	.35615-19	.28361+00	.14600-22	.92558-19
H	.27800-10	.33176-10	.33176-09	.26419+10	.44201-14	.28022-10
NO ₃	.00000	.00000	.00000	.00000	.00000	.00000
NO ₂	.17816-28	.21261-28	.21261-27	.16931-08	.12928-30	.81961-27
NO	.80248-17	.95766-17	.95766-16	.76261+03	.37982-19	.24079-15
N	.50410-25	.60158-25	.60158-24	.47905-05	.11138-27	.70609-24
O ₂	.95527-23	.11400-22	.11400-21	.90781-03	.48216-25	.30568-21
O	.10843-22	.12701-22	.12701-21	.10114-02	.26859-25	.17028-21
NH	.14803-21	.17666-21	.17666-20	.14068-01	.35061-24	.22227-20
OH	.46803-13	.55853-13	.55853-12	.44477+07	.12555-15	.79597-12

CO 0.3709
 H₂ 0.2477
 CH₄ 0.0012
 CO₂ 0.0739
 H₂O 0.3000
 N₂ 0.0062

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.72791-01	.89809-01	.89809+00	.71517+19	.19044-03	.11676+01
CO ₂	.24840+00	.30647+00	.30647+01	.24405+20	.17827-02	.10932+02
CO	.79673-01	.97065-01	.97065+00	.77295+19	.35937-03	.22037+01
NH ₃	.61712-04	.76140-04	.76140-03	.60632+16	.17140-06	.10510-02
H ₂ O	.24324+00	.30010+00	.30010+01	.23898+20	.71459-03	.43819+01
H ₂	.16119+00	.19887+00	.19887+01	.15837+20	.52993-04	.32496+00
N ₂	.61691-02	.76114-02	.76114-01	.60611+18	.28182-04	.17282+00
C	S .46140-01	.10000+01	.00000	.00000	.00000	.55419+00

THE TRACE VALUES ARE

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
HCN	.40640-07	.50141-07	.50141-06	.39929+13	.17911-09	.10983-05
CH ₃	.24237-09	.29903-09	.29903-08	.23813+11	.59426-12	.36440-08
C	.33518-33	.41354-33	.41354-32	.32931-13	.65652-36	.40258-32
NH ₂	.18302-12	.22581-12	.22581-11	.17982+08	.47824-15	.29326-11
HN ₃	.41417-25	.51100-25	.51100-24	.40692-05	.29062-27	.17821-23
HN ₃	.27415-37	.33825-37	.33825-36	.26935-17	.00000	.17275-35
HN ₂	.45492-25	.56127-25	.56127-24	.44695-05	.34878-27	.21387-23
HN ₂	.60663-25	.74845-25	.74845-24	.59601-05	.46509-27	.28519-23
HN ₂	.30729-20	.37913-20	.37913-19	.30191+00	.15542-22	.95303-19
H	.26571-10	.32782-10	.32782-09	.26106+10	.43678-14	.26783-10
NO ₃	.00000	.00000	.00000	.00000	.00000	.00000
NO ₂	.18854-28	.23262-28	.23262-27	.18524-08	.14145-30	.86737-27
NO	.83618-17	.10317-16	.10317-15	.82154+03	.40917-19	.25090-15
N	.51719-25	.63810-25	.63810-24	.50614-05	.11814-27	.72443-24
O ₂	.95307-23	.11759-22	.11759-21	.93639-03	.46734-25	.30497-21
O	.10455-22	.12899-22	.12899-21	.10272-02	.27278-25	.16727-21
NH	.15008-21	.18516-21	.18516-20	.14745-01	.36748-24	.22534-20
OH	.45432-13	.56053-13	.56053-12	.44637+07	.12600-15	.77266-12

Table 49 (cont'd)

Texaco Entrained Oxygen-Blown Gas (Cont'd)

CO 0.3974
 H₂ 0.2654
 CH₄ 0.0013
 CO₂ 0.0792
 H₂O 0.2500
 N₂ 0.0066

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.06750-01	.85252-01	.85252+00	.67889+19	.18078-03	.10709+01
CO ₂	.24792+00	.31665+00	.31665+01	.25215+20	.18470-02	.10911+02
CO	.77251-01	.98664-01	.98664+00	.78569+19	.36530-03	.21639+01
NH ₃	.60196-04	.76883-04	.76883-03	.61224+16	.17307-06	.10252-02
H ₂ O	.23270+00	.29721+00	.29721+01	.23867+20	.70770-03	.41921+01
H ₂	.15171+00	.19376+00	.19376+01	.15430+20	.51632-04	.30585+00
N ₂	.65699-02	.83911-02	.83911-01	.66820+18	.31069-04	.18404+00
C	S .85976-01	.10000+01	.00000	.00000	.00000	.10327+01

THE TRACE VALUES ARE

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
HCN	.40687-07	.51966-07	.51966-06	.41382+13	.18563-09	.10996-05
CH ₃	.22517-09	.28758-09	.28758-08	.22901+11	.57150-12	.33654-08
C	.32379-33	.41354-33	.41354-32	.32931-13	.65652-36	.38890-32
NH ₂	.18087-12	.23100-12	.23100-11	.18395+08	.48923-15	.28980-11
HN ₃	.45713-25	.58385-25	.58385-24	.46493-05	.33205-27	.19669-23
HN ₃	.28626-37	.36817-37	.36817-36	.29318-17	.00000	.18164-35
HN ₃	.47058-25	.60102-25	.60102-24	.47861-05	.37348-27	.22123-23
HN ₃	.62751-25	.80146-25	.80146-24	.63822-05	.49803-27	.29501-23
HN ₃	.31271-20	.39940-20	.39940-19	.31805+00	.16373-22	.96985-19
H	.25336-10	.32359-10	.32359-09	.25768+10	.43113-14	.25538-10
NO ₃	.00000	.00000	.00000	.00000	.00000	.00000
NO ₂	.19758-28	.25235-28	.25235-27	.20096-08	.15345-30	.90898-27
NO	.86209-17	.11011-16	.11011-15	.87680+03	.43669-19	.25868-15
N	.52458-25	.66999-25	.66999-24	.53353-05	.12604-27	.73478-24
O ₂	.95126-23	.12149-22	.12149-21	.96749-03	.51387-25	.30439-21
O	.10266-22	.13112-22	.13112-21	.10441-02	.27728-25	.16425-21
NH	.15025-21	.19190-21	.19190-20	.15282-01	.38086-24	.22561-20
OH	.44034-13	.56240-13	.56240-12	.44785+07	.12642-15	.74689-12

CO 0.4100
 H₂ 0.2740
 CH₄ 0.0010
 CO₂ 0.0820
 H₂O 0.2260
 N₂ 0.0070

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
CH ₄	.03742-01	.82805-01	.82805+00	.65940+19	.17559-03	.10226+01
CO ₂	.24798+00	.32215+00	.32215+01	.25653+20	.18740-02	.10914+02
CO	.76607-01	.99517-01	.99517+00	.79248+19	.36845-03	.21458+01
NH ₃	.60149-04	.78138-04	.78138-03	.62223+16	.17590-06	.10244-02
H ₂ O	.22743+00	.29544+00	.29544+01	.23527+20	.70349-03	.40971+01
H ₂	.14700+00	.19096+00	.19096+01	.15207+20	.50885-04	.29635+00
N ₂	.69699-02	.90543-02	.90543-01	.72102+18	.33525-04	.19525+00
C	S .10467+00	.10000+01	.00000	.00000	.00000	.12572+01

THE TRACE VALUES ARE

SPECIES NAME	MOLES	MOLE FRAC	PRESSURE	PART/CC	DENSITY	MASS
HCN	.41252-07	.53589-07	.53589-06	.42674+13	.19143-09	.11149-05
CH ₃	.21659-09	.28137-09	.28137-08	.22406+11	.55915-12	.32565-08
C	.31634-33	.41354-33	.41354-32	.32931-13	.65653-36	.38236-32
NH ₂	.18205-12	.23649-12	.23649-11	.18832+08	.50005-15	.29169-11
HN ₃	.50011-25	.64967-25	.64967-24	.51735-05	.36949-27	.21519-23
HN ₃	.29991-37	.38960-37	.38960-36	.31025-17	.00000	.18898-35
HN ₃	.48539-25	.63055-25	.63055-24	.50213-05	.39183-27	.22620-23
HN ₃	.64727-25	.84084-25	.84084-24	.66958-05	.52250-27	.30430-23
HN ₃	.31979-20	.41543-20	.41543-19	.33082+00	.17030-22	.99181-19
H	.24728-10	.32124-10	.32124-09	.25581+10	.42600-14	.24926-10
NO ₃	.00000	.00000	.00000	.00000	.00000	.00000
NO ₂	.20529-28	.26669-28	.26669-27	.21237-08	.16217-30	.94445-27
NO	.08800-17	.11536-16	.11536-15	.91667+03	.45754-19	.26647-15
N	.53575-25	.69596-25	.69596-24	.55422-05	.12885-27	.75042-24
O ₂	.51149-23	.12360-22	.12360-21	.98429-03	.52279-25	.30447-21
O	.10181-22	.13225-22	.13225-21	.10532-02	.27967-25	.16288-21
NH	.15234-21	.19790-21	.19790-20	.15759-01	.39275-24	.22874-20
OH	.43350-13	.56315-13	.56315-12	.44645+07	.12659-15	.73726-12

Table 50

MOLE FRACTIONS OF MAJOR AND TRACE CONSTITUENTS IN THE MCFC ANODE INLET GAS

Rockwell Molten Carbonate Air-Blown Gas	Rockwell Molten Carbonate Air-Blown Gas Zinc Oxide Polished	METC Gravitating Bed Air-Blown Gas FeO/ZnO Desulfurization and Filtered	METC Gravitating Bed Air-Blown Gas FeO Desulfurization	Westinghouse Fluidized Bed Oxygen-Blown Gas Dolomite/ZnO Desulfurization	Westinghouse Fluidized Bed Oxygen-Blown Gas Selexol/ZnO Desulfurization	Texaco Entrained Oxygen-Blown Gas Benfield/ZnO Desulfurization	Texaco Entrained Oxygen-Blown Gas Molten Carbonate/ ZnO Desulfurization
CO 0.2192	CO 0.2192	CO 0.1714	CO 0.1714	CO 0.3186	CO 0.3186	CO 0.3391	CO 0.3391
H ₂ 0.0916	H ₂ 0.0916	H ₂ 0.1248	H ₂ 0.1248	H ₂ 0.1593	H ₂ 0.1593	H ₂ 0.2265	H ₂ 0.2265
CH ₄ 0.0130	CH ₄ 0.0130	CH ₄ 0.0237	CH ₄ 0.0237	CH ₄ 0.0295	CH ₄ 0.0295	CH ₄ 0.0011	CH ₄ 0.0011
CO ₂ 0.0214	CO ₂ 0.0214	CO ₂ 0.0537	CO ₂ 0.0537	CO ₂ 0.0797	CO ₂ 0.0797	CO ₂ 0.0676	CO ₂ 0.0676
H ₂ O 0.2500	H ₂ O 0.2500	H ₂ O 0.2100	H ₂ O 0.2100	H ₂ O 0.4100	H ₂ O 0.4100	H ₂ O 0.3600	H ₂ O 0.3600
N ₂ 0.4048	N ₂ 0.4048	N ₂ 0.4163	N ₂ 0.4163	N ₂ 0.0030	N ₂ 0.0030	N ₂ 0.0056	N ₂ 0.0056
NH ₃ 13.2 ppm	NH ₃ 13.2 ppm	NH ₃ 3477.1 ppm	NH ₃ 3477.1 ppm	NH ₃ 207.7 ppm	NH ₃ -	NH ₃ -	NH ₃ 1239.4 ppm
H ₂ S 132.0 ppm	H ₂ S 66.0 ppb	H ₂ S 69.5 ppb	H ₂ S 139.1 ppm	H ₂ S 51.9 ppb	H ₂ S 51.9 ppb	H ₂ S 56.3 ppb	H ₂ S 56.3 ppb
Na ₂ CO ₃ 396.1 ppm	Na ₂ CO ₃ 4.0 ppm	HCl 695.4 ppm	HCl 695.4 ppm	HCl 415.5 ppm	HCl -	HCl -	HCl -
HCl -	HCl -	Pb 1.7 ppm	Pb 1.7 ppm	Pb 1.0 ppm	Pb 103.9 ppb	Pb 1.1 ppm	Pb 1.1 ppm
Pb 1.3 ppm	Pb 1.3 ppm	C 4.2 ppm	C 278.2 ppm	As 5.2 ppm	As 103.9 ppb	As 3.4 ppm	As 5.6 ppm
As 6.6 ppm	As 6.6 ppm	Tar 5563.3 ppm	Tar 5563.3 ppm	C 3.1 ppm	C 18.7 ppm	C 3.4 ppm	C 3.4 ppm
	ZnO 132.0 ppb	ZnO 139.1 ppb			Poly- 103.9ppb ethylene glycol in ether	K ₂ CO ₃ 20.3 ppm	Na ₂ CO ₃ 338.0ppm

Table 51
OXIDANT COMPOSITION,
mole fractions

<u>Bulk Gas Constituent</u>	<u>Air-Blown Coal Gas</u>	<u>Oxygen-Blown Coal Gas</u>
CO ₂	0.1214	0.13
H ₂ O	0.1488	0.17
N ₂	0.6641	0.63
O ₂	0.0656	0.07

containing x_i moles of the i^{th} species, the free energy can be expressed as:

$$F(X) = \sum_{i=1}^n f_i, \quad (195)$$

where $X = (x_1, x_2, \dots, x_n)$, the mole numbers,

$$f_i = x_i [c_i + \ln(x_i/\bar{x})], \quad (196)$$

$$c_i = (G^0/RT)_i + \ln P, \quad (197)$$

P = total pressure, atm, and

$$\bar{x} = \sum_{i=1}^n x_i. \quad (198)$$

The equilibrium composition results from the nonnegative set of x_i values that minimizes $F(X)$ and satisfies the mass balance constraints of

$$\sum_{i=1}^n a_{ij} = b_j \quad (j = 1, 2, \dots, m), \quad (199)$$

where m = different types of atoms

a_{ij} = formula numbers indicating the number of atoms of element j in a molecule of species i

b_j = total number of atomic weights of element j originally present in the mixture.

At temperatures between 873 and 1023 K (1112 and 1382°F), quantitative measurements using galvanic cells of the type

have shown a nearly linear relation of the cell emf and the logarithm of the oxygen partial pressure.^{68,69} The oxygen partial pressure in a mixture of nonreactive gases containing only nitrogen, argon, or carbon dioxide could be measured, as could the residual oxygen pressure resulting from the reaction of hydrocarbons, carbon monoxide, hydrogen, and other gases with oxygen within the cell. The theoretical open circuit potential (OCP)_T difference in volts between the two electrodes in the cell was related to the oxygen pressure in the fuel gas and to air at the counterelectrode by the following equation:

$$E = E_r - E_l = RT/nF(\ln P_r/P_l) = 4.96 \times 10^{-5} T_1 (\log P_r/P_l), \quad (201)$$

where n , the number of electrons, is equal to 4 on the basis of the reversible reaction

Given the molar percentages of H_2O , H_2 , CO_2 , and CO in the fuel gas, the equilibrium partial pressure of oxygen can be established through the following equilibrium constant (K_p) relations:

$$K_p = \frac{[\text{H}_2\text{O}]}{[\text{H}_2][\text{O}_2]^{1/2}} ; K_p(1)[\text{O}_2]^{1/2} = \frac{[\text{H}_2\text{O}]}{[\text{H}_2]} \quad (204)$$

* Brackets indicate concentration or partial pressure.

$$K_p = \frac{[\text{CO}_2]}{[\text{CO}][\text{O}_2]^{1/2}} \quad ; \quad K_p(2)[\text{O}_2]^{1/2} = \frac{[\text{CO}_2]}{[\text{CO}]} \quad (206)$$

In order to define the chemical stability of the nickel anode when it is exposed to fuel gases containing sulfur, the partial pressure or concentration of sulfur must be determined. The total sulfur content is defined as:

$$[\text{S}] = 2[\text{S}_2] + [\text{COS}] + 2[\text{CS}_2] + [\text{H}_2\text{S}] + [\text{SO}_2] \quad (207)$$

and can be related to the partial pressures of the bulk gas constituents and to the established oxygen partial pressure through the following K_p relations:

$$K_p = \frac{[\text{SO}_2][\text{H}_2]}{[\text{H}_2\text{S}][\text{O}_2]} \quad ; \quad K_p(3) \frac{[\text{O}_2]}{[\text{H}_2]} = \frac{[\text{SO}_2]}{[\text{H}_2\text{S}]} \quad (209)$$

$$K_p = \frac{[\text{H}_2\text{O}]^2 [\text{CS}_2]}{[\text{H}_2\text{S}]^2 [\text{CO}_2]} \quad ; \quad K_p(4) \frac{[\text{CO}_2]}{[\text{H}_2\text{O}]^2} = \frac{[\text{CS}_2]}{[\text{H}_2\text{S}]^2} \quad (211)$$

$$K_p = \frac{[\text{COS}][\text{H}_2\text{O}]}{[\text{H}_2\text{S}][\text{CO}_2]} \quad ; \quad K_p(5) \frac{[\text{CO}_2]}{[\text{H}_2\text{O}]} = \frac{[\text{COS}]}{[\text{H}_2\text{S}]} \quad (213)$$

$$K_p = \frac{[H_2S]}{[S_2]^{1/2} [H_2]} ; \frac{[H_2S]}{K_p^2(6) [H_2]} = \frac{[S_2]}{[H_2S]} \quad (215)$$

Having established the partial pressure of oxygen and sulfur in the fuel gas, we can evaluate the stability of the various nickel phases (metallic Ni, NiS, Ni₃S₂, NiO, and NiSO₄) on the basis of their free energy of formation.

Preliminary calculations using this model were performed for the Rockwell molten carbonate gasifier air-blown coal gas supplied to a 923 K (1202°F), 10.5 atm MCFC system. Note that this model does not account for the presence of CH₄, NH₃, or solid carbon, or the effects of chemisorption. In the absence of trace contaminants, the model indicates that if the nickel anode were exposed to the 100 ppm sulfur fuel gas, an OCP_T of less than 0.7 or more than 0.94 V would be required in order to avoid sulfidation of the inlet anode material surface (Figure 25). Nickel oxide (NiO) is projected to form as the stable anode phase for OCP_Ts of less than 0.7 V, while metallic Ni results when the OCP_T exceeds 0.94 V. The transition of Ni₃S₂ to Ni as a function of the fuel gas sulfur content is independent of the cell operating pressure (1.0 to 10.5 atm) when an OCP_T of 0.8 to 1.0 V is maintained. At an OCP_T below 0.7 V, 53.76, 106.1 and more than 150 ppm of sulfur in the 923 K (1202°F) inlet fuel gas is required to convert NiO into Ni₃S₂ for cells operating at 10.5, 5, and 1 atm, respectively (Table 52).

The presence of trace constituents Pb, As, and Na does not perturb the NiO-Ni₃S₂-Ni phase stability as a function of the total sulfur content and OCP_T (Figure 26). At low OCP_T trace constituents may condense along the anode surface, principally as lead sulfate (PbSO₄ or 2PbO·PbSO₄), arsenic pentoxide (As₂O₅), and sodium sulfate (Na₂SO₄). As the OCP_T is increased, lead and arsenic exist predominantly as volatiles [Pb(g), AsO(g)]. Within the Ni₃S₂ regime the fuel gas sodium forms both

Figure 25 -- Relation of Theoretical Open-Circuit Potential to Sulfur Concentration at the Nickel Anode in the Rockwell Molten Carbonate Gasifier Air-Blown MCFC at 923 K (1202°F) and 10.5 atm

as the sulfate (Na_2SO_4) and as the carbonate (Na_2CO_3) species. The projected $\text{Na}_2\text{SO}_4 \rightarrow \text{Na}_2\text{CO}_3$ transition occurs between 0.74 and 0.785 V, depending on the total sulfur content of the inlet fuel gas. A sharp transition of the solid Na_2CO_3 phase to volatile Na is projected for a cell OCP_T greater than 0.92 V.

In order to demonstrate the stability of the electrolyte when exposed to fuel gases containing sulfur and trace contaminants, we used the model. It projected a transition of the electrolyte K_2CO_3 into K_2SO_4 within the LiAlO_2 matrix below OCP_T of 0.8 V when exposed to sulfur concentrations ranging from 0 to 150 ppm (Figure 27). From the phase stability diagram in Figure 28, the electrolyte containing 62 wt% Li_2CO_3 /38 wt% K_2CO_3 at 923 K (1202°F) cell operating temperatures is expected to exist as a liquid melt. The literature does not detail the solubilities of either volatile or condensed contaminant phases within this melt. We have chosen to estimate the thermodynamic properties for

Table 52

PROJECTED SULFUR CONCENTRATIONS REQUIRED TO PROMOTE PHASE
TRANSITIONS OF THE NICKEL ANODE MATERIAL AS A FUNCTION
OF THE THEORETICAL OPEN CIRCUIT POTENTIAL AND MCFC
TOTAL PRESSURE

System Pressure								
1 atm			5 atm			10.5 atm		
emf, V	Phase	Sulfur, ppm	emf, V	Phase	Sulfur, ppm	emf, V	Phase	Sulfur, ppm
0.10	NiO	—	0.10	NiO	—	0.10	NiO	—
0.20	NiO	—	0.20	NiO	—	0.20	NiO	—
0.30	NiO	—	0.30	NiO	—	0.30	NiO	—
0.40	NiO	—	0.40	NiO	—	0.40	NiO	—
0.50	NiO	—	0.50	NiO	—	0.50	NiO	—
0.60	NiO	—	0.60	NiO	—	0.60	NiO	—
0.70	NiO*	—	0.70	NiO/Ni ₃ S ₂	106.10	0.70	NiO/Ni ₃ S ₂	53.76
0.72	NiO/Ni ₃ S ₂	90.81	0.72	NiO/Ni ₃ S ₂	22.01	0.72	NiO/Ni ₃ S ₂	12.99
0.74	NiO/Ni ₃ S ₂	18.54	0.74	Ni ₃ S ₂	—	0.74	Ni ₃ S ₂	—
0.76	Ni ₃ S ₂	—	0.76	Ni ₃ S ₂	—	0.76	Ni ₃ S ₂	—
0.78	Ni ₃ S ₂	—	0.78	Ni ₃ S ₂	—	0.78	Ni ₃ S ₂	—
0.80	Ni ₃ S ₂	—	0.80	Ni ₃ S ₂	—	0.80	Ni ₃ S ₂	—
0.82	Ni ₃ S ₂	—	0.82	Ni ₃ S ₂	—	0.82	Ni ₃ S ₂	—
0.84	Ni/Ni ₃ S ₂	10.98	0.84	Ni/Ni ₃ S ₂	10.96	0.84	Ni/Ni ₃ S ₂	10.96
0.86	Ni/Ni ₃ S ₂	17.85	0.86	Ni/Ni ₃ S ₂	17.85	0.86	Ni/Ni ₃ S ₂	17.85
0.88	Ni/Ni ₃ S ₂	28.79	0.88	Ni/Ni ₃ S ₂	28.79	0.88	Ni/Ni ₃ S ₂	28.79
0.90	Ni/Ni ₃ S ₂	45.76	0.90	Ni/Ni ₃ S ₂	45.76	0.90	Ni/Ni ₃ S ₂	45.76
0.92	Ni/Ni ₃ S ₂	71.13	0.92	Ni/Ni ₃ S ₂	71.13	0.92	Ni/Ni ₃ S ₂	71.13
0.94	Ni/Ni ₃ S ₂	107.05	0.94	Ni/Ni ₃ S ₂	107.05	0.94	Ni/Ni ₃ S ₂	107.05
0.96	Ni	—	0.96	Ni	—	0.96	Ni	—
0.98	Ni	—	0.98	Ni	—	0.98	Ni	—
1.00	Ni	—	1.00	Ni	—	1.00	Ni	—

Figure 26 -- Effect of Lead, Arsenic, and Sodium Contaminants on the Stability of the Nickel Anode Material in the Rockwell Molten Carbonate Gasifier Air-Blown MCFC at 923 K (1202°F) and 10.5 atm

the eutectic mixture and project its phase stability in the sulfur-containing environments.

Although this model is able to project phase stabilities of electrode materials as a function of sulfur concentrations and OCP_T , several revisions were required in order to be able to:

- Consider the presence of CO_2 in the oxidant gases, a principal constituent in the MCFC cathode half-cell reaction.
- Incorporate the potential for carbon deposition along the anode channel. Although the initial fuel gas composition has been humidified, minimizing carbon formation at the anode inlet,

Figure 27 -- Phase Stability of the 62% Li_2CO_3 /38% K_2CO_3
Electrolyte to the Rockwell Molten Carbonate Gasifier
Air-Blown Fuel Gases in the 923 K (1202°F) and 10.5 atm
MCFC

Figure 28 -- K_2CO_3 / Li_2CO_3 Phase Stability Diagram⁷⁰

compositional changes within the fuel gas may occur, so that at equilibrium, carbon may form as a stable product.

- Project the resulting equilibrium fuel and oxidant gas composition as a function of position in the cocurrent electrode system. Linear step gradients in anode and cathode temperature will be assumed in the constant pressure MCFC. The resulting phase stability of nickel along the anode and the resulting current and cell voltage will be used in routines that ultimately rank cell performance for the various MCFC. These revisions are described below and constitute the model upon which this study is based.

In an anode-fuel gas reaction model revision, the fuel gas is considered to consist of eight gas species: H_2 , H_2O , CO , CO_2 , CH_4 , N_2 , NH_3 , and O_2 , with the possible formation of solid carbon.* Ammonia and oxygen in this investigation are assumed to be present in trace proportions. The reactions of H_2 and CO with the electrolyte carbonate ion generate electrons, as shown in reactions (216) and (217):

or, more conveniently,

In addition, fuel gas species reactions occur simultaneously. These include:

* Carbon as graphite.

The atomic molar mass balances (C, H, N, O) in the fuel gas are

$$b_H = (2[\text{H}_2] + 2[\text{H}_2\text{O}] + 4[\text{CH}_4] + 3[\text{NH}_3])\lambda/P \quad (224)$$

$$b_C = ([\text{CO}] + [\text{CO}_2] + [\text{CH}_4])\lambda/P \quad (225)$$

$$b_O = ([\text{CO}] + 2[\text{CO}_2] + [\text{H}_2\text{O}] + 2[\text{O}_2])\lambda/P \quad (226)$$

$$b_N = (2[\text{N}_2] + [\text{NH}_3])\lambda/P, \quad (227)$$

where $[\text{H}_2]$, $[\text{H}_2\text{O}]$, and so on are the species partial pressure, λ the total number of gaseous moles in the fuel gas ($PV = \lambda RT$), and P the total gas pressure at temperature T . The total gas pressure in the fuel gas stream is:

$$P = [\text{H}_2] + [\text{H}_2\text{O}] + [\text{CO}] + [\text{CO}_2] + [\text{CH}_4] + [\text{N}_2] + [\text{O}_2] + [\text{NH}_3]. \quad (228)$$

From this equation one obtains:

$$\lambda = (b_H/2 + b_N/2 + b_C)/(1 + 2[\text{CH}_4]/P). \quad (229)$$

Solving the above equations simultaneously with the mass action laws, we can determine the values of $[\text{H}_2]$, $[\text{H}_2\text{O}]$, $[\text{CO}]$, $[\text{CO}_2]$, $[\text{CH}_4]$, $[\text{N}_2]$, and λ .

The oxidant considered in this study consists of four chemical species: O_2 , CO_2 , H_2O , and N_2 . The reaction of O_2 and CO_2 with

externally supplied electrons produces the carbonate ion. This reaction is written as:

or, more conveniently,

In the oxidant, the atomic molar mass balances are:

$$b_H = 2[\text{H}_2\text{O}]\lambda/P \quad (232)$$

$$b_C = [\text{CO}_2]\lambda/P \quad (233)$$

$$b_O = (2[\text{CO}_2] + 2[\text{O}_2] + [\text{H}_2\text{O}])\lambda/P \quad (234)$$

$$b_N = 2[\text{N}_2]\lambda/P, \quad (235)$$

where $[\text{H}_2\text{O}]$, $[\text{CO}_2]$, and so on, are the species partial pressure, λ the total number of gaseous moles in the oxidant ($PV = \lambda RT$), and P the total gas pressure at temperature T . The total gas pressure is:

$$P = [\text{H}_2\text{O}] + [\text{O}_2] + [\text{CO}_2] + [\text{N}_2], \quad (236)$$

and, from the above,

$$\lambda = \frac{1}{2} (b_O + \frac{1}{2} b_N + \frac{1}{2} b_H). \quad (237)$$

If the total pressure and the b_j ($j = \text{H}, \text{C}, \text{O}, \text{N}$) values are known, the above equations can be solved simultaneously, and values of $[\text{H}_2\text{O}]$, $[\text{CO}_2]$, $[\text{O}_2]$, $[\text{N}_2]$, and λ can be determined.

Neglecting diffusion, we can describe the gas flow of both the fuel gas and the oxidant streams in terms of the continuity equation of the individual chemical species. For example,

$$\frac{\partial N_i}{\partial t} + \frac{\partial N_i V_s}{\partial x} = K_i, \quad (238)$$

where $N_i = P_i/kT$ is the i 'th chemical species number density, K_i its net rate of formation, and V_s the mass-averaged stream velocity. In this study, the K_i values are expressed in terms of their ionic current flows, J_i , in the electrolyte:

$$K_i = \frac{N_o}{\ell F} \left(\frac{J}{n} \right)_i, \quad (239)$$

where $J_i \equiv J$, and n is the electron equivalent number (the stoichiometry number of electrons in reactions (216), (217), and (230)). N_o is the Avagadro number, F is Faraday's constant, and ℓ is the thickness of the gas stream channel.

In terms of the atomic molar values, b_j , equation (230) is rewritten as:

$$\frac{\partial (b_j N / \lambda)}{\partial t} + \frac{\partial (b_j \frac{NV_s}{\lambda})}{\partial x} = \frac{N_o}{\ell F} \sum a_{ij} \left(\frac{J}{n} \right)_i, \quad (240)$$

where the a_{ij} coefficients are values indicating the number of atomic elements of type j in species i . At steady-state conditions a special case:

$$\left(\frac{\partial b_j}{\partial x} = 0 \right)$$

gives

$$\frac{\partial \ln \lambda}{\partial x} = \frac{N_o}{\ell F N V_s} \sum \left(\frac{J}{n} \right)_i. \quad (241)$$

This equation results because either the a_{ij} or the $\left(\frac{J}{n} \right)_i$ terms are zero for the i 'th species when

$$\frac{\partial b_j}{\partial x} = 0.$$

In general,

$$\frac{\partial b_j}{\partial x} = \frac{N_o}{\ell F} \frac{\lambda}{NV_s} \sum a_{ij} \left(\frac{J}{n}\right)_i \quad (242)$$

and

$$\frac{\partial NV_s}{\partial x} = \frac{N_o}{\ell F} \sum \left(\frac{J}{n}\right)_i \quad (243)$$

or

$$\frac{\partial \bar{b}_j}{\partial x} = \frac{N_o}{\ell F NV_s} \left\{ \sum_i a_{ij} \left(\frac{J}{n}\right)_i - \bar{b}_j \sum_i \left(\frac{J}{n}\right)_i \right\}, \quad (244)$$

where

$$\bar{b}_j \equiv b_j / \lambda. \quad (245)$$

Using the above gas flow dependent equations, we find that the elemental molar changes in the fuel gas and oxidant streams caused by chemical reactions with the carbonate ion are:

(1) Anode*

$$\frac{\partial b_O^a}{\partial x} = \left(\frac{\lambda}{NV_s}\right)_a \frac{N_o}{\ell F} \frac{3}{2} J_a \quad (246)$$

$$\frac{\partial b_C^a}{\partial x} = \left(\frac{\lambda}{NV_s}\right)_a \frac{N_o}{\ell F} \frac{1}{2} J_a \quad (247)$$

$$\frac{\partial b_H^a}{\partial x} = 0 \quad (248)$$

$$\frac{\partial b_N^a}{\partial x} = 0 \quad (249)$$

*The superscripts (a) and (c) refer to the conditions in the gases at the anode and the cathode, respectively.

$$\frac{\partial NV_s}{\partial x} = \frac{N_o}{\ell F} 1/2 J_a \quad (250)$$

$$\frac{\partial \lambda}{\partial x} = \frac{N_o}{\ell F} \frac{\lambda}{NV_s} 1/2 J_a , \quad (251)$$

where J_a is the ionic flow at the anode.

(2) Cathode

$$\frac{\partial b_O^c}{\partial x} = - \left(\frac{\lambda}{NV_s} \right)_c \frac{N_o}{\ell F} 3/2 J_c \quad (252)$$

$$\frac{\partial b_C^c}{\partial x} = - \left(\frac{\lambda}{NV_s} \right)_c \frac{N_o}{\ell F} 1/2 J_c \quad (253)$$

$$\frac{\partial b_H^c}{\partial x} = 0 \quad (254)$$

$$\frac{\partial b_N^c}{\partial x} = 0 \quad (255)$$

$$\frac{\partial NV_s}{\partial x} = - \frac{N_o}{\ell F} \frac{3}{4} J_c \quad (256)$$

$$\frac{\partial \lambda}{\partial x} = - \frac{N_o}{\ell F} \frac{\lambda}{NV_s} \frac{3}{4} J_c , \quad (257)$$

where J_c is the ionic flow at the cathode.

The anode and cathode ionic flows are related by the following definition:

$$J_a = \epsilon_I J_c , \quad (258)$$

where ϵ_I is the current efficiency. Ideally, the overall relations of carbon and oxygen in the fuel cell are:

$$b_O^a + b_O^c = C_1(\text{constant}) \quad (259)$$

$$b_C^a + b_C^c = C_2(\text{constant}) , \quad (260)$$

or

$$\frac{\partial b_O^a}{\partial x} = - \frac{\partial b_O^c}{\partial x} \quad (261)$$

and

$$\frac{\partial b_C^a}{\partial x} = - \frac{\partial b_C^c}{\partial x} . \quad (262)$$

The above chemical reactions involving the electrolyte carbonate ion determine the overall electrochemical expression for the fuel cell, which can be expressed in terms of the Nernst equation:

$$E = E^O + \frac{RT_a}{4F} \ln \left(\frac{[H_2][CO]}{[H_2O][CO_2]^3} \right)_a + \frac{RT_c}{4F} \ln ([CO]^2[O_2])_c, \quad (263)$$

where T_a is the fuel gas temperature and T_c the oxidant temperature, R the universal gas constant, and F the Faraday constant. The E^O parameter represents a change in the chemical potential across the overall chemical reaction. That is,

$$E^O = -\Delta G^O/4F, \quad (264)$$

with

$$\Delta G^O = -(G_{H_2}^O + G_{CO}^O - G_{H_2O}^O - 3G_{CO_2}^O)_a - (2G_{CO_2}^O + G_{O_2}^O)_c, \quad (265)$$

where G_x^0 ($x = H_2, CO, H_2O, CO_2, O_2$) are the standard Gibbs free energies (chemical potentials) of the species in both the fuel gas and oxidant streams.

The potential balance across the fuel cell at a distance x from either the anode or cathode inlet is defined as:

$$E = V_0 + ZJ(x), \quad (266)$$

where J is the current density, and V_0 is the terminal voltage. In the above equation Z is defined as the total effective cell impedance at distance x :

$$Z \equiv R_\Omega dA + Z_A + Z_C, \quad (267)$$

where $dA = (W)dx$ is an incremental area at distance x , W is the fuel cell width, R_Ω is the ohmic cell resistance, and Z_A the activation and Z_C the concentration polarization resistance.

Equilibrium concentrations of chemical species in gas streams subjected to pressure and/or temperature gradients are best determined by integrative means, in particular for processes involving mass transfer. We have, therefore, adapted this scheme to the fuel cell model used in this study. The integration methods employed are either the Hamming or the Euler predictor corrector routines.

In the present model we neglect diffusion processes and consider only one-dimensional gas flow. Integration of the chemical species concentrations (partial pressures) is performed along the gas stream, starting with known inlet concentrations and terminating at one or more predetermined boundary conditions (i.e., cell length, fuel or oxidant gas utilization, total cell current, average current density, and terminal voltage).

Since most computer libraries contain very reliable integration routines, we will limit our present discussion to formulae that define only the gradients that are to be integrated. We determine these concentration gradients at each integration point by solving simultaneously a set of linear independent equations that describe the chemical reactions taking place and the mass balances that must be satisfied. For each chemical reaction the mass action law can be written as:

$$\sum_{i=1}^{i=N_s} \eta_i^{(K)} \frac{\partial \ln P_i}{\partial x} = \frac{\Delta H_r^{(K)}}{RT^2} \frac{dT}{dx} ; \quad K = 1, 2, 3, \dots N_r , \quad (268)$$

where $\eta_i^{(K)}$ are the stoichiometric coefficients of the K^{th} chemical reaction for each (i^{th}) chemical species in the mixture, P_i the species partial pressure, $\Delta H_r^{(K)}$ the enthalpy change across the reaction, T the gas temperature, $\frac{dT}{dx}$ the temperature gradient, and R the universal gas constant. In addition, the elemental molar mass constraints are represented as:

$$\sum_i a_{ij} P_i \frac{\partial \ln P_i}{\partial x} = F_j ; \quad j = 1, 2, 3, \dots N_e , \quad (269)$$

where, by use of the continuity equation,

$$F_j = \frac{N_o}{\lambda F} \frac{P}{NV_s} \left\{ \sum_{i,j} a_{ij} \left(\frac{J}{n} \right)_i - \frac{b_j}{\lambda} \sum \left(\frac{J}{n} \right)_i \right\} . \quad (270)$$

In the above expression the value of each parameter is known at each successive integration point. Thus, equations (262) and (263) represent N_r and N_e independent equations, which are linear with respect to $\frac{\partial \ln P_i}{\partial x}$. For ideal gas mixtures the total number of gas species, N_s , equals N_r and N_e , and the above equations can be solved simultaneously for the $\frac{\partial \ln P_i}{\partial x}$ gradients. If, however, a condensed state is present and in equilibrium with the gas species, a slight modification of

the above set of equations is necessary, and again the $\frac{\partial \ln P_i}{\partial x}$ are determined simultaneously.

In the integration of dependent variables and solution of cell efficiencies, the following variables are evaluated simultaneously along the fuel cell length:

<u>Anode</u>		<u>Cathode</u>	
T	[H ₂ O]	T	
NV _s	[CO]	NV _s	
λ	[CO ₂]	b _O	
b _O	[CH ₄]	b _C	
b _C	[NH ₃]		
[O ₂]	[N ₂]		
[H ₂]			

In addition, the total cell current is determined as

$$I_a = \epsilon_I W \int_0^L J_c dx . \quad (271)$$

The cell efficiencies and/or percentage of fuel and oxidant utilization are determined as shown below:

- H₂ utilization at the anode:

$$n_{H_2} = \left[1 - \frac{[H_2]_x}{[H_2]_o} \right] 100 , \quad (272)$$

where [H₂]_x is the equilibrium concentration of H₂ in the fuel gas at distance x from the anode inlet, and [H₂]_o is the initial H₂ concentration within the fuel gas entering the MCFC.

- CO utilization at the anode:

$$n_{CO} = \left[1 - \frac{[CO]_x}{[CO]_o} \right] 100. \quad (273)$$

- H_2 and CO utilization at the anode:

$$n_{H_2 + CO} = \left[1 - \frac{[H_2]_x [CO]_x}{[H_2]_o [CO]_o} \right] 100. \quad (274)$$

- CO_2 utilization at the cathode:

$$n_{CO_2} = \left[1 - \frac{[CO_2]_x}{[CO_2]_o} \right] 100. \quad (275)$$

- O_2 utilization at the cathode:

$$n_{O_2} = \left[1 - \frac{[O_2]_x}{[O_2]_o} \right] 100. \quad (276)$$

In order to provide a means by which cell performance can be evaluated, thermodynamic, voltage, current, and overall efficiencies for each gasifier/gas-cleanup fuel cell system have been determined. The enthalpy change across reaction (265) is:

$$\Delta H_\epsilon = (H_{H_2} + H_{CO} - 3H_{CO_2})_a - (2H_{CO_2} + H_{O_2})_c. \quad (277)$$

Hence, the thermodynamic cell efficiency at distance x is:

$$\epsilon_{th} = \Delta G / \Delta H_\epsilon = -E / \Delta H_\epsilon. \quad (278)$$

As previously discussed, at equilibrium conditions when a net current is drawn, driving an external load, inefficiencies result, reducing the overall cell voltage to a value that is less than the thermodynamic equilibrium, E , or OCP_T . The voltage efficiency is defined as:

$$\epsilon_v = \frac{V_o}{E}, \quad (279)$$

where V_o = actual cell voltage under load conditions, and
 E = theoretical open-circuit equilibrium potential.

The quantity of current produced by the electrochemical reactions is obtained from Faraday's law:

$$I_F = nF \frac{df}{dt}, \quad (280)$$

where df/dt is the molar flow rate of the fuel gas. Fuel cells normally operate at less than 100% utilization of H_2 or CO in the fuel gas and CO_2 or O_2 in the oxidant stream in order to minimize diffusion losses within the cell. The resulting current related to the quantity of fuel consumed (fuel or oxidant utilization) is:

$$I = nF \left[\frac{df}{dt} \right]_{\text{consumed}} \cdot \quad (281)$$

The current efficiency (ϵ_I), therefore, is defined as:

$$\epsilon_I = \frac{I}{I_F}. \quad (282)$$

The electrochemical efficiency (ϵ_E) of the fuel cell is, therefore, defined as the product of all three efficiency terms:

$$\epsilon_E = (\epsilon_{th})(\epsilon_v)(\epsilon_I). \quad (283)$$

Two final efficiencies are determined. These are the heating value efficiency at the anode (ϵ_H) and the overall fuel cell efficiency (ϵ_F), which will be used to rank cell performance when the MCFC is operated with either Rockwell, METC, Westinghouse, or Texaco fuel gases. They have been defined as follows:

$$\epsilon_H = \frac{X_{H_2} \Delta H_C [H_2]}{X_{H_2} \Delta H_C [H_2] + X_{CH_4} \Delta H_C [CH_4] + X_{CO} \Delta H_C [CO]} \quad (284)$$

and

$$\epsilon_F = (\epsilon_E)(\epsilon_H), \quad (285)$$

where X_Z ($Z = H_2$, CH_4 , and CO) is the species mole fraction, and ΔH_C is the species heat of combustion. The heat of combustion for H_2 , CH_4 , and CO is determined by calculating the enthalpy change across the chemical reactions defined in equations (219) through (220).

At each successive integration point along the fuel gas channel, equilibrium concentrations of sulfur-bearing gas species (i.e., H_2S , SO_2 , CS_2 , COS , and S_2) are determined. These latter calculations neglect chemisorption and assume that various sulfur impurities are present within the fuel gas and are defined either by the partial pressure of S_2 or in terms of the total molar sulfur concentration in ppm. For either case the sulfur equilibrium distribution and the fuel gas calculations are used to determine the material stability at the anode/fuel gas interface. These results are illustrated in the form of phase stability diagrams, not only of the anode material, but also of trace contaminants such as Pb, As, Zn, and Cl within the fuel gas as a function of total sulfur concentration versus cell length, cell emf, or average current density.

Four assumptions have been made in the cocurrent flow MCFC model derived above. These are:

- Chemisorption effects are not included in the model.
- All fuel gases entering at the anode inlet of the MCFC have been humidified to the extent that carbon will not form at equilibrium from either the Boudouard or water gas shift reaction in the bulk gas. Carbon or tar particles entrained in the fuel gas, present as trace constituents, are not accounted for in the initial bulk gas humidification. As trace constituents, the carbon and tar contaminants can remain as intact solid or condensed phases within the reducing environment or react with or volatilize into the bulk gas stream.
- The projected partial pressure of ammonia is established by the equilibrium fuel gas composition. In processes using the Selexol or Benfield desulfurization procedure, both the ammonia and sulfur concentrations are simultaneously reduced. The projections reflect the equilibrium NH_3 partial pressures, with the exception of the Westinghouse Selexol and Texaco Benfield systems, where a 100-fold decrease in the initial NH_3 content has been defined for the inlet anode condition.
- The total atomic concentrations of the trace element constituents remains constant throughout the anode gas channel. Solid or condensed products may be predicted at a specific location along the anode surface, but deposition (depletion of the trace constituent from the bulk gas stream) is unaccounted for in the equilibrium model, since particle arrival rates to the anode surface have not been considered.

3.3.4 Modeling and Assessment of Fuel Cell Performance

Fuel gases from the Rockwell, METC, Westinghouse, and Texaco gasifiers were humidified to minimize carbon deposition at the anode inlet. In an initial attempt to optimize the Rockwell molten carbonate air-blown fuel cell performance, cell dimensions of 121.9 cm by 121.9 cm (4 ft by 4 ft), with a gas stream channel thickness of 0.254 cm (0.1 in), were chosen. Inlet anode temperatures were defined as 923 K (1202°F) and cathode temperatures as 894 K (1150°F). A linear step-gradient was established along the electrodes with preselected outlet anode and cathode temperatures of 953 K (1256°F). Resistances through the 10 atm pressurized cell operating at a terminal voltage of 0.8 V were specified as follows: cell resistance, 0.1345×10^{-4} ohms; total cell impedance ($\eta_a + \eta_c$), $0.400 \text{ ohm}\cdot\text{cm}^2$; and cell flow efficiency, 100%. The effects of the anode and cathode gas velocity on H_2 and CO fuel gas, and O_2 oxidant

gas utilization as a function of both position within the 1.486×10^4 sq cm (16 sq ft) cell and nickel anode material stability were evaluated and are summarized in Figure 29.

For a constant fuel gas stream velocity of 7.31 cm/s (0.24 ft/sec), oxidant gas velocities of 17.57 cm/s (0.58 ft/sec) are sufficient to achieve 45.63% utilization of the oxidant within 15.80 cm (6.22 in) of the anode inlet, while only 26.12% of the H_2 and CO within the fuel gas are consumed. Increasing the oxidant gas velocity to 35.05 cm/s (1.15 ft/sec) achieves 82.7% utilization of the fuel gas and, optimally, 45.3% of the oxidant gas within the first third of the cell. A continued increase in the oxidant gas velocity to 70.10 cm/s (2.30 ft/sec) reduces the oxidant utilization, while 85% of the fuel gas is utilized within 40.10 cm (1.32 ft).

Standard gas velocities of 14.65 cm/s (0.5 ft/sec) of fuel gas and 35.05 cm/s (1.15 ft/sec) of oxidant gas are projected to achieve a 24.84% fuel gas utilization and a 45.53% oxidant gas utilization within 32 cm (1.05 ft) of the cell inlet. An increase in the velocity of the oxidant stream to 70.10 cm/s (2.30 ft/sec) is required in order to achieve 82.5% fuel gas utilization and 45.4% oxidant gas utilization within the entire 1.486×10^4 sq cm (16 sq ft) fuel cell for the cell parameters and conditions previously defined.

Alternatively, for a 29.26 cm/s (0.96 ft/sec) fuel gas velocity and a 70.10 cm/s (2.30 ft/sec) oxidant gas velocity, 22.6% of the fuel gas is utilized, and 45.4% of the oxidant is consumed within 68 cm (2.23 ft) of the cell. Increasing the oxidant stream to 140.2 cm/s (4.59 ft/sec) while maintaining the 29.26 cm/s (0.96 ft/sec) fuel gas stream requires a larger cell to achieve optimum fuel and oxidant gas utilization.

In cell operations with a terminal voltage of 0.8 V, the NiO anode material is reduced to the metal when contacted with fuel gases under equilibrium conditions. Figure 29 defines the stability of the nickel anode material in fuel gases containing sulfur. To the left of

Rockwell Molten Carbonate Air-Blown MCFC

Total Gas Pressure: 10 atm

Cell Resistance: 0.1345-4 ohms*

Total Electrode Impedance: 0.4 ohms-cm²

Terminal Voltage: 0.8 Volts

Current Flow Efficiency: 100 %

Cell Dimensions: Length = 121.9 cm

Width = 121.9 cm

Thickness = 0.254 cm

	Fuel Gas Velocity, cm/sec	% (H ₂ +CO) Utilization	Oxidant Gas Velocity, cm/sec	%O ₂ Utilization	%CO ₂ Utilization	Average Current Density, Amp/cm ²	Stream Distance, cm
(A)	7.31	26.12	17.57	45.63	50.22	0.4981	15.80
(B)	7.31	82.71	35.05	45.47	50.04	0.3622	43.20
(C)	7.31	85.12	70.10	21.98	24.19	0.3979	40.10
(D)	14.63	24.84	35.05	45.53	50.11	0.4865	32.20
(E)	14.63	82.49	70.10	45.42	49.98	0.2563	122.20
(F)	29.26	22.66	70.10	45.44	50.11	0.4599	68.00
(G)	29.26	50.71	140.20	33.16	36.49	0.3846	122.20

Figure 29 - Anode Stability in Rockwell Fuel Gases Containing Sulfur in Various Fuel and Oxidant Gas Stream Velocities

each cell parameter line, nickel is projected to exist as the stable equilibrium phase, while to the right of each line, Ni_3S_2 forms as the preferred equilibrium species. As shown in Figure 29, the slower the flow of fuel gases through the anode gas channel, the earlier (closer to the anode inlet) bulk sulfidation will result for fixed fuel gas sulfur concentrations.

For the Rockwell fuel gas containing 132 ppm total sulfur, bulk sulfidation of the material is projected to occur after the 7.31 cm/s fuel gas has migrated 20 cm through the anode channel, while in the 14.63 cm/s fuel gas it is projected to occur at distances greater than 48 cm from the anode inlet. Although only achieving 50% and 33% utilization of the available fuel and oxidant gases, the 29.26 cm/s fuel gas system is projected to be virtually free of sulfidation. With only 66 ppm total sulfur in the Rockwell fuel gas, the initial 32 to 35 cm from the anode inlet will not sulfidize in the 7.31 cm/s stream, the initial 76 cm will not sulfidize in the 14.63 cm/s stream, and the entire anode will remain virtually unaffected when fuel gas streams approach 29.26 cm/s.

A tabulation of the projected equilibrium partial pressures of volatile species within the fuel and oxidant gases as well as of the fuel cell emf (volts), stream velocities (cm/s), local current density (A/cm^2) as a function of distance from the electrode inlet and metal temperature, the total cell current (A), and average current density (A/cm^2) is given in Table 53 for the MCFC with initial fuel gas velocities of 14.63 cm/s and oxidant gas velocities of 70.10 cm/s. Estimates of each MCFC voltage, thermodynamic, electrochemical, heating value, and overall fuel cell efficiency as a function of position along the electrode follows the main section of Table 53, with a final tabulation of the sulfur species distribution (in ppm) as a function of total sulfur within the fuel gas and electrode distance.

Hydrogen utilization continuously increases as the fuel gas permeates the anode channel, while CO reacts initially with the

Table 53

MODEL PROJECTIONS FOR THE ROCKWELL MOLTEN CARBONATE FUEL GAS MCFC

TEST CASE WITH ANODE MATERIAL - ROCKWELL/AIR BLOWN MCFC									
VAPOR PRESSURE (ATM) DATA AT ELECTRODES (TERMINAL VOLTAGE : .80000+00 VOLTS)									
TOTAL GAS PRESSURE 10.00 ATMOSPHERE									
LENGTH (CM)	.0000	.1550+02	.4050+02	.4580+02	.6100+02	.7620+02	.9150+02	.1067+03	.1220+03
FUEL CELL EMF (V)	.1054+01	.1005+01	.9652+00	.9275+00	.8919+00	.8599+00	.8334+00	.8139+00	.8010+00
CATHODE :									
TEMPERATURE DEG. K	894.00	901.41	908.76	916.17	923.52	930.88	938.29	945.64	953.05
CURRENT(AMP/CM2)	.6342+00	.5121+00	.4128+00	.3187+00	.2298+00	.1498+00	.8344-01	.3484-01	.2471-02
VELOCITY (CM/SEC)	.7010+02	.6871+02	.6767+02	.6693+02	.6650+02	.6636+02	.6647+02	.6679+02	.6725+02
H2O	.1488+01	.1531+01	.1567+01	.1597+01	.1620+01	.1637+01	.1647+01	.1652+01	.1654+01
CO2	.1214+01	.1057+01	.9247+00	.8143+00	.7294+00	.6693+00	.6318+00	.6130+00	.6073+00
N2	.6642+01	.6832+01	.6994+01	.7129+01	.7232+01	.7305+01	.7351+01	.7374+01	.7381+01
O2	.6561+00	.5791+00	.5140+00	.4597+00	.4180+00	.3886+00	.3702+00	.3609+00	.3581+00
TOTAL GAS MOLES	.4669+01	.4538+01	.4433+01	.4350+01	.4288+01	.4245+01	.4218+01	.4205+01	.4201+01
X O2 CONSUMED	.0000	.1172+02	.2166+02	.2992+02	.3628+02	.4077+02	.4358+02	.4499+02	.4542+02
X CO2 CONSUMED	.0000	.1290+02	.2384+02	.3293+02	.3993+02	.4487+02	.4796+02	.4951+02	.4998+02
ANODE :									
TEMPERATURE DEG. K	923.00	926.77	930.51	934.27	938.01	941.75	945.52	949.26	953.02
CURRENT(AMP/CM2)	.6342+00	.5121+00	.4128+00	.3187+00	.2298+00	.1498+00	.8344-01	.3484-01	.2471-02
VELOCITY (CM/SEC)	.1463+02	.1604+02	.1720+02	.1815+02	.1887+02	.1940+02	.1976+02	.1997+02	.2010+02
O2	.6872-22	.1678-21	.5254-21	.1489-20	.4372-20	.1218-19	.2915-19	.5473-19	.8062-19
H2	.1427+01	.1192+01	.9434+00	.6907+00	.4815+00	.3373+00	.2514+00	.2094+00	.1958+00
H2O	.1595+01	.1983+01	.2247+01	.2435+01	.2561+01	.2639+01	.2684+01	.2706+01	.2713+01
CO	.6749+00	.7044+00	.6302+00	.5022+00	.3727+00	.2738+00	.2114+00	.1807+00	.1724+00
CO2	.1578+01	.2405+01	.3025+01	.3503+01	.3852+01	.4089+01	.4231+01	.4301+01	.4321+01
CH4	.4247+00	.1845+00	.6416-01	.1647-01	.3507-02	.7661-03	.2149-03	.9406-04	.6538-04
NH3	.3474-02	.2466-02	.1633-02	.9696-03	.5191-03	.3038-03	.1888-03	.1391-03	.1223-03
N2	.4287+01	.3926+01	.3677+01	.3500+01	.3379+01	.3300+01	.3254+01	.3231+01	.3224+01
C (C)	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
[H2O]/[H2]	.1117+01	.1663+01	.2382+01	.3525+01	.5319+01	.7625+01	.1068+02	.1292+02	.1385+02
[CO2]/[CO]	.2323+01	.3393+01	.4773+01	.6932+01	.1027+02	.1484+02	.1988+02	.2565+02	.2461+02
[SO2]/[H2S]	.6802-08	.2029-07	.5908-07	.1985-06	.7268-06	.2516-05	.7033-05	.1383-04	.1901-04
[CS2]/[H2S]*.2)	.3818-04	.3904-04	.3964-04	.4051-04	.4173-04	.4318-04	.4475-04	.4632-04	.4791-04
[COS]/[H2S]	.1620-01	.2022-01	.2285-01	.2486-01	.2646-01	.2773-01	.2872-01	.2946-01	.3004-01
TOTAL GAS MOLES	.9438+00	.1031+01	.1101+01	.1156+01	.1198+01	.1227+01	.1244+01	.1253+01	.1255+01
X GRAPHITE IN MIX	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
X H2 CONSUMED	.0000	.1646+02	.3390+02	.5161+02	.6627+02	.7637+02	.8239+02	.8533+02	.8628+02
X CO CONSUMED	.0000	.4366+01	.6631+01	.2559+02	.4477+02	.5944+02	.6867+02	.7322+02	.7446+02
X CO+H2 CONSUMED	.0000	.9774+01	.2515+02	.4325+02	.5937+02	.7094+02	.7798+02	.8144+02	.8249+02
TOTAL CELL CURRENT (AMPS) :	.3811+04								
AVERAGE CURRENT DENSITY :	.2563+00 AMPS/CM2								
FUEL CELL PLATE DIMENSIONS (CM) : WIDTH	.1219+03			LENGTH	.1219+03		THICKNESS	.2540+00	
CELL RESISTANCE :	.13450-04 OHMS								
TOTAL ELECTRODE (2A+2C) IMPEDANCE :	.40000+00 OHMS.CM2								

Table 53 (Continued)

HEAT OF C. (KCAL/POLE)	-.2112+02	-.1534+02	-.1107+02	-.7795+01	-.5434+01	-.3660+01	-.2920+01	-.2462+01	-.2325+01
THE FOLLOWING EFFICIENCIES ARE IN FRACTIONAL UNITS									
VOLTAGE EFFICIENCY	.7592+00	.7961+00	.8288+00	.8625+00	.8969+00	.9303+00	.9599+00	.9829+00	.9988+00
THERMODYNAMIC EFFICIENCY	.7727+00	.7361+00	.7063+00	.6781+00	.6514+00	.6274+00	.6075+00	.5927+00	.5827+00
ELECTROCHEMICAL EFF.	.5866+00	.5860+00	.5854+00	.5849+00	.5843+00	.5837+00	.5831+00	.5825+00	.5820+00
HEATING VALUE EFFICIENCY	.7095+00	.4596+00	.5041+00	.5240+00	.5240+00	.5168+00	.5092+00	.5031+00	.4984+00
FUEL CELL EFFICIENCY	.2343+00	.2693+00	.2951+00	.3065+00	.3062+00	.3017+00	.2969+00	.2931+00	.2900+00

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+01								
H2S	.5842+00	.9803+00	.9778+00	.9758+00	.9743+00	.9731+00	.9722+00	.9715+00	.9709+00
SO2	.6694-06	.1989-07	.5777-07	.1937-06	.7082-06	.2448-05	.6838-05	.1344-04	.1846-03
CS2	.3675-09	.3728-09	.3766-09	.3834-09	.3937-09	.4064-09	.4203-09	.4345-09	.4488-09
COS	.1584-01	.1970-01	.2221-01	.2411-01	.2562-01	.2682-01	.2775-01	.2844-01	.2898-01
S2	.4409-10	.6894-10	.1204-09	.2456-09	.5528-09	.1232-08	.2424-08	.3819-08	.4773-08
H2/H2S	.1450+06	.1216+06	.9649+05	.7078+05	.4941+05	.3466+05	.2586+05	.2155+05	.2017+05

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+01								
H2S	.4921+01	.4901+01	.4889+01	.4879+01	.4872+01	.4866+01	.4861+01	.4857+01	.4855+01
SO2	.3347-07	.9945-07	.2889-06	.9686-06	.3341-05	.1224-04	.3419-04	.6719-04	.9229-04
CS2	.9186-08	.9320-08	.9414-08	.9585-08	.9842-08	.1016-07	.1051-07	.1086-07	.1122-07
COS	.7919-01	.9849-01	.1110+00	.1206+00	.1261+00	.1341+00	.1387+00	.1422+00	.1449+00
S2	.1102-06	.1724-06	.3009-06	.6140-06	.1382-07	.3079-07	.6060-07	.9547-07	.1193-06
H2/H2S	.2901+05	.2433+05	.1930+05	.1416+05	.9883+04	.6931+04	.5172+04	.4311+04	.4034+04

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+02								
H2S	.9842+01	.9803+01	.9778+01	.9759+01	.9743+01	.9731+01	.9722+01	.9715+01	.9709+01
SO2	.6694-07	.1989-06	.5777-06	.1937-05	.7082-05	.2448-04	.6838-04	.1344-03	.1846-03
CS2	.3675-07	.3728-07	.3766-07	.3834-07	.3937-07	.4064-07	.4203-07	.4345-07	.4488-07
COS	.1584+00	.1970+00	.2221+00	.2411+00	.2562+00	.2682+00	.2775+00	.2844+00	.2898+00
S2	.4409-08	.6894-08	.1204-07	.2456-07	.5528-07	.1232-06	.2424-06	.3819-06	.4773-06
H2/H2S	.1450+05	.1216+05	.9649+04	.7078+04	.4941+04	.3466+04	.2586+04	.2155+04	.2017+04

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+02								
H2S	.4921+02	.4901+02	.4889+02	.4879+02	.4872+02	.4866+02	.4861+02	.4857+02	.4855+02
SO2	.3347-06	.9945-06	.2889-05	.9686-05	.3341-04	.1224-03	.3419-03	.6719-03	.9229-03
CS2	.9186-06	.9320-06	.9414-06	.9585-06	.9842-06	.1016-05	.1051-05	.1086-05	.1122-05
COS	.7919+00	.9849+00	.1110+01	.1206+01	.1261+01	.1341+01	.1387+01	.1422+01	.1449+01
S2	.1102-06	.1724-06	.3009-06	.6140-06	.1382-05	.3079-05	.6060-05	.9547-05	.1193-04
H2/H2S	.2901+04	.2433+04	.1930+04	.1416+04	.9883+03	.6931+03	.5172+03	.4311+03	.4034+03

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+03								
H2S	.5842+02	.9803+02	.9778+02	.9759+02	.9743+02	.9731+02	.9722+02	.9715+02	.9710+02
SO2	.6694-06	.1989-05	.5777-05	.1937-04	.7082-04	.2448-03	.6838-03	.1344-02	.1846-02
CS2	.3675-05	.3728-05	.3766-05	.3834-05	.3937-05	.4064-05	.4203-05	.4345-05	.4488-05
COS	.1584+01	.1970+01	.2221+01	.2411+01	.2562+01	.2682+01	.2775+01	.2845+01	.2898+01
S2	.4409-06	.6894-06	.1204-05	.2456-05	.5528-05	.1232-04	.2424-04	.3819-04	.4773-04
H2/H2S	.1450+04	.1216+04	.9649+03	.7078+03	.4941+03	.3466+03	.2586+03	.2155+03	.2017+03

Table 53 (Continued)

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1500+03									
H2S	.1476+03	.1470+03	.1467+03	.1464+03	.1462+03	.1460+03	.1458+03	.1457+03	.1456+03	
SO2	.1004-05	.2984-05	.8666-05	.2906-04	.1062-03	.3672-03	.1028-02	.2016-02	.2789-02	
CS2	.8268-05	.8588-05	.8473-05	.8626-05	.8858-05	.9143-05	.9456-05	.9776-05	.1010-04	
COS	.2376+01	.2955+01	.3531+01	.3617+01	.3843+01	.4023+01	.4162+01	.4267+01	.4347+01	
S2	.5921-06	.1551-05	.2708-05	.5526-05	.1244-04	.2771-04	.5454-04	.8593-04	.1074-03	
H2/H2S	.5669+03	.6109+03	.6433+03	.4719+03	.3294+03	.2310+03	.1724+03	.1437+03	.1345+03	

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.2000+03									
H2S	.1968+03	.1961+03	.1956+03	.1952+03	.1949+03	.1946+03	.1944+03	.1941+03	.1940+03	
SO2	.1339-05	.3978-05	.1153-04	.3874-04	.1416-03	.4896-03	.1368-02	.2667-02	.1692-02	
CS2	.1470-04	.1451-04	.1506-04	.1534-04	.1575-04	.1625-04	.1681-04	.1738-04	.1795-04	
COS	.3168+01	.3940+01	.4441+01	.4822+01	.5125+01	.5364+01	.5550+01	.5689+01	.5796+01	
S2	.1764-05	.2758-05	.4814-05	.9823-05	.2211-04	.4927-04	.9697-04	.1528-03	.1909-03	
H2/H2S	.7252+03	.6082+03	.4824+03	.3539+03	.2471+03	.1733+03	.1293+03	.1078+03	.1008+03	

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.2500+03									
H2S	.2460+03	.2451+03	.2444+03	.2440+03	.2436+03	.2433+03	.2431+03	.2429+03	.2427+03	
SO2	.1673-05	.2973-05	.1444-04	.4843-04	.1770-03	.6120-03	.1709-02	.3359-02	.4615-02	
CS2	.2297-04	.2330-04	.2354-04	.2396-04	.2460-04	.2540-04	.2627-04	.2715-04	.2805-04	
COS	.3960+01	.4925+01	.5551+01	.6028+01	.6406+01	.6705+01	.6937+01	.7111+01	.7245+01	
S2	.2756-05	.4309-05	.7522-05	.1535-04	.3455-04	.7698-04	.1515-03	.2387-03	.2983-03	
H2/H2S	.5803+03	.4866+03	.3860+03	.2831+03	.1977+03	.1386+03	.1034+03	.8622+02	.8068+02	

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.3000+03									
H2S	.4921+03	.4901+03	.4889+03	.4879+03	.4872+03	.4866+03	.4861+03	.4857+03	.4855+03	
SO2	.3347-05	.9946-05	.2889-04	.9666-04	.3541-03	.1224-02	.3419-02	.6719-02	.9229-02	
CS2	.9186-04	.9320-04	.9414-04	.9585-04	.9842-04	.1016-03	.1051-03	.1086-03	.1122-03	
COS	.7919+01	.9849+01	.1110+02	.1206+02	.1281+02	.1341+02	.1387+02	.1422+02	.1446+02	
S2	.1102-04	.1724-04	.3009-04	.6140-04	.1382-03	.3079-03	.6061-03	.9547-03	.1193-02	
H2/H2S	.2901+03	.2433+03	.1930+03	.1416+03	.9883+02	.6931+02	.5172+02	.4311+02	.4034+02	

carbonate ions from the electrolyte to form CO_2 and at equilibrium dissociates into CO and $\frac{1}{2} \text{O}_2$, indicative of the increase in the partial pressure of CO at 15.30 cm from the anode inlet, as shown in Table 53. Thereafter, the utilization of the fuel gas CO with secondary dissociation reactions occurs as distance from the anode inlet and metal temperature increases. Both $p_{\text{H}_2\text{O}}$ and p_{CO_2} are shown to increase as a function of anode distance, with equilibrium dissociation contributing to the slight increase in p_{O_2} . The partial pressures of CH_4 , NH_3 , and N_2 decrease as a function of anode distance, partly because of the chemical equilibrium reactions and of the dilution effect observed when the total moles of fuel gas increase as the equivalent total moles of oxidant gas decrease.

The efficiency calculations will be used to compare cell operating parameters for the various gasification systems, and, therefore, will not be discussed at this time.

Reviewing the tabulated sulfur distributions projected in Table 53, we observed that as a function of distance from the anode inlet, the principal sulfur constituent, H_2S , decreases, while the secondary sulfur constituent, COS , increases. Trace constituent concentrations of SO_2 , carbon disulfide (CS_2), and S_2 also increase as the fuel gas flows toward the anode outlet.

In order to represent the MCFC in which the oxidant gases are recycled and cooled, an expanded cathode temperature gradient must be assigned. In this set of parameter optimization calculations, similar cell resistances, terminal voltage, cell dimensions, and MCFC pressures are maintained as in the previous discussion, but the cathode inlet temperature is lowered to 866 K (1100°F) and the outlet temperature increased to 977 K (1300°F), while the original 923 K (1200°F) anode inlet temperature is maintained and equivalent temperatures at the anode and cathode outlet are assumed. Table 54 illustrates the effect of fuel and oxidant gas velocities on utilization distance along the electrodes in the Rockwell air-blown cell model. Maintaining a constant oxidant

Table 54

EFFECT OF TEMPERATURE AND STREAM VELOCITIES ON FUEL AND OXIDANT
UTILIZATION, AND METAL SULFIDATION REACTIONS IN THE ROCKWELL
MOLTEN CARBONATE AIR-BLOWN MCFC

Rockwell Molten Carbonate Air-Blown MCFC

Total Gas Pressure: 10 atm

Cell Resistance: 0.1345-4 ohms

Total Electrode Impedance: 0.4 ohms-cm²

Terminal Voltage: 0.8 Volts

Current Flow Efficiency: 100 %

Cell Dimensions: Length = 121.9 cm

Width = 121.9 cm

Thickness = 0.254 cm

	Temperature, K				Stream Velocity, cm/sec		Utilization			Distance From Anode Inlet Where Utilization is Achieved, cm	Total Sulfur Concentration for Ni - Ni ₃ S ₂ ppm								
	Anode		Cathode		Anode	Cathode	%H ₂ + CO	%CO ₂	%O ₂		Distance From Anode Inlet, cm								
	Inlet	Outlet	Inlet	Outlet							0	15.30	30.50	45.80	61.00	76.20	91.50	106.70	122.20
(A)	923	977	866	977	14.00	70.10	85.03	47.02	42.72	72.60	252.83	210.24	152.36	93.73	53.99	-	-	-	-
(B)	923	977	866	977	14.63	70.10	85.03	49.37	44.36	79.80	252.83	213.17	199.15	102.65	62.45	40.53	37.60 (79.8)	-	-
(C)	923	977	866	977	15.00	70.10	83.39	50.01	45.45	79.40	252.83	214.76	162.88	107.68	67.37	44.63	41.77 (79.4)	-	-
(D)	923	977	866	977	16.46	70.10	72.14	50.01	45.45	70.00	252.83	220.30	175.86	126.01	85.21	69.73 (70.0)	-	-	-
(E)	920	977	866	977	15.00	70.10	76.28	50.02	45.45	75.00	247.52	216.47	172.78	122.56	82.53	58.70 (75.5)	-	-	-
(F)	923	977	866	977	14.63	35.05	25.49	50.13	45.13	26.40	252.83	214.41	180.09 (26.4)	-	-	-	-	-	-
(G)	923	977	866	977	21.94	70.10	42.93	50.00	45.44	60.70	252.83	234.21	208.35	176.13	145.20 (60.7)	-	-	-	-
(H)	923	977	866	977	21.94	35.05	10.99	50.13	45.44	25.20	252.83	234.98	221.07 (25.2)	-	-	-	-	-	-
(I)	866	977	866	977	14.63	70.10	-83.74	50.04	45.48	72.50	163.27	191.54	225.37	265.44	311.62	351.20 (72.5)	-	-	-
(J)	900	977	866	977	14.63	70.10	-32.82	50.04	45.48	61.20	213.79	218.72	229.63	244.74	263.18	263.44 (61.2)	-	-	-
(K)	918	977	866	977	14.63	70.10	-15.20	50.05	45.44	55.70	244.01	231.98	229.58	232.54	236.60 (55.7)	-	-	-	-
(L)	921	977	866	977	14.63	70.10	84.63	51.30	46.66	91.50	249.28	214.48	166.04	112.61	72.27	48.84	39.10	-	-
(M)	922	977	866	977	14.63	70.10	84.14	50.00	45.40	82.00	251.08	213.84	162.63	107.60	67.28	44.57	39.83 (82.0)	-	-
(N)	923	977	866	977	14.63	70.10	85.03	49.37	44.86	79.80	252.83	213.17	199.15	102.63	62.45	40.53	37.60 (79.8)	-	-
(O)	926	977	866	977	14.63	70.10	85.02	46.51	42.26	68.40	258.23	210.82	148.38	88.22	48.93	37.43 (68.4)	-	-	-
(P)	947	977	866	977	14.63	70.10	85.09	33.50	30.40	37.10	297.88	182.17	72.73	40.23 (37.1)	-	-	-	-	-

velocity of 70.10 cm/s while increasing the fuel gas flow from 14.00 to 16.46 cm/s (Table 54 A-D) we observed that a maximum distance of 79.80 cm from the anode inlet will achieve 85% H₂ and CO fuel gas utilization and 50% CO₂ or O₂ oxidant gas utilization when the fuel gas velocity is 14.63 cm/s, as shown in the initial set of calculations. Migration through the cell to a location 91.5 cm from the anode and cathode inlets, however, promotes 87.23% utilization of the H₂ and CO in the fuel gas, and 50.35% CO₂ and 45.75% O₂ in the oxidant gases. Continued progression of the gases through the respective channels promotes the reforming of H₂ and CO in the fuel gas, primarily through the H₂O and CO₂ dissociation equilibrium reactions. Ultimately, 84.88% H₂ and CO, and 49.30% CO₂ and 44.80% O₂ is utilized over the 1.486×10^4 sq cm electrodes.

In order to establish the effect of both fuel gas velocity and inlet anode temperature (Table 54 C, E) the fuel gas velocity was arbitrarily selected at 15.00 cm/s. Under these conditions the prescribed 50% utilization of the oxidant gas was achieved at a location closer to the cathode inlet (75.00 cm) for anode inlet temperatures of 920 K (1196°F), while the 50% oxidant utilization was achieved at 79.40 cm from the cathode inlet for anode inlet temperatures of 923 K (1202°F).

Series B, F, G, H in Table 54 demonstrates that variation of the gas stream velocities is optimized for 14.63 cm/s fuel gas and 70.10 cm/s oxidant gas flows. In order to define the optimal anode inlet temperature for this system, we generated series I through P. At anode inlet temperatures of 866 to ~ 920 K (1099 to ~ 1196°F), carbonate ions migrating through the electrolyte react with the H₂ and CO in the fuel gas to form H₂O and CO₂ but are automatically reconverted into H₂, CO₂, and O₂. The released oxygen reacts with fuel gas CH₄ to yield an additional quantity of CO₂ and H₂O along the anode surface, which dissociates into H₂ and CO. In this manner the apparent negative fuel gas utilization shown in Table 54 (I, J, K) represents this series of complex reactions, ultimately producing a greater concentration of H₂ and CO in the fuel gas than was present in the initial inlet composition. As

the anode inlet temperature increases, this effect is minimized. Optimal temperatures of 921 K (1198°F) achieve the prescribed fuel and oxidant gas utilization at 91.50 cm from the anode and cathode inlets for the 14.63 cm/s fuel gas and 70.10 cm/s oxidant gas stream velocities. A maximum utilization of 83.34% H₂ and CO, 50.71% CO₂, and 46.08% O₂ is achieved for this system after the gas has permeated the entire 1.486×10^4 sq cm MCFC.

As shown in Table 54, the concentration of total sulfur required to convert the Ni into Ni₃S₂ is sensitive not only to hydrogen utilization in the fuel gas stream, but also to the inlet anode operating temperature and to the distance from the anode inlet. The principal volatile sulfur phase in the anode gas channel is that of H₂S. A [H₂]/[H₂S] ratio of 573.64 (252.8 ppm S) at the 923 K (1202°F) anode inlet is sufficient to sulfidize the metal (Table 54, B). At a distance of 15.3 cm from the anode inlet, a [H₂]/[H₂S] ratio of 547.04 (213.17 ppm S) will promote anode sulfidation. As the fuel gas progresses through the cell toward the outlet, hydrogen is consumed and the maximum [H₂]/[H₂S] ratio at which anode sulfidation occurs is simultaneously lowered. For this reason a lower sulfur concentration in the fuel gas at the MCFC outlet will enhance formation of Ni₃S₂, as compared with the higher sulfur tolerance at the anode inlet. Sulfur tolerances are tabulated in Table 54 only up to the point where the fuel or oxidant utilization has been achieved.

The [H₂]/[H₂S] ratio required to sulfidize the nickel anode is highly sensitive to inlet temperatures and temperature gradients along the electrode. As the anode inlet temperature increases from 866 to 947 K (1099 to 1245°F), we observe that the concentration of sulfur required to convert Ni to Ni₃S₂ increases. For systems I, J, K, where reactions within the anode gas channel promote formation, as opposed to hydrogen utilization as a function of distance, the concentration of sulfur required to sulfidize the anode increases. Under normal operations, however, where hydrogen is consumed along the anode, the sulfur tolerance markedly decreases, as we previously discussed.

The stability of the nickel anode material when exposed to Rockwell fuel gases was evaluated for cell terminal voltage operations ranging from 0.7 to 0.9 V. Anode inlet temperatures were maintained at 921 K (1198°F), with a linear-step gradient assumed up to the 977 K (1299°F) outlet. Cathode temperatures were established simultaneously at 866 K (1099°F) at the inlet and at 977 K (1299°F) at the outlet for the 10 atm, 1.486×10^4 sq cm MCFC, with cell resistances of 0.1345×10^{-4} ohms and total electrode impedances of $0.4 \text{ ohms} \cdot \text{cm}^2$. As illustrated in Figure 30, at constant stream velocities (fuel gas 14.63 cm/s; oxidant gas 70.10 cm/s) a substantially higher concentration of sulfur is required within the fuel gas prior to bulk anode sulfidation. Also, at terminal voltage operations of more than 0.8 V, utilization of H_2 and CO at the anode is apparently diminished throughout the cell. At between 90 and 100 cm these concentrations within the fuel gas stream increase, resulting from the dissociation of the H_2O and CO_2 reaction products at increased electrode temperatures. Stream velocities once again need to be readjusted for MCFC operations at ~ 8.5 to 9.0 V in order to achieve 85% H_2 and CO, and 50% O_2 or 50% CO_2 utilization.

Reduction in the cell terminal voltage at these stream velocities indicates that the anode material is highly sensitive to sulfur concentration and will be sulfided at 40 cm from the inlet when the fuel gas contains ~ 55 to 85 ppm for the 0.7 and 0.75 terminal voltage MCFC, respectively. Also in Figure 30, for terminal voltage operations below 0.8 V, 85% H_2 and CO, and 50% CO_2 or 50% O_2 utilization is apparently achieved before the fuel or oxidant streams traverse the entire channel length.

For the conditions specified in Figure 30, we were unable to attain the required 0.160 A/cm^2 average current density for MCFC operations. We then performed the reverse calculations in which the average current density is specified and the terminal voltage and utilization are generated on the basis of defined stream velocities (Table 55). With anode inlet and outlet temperatures of 866 and 977 K, distances of not more than 91.50 cm from the anode inlet are achieved before the average local current density approaches the limiting current

Rockwell Molten Carbonate Air-Blown MCFC

Total Gas Pressure: 10 atm

Cell Resistance: 0.1345-4 ohms

Total Electro Impedance: 0.4 ohms-cm²

Terminal Voltage: 0.7, 0.75, 0.8, 0.85, 0.9 volts

Current Flow Efficiency: 100 %

Cell Dimensions: Length = 121.9 cm

Width = 121.9 cm

Thickness = 0.254 cm

Stream Velocities: Fuel Gas = 0.1463 + 2 cm/sec

Oxidant Gas = 0.7010 + 2 cm/sec

	Terminal Voltage, Volts	Utilization			Estimated Current Density, Amp/cm ²
		% (H ₂ + CO)	% CO ₂	% O ₂	
(A)	0.7	81.81	50.02	45.45	0.7407 (43.60 cm)
(B)	0.75	81.78	50.01	45.44	0.5914 (54.60 cm)
(C)	0.80	83.34	50.71	46.01	0.2680 (121.9 cm)
(D)	0.85	62.99	42.03	38.19	0.2261 (121.9 cm)
(E)	0.90	34.67	31.10	28.26	0.1771 (121.9 cm)

Figure 30 -- Effect of Terminal Voltage on Anode Stability for the Rockwell Molten Carbonate Air-Blown MCFC

Table 55

FUEL AND OXIDANT GAS UTILIZATION PROJECTIONS IN THE ROCKWELL MOLTEN
CARBONATE FUEL GAS AIR-BLOWN MCFC

Dwg. 4251882

	Temperature, K				Stream Velocity, cm/sec		Utilization			Average Current Density, Amps/cm ²	Terminal Voltage, Volts	Approximate Distance From Anode Inlet Prior to Reverse Polarization, cm
	Anode Inlet	Anode Outlet	Cathode Inlet	Cathode Outlet	Fuel Gas	Oxidant Gas	% (H ₂ + CO)	% CO ₂	% O ₂			
Ⓐ	923	977	866	977	14.63	70.10	35.84	29.70	26.99	0.1572	0.9184	91.5
Ⓑ	923	977	866	977	14.63	50.00	36.67	43.25	39.30	0.1572	0.9003	91.5
Ⓒ	923	977	866	977	20.00	70.10	13.26	29.03	26.38	0.1572	0.9292	91.5
Ⓓ	923	977	866	977	12.31	70.10	53.22	30.18	27.42	0.1572	0.8947	91.5
Ⓔ	923	977	866	977	12.31	50.00	52.86	42.26	39.31	0.1572	0.8848	76.2
Ⓕ	923	977	866	977	14.63	70.10	12.26	19.86	18.05	0.0999	0.9569	76.2
Ⓖ	923	977	866	977	14.63	70.10	56.18	37.47	34.05	0.1999	0.8724	91.5
Ⓗ	923	953	894	953	14.63	70.10	9.92	18.45	16.77	0.0999	0.9393	106.7
Ⓙ	923	953	894	953	14.63	70.10	33.31	29.39	26.71	0.1572	0.8947	121.9
Ⓚ	923	953	894	953	14.63	70.10	34.62	29.94	27.20	0.1599	0.8925	121.9
Ⓛ	923	953	894	953	14.63	70.10	54.52	38.05	34.57	0.1998	0.8586	121.9

density or zero current, then shifts through a reverse polarization. For this to occur, an external power source would be required to continue to generate current after the limiting current density has been obtained, but provisions for this have not been considered in this study.

For fuel and oxidant stream velocities of 14.63 and 70.10 cm/s the $\sim 0.160 \text{ A/cm}^2$ MCFC utilizes only 35.84% H_2 and CO, and 29.70% CO_2 and 26.99% O_2 within 91.50 cm from the inlet. The terminal voltage of 0.9184 V results with a dead space of 30.40 cm from the electrode outlet in which the fuel and oxidant are no longer utilized and current is no longer generated (Table 55A). Decreasing the oxidant flow rate to 50 cm/s while maintaining the electrode temperature and average current density marginally enhances fuel and oxidant utilization for the 0.9003 V MCFC (Table 55B). If the fuel gas stream velocity is increased to 20.00 cm/s while the oxidant stream is maintained at 70.10 cm/s, the percent H_2 and CO consumption decreases as the cell terminal voltage increases to 0.9292 V (Table 55C).

In order to maximize utilization, the anode gas stream velocity is decreased to 12.31 cm/s, which promotes 53.22% utilization of the H_2 and CO, 30.18% CO_2 , and 27.42% O_2 within the first 91.50 cm of the 0.8947 V cell. One would suspect that with the 12.31 cm/s fuel gas stream velocity maintained and the oxidant gas stream velocity reduced to 50 cm/s, an increased utilization should result. As shown in Table 55E, oxidant utilization increases, with a slight decrease in the fuel utilization for the 0.8848 V cell under these operating conditions. The limiting current density, however, is achieved at 76.20 cm from the anode inlet.

Although the percentage of utilization of the fuel and oxidant gas constituents for the 0.160 A/cm^2 cell operating with an inlet fuel gas stream velocity of 14.63 cm/s and oxidant stream velocity of 70.10 cm/s was relatively low, utilization can be increased if the MCFC average current density is increased to 0.200 A/cm^2 (Table 55 A,F,G).

With only 0.200 A/cm^2 , however, the 0.8724 V cell again achieves an exchange current density of zero within 91.50 cm from the anode inlet. In order to attain maximum utilization of the fuel and oxidant gases over the entire length of 121.9 cm , an average current density of $\sim 0.250 \text{ A/cm}^2$ would be required.

Alternatively, to achieve maximum utilization of the cell length, a less severe temperature gradient must be imposed along the cathode. This need becomes evident in Table 55 when we compare F and H, A and I, and G and K. Although the fuel and oxidant utilizations change very little, the entire 121.9 cm length of the MCFC is used when the cathode temperatures are 894 K at the inlet and 953 K at the outlet, versus a maximum length of only 91.50 cm used for the 866 to 977 K cathode when similar fuel and oxidant stream velocities are maintained. With the smaller temperature gradient, average current densities greater than 0.200 A/cm^2 but less than 0.250 A/cm^2 are projected to achieve the $85\% \text{ H}_2$ and CO , $50\% \text{ CO}_2$, and $50\% \text{ O}_2$ utilization over the entire cell length.

In order to demonstrate the effect of resistance on cell performance and material stability, a final series of calculations was made using the Rockwell molten carbonate air-blown MCFC system. For this series the fuel gas and oxidant stream velocities were maintained at 14.63 and 70.10 cm/s over the 923 to 977 K anode and the 866 to 977 K cathode. Multiples of the $0.1345 \times 10^{-4} \text{ ohm}$ cell resistance and the $0.4 \text{ ohm}\cdot\text{cm}^2$ total electrode impedance were selected for the MCFC operating at an average current density of ~ 0.160 , 0.200 , and 0.250 A/cm^2 . Table 56 summarizes the projected terminal voltages, $\% \text{ H}_2$ and CO , CO_2 , and O_2 utilizations, approximate location (if applicable) where reverse polarization occurs, and the total concentration of sulfur as a function of distance that must be present within the fuel gas in order to sulfidize the nickel anode. With cell resistances of $0.1345 \times 10^{-4} \text{ ohms}$ and total electrode impedance of $0.4 \text{ ohms}\cdot\text{cm}^2$, less than 60% of the fuel gas H_2 and CO is used before reverse polarization takes place within 100 cm of the cell operating with an average current density of

Table 56

Dwg. 5600C02

EFFECT OF CELL RESISTANCE ON THE ROCKWELL MOLTEN CARBONATE
AIR-BLOWN MCFC PERFORMANCE AND ANODE MATERIAL STABILITY

Rockwell Molten Carbonate Air-Blown MCFC

Fuel Gas Velocity: 14.63 cm/sec
Oxidant Gas Velocity: 70.10 cm/sec
Anode Inlet Temperature: 923K
Anode Outlet Temperature: 977K
Cathode Inlet Temperature: 866K
Cathode Outlet Temperature: 977K

Ⓐ Cell Resistance: 0.1345×10^{-4} ohms

Total Electrode Impedance: $0.4 \text{ ohms} \cdot \text{cm}^2$

	Average Current Density, Amps/cm ²	Terminal Voltage, Volts	Utilization			Approximate Distance From Anode Inlet Prior to Reverse Polarization, cm	Total Sulfur Concentration for Ni → Ni ₃ S ₂ , ppm								
			% (H ₂ + CO)	%CO ₂	%O ₂		Distance From Anode Inlet, cm								
							0	15.30	30.50	45.80	61.00	76.20	91.50	106.70	122.20
A-1	0.1572	0.9167	32.35	28.41	25.82	91.7	252.83	238.62	222.33	205.37	191.89	185.03	-	-	-
A-2	0.1999	0.8769	54.28	36.76	33.40	100.6	252.83	230.29	202.26	171.49	145.74	129.61	124.55	-	-
A-3	0.2498	0.8236	79.38	46.91	42.63	101.2	252.83	218.56	172.90	123.61	86.12	64.11	54.39	-	-

Ⓑ Cell Resistance: 0.2690×10^{-4} ohms

Total Electrode Impedance: $0.8 \text{ ohms} \cdot \text{cm}^2$

	Average Current Density, Amps/cm ²	Terminal Voltage, Volts	Utilization			Approximate Distance From Anode Inlet Prior to Reverse Polarization, cm	Total Sulfur Concentration for Ni → Ni ₃ S ₂ , ppm								
			% (H ₂ + CO)	%CO ₂	%O ₂		Distance From Anode Inlet, cm								
							0	15.30	30.50	45.80	61.00	76.20	91.50	106.70	122.20
B-1	0.1599	0.8583	33.07	28.93	26.29	+121.9	252.83	250.19	244.78	236.21	225.45	214.22	204.54	198.22	196.08
B-2	0.1999	0.8103	54.18	36.76	33.40	+121.9	252.83	245.21	232.92	215.11	193.70	171.99	153.11	139.06	130.24
B-3	0.2498	0.7458	79.37	46.91	42.62	+121.9	252.83	238.36	215.99	184.64	149.08	115.88	88.91	69.38	56.59

Ⓒ Cell Resistance: 0.4035×10^{-4} ohms

Total Electrode Impedance: $1.2 \text{ ohms} \cdot \text{cm}^2$

	Average Current Density, Amps/cm ²	Terminal Voltage, Volts	Utilization			Approximate Distance From Anode Inlet Prior to Reverse Polarization, cm	Total Sulfur Concentration for Ni → Ni ₃ S ₂ , ppm									
			% (H ₂ O+CO)	%CO ₂	%O ₂		Distance From Anode Inlet, cm									
							0	15.30	30.50	45.80	61.00	76.20	91.50	106.70	122.20	
C-1	0.1599	0.7990	33.08	28.93	26.29	+121.9	252.83	254.11	252.65	247.73	239.48	228.64	216.70	205.46	196.08	
C-2	0.1998	0.7361	54.18	36.76	33.40	+121.9	252.83	249.77	242.31	229.24	210.97	189.37	167.16	147.12	130.25	
C-3	0.2498	0.6540	79.37	46.91	42.62	+121.9	252.83	243.98	228.17	203.43	171.57	137.30	105.28	78.31	56.60	

~ 0.160 to 0.200 A/cm^2 . By increasing the average current density to 0.250 A/cm^2 , 79% of the fuel gas H_2 and CO , and 50% of the CO_2 are utilized, but the current shown to be generated is only within the first 101 cm of the cell.

Increasing the cell resistance and total electrode impedance by a factor of two decreases fuel utilization per unit cell length for a given current generation. Also, as the average current density increases from 0.160 to 0.250 , so does the % H_2 and CO , CO_2 , and O_2 utilization. Although the percentage of fuel or oxidant consumed does not dramatically vary for cell resistances of 0.269×10^{-4} to 0.4035×10^{-4} ohms or for total electrode impedances of 0.8 to $1.2 \text{ ohms}\cdot\text{cm}^2$, Figure 31 illustrates that as the ohmic and polarization resistances increase as a function of increasing average current density, a decrease in the terminal voltage of the MCFC is obtained.

The overall stability of the anode material in the Rockwell fuel gas is illustrated in Figure 32. As the average current density of the cell is increased, the sulfur tolerance (the concentration of sulfur required to sulfidize the material) is lowered considerably. For a cell with a resistance of 0.1345×10^{-4} ohms and total electrode impedance of $0.4 \text{ ohms}\cdot\text{cm}^2$, at 70 cm from the anode inlet 187, 134, and 70 ppm sulfur must be present within the fuel gas prior to sulfidation for cells operating with average current densities of ~ 0.160 , 0.200 , and 0.250 A/cm^2 . For cells operating with similar current densities but with higher resistances of either 0.269×10^{-4} or 0.4035×10^{-4} ohms and total electrode impedance of 0.8 or $1.2 \text{ ohms}\cdot\text{cm}^2$, 196, 130, and 56 ppm sulfur must be present within the fuel gases prior to sulfidation of the anode outlet.

The previous discussion has briefly illustrated the effects that variation in fuel and oxidant gas stream velocities, anode and cathode temperature gradients, terminal voltage, average current density, and cell resistance have on fuel and oxidant utilization and on material stability. Variation in any one of these parameters ultimately affects

Figure 31 -- Relation of Average Current Density and Terminal Voltage in the Rockwell Molten Carbonate Air-Blown MCFC as a Function of Cell Resistance

Rockwell Molten Carbonate Air-Blown MCFC

Fuel Gas Velocity: 14.63 cm/sec

Oxidant Gas Velocity: 70.10 cm/sec

Anode Inlet Temperature: 923K

Anode Outlet Temperature: 977K

Cathode Inlet Temperature: 860K

Cathode Outlet Temperature: 977K

Figure 32 -- Stability of Nickel Anode Materials in the Rockwell Molten Carbonate Air-Blown MCFC as a Function of Average Current Density for Various Cell Resistances and Impedances

both utilization and material stability. The following sections will consider only two cell models and will assess the cells' efficiencies, anode material stability, and trace constituent reactions when Rockwell molten carbonate, METC gravitating-bed, Westinghouse fluidized-bed, and Texaco entrained fuel gases are used in either an air- or oxygen-blown gasifier.

The cell models are primarily based on the 1:5 ratio of fuel to oxidant gas stream velocities and assume inlet anode temperatures of 923 K, with cathode temperatures subjected to oxidant recycle and cooling. Because of the physical thickness of the electrode and contact with the thin electrolyte matrix, anode outlet temperatures are assumed to be equivalent to those at the cathode outlet. Both models are maintained at 10 atm total pressure, while two criteria are established for the average current density, cell resistance, and total electrode impedance. The two-cell models are defined as:

<u>MCFC-1</u>	<u>MCFC-2</u>
Fuel Gas Velocity: 14.63 cm/s	Fuel Gas Velocity: 14.63 cm/s
Oxidant Gas Velocity: 70.10 cm/s	Oxidant Gas Velocity: 70.10 cm/s
Anode Inlet Temperature: 923 K	Anode Inlet Temperature: 923 K
Anode Outlet Temperature: 977 K	Anode Outlet Temperature: 977 K
Cathode Inlet Temperature: 866 K	Cathode Inlet Temperature: 866 K
Cathode Outlet Temperature: 977 K	Cathode Outlet Temperature: 977 K
Average Current Density: 0.160 A/cm ²	Average Current Density: 0.250 A/cm ²
Cell Resistance: 0.1345 x 10 ⁻⁴ ohms	Cell Resistance: 0.4035 x 10 ⁻⁴ ohms
Total Electrode Impedance: 0.4 ohms·cm ²	Total Electrode Impedance: 1.2 ohms·cm ²
Total Cell Pressure: 10 atm	Total Cell Pressure: 10 atm

3.3.4.1 Evaluation of the Molten Carbonate Air-Blown Gas to MCFC

The MCFC models for operations with ~ 0.160 A/cm² with a cell resistance of 0.1345 x 10⁻⁴ ohms and a total electrode impedance of 0.400 ohms·cm² are presented in Table 57. As described previously, the limiting current density is attained within the initial 95 cm of the

Table 57

FUEL AND OXIDANT GAS COMPOSITIONS AND UTILIZATIONS AS A FUNCTION
OF LOCATION IN THE ROCKWELL 0.160 A/cm² MOLTEN
CARBONATE AIR-BLOWN MCFC

TEST CASE WITH ANODE MATERIAL - ROCKWELL/AIR BLOWN MCFC									
VAPOR PRESSURE (ATM) DATA AT ELECTRODES (TERMINAL VOLTAGE : .91667+00 VOLTS)									
TOTAL GAS PRESSURE 10.00 ATMOSPHERE									
LENGTH (CM)	.0000	.1530+02	.3050+02	.4580+02	.6100+02	.7620+02	.9500+02	.1067+03	.1220+03
FUEL CELL EMF (V)	.1109+01	.1064+01	.1027+01	.9939+00	.9654+00	.9410+00	.9166+00	.9167+00	.9167+00
CATHODE :									
TEMPERATURE DEG. K	866.00	879.93	893.77	907.70	921.55	935.39	952.51	963.16	977.09
CURRENT (AMP/CM2)	.4812+00	.3672+00	.2747+00	.1930+00	.1217+00	.6082-01	.0000	.0000	.0000
VELOCITY (CM/SEC)	.7010+02	.6980+02	.6981+02	.7008+02	.7060+02	.7134+02	.7251+02	.7333+02	.7439+02
H2O	.1488+01	.1519+01	.1542+01	.1560+01	.1572+01	.1579+01	.1582+01	.1582+01	.1582+01
O2	.1214+01	.1103+01	.1016+01	.9502+00	.9056+00	.8796+00	.8691+00	.8691+00	.8691+00
N2	.6642+01	.6777+01	.6883+01	.6963+01	.7017+01	.7049+01	.7062+01	.7062+01	.7062+01
O2	.6561+00	.6014+00	.5587+00	.5265+00	.5046+00	.4918+00	.4867+00	.4867+00	.4867+00
TOTAL GAS MOLES	.4820+01	.4723+01	.4651+01	.4597+01	.4562+01	.4541+01	.4533+01	.4533+01	.4533+01
% O2 CONSUMED	.0000	.8335+01	.1484+02	.1975+02	.2309+02	.2504+02	.2582+02	.2582+02	.2582+02
% CO2 CONSUMED	.0000	.9173+01	.1634+02	.2173+02	.2541+02	.2755+02	.2841+02	.2841+02	.2841+02
ANODE :									
TEMPERATURE DEG. K	923.00	929.78	936.51	943.29	950.02	956.76	965.08	970.27	977.04
CURRENT (AMP/CM2)	.4812+00	.3672+00	.2747+00	.1930+00	.1217+00	.6082-01	.0000	.0000	.0000
VELOCITY (CM/SEC)	.1463+02	.1574+02	.1662+02	.1730+02	.1780+02	.1815+02	.1840+02	.1849+02	.1862+02
O2	.6872-22	.1919-21	.4720-21	.1092-20	.2323-20	.4447-20	.8422-20	.1185-19	.1846-19
H2	.1427+01	.1281+01	.1159+01	.1001+01	.8937+00	.8321+00	.7924+00	.7898+00	.7856+00
H2O	.1595+01	.1890+01	.2090+01	.2229+01	.2320+01	.2474+01	.2401+01	.2407+01	.2415+01
CO	.6749+00	.7319+00	.7267+00	.6926+00	.6550+00	.6307+00	.6298+00	.6394+00	.6513+00
CO2	.1578+01	.2185+01	.2616+01	.2921+01	.3120+01	.3231+01	.3267+01	.3259+01	.3249+01
CH4	.4247+00	.2266+00	.1154+00	.5733-01	.3021-01	.1824-01	.1254-01	.1082-01	.8905-02
NH3	.3474-02	.2712-02	.2106-02	.1628-02	.1293-02	.1083-02	.9602-03	.9212-03	.8717-03
N2	.4287+01	.4014+01	.3830+01	.3706+01	.3627+01	.3583+01	.3566+01	.3566+01	.3566+01
C(C)	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
[H2O]/[H2]	.1117+01	.1476+01	.1839+01	.2226+01	.2596+01	.2880+01	.3030+01	.3048+01	.3075+01
[CO2]/[CO]	.2323+01	.2967+01	.3577+01	.4190+01	.4733+01	.5090+01	.5154+01	.5063+01	.4957+01
[SO2]/[H2S]	.6802-08	.1635-07	.3515-07	.7179-07	.1338-06	.2179-06	.3195-06	.3763-06	.4663-06
[CO2]/([H2S]**2)	.3818-04	.4818-04	.5194-04	.4387-04	.4203-04	.4841-04	.5151-04	.5354-04	.5625-04
[CO5]/[H2S]	.1620-01	.1956-01	.2186-01	.2363-01	.2502-01	.2611-01	.2709-01	.2759-01	.2823-01
TOTAL GAS MOLES	.9438+00	.1008+01	.1057+01	.1092+01	.1116+01	.1130+01	.1135+01	.1135+01	.1135+01
% GRAPHITE IN MIX	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
% H2 CONSUMED	.0000	.1029+02	.2037+02	.2984+02	.3739+02	.4227+02	.4448+02	.4467+02	.4496+02
% CO CONSUMED	.0000	.8438+01	.7679+01	.2621+01	.2958+01	.6545+01	.6683+01	.5266+01	.3504+01
% CO+H2 CONSUMED	.0000	.4274+01	.1136+02	.1942+02	.2634+02	.3080+02	.3235+02	.3202+02	.3165+02
TOTAL CELL CURRENT (AMPS) :	.2338+04								
AVERAGE CURRENT DENSITY :	.1572+00 AMPS/CM2								
FUEL CELL PLATE DIMENSIONS (CM) : WIDTH	.1219+03								
CELL RESISTANCE : 13450-04 OHMS									
TOTAL ELECTRODE (2A+2C) IMPEDANCE :	.40000+00 OHMS.CM2								

Table 57 (Continued)

HEAT OF C. (KCAL/MOLE)	-.2112+02	-.1685+02	-.1384+02	-.1170+02	-.1029+02	-.9488+01	-.9186+01	-.9202+01	-.9222+01
THE FOLLOWING EFFICIENCIES ARE IN FRACTIONAL UNITS									
VOLTAGE EFFICIENCY	.8264+00	.8618+00	.8929+00	.9223+00	.9495+00	.9741+00	.1000+01	.1000+01	.1000+01
THERMODYNAMIC EFFICIENCY	.8194+00	.7842+00	.7554+00	.7300+00	.7077+00	.6885+00	.6690+00	.6680+00	.6667+00
ELECTROCHEMICAL EFF.	.6772+00	.6759+00	.6746+00	.6733+00	.6720+00	.6707+00	.6690+00	.6680+00	.6667+00
HEATING VALUE EFFICIENCY	.3995+00	.4493+00	.4856+00	.5062+00	.5137+00	.5139+00	.5106+00	.5080+00	.5044+00
FUEL CELL EFFICIENCY	.2705+00	.3036+00	.3276+00	.3408+00	.3452+00	.3447+00	.3416+00	.3394+00	.3363+00

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+01								
H2S	.9842+00	.9809+00	.9787+00	.9770+00	.9757+00	.9747+00	.9737+00	.9733+00	.9727+00
SO2	.6694-08	.1604-07	.3440-07	.7014-07	.1306-06	.2124-06	.2111-06	.2090-06	.2088-06
CS2	.3675-09	.3842-09	.3992-09	.4161-09	.4355-09	.4570-09	.4856-09	.5040-09	.5288-09
COS	.1584-01	.1906-01	.2126-01	.2294-01	.2426-01	.2529-01	.2622-01	.2668-01	.2729-01
S2	.4409-10	.6456-10	.9644-10	.1462-09	.2154-09	.2968-09	.3895-09	.4417-09	.4720-09
H2/H2S	.1450+06	.1305+06	.1161+06	.1025+06	.9159+05	.8455+05	.8138+05	.8115+05	.8077+05

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+01								
H2S	.4921+01	.4905+01	.4894+01	.4885+01	.4879+01	.4873+01	.4869+01	.4866+01	.4863+01
SO2	.3347-07	.8018-06	.1720-06	.3507-06	.6528-05	.1062-04	.1555-04	.1831-04	.2268-04
CS2	.9186-08	.9605-08	.9980-08	.1040-07	.1089-07	.1143-07	.1214-07	.1260-07	.1322-07
COS	.7919+00	.9531+00	.1063+01	.1147+01	.1213+01	.1264+01	.1311+01	.1334+01	.1364+01
S2	.1102-08	.1614-08	.2441-08	.3655-08	.5385-08	.7420-08	.9738-08	.1204-07	.1501-07
H2/H2S	.2901+05	.2611+05	.2323+05	.2050+05	.1832+05	.1691+05	.1628+05	.1623+05	.1613+05

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+02								
H2S	.9842+01	.9809+01	.9787+01	.9770+01	.9757+01	.9747+01	.9737+01	.9733+01	.9727+01
SO2	.6694-08	.1604-07	.3440-07	.7014-07	.1306-06	.2124-06	.2111-06	.2090-06	.2088-06
CS2	.3675-09	.3842-09	.3992-09	.4161-09	.4355-09	.4570-09	.4856-09	.5040-09	.5288-09
COS	.1584+00	.1906+00	.2126+00	.2294+00	.2426+00	.2529+00	.2622+00	.2668+00	.2729+00
S2	.4409-10	.6456-10	.9644-10	.1462-09	.2154-09	.2968-09	.3895-09	.4417-09	.4720-09
H2/H2S	.1450+06	.1305+06	.1161+06	.1025+06	.9159+05	.8455+05	.8138+05	.8115+05	.8077+05

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+02								
H2S	.4921+02	.4905+02	.4894+02	.4885+02	.4879+02	.4873+02	.4869+02	.4866+02	.4863+02
SO2	.3347-06	.8018-06	.1720-05	.3507-05	.6528-05	.1062-04	.1555-04	.1831-04	.2268-04
CS2	.9186-06	.9605-06	.9980-06	.1040-05	.1089-05	.1143-05	.1214-05	.1260-05	.1322-05
COS	.7919+00	.9531+00	.1063+01	.1147+01	.1213+01	.1264+01	.1311+01	.1334+01	.1364+01
S2	.1102-08	.1614-08	.2441-08	.3655-08	.5385-08	.7420-08	.9738-08	.1204-07	.1501-07
H2/H2S	.2901+04	.2611+04	.2323+04	.2050+04	.1832+04	.1691+04	.1628+04	.1623+04	.1613+04

Table 57 (Continued)

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+03									
H2S	.9842+02	.9809+02	.9787+02	.9770+02	.9757+02	.9747+02	.9737+02	.9733+02	.9727+02	
SO2	.8694-05	.1404-05	.3440-05	.7014-05	.1306-04	.2124-04	.3111-04	.3662-04	.4535-04	
CS2	.3675-05	.3842-05	.3992-05	.4162-05	.4355-05	.4570-05	.4856-05	.5040-05	.5288-05	
COS	.1584+01	.1906+01	.2126+01	.2294+01	.2426+01	.2529+01	.2622+01	.2668+01	.2729+01	
S2	.4409-06	.6456-06	.9644-06	.1262-05	.2154-05	.2968-05	.3895-05	.4417-05	.5005-05	
H2/H2S	.1450+04	.1305+04	.1161+04	.1025+04	.9159+03	.8455+03	.8138+03	.8115+03	.8077+03	

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1500+03									
H2S	.1476+03	.1471+03	.1468+03	.1466+03	.1464+03	.1462+03	.1461+03	.1460+03	.1459+03	
SO2	.1004-05	.1405-05	.5161-05	.1052-04	.1958-04	.3186-04	.4666-04	.5493-04	.6803-04	
CS2	.8208-05	.8645-05	.8982-05	.9361-05	.9799-05	.1028-04	.1093-04	.1131-04	.1190-04	
COS	.3176+01	.2859+01	.3189+01	.3441+01	.3638+01	.3793+01	.3932+01	.4005+01	.4099+01	
S2	.9921-06	.1453-05	.2170-05	.3289-05	.4847-05	.6678-05	.8764-05	.9937-05	.1171-04	
H2/H2S	.9669+03	.8703+03	.7742+03	.6833+03	.6106+03	.5636+03	.5425+03	.5410+03	.5385+03	

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.2000+03									
H2S	.1968+03	.1962+03	.1957+03	.1954+03	.1951+03	.1949+03	.1947+03	.1947+03	.1945+03	
SO2	.1339-05	.1207-05	.8881-05	.1403-04	.2611-04	.4248-04	.6222-04	.7324-04	.9071-04	
CS2	.1470-04	.1537-04	.1597-04	.1665-04	.1742-04	.1828-04	.1942-04	.2016-04	.2115-04	
COS	.1168+01	.3813+01	.4252+01	.4588+01	.4851+01	.5058+01	.5243+01	.5336+01	.5458+01	
S2	.1764-05	.2582-05	.3858-05	.5848-05	.8616-05	.1167-04	.1558-04	.1767-04	.2032-04	
H2/H2S	.7252+03	.6527+03	.5807+03	.5125+03	.4580+03	.4227+03	.4069+03	.4057+03	.4039+03	

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.2500+03									
H2S	.2460+03	.2452+03	.2447+03	.2443+03	.2439+03	.2437+03	.2434+03	.2433+03	.2432+03	
SO2	.1673-05	.4009-05	.8601-05	.1754-04	.2264-04	.5311-04	.7777-04	.9155-04	.1134-03	
CS2	.2297-04	.2401-04	.2495-04	.2601-04	.2722-04	.2856-04	.3035-04	.3150-04	.3305-04	
COS	.3960+01	.4766+01	.5315+01	.5735+01	.6064+01	.6322+01	.6554+01	.6670+01	.6822+01	
S2	.2756-05	.4035-05	.6028-05	.9137-05	.1346-04	.1855-04	.2434-04	.2760-04	.3253-04	
H2/H2S	.5801+03	.5222+03	.4645+03	.4100+03	.3664+03	.3382+03	.3255+03	.3246+03	.3231+03	

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+03									
H2S	.4921+03	.4905+03	.4894+03	.4885+03	.4879+03	.4873+03	.4869+03	.4866+03	.4863+03	
SO2	.3347-05	.8018-05	.1720-04	.3507-04	.6528-04	.1062-03	.1555-03	.1831-03	.2268-03	
CS2	.9186-04	.9605-04	.9980-04	.1040-03	.1089-03	.1143-03	.1214-03	.1260-03	.1322-03	
COS	.7919+01	.9531+01	.1063+02	.1147+02	.1213+02	.1264+02	.1311+02	.1334+02	.1364+02	
S2	.1102-04	.1614-04	.2411-04	.3655-04	.5385-04	.7420-04	.9738-04	.1104-03	.1301-03	
H2/H2S	.2901+03	.2611+03	.2323+03	.2050+03	.1832+03	.1691+03	.1628+03	.1623+03	.1615+03	

cell. The projected gas composition along both the anode and cathode as a function of distance indicates that only 31.65% and less than 30% of the fuel gas and the oxidant are utilized for the $\sim 0.160 \text{ A/cm}^2$, 0.9160 V MCFC.

Table 58 defines the cell operating with an average current density of $\sim 0.250 \text{ A/cm}^2$, cell resistances of $0.4035 \times 10^{-4} \text{ ohms}$, total electrode impedances of $1.200 \text{ ohms}\cdot\text{cm}^2$ and a resulting terminal voltage of 0.6540 V. The second model cell is shown to achieve 80% utilization of the fuel gas, and 43% O_2 and 47% CO_2 utilization of the oxidant gas over all the electrode surfaces, and to eliminate the occurrence of limiting current.

Initially, in both Rockwell molten carbonate air-blown cells, as hydrogen is being utilized, producing CO_2 and H_2O from reaction with the electrolyte ions, CO_2 simultaneously dissociates into CO, increasing its total concentration within the fuel gas stream. This dissociation is evident in the negative CO consumption in the first 61 cm from the anode inlet.

Although maximum fuel and oxidant utilizations within the 0.160 A/cm^2 Rockwell molten carbonate fuel gas cell were not achieved, the cell's overall fuel cell efficiency is ~ 1.5 times that of the 0.250 A/cm^2 cell that achieved maximum utilization. This effect is primarily the result of the lowered voltage efficiency in the 0.250 A/cm^2 cell. In accounting for only 78.5% use of the 121.9 cm anode length, the 0.160 A/cm^2 cell appears marginally more efficient than the 0.250 A/cm^2 cell.

The stability of the nickel anode material and the trace contaminant composition of As, Na, and Pb in the Rockwell molten carbonate fuel gas environment were established for both cell models and are illustrated in Figures 33 and 34. After 50 cm the tolerance of the anode in the 0.250 A/cm^2 cell is shown to become increasingly sensitive to low levels of sulfur present within the fuel gases. Sulfidation of the anode outlet for the 0.250 A/cm^2 cell results in the presence of

Table 58

FUEL AND OXIDANT GAS COMPOSITIONS AND UTILIZATIONS AS A FUNCTION
OF LOCATION IN THE ROCKWELL 0.250 A/cm² MOLTEN
CARBONATE AIR-BLOWN MCFC

TEST CASE WITH ANODE MATERIAL - ROCKWELL/AIR BLOWN MCFC

VAPOR PRESSURE (ATM) DATA AT ELECTRODES (TERMINAL VOLTAGE : .65403*00 VOLTS)

TOTAL GAS PRESSURE 10.00 ATMOSPHERE

LENGTH (CM)	.0000	.1530+02	.3050+02	.4580+02	.6100+02	.7620+02	.9150+02	.1067+03	.1220+03
FUEL CELL EMF (V)	.1109+01	.1068+01	.1030+01	.9929+00	.9552+00	.9167+00	.8773+00	.8379+00	.7982+00

CATHODE :

TEMPERATURE DEG. K	866.00	879.93	893.77	907.70	921.55	935.39	949.32	963.16	977.09
CURRENT (AMP/CM2)	.3792+00	.3447+00	.3133+00	.2823+00	.2509+00	.2188+00	.1860+00	.1532+00	.1201+00
VELOCITY (CM/SEC)	.7010+02	.7001+02	.6998+02	.7004+02	.7017+02	.7038+02	.7069+02	.7110+02	.7161+02
H2O	.1488+01	.1514+01	.1538+01	.1561+01	.1582+01	.1601+01	.1618+01	.1632+01	.1644+01
CO2	.1214+01	.1119+01	.1038+01	.9423+00	.8698+00	.8008+00	.7355+00	.6875+00	.6446+00
N2	.6642+01	.6758+01	.6866+01	.6968+01	.7061+01	.7145+01	.7220+01	.7283+01	.7335+01
O2	.6561+00	.6093+00	.5656+00	.5246+00	.4870+00	.4531+00	.4230+00	.3975+00	.3764+00
TOTAL GAS MOLES	.4820+01	.4737+01	.4662+01	.4594+01	.4534+01	.4480+01	.4434+01	.4395+01	.4364+01
% O2 CONSUMED	.0000	.7127+01	.1376+02	.2004+02	.2577+02	.3094+02	.3552+02	.3942+02	.4262+02
% CO2 CONSUMED	.0000	.7843+01	.1517+02	.2206+02	.2836+02	.3405+02	.3909+02	.4338+02	.4691+02

ANODE :

TEMPERATURE DEG. K	923.00	929.78	936.51	943.29	950.02	956.76	963.53	970.27	977.04
CURRENT (AMP/CM2)	.3792+00	.3447+00	.3133+00	.2823+00	.2509+00	.2188+00	.1860+00	.1532+00	.1201+00
VELOCITY (CM/SEC)	.1463+02	.1560+02	.1650+02	.1733+02	.1810+02	.1880+02	.1944+02	.1999+02	.2047+02

O2	.6872-22	.1759-21	.4350-21	.1121-20	.3049-20	.8984-20	.2782-19	.8874-19	.2941-18
H2	.1427+01	.1310+01	.1167+01	.9918+00	.7985+00	.6106+00	.4476+00	.3167+00	.2206+00
H2O	.1595+01	.1851+01	.2060+01	.2236+01	.2383+01	.2500+01	.2591+01	.2658+01	.2707+01
CO	.6749+00	.7341+00	.7364+00	.6881+00	.6004+00	.4935+00	.3865+00	.2919+00	.2132+00
CO2	.1578+01	.2098+01	.2545+01	.2939+01	.3288+01	.3593+01	.3856+01	.4072+01	.4245+01
CH4	.4247+00	.2484+00	.1284+00	.5515-01	.1924-01	.5512-02	.1345-02	.2939-03	.5757-04
NH3	.3474-02	.2818-02	.2198-02	.1604-02	.1083-02	.6789-03	.4007-03	.2271-03	.1237-03
N2	.4287+01	.4051+01	.3859+01	.3699+01	.3567+01	.3459+01	.3370+01	.3300+01	.3244+01

C (C)	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
[H2O]/[H2]	.1117+01	.1413+01	.1765+01	.2222+01	.2924+01	.4094+01	.5788+01	.8341+01	.1227+02
[CO2]/[CO]	.2323+01	.2840+01	.3433+01	.4245+01	.5244+01	.6542+01	.8198+01	.1038+02	.1379+02
[SO2]/[H2S]	.6802-08	.1465-07	.3156-07	.7439-07	.1979-06	.5942-06	.1973-05	.6983-05	.2646-04
[CS2]/[CH2S]**2)	.3818-04	.4025-04	.4201-04	.4386-04	.4599-04	.4854-04	.5153-04	.5487-04	.5852-04
[COS]/[H2S]	.1620-01	.1918-01	.2158-01	.2370-01	.2567-01	.2757-01	.2943-01	.3122-01	.3292-01

TOTAL GAS MOLES	.9438+00	.9989+00	.1049+01	.1094+01	.1135+01	.1170+01	.1201+01	.1227+01	.1248+01
% GRAPHITE IN MIX	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
% H2 CONSUMED	.0000	.8238+01	.1826+02	.3051+02	.4405+02	.5722+02	.6864+02	.7767+02	.8455+02
% CO CONSUMED	.0000	.8776+01	.9115+01	.1950+01	.1103+01	.2688+02	.4274+02	.5674+02	.6841+02
% CO+H2 CONSUMED	.0000	.2776+01	.9469+01	.2009+02	.3345+02	.4748+02	.6032+02	.7095+02	.7937+02
TOTAL CELL CURRENT (AMPS) :	.3715+04								

AVERAGE CURRENT DENSITY : .2498+00 AMPS/CM2

FUEL CELL PLATE DIMENSIONS (CM) : WIDTH	.1219+03	LENGTH	.1219+03	THICKNESS	.2540+00
CELL RESISTANCE : .40350-04 OHMS					
TOTAL ELECTRODE (2A+2C) IMPEDANCE :	.12000+01 OHMS.CM2				

Table 58 (Continued)

HEAT OF C. (KCAL/MOLE)	-.2112+02	-.1746+02	-.1433+02	-.1157+02	-.9151+01	-.7054+01	-.5287+01	-.3865+01	-.2747+01
THE FOLLOWING EFFICIENCIES ARE IN FRACTIONAL UNITS									
VOLTAGE EFFICIENCY	.5896+00	.6125+00	.6349+00	.6587+00	.6847+00	.7135+00	.7455+00	.7805+00	.8194+00
THERMODYNAMIC EFFICIENCY	.8194+00	.7873+00	.7580+00	.7292+00	.7002+00	.6707+00	.6406+00	.6107+00	.5806+00
ELECTROCHEMICAL EFF.	.4831+00	.4822+00	.4813+00	.4804+00	.4794+00	.4785+00	.4776+00	.4766+00	.4757+00
HEATING VALUE EFFICIENCY	.3995+00	.4436+00	.4814+00	.5069+00	.5163+00	.5122+00	.5011+00	.4881+00	.4753+00
FUEL CELL EFFICIENCY	.1930+00	.2139+00	.2317+00	.2435+00	.2475+00	.2451+00	.2393+00	.2326+00	.2261+00

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+01								
H2S	.9842+00	.9813+00	.9790+00	.9770+00	.9751+00	.9733+00	.9715+00	.9698+00	.9682+00
SO2	.6694-08	.1437-07	.3089-07	.7268-07	.1929-08	.5784-08	.1517-05	.6772-05	.2562-04
CS2	.3675-09	.3851-09	.4001-09	.4159-09	.4345-09	.4569-09	.4833-09	.5129-09	.5452-09
COS	.1584-01	.1870-01	.2099-01	.2301-01	.2487-01	.2667-01	.2842-01	.3008-01	.3167-01
S2	.4409-10	.6176-10	.9157-10	.1490-09	.2694-09	.5390-09	.1172-08	.2694-08	.6543-08
H2/H2S	.1450+06	.1335+06	.1192+06	.1015+06	.8189+05	.6274+05	.4608+05	.3286+05	.2278+05

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+01								
H2S	.4921+01	.4906+01	.4895+01	.4885+01	.4875+01	.4866+01	.4858+01	.4849+01	.4841+01
SO2	.3347-07	.7185-07	.1515-06	.3234-06	.9244-06	.2882-05	.9584-05	.3386-04	.1281-03
CS2	.9186-08	.9629-08	.1000-07	.1040-07	.1086-07	.1142-07	.1208-07	.1282-07	.1363-07
COS	.7919-01	.9351-01	.1050+00	.1150+00	.1244+00	.1333+00	.1421+00	.1504+00	.1584+00
S2	.1102-08	.1544-08	.2289-08	.3725-08	.6736-08	.1348-07	.2930-07	.6734-07	.1636-06
H2/H2S	.2901+05	.2669+05	.2384+05	.2030+05	.1638+05	.1255+05	.9215+04	.6572+04	.4556+04

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+02								
H2S	.9842+01	.9813+01	.9790+01	.9770+01	.9751+01	.9733+01	.9715+01	.9698+01	.9682+01
SO2	.6694-08	.1437-07	.3089-07	.7268-07	.1929-08	.5784-08	.1517-05	.6772-05	.2562-04
CS2	.3675-07	.3851-07	.4001-07	.4159-07	.4345-07	.4569-07	.4834-07	.5129-07	.5452-07
COS	.1584+00	.1870+00	.2099+00	.2301+00	.2487+00	.2667+00	.2842+00	.3008+00	.3167+00
S2	.4409-08	.6176-08	.9157-08	.1490-07	.2694-07	.5390-07	.1172-06	.2694-06	.6543-06
H2/H2S	.1450+05	.1335+05	.1192+05	.1015+05	.8189+04	.6274+04	.4608+04	.3286+04	.2278+04

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+02								
H2S	.4921+02	.4906+02	.4895+02	.4885+02	.4875+02	.4866+02	.4858+02	.4849+02	.4841+02
SO2	.3347-08	.7185-08	.1515-06	.3234-06	.9244-06	.2882-05	.9588-05	.3386-04	.1281-03
CS2	.9186-06	.9629-06	.1000-05	.1040-05	.1086-05	.1142-05	.1208-05	.1282-05	.1363-05
COS	.7919+00	.9351+00	.1050+01	.1150+01	.1244+01	.1333+01	.1421+01	.1504+01	.1584+01
S2	.1102-06	.1544-06	.2289-06	.3725-06	.6736-06	.1348-05	.2930-05	.6734-05	.1636-04
H2/H2S	.2901+04	.2669+04	.2384+04	.2030+04	.1638+04	.1255+04	.9215+03	.6572+03	.4556+03

Table 58 (Continued)

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+03								
H ₂ S	.9862+02	.9813+02	.9790+02	.9770+02	.9751+02	.9732+02	.9715+02	.9698+02	.9682+02
SO ₂	.8694+02	.1437-05	.3089-05	.7268-05	.1926-04	.5784-04	.1917-03	.6772-03	.2565-03
CS ₂	.3675-05	.3852-05	.4001-05	.4160-05	.4345-05	.4569-05	.4834-05	.5129-05	.5474-05
COS	.1584+01	.1870+01	.2099+01	.2301+01	.2487+01	.2667+01	.2842+01	.3009+01	.3167+01
S ₂	.4409-04	.6176-06	.9157-06	.1490-05	.2694-05	.5390-05	.1172-04	.3094-04	.6543-04
H ₂ /H ₂ S	.1450+04	.1335+04	.1192+04	.1015+04	.8189+03	.6274+03	.4608+03	.3286+03	.2278+03

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1500+03								
H ₂ S	.1476+03	.1472+03	.1468+03	.1465+03	.1463+03	.1460+03	.1457+03	.1455+03	.1452+03
SO ₂	.1004-05	.2156-05	.4634-05	.1090-04	.2894-04	.8675-04	.2875-03	.1016-02	.3842-02
CS ₂	.8268-05	.8666-05	.9002-05	.9359-05	.9776-05	.1028-04	.1088-04	.1154-04	.1227-04
COS	.2376+01	.2605+01	.3149+01	.3451+01	.3731+01	.4000+01	.4263+01	.4513+01	.4751+01
S ₂	.6921-04	.1390-05	.2060-05	.3353-05	.6063-05	.1213-04	.2637-04	.5061-04	.1472-03
H ₂ /H ₂ S	.9669+03	.8598+03	.7945+03	.6768+03	.5460+03	.4182+03	.3072+03	.2191+03	.1519+03

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.2000+03								
H ₂ S	.1968+03	.1963+03	.1958+03	.1954+03	.1950+03	.1947+03	.1943+03	.1940+03	.1936+03
SO ₂	.1339-05	.2874-05	.6179-05	.1454-04	.3859-04	.1157-03	.3841-03	.1352-02	.5123-02
CS ₂	.1470-04	.1541-04	.1600-04	.1664-04	.1738-04	.1828-04	.1933-04	.2052-04	.2181-04
COS	.3166+01	.3741+01	.4199+01	.4602+01	.4974+01	.5333+01	.5688+01	.6017+01	.6335+01
S ₂	.1764-05	.2470-05	.3663-05	.5460-05	.1078-04	.2196-04	.4688-04	.1078-03	.2617-03
H ₂ /H ₂ S	.7252+03	.6674+03	.5959+03	.5076+03	.4095+03	.3137+03	.2304+03	.1643+03	.1139+03

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.2500+03								
H ₂ S	.2460+03	.2453+03	.2447+03	.2442+03	.2438+03	.2433+03	.2429+03	.2425+03	.2421+03
SO ₂	.1673-05	.3593-05	.7724-05	.1817-04	.4823-04	.1446-03	.4792-03	.1693-02	.6404-02
CS ₂	.2297-04	.2407-04	.2501-04	.2600-04	.2716-04	.2856-04	.3021-04	.3206-04	.3408-04
COS	.3960+01	.4676+01	.5248+01	.5752+01	.6218+01	.6667+01	.7104+01	.7521+01	.7918+01
S ₂	.2756-05	.3860-05	.5723-05	.9313-05	.1684-04	.3369-04	.7325-04	.1684-03	.4090-03
H ₂ /H ₂ S	.5801+03	.5339+03	.4767+03	.4061+03	.3276+03	.2509+03	.1843+03	.1314+03	.9112+02

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+03								
H ₂ S	.4921+03	.4906+03	.4895+03	.4885+03	.4875+03	.4866+03	.4858+03	.4849+03	.4841+03
SO ₂	.3347-05	.7183-05	.1545-04	.3634-04	.9646-04	.2892-03	.9584-03	.3386-03	.1281-02
CS ₂	.9186-04	.9629-04	.1000-03	.1040-03	.1086-03	.1142-03	.1208-03	.1282-03	.1364-03
COS	.7919+01	.9351+01	.1050+02	.1150+02	.1244+02	.1333+02	.1421+02	.1504+02	.1584+02
S ₂	.1102-04	.1544-04	.2289-04	.3725-04	.6736-04	.1348-03	.2930-03	.6334-03	.1636-02
H ₂ /H ₂ S	.2901+03	.2669+03	.2384+03	.2030+03	.1638+03	.1253+03	.9215+02	.6572+02	.4556+02

56 ppm sulfur, while in the 0.160 A/cm^2 cell 184 to 208 ppm sulfur must be present in the fuel gases prior to the formation of Ni_3S_2 .

In both cells As exists as volatile As_4 , with Na having the potential to deposit as sodium carbonate (Na_2CO_3). The current MCFC model does not account for deposition of solid phases. In this manner the initial concentration of Na remains within the fuel gas channel, and the most stable equilibrium Na phase is established within the local fuel gas environment. Although sulfur is also present within the local fuel gas, sodium is not considered to be the most active element to react with it, forming the sulfate (Na_2SO_4), but exists predominantly as the carbonate in the presence of the more active sulfided nickel anode material.

In fuel gas containing 0 to 500 ppm sulfur, Pb is projected to exist as a solid within the first 50 cm of the MCFC. Only minor variation in the stability of the solid Pb complex is projected in the presence of sulfur. For example, within the 0.160 A/cm^2 cell, 385.9 ppm S is required to maintain the stability of solid Pb at 15.3 cm from the anode, and 306.6 ppm S at 30.5 cm, while within the 0.250 A/cm^2 cell, 413.1 ppm S at 15.3 cm, and 300.6 ppm S at 30.5 cm are required to convert solid lead into the volatile lead sulfide (PbS) complex. After 50 cm complete volatilization of the solid occurs, forming elemental gaseous lead (Pb) or PbS , depending on the local sulfur concentration in the fuel gas stream. As shown in Table 59, the Pb to PbS transition is strongly dependent on the surrounding sulfur concentration in the fuel gas approaching the anode outlet.

Initial concentration of 132 ppm total sulfur in the Rockwell molten carbonate fuel gas will have virtually no effect on sulfidation of the anode material and on subsequent cell performance when the MCFC is operated at an average current density of 0.160 A/cm^2 (Figure 33). These levels are shown in Figure 34, however, to enhance sulfidation after the gas has traversed 75 cm of the anode gas channel. In order to minimize sulfur concentration in the fuel gases and simultaneously to

Curve 731010-B

Rockwell Molten Carbonate Air-Blown MCFC

Fuel Gas Velocity: 14.63 cm/sec
 Oxidant Gas Velocity: 70.10 cm/sec
 Anode Inlet Temperature: 923K
 Anode Outlet Temperature: 977K
 Cathode Inlet Temperature: 866K
 Cathode Outlet Temperature: 977K
 Cell Resistance: 0.1345-4 ohms

Total Electrode Impedance: 0.4 ohms·cm²
 Average Current Density: 0.157 Amps/cm²
 Terminal Voltage: 0.9167 Volts

Figure 33 -- Nickel Anode and Trace Element Sulfur Tolerance in the Rockwell Molten Carbonate Air-Blown 0.160 A/cm² MCFC

Figure 34 -- Nickel Anode and Trace Element Sulfur Tolerance in the Rockwell Molten Carbonate Air-Blown 0.250 A/cm² MCFC

Table 59

PROJECTED LEAD SPECIES AS A FUNCTION OF LOCATION IN THE
ROCKWELL MOLTEN CARBONATE AIR-BLOWN MCFC

Distance From Anode Inlet, cm	Total Sulfur Concentration, ppm							
	1	5	10	50	100	150	200	500
0					Pb (s)			
15.3					Pb (s)			PbS (g)
30.5					Pb (s)			PbS (g)
45.8					Pb (s)			PbS (g)
61.0				Pb (g)				PbS (g)
76.2				Pb (g)				PbS (g)
91.5				Pb (g)				PbS (g)
106.7			Pb (g)					PbS (g)
122.0			Pb (g)					PbS (g)

minimize anode sulfidation, desulfurization using regenerative heat exchange and ZnO polishing is employed. In this manner we estimate that sulfur may be reduced from 132 ppm as H_2S to levels of 66 ppb. Simultaneously Na_2CO_3 is reduced from 396.1 ppm to 4 ppm, while the concentrations of Pb and As are assumed to be unaffected. Although desulfurization can be achieved using this technique, contaminants of ZnO are likely to become entrained in the scrubbed effluent. The models were reevaluated on this basis. Tables 60 and 61 indicate that no change is evident in the bulk gas composition when either raw Rockwell or ZnO polished gases are used as fuel gas reactants. Similarly, phase stabilities of the solid Pb and Na complexes are identical with those previously discussed for either the 0.160 or 0.150 A/cm^2 MCFC. Arsenic exists predominantly as gaseous As_4 throughout the cell, while Pb undergoes volatile transitions similar to those shown in Table 59.

Table 60

FUEL AND OXIDANT GAS COMPOSITIONS AND UTILIZATIONS AS A
FUNCTION OF LOCATION IN THE ROCKWELL 0.160 A/cm² MOLTEN
CARBONATE AIR-BLOWN ZnO POLISHED MCFC

TEST CASE WITH ANODE MATERIAL - ROCKWELL/AIR BLOWN MCFC/ZINC OXIDE POLISHED										
VAPOR PRESSURE (ATM) DATA AT ELECTRODES (TERMINAL VOLTAGE : .91667+00 VOLTS)										
TOTAL GAS PRESSURE 10.00 ATMOSPHERE										
LENGTH (CM)	.0000	.1530+02	.3050+02	.4580+02	.6100+02	.7620+02	.9100+02	.1067+03	.1220+03	
FUEL CELL EMF (V)	.1109+01	.1064+01	.1027+01	.9939+00	.9654+00	.9410+00	.9166+00	.9167+00	.9167+00	
CATHODE :										
TEMPERATURE DEG. K	866.00	879.93	893.77	907.70	921.55	935.39	952.51	963.16	977.09	
CURRENT (AMP/CM ²)	.4812+00	.3672+00	.2747+00	.1930+00	.1217+00	.6082-01	.0000	.0000	.0000	
VELOCITY (CM/SEC)	.7010+02	.6960+02	.6981+02	.7008+02	.7060+02	.7134+02	.7251+02	.7333+02	.7439+02	
H ₂ O	.1488+01	.1519+01	.1542+01	.1560+01	.1572+01	.1579+01	.1582+01	.1582+01	.1582+01	
O ₂	.1214+01	.1193+01	.1016+01	.9502+00	.9056+00	.8796+00	.8691+00	.8691+00	.8691+00	
N ₂	.6642+01	.6777+01	.6881+01	.6963+01	.7017+01	.7049+01	.7062+01	.7062+01	.7062+01	
O ₂	.6561+00	.6014+00	.5587+00	.5265+00	.5046+00	.4918+00	.4867+00	.4867+00	.4867+00	
TOTAL GAS MOLES	.4820+01	.4723+01	.4651+01	.4597+01	.4562+01	.4541+01	.4533+01	.4533+01	.4533+01	
X O ₂ CONSUMED	.0000	.8335+01	.1484+02	.1975+02	.2309+02	.2504+02	.2582+02	.2582+02	.2582+02	
X CO ₂ CONSUMED	.0000	.9173+01	.1634+02	.2173+02	.2541+02	.2755+02	.2841+02	.2841+02	.2841+02	
ANODE :										
TEMPERATURE DEG. K	923.00	929.78	936.51	943.29	950.02	956.76	965.08	970.27	977.04	
CURRENT (AMP/CM ²)	.4812+00	.3672+00	.2747+00	.1930+00	.1217+00	.6082-01	.0000	.0000	.0000	
VELOCITY (CM/SEC)	.1463+02	.1574+02	.1662+02	.1730+02	.1780+02	.1815+02	.1840+02	.1849+02	.1862+02	
O ₂	.6872-22	.1919-21	.4720-21	.1092-20	.2323-20	.4447-20	.8432-20	.1185-19	.1846-19	
H ₂ O	.1427+01	.1281+01	.1137+01	.1001+01	.8937+00	.8241+00	.7924+00	.7896+00	.7856+00	
H ₂ O	.1555+01	.1690+01	.1800+01	.2229+01	.2320+01	.2374+01	.2401+01	.2407+01	.2415+01	
CO	.6749+00	.7319+00	.7267+00	.6926+00	.6550+00	.6307+00	.6298+00	.6394+00	.6513+00	
CO ₂	.1578+01	.2185+01	.2616+01	.2921+01	.3120+01	.3231+01	.3267+01	.3259+01	.3246+01	
CH ₄	.4247+00	.2266+00	.1154+00	.5733-01	.3021-01	.1824-01	.1254-01	.1082-01	.8905-02	
NH ₃	.3474-02	.2712-02	.2106-02	.1628-02	.1293-02	.1083-02	.9602-03	.9212-03	.8717-03	
N ₂	.4287+01	.4014+01	.3630+01	.3706+01	.3627+01	.3583+01	.3566+01	.3566+01	.3566+01	
C(C)	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	
[H ₂ O]/[H ₂]	.1117+01	.1476+01	.1839+01	.2226+01	.2596+01	.2880+01	.3030+01	.3048+01	.3075+01	
[CO ₂]/[CO]	.2323+01	.2967+01	.3577+01	.4190+01	.4733+01	.5090+01	.5154+01	.5065+01	.4957+01	
[SO ₂]/[H ₂ S]	.6802-08	.1635-07	.3515-07	.7179-07	.1338-06	.2179-06	.3195-06	.3763-06	.4463-06	
[CS ₂]/[H ₂ S+2]	.3818-04	.4018-04	.4194-04	.4367-04	.4603-04	.4841-04	.5153-04	.5354-04	.5625-04	
[CO ₂]/[H ₂ S]	.1620-01	.1956-01	.2186-01	.2363-01	.2502-01	.2611-01	.2709-01	.2759-01	.2823-01	
TOTAL GAS MOLES	.9438+00	.1008+01	.1057+01	.1092+01	.1116+01	.1130+01	.1135+01	.1135+01	.1135+01	
X GRAPHITE IN MIX	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	
X H ₂ CONSUMED	.0000	.1029+02	.2037+02	.2984+02	.3739+02	.4227+02	.4448+02	.4467+02	.4466+02	
X CO CONSUMED	.0000	.8438+01	.7679+01	.2621+01	.2958+01	.6545+01	.6683+01	.5266+01	.3504+01	
X CO+H ₂ CONSUMED	.0000	.4274+01	.1136+02	.1942+02	.2634+02	.3080+02	.3235+02	.3202+02	.3165+02	
TOTAL CELL CURRENT (AMPS) :	.2338+04									
AVERAGE CURRENT DENSITY :	.1572+00 AMPS/CM ²									
FUEL CELL FLATE DIMENSIONS (CM) : WIDTH	.1219+03									
CELL RESISTANCE :	.19450-04 OHMS									
TOTAL ELECTRODE (2A+2C) IMPEDANCE :	.40000+00 OHMS.CM ²									

Table 60 (Continued)

HEAT OF C. (KCAL/MOLE)	-.2112+02	-.1685+02	-.1384+02	-.1170+02	-.1029+02	-.9488+01	-.9186+01	-.9202+01	-.9222+01
THE FOLLOWING EFFICIENCIES ARE IN FRACTIONAL UNITS									
VOLTAGE EFFICIENCY	.8264+00	.8618+00	.8929+00	.9223+00	.9495+00	.9741+00	.1000+01	.1000+01	.1000+01
THERMODYNAMIC EFFICIENCY	.8194+00	.7842+00	.7554+00	.7300+00	.7077+00	.6885+00	.6690+00	.6680+00	.6667+00
ELECTROCHEMICAL EFF.	.6772+00	.6759+00	.6746+00	.6733+00	.6720+00	.6707+00	.6690+00	.6680+00	.6667+00
HEATING VALUE EFFICIENCY	.3995+00	.4493+00	.4856+00	.5062+00	.5137+00	.5139+00	.5106+00	.5080+00	.5044+00
FUEL CELL EFFICIENCY	.2705+00	.3036+00	.3276+00	.3408+00	.3452+00	.3447+00	.3416+00	.3394+00	.3363+00

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+01								
H2S	.9842+00	.9809+00	.9787+00	.9770+00	.9757+00	.9747+00	.9737+00	.9733+00	.9727+00
SO2	.6694+00	.1604+07	.3440+07	.7014+07	.1306+08	.2124+08	.3111+08	.3662+08	.4335+08
CS2	.3675+09	.3842+09	.3992+09	.4161+09	.4335+09	.4520+09	.4856+09	.5040+09	.5288+09
COS	.1584+01	.1906+01	.2126+01	.2294+01	.2426+01	.2529+01	.2622+01	.2668+01	.2699+01
S2	.4405+10	.6456+10	.6644+10	.6622+09	.5154+09	.5988+09	.6895+09	.7216+09	.5205+09
H2/H2S	.1450+06	.1305+06	.1161+06	.1025+06	.9159+05	.8455+05	.8138+05	.8115+05	.8077+05

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+01								
H2S	.4921+01	.4905+01	.4894+01	.4885+01	.4879+01	.4873+01	.4869+01	.4866+01	.4863+01
SO2	.3347+06	.8018+06	.1720+06	.3507+06	.6528+06	.1062+07	.1555+07	.1831+07	.2228+07
CS2	.9186+08	.9605+08	.9980+08	.1040+08	.1089+08	.1143+08	.1214+08	.1260+08	.1322+08
COS	.7915+00	.9531+00	.1063+01	.1147+01	.1213+01	.1264+01	.1311+01	.1334+01	.1364+01
S2	.1102+08	.1614+08	.2411+08	.3655+08	.5385+08	.7420+08	.9737+08	.1164+09	.1501+09
H2/H2S	.2901+05	.2611+05	.2323+05	.2050+05	.1832+05	.1691+05	.1628+05	.1623+05	.1615+05

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+02								
H2S	.9842+01	.9809+01	.9787+01	.9770+01	.9757+01	.9747+01	.9737+01	.9733+01	.9727+01
SO2	.6694+07	.1604+06	.3440+06	.7014+06	.1306+07	.2124+07	.3111+07	.3662+07	.4335+07
CS2	.3675+07	.3842+07	.3992+07	.4161+07	.4335+07	.4520+07	.4856+07	.5040+07	.5288+07
COS	.1584+00	.1906+00	.2126+00	.2294+00	.2426+00	.2529+00	.2622+00	.2668+00	.2699+00
S2	.4405+08	.6456+08	.6644+08	.6622+07	.5154+07	.5988+07	.6895+07	.7216+07	.5205+07
H2/H2S	.1450+05	.1305+05	.1161+05	.1025+05	.9159+04	.8455+04	.8138+04	.8115+04	.8077+04

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+02								
H2S	.4921+02	.4905+02	.4894+02	.4885+02	.4879+02	.4873+02	.4869+02	.4866+02	.4863+02
SO2	.3347+06	.8018+06	.1720+05	.3507+05	.6528+05	.1062+06	.1555+06	.1831+06	.2228+06
CS2	.9186+08	.9605+08	.9980+08	.1040+08	.1089+08	.1143+08	.1214+08	.1260+08	.1322+08
COS	.7915+00	.9531+00	.1063+01	.1147+01	.1213+01	.1264+01	.1311+01	.1334+01	.1364+01
S2	.1102+08	.1614+08	.2411+08	.3655+08	.5385+08	.7420+08	.9737+08	.1164+09	.1501+09
H2/H2S	.2901+04	.2611+04	.2323+04	.2050+04	.1832+04	.1691+04	.1628+04	.1623+04	.1615+04

Table 60 (Continued)

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR .1000+03

H2S	.9842+02	.9809+02	.9787+02	.9770+02	.9727+02	.9747+02	.9737+02	.9733+02	.9727+02
SO2	.6694-06	.1604-05	.3444-05	.7014-05	.1306-04	.2124-04	.3111-04	.3662-04	.4535-04
CS2	.5672-05	.3842-05	.3992-05	.4162-05	.4355-05	.4570-05	.4836-05	.5040-05	.5288-05
COS	.1584+01	.1406+01	.2122+01	.2294+01	.2426+01	.2529+01	.2622+01	.2668+01	.2729+01
S2	.4405-06	.6456-04	.9644-06	.1462+05	.2154-03	.2968-05	.3895+05	.4417-03	.5205+05
H2/H2S	.1450+04	.1305+04	.1161+04	.1025+04	.9159+03	.8455+03	.8138+03	.8115+03	.8077+03

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR .1500+03

H2S	.1476+03	.1471+03	.1466+03	.1466+03	.1464+03	.1462+03	.1461+03	.1460+03	.1459+03
SO2	.1004-05	.2405-05	.5161-05	.1052-04	.1958-04	.3186-04	.4666-04	.5493-04	.6803-04
CS2	.8268-05	.8645-05	.8986-05	.9363-05	.9799-05	.1028-04	.1093-04	.1134-04	.1190-04
COS	.2776+01	.2859+01	.3189+01	.3441+01	.3638+01	.3793+01	.3932+01	.4002+01	.4093+01
S2	.6921-06	.1453-05	.2170-05	.3289-05	.4847-05	.6678-05	.8764-05	.9937-05	.1171-04
H2/H2S	.6665+03	.8703+03	.7742+03	.6833+03	.6106+03	.5636+03	.5425+03	.5410+03	.5385+03

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR .2000+03

H2S	.1968+03	.1962+03	.1957+03	.1954+03	.1951+03	.1949+03	.1947+03	.1947+03	.1945+03
SO2	.1339-05	.3207-05	.6681-05	.1403-04	.2611-04	.4248-04	.6222-04	.7324-04	.9071-04
CS2	.1470-04	.1537-04	.1597-04	.1665-04	.1742-04	.1828-04	.1942-04	.2016-04	.2115-04
COS	.1168+01	.3813+01	.4252+01	.4588+01	.4851+01	.5058+01	.5243+01	.5336+01	.5458+01
S2	.1764-05	.2582-05	.3858-05	.5848-05	.8616-05	.1187-04	.1558-04	.1767-04	.2082-04
H2/H2S	.7252+03	.6527+03	.5807+03	.5125+03	.4580+03	.4227+03	.4069+03	.4057+03	.4039+03

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR .2500+03

H2S	.2460+03	.2452+03	.2447+03	.2443+03	.2439+03	.2437+03	.2434+03	.2433+03	.2432+03
SO2	.1673-05	.4009-05	.8601-05	.1754-04	.3264-04	.5311-04	.7777-04	.9155-04	.1134-03
CS2	.2297-04	.2401-04	.2495-04	.2601-04	.2722-04	.2856-04	.3035-04	.3150-04	.3305-04
COS	.1560+01	.4766+01	.5315+01	.5735+01	.6064+01	.6322+01	.6554+01	.6670+01	.6822+01
S2	.2756-05	.4035-05	.6028-05	.9137-05	.1346-04	.1855-04	.2434-04	.2700-04	.3253-04
H2/H2S	.5801+03	.5222+03	.4645+03	.4100+03	.3664+03	.3382+03	.3255+03	.3246+03	.3231+03

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR .5000+03

H2S	.4921+03	.4905+03	.4894+03	.4885+03	.4879+03	.4873+03	.4865+03	.4866+03	.4863+03
SO2	.3347-05	.8018-05	.1726-04	.3507-04	.6528-04	.1062-03	.1555-03	.1831-03	.2268-03
CS2	.9186-04	.9605-04	.9986-04	.1040-03	.1089-03	.1143-03	.1212-03	.1260-03	.1322-03
COS	.7919+01	.9531+01	.1063+02	.1147+02	.1213+02	.1264+02	.1311+02	.1334+02	.1364+02
S2	.1102-04	.1614-04	.2411-04	.3655-04	.5385-04	.7420-04	.9738-04	.1104-03	.1301-03
H2/H2S	.2901+03	.2611+03	.2323+03	.2050+03	.1832+03	.1691+03	.1628+03	.1623+03	.1615+03

Table 61

FUEL AND OXIDANT GAS COMPOSITIONS AND UTILIZATIONS AS A
FUNCTION OF LOCATION IN THE ROCKWELL 0.250 A/cm² MOLTEN
CARBONATE AIR-BLOWN ZnO POLISHED MCFC

TEST CASE WITH ANODE MATERIAL - ROCKWELL/AIR BLCHN MCFC/ZINC OXIDE POLISHED

VAPOR PRESSURE (ATM) DATA AT ELECTRODES (TERMINAL VOLTAGE : .65403+00 VOLTS)

TOTAL GAS PRESSURE 10.00 ATMOSPHERE

LENGTH (CM)	.0000	.1530+02	.3050+02	.4580+02	.6100+02	.7620+02	.9150+02	.1067+03	.1220+03
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FUEL CELL EMF (V)	.1109+01	.1068+01	.1030+01	.9929+00	.9552+00	.9167+00	.8773+00	.8379+00	.7982+00
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CATHODE :

TEMPERATURE DEG. K	866.00	879.93	893.77	907.70	921.55	935.39	949.32	963.16	977.09
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TIME (SEC)	0	1	2	3	4	5	6	7	8	9
CURRENT (AMP/CM2)	.3792+00	.3447+00	.3133+00	.2823+00	.2509+00	.2188+00	.1860+00	.1532+00	.1201+00	

VELOCITY (CM/SEC)	.7010+02	.7001+02	.6998+02	.7004+02	.7017+02	.7038+02	.7069+02	.7110+02	.7161+02
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W20	.1488+01	.1514+01	.1538+01	.1561+01	.1582+01	.1601+01	.1618+01	.1632+01	.1644+01
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C02	.1214+01	.1119+01	.1030+01	.9463+00	.8898+00	.8008+00	.7393+00	.6873+00	.6448+00
N2	.6642+01	.6758+01	.6866+01	.6968+01	.7061+01	.7145+01	.7220+01	.7283+01	.7335+01

02 .6561+00 .6093+00 .5656+00 .5246+00 .4870+00 .4531+00 .4230+00 .3973+00 .3764+00

TOTAL GAS MOLES	.4820+01	.4737+01	.4662+01	.4594+01	.4534+01	.4480+01	.4434+01	.4395+01	.4364+01
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7 02 CONSUMED	.0000	.7127+01	.1378+02	.2004+02	.2577+02	.3094+02	.3552+02	.3942+02	.4282+02
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% CO2 CONSUMED	.0000	.7843+01	.1517+02	.2206+02	.2836+02	.3405+02	.3909+02	.4338+02	.4691+02
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ANCDE :

TEMPERATURE DEG. K	923.00	929.78	936.51	943.29	950.02	956.76	963.53	970.27	977.04
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CURRENT (AMP/CM ²)	.3792+00	.3447+00	.3133+00	.2823+00	.2509+00	.2188+00	.1860+00	.1532+00	.1201+00
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VELOCITY (CM/SEC)	.1463+C2	.1560+02	.1650+02	.1733+02	.1810+02	.1880+02	.1944+C2	.1999+C2	.2047+C2
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02 .4872-22 .1759-21 .4350-21 .1121-20 .3069-20 .8984-20 .2782-19 .8874-19 .2541-18

H2	.1427+01	.1310+01	.1187+01	.9918+00	.7985+00	.6108+00	.4478+00	.3187+00	.2208+00
H2O	.1595+01	.1851+01	.2060+01	.2236+01	.2383+01	.2500+01	.2591+01	.2658+01	.2707+01

28	.6749+00	.7341+00	.7364+00	.6881+00	.6004+00	.4935+00	.3883+00	.2919+00	.2132+00
02	.1578+01	.2098+01	.2545+01	.2939+01	.3288+01	.3593+01	.3856+01	.4072+01	.4245+01

CH4	.4247+00	.2484+00	.1284+00	.5515-01	.1924-01	.5512-02	.1345-02	.2939-03	.5757-04
NH3	.3131-02	.2818-02	.2108-02	.1606-02	.1083-02	.6288-03	.4002-03	.2221-03	.1232-03

N2	.4287+01	.4051+01	.3859+01	.3699+01	.3567+01	.3459+01	.3370+01	.3300+01	.3244+01
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(C) .0000 .0000 .0000 .0000 .0000 .0000 .0000 .0000 .0000

[H20]/[H2] .1117+01 .1413+01 .1765+01 .2255+01 .2984+01 .4094+01 .5788+01 .8341+01 .1227+02

[002]/[001]	.2522-01	.2840-01	.3433-01	.4243-01	.5441-01	.7133-01	.7773-01	.9388-01	.9777-01
[102]/[101]	.4802-08	.1465-07	.3156-07	.7439-07	.1979-06	.5942-06	.1973-05	.6983-05	.2646-04

[C23]/[H2S]	.3818-04	.4025-04	.4201-04	.4388-04	.4599-04	.4834-04	.5133-04	.5487-04	.5892-04
[C05]/[H2S]	.1620-01	.1918-01	.2158-01	.2370-01	.2567-01	.2757-01	.2943-01	.3122-01	.3292-01

TOTAL GAS MOLES	.6478+00	.9989+00	.1049+01	.1094+01	.1135+01	.1170+01	.1201+01	.1227+01	.1248+01
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% GRAPHITE IN MIX	.6000	.8000	.6000	.9000	.7000	.9000	.8000	.8000
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7	W2 CONSUMED	0000	8238+01	-1826+02	-3051+02	.4405+02	.5722+02	.6864+02	.7767+02	.8455+02
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7 CO CONSUMED	6000	= 8274+01	= 8115+01	= 1950+01	= 1103+02	= 2688+02	= 4274+02	= 5674+02	= 6841+02
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8. FARMER CONSUMED	6000	2374+01	6110+01	2600+02	3345+02	4748+02	6032+02	7095+02	7537+02
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[illegible]

INCREASED CURRENT ASSETS 1,571,504

AVERAGE CURRENT DENSITY : .2498*00 AMPS/CM2

LL CELL PLATE DIMENSIONS (CM) : WIDTH .1219+05 LENGTH .1219+05 THICKNESS .0254+05
LL RESISTANCE : .40350-C4 CHMS

TOTAL ELECTRODE (2A+2C) IMPEDANCE : .12000+CI OHMS.CM2

Table 61 (Continued)

HEAT OF C. (KCAL/MOLE)	-.2112+02	-.1746+02	-.1433+02	-.1157+02	-.9151+01	-.7054+01	-.5287+01	-.3865+01	-.2747+01
THE FOLLOWING EFFICIENCIES ARE IN FRACTIONAL UNITS									
VOLTAGE EFFICIENCY	.5896+00	.6125+00	.6349+00	.6587+00	.6847+00	.7135+00	.7455+00	.7805+00	.8194+00
THERMODYNAMIC EFFICIENCY	.8194+00	.7873+00	.7580+00	.7292+00	.7002+00	.6707+00	.6406+00	.6107+00	.5806+00
ELECTROCHEMICAL EFF.	.4831+00	.4822+00	.4813+00	.4804+00	.4794+00	.4785+00	.4776+00	.4766+00	.4757+00
HEATING VALUE EFFICIENCY	.3955+00	.4436+00	.4814+00	.5069+00	.5163+00	.5122+00	.5011+00	.4881+00	.4753+00
FUEL CELL EFFICIENCY	.1930+00	.2139+00	.2317+00	.2435+00	.2475+00	.2451+00	.2393+00	.2326+00	.2261+00

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+01								
H2S	.9842+00	.9813+00	.9790+00	.9770+00	.9751+00	.9733+00	.9715+00	.9698+00	.9682+00
SO2	.6694-08	.1437-07	.3085-07	.7268-07	.1929-06	.5784-06	.1917-05	.6772-05	.2562-04
CS2	.3675-09	.3851-09	.4001-09	.4159-09	.4345-09	.4569-09	.4833-09	.5126-09	.5452-09
COS	.1584-01	.1870-01	.2095-01	.2301-01	.2487-01	.2667-01	.2842-01	.3008-01	.3167-01
S2	.4405-08	.6176-10	.9157-10	.1490-09	.2694-09	.5390-09	.1172-08	.2654-08	.6343-08
H2/H2S	.1450+05	.1335+06	.1192+06	.1015+06	.8189+05	.6274+05	.4608+05	.3286+05	.2278+05

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+01								
H2S	.4921+01	.4906+01	.4895+01	.4885+01	.4875+01	.4866+01	.4858+01	.4849+01	.4841+01
SO2	.3347-07	.7185-07	.1545-06	.3634-06	.9646-06	.2892-05	.9584-05	.3386-04	.1281-03
CS2	.9186-08	.9629-08	.1000-07	.1040-07	.1086-07	.1142-07	.1208-07	.1282-07	.1363-07
COS	.7919-01	.9351-01	.1050+00	.1150+00	.1244+00	.1333+00	.1421+00	.1504+00	.1584+00
S2	.1102-08	.1544-08	.2285-08	.3725-08	.6736-08	.1348-07	.2950-06	.6734-07	.1686-06
H2/H2S	.2901+05	.2669+05	.2384+05	.2030+05	.1638+05	.1255+05	.9215+04	.6572+04	.4556+04

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+02								
H2S	.9842+01	.9813+01	.9790+01	.9770+01	.9751+01	.9733+01	.9715+01	.9698+01	.9682+01
SO2	.6694-07	.1437-06	.3085-06	.7268-06	.1929-05	.5784-05	.1917-04	.6772-04	.2562-03
CS2	.3675-07	.3851-07	.4001-07	.4159-07	.4345-07	.4569-07	.4833-07	.5126-07	.5452-07
COS	.1584+00	.1870+00	.2095+00	.2301+00	.2487+00	.2667+00	.2842+00	.3008+00	.3167+00
S2	.4405-08	.6176-08	.9157-08	.1490-07	.2694-07	.5390-07	.1172-06	.2654-06	.6343-06
H2/H2S	.1450+05	.1335+05	.1192+05	.1015+05	.8189+04	.6274+04	.4608+04	.3286+04	.2278+04

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+02								
H2S	.4921+02	.4906+02	.4895+02	.4885+02	.4875+02	.4866+02	.4858+02	.4849+02	.4841+02
SO2	.3347-06	.7185-06	.1545-05	.3634-05	.9646-05	.2892-04	.9584-04	.3386-03	.1281-02
CS2	.9186-06	.9629-06	.1000-05	.1040-05	.1086-05	.1142-05	.1208-05	.1282-05	.1363-05
COS	.7919+00	.9351+00	.1050+01	.1150+01	.1244+01	.1333+01	.1421+01	.1504+01	.1584+01
S2	.1102-06	.1544-06	.2285-06	.3725-06	.6736-06	.1348-05	.2950-05	.6734-05	.1686-04
H2/H2S	.2901+04	.2669+04	.2384+04	.2030+04	.1638+04	.1255+04	.9215+03	.6572+03	.4556+03

Table 61 (Continued)

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR .1000+03

H2S	.9842+02	.9813+02	.9790+02	.9770+02	.9751+02	.9733+02	.9715+02	.9696+02	.9682+02
SO2	.6694-06	.1437-05	.3085-05	.7268-05	.1929-04	.5784-04	.1917-03	.6772-03	.2562-02
CS2	.7675-05	.3852-05	.4001-05	.4160-05	.4345-05	.4569-05	.4834-05	.5125-05	.5453-05
COS	.1584+01	.1870+01	.2095+01	.2301+01	.2487+01	.2667+01	.2842+01	.3009+01	.3167+01
S2	.4405-06	.6176-06	.9157-06	.1490-05	.2694-05	.5390-05	.1172-04	.2664-04	.6544-04
H2/H2S	.1450+04	.1335+04	.1192+04	.1015+04	.8189+03	.6274+03	.4608+03	.3286+03	.2278+03

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR .1500+03

H2S	.1476+03	.1472+03	.1466+03	.1465+03	.1463+03	.1460+03	.1457+03	.1455+03	.1452+03
SO2	.1004-05	.2156-05	.4634-05	.1090-04	.6894-04	.8675-04	.10875-04	.1016-03	.3825-02
CS2	.8268-05	.8666-05	.9002-05	.9359-05	.9776-05	.1028-04	.1088-04	.1154-04	.1227-04
COS	.2376+01	.2805+01	.3145+01	.3451+01	.3731+01	.4000+01	.4263+01	.4513+01	.4751+01
S2	.9921-06	.1390-05	.2060-05	.3353-05	.6063-05	.1213-04	.2637-04	.6061-04	.1472-03
H2/H2S	.9665+03	.8898+03	.7945+03	.6766+03	.5460+03	.4182+03	.3072+03	.2191+03	.1549+03

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR .2000+03

H2S	.1966+03	.1963+03	.1958+03	.1954+03	.1950+03	.1947+03	.1943+03	.1940+03	.1936+03
SO2	.1335-05	.2874-05	.6175-05	.1454-04	.3859-04	.1157-03	.3834-03	.1354-02	.5123-02
CS2	.1470-04	.1541-04	.1600-04	.1664-04	.1738-04	.1828-04	.1933-04	.2052-04	.2181-04
COS	.3168+01	.3741+01	.4195+01	.4602+01	.4974+01	.5333+01	.5683+01	.6017+01	.6335+01
S2	.1764-05	.2470-05	.3663-05	.5960-05	.1078-04	.2156-04	.4688-04	.1078-03	.2617-03
H2/H2S	.7252+03	.6674+03	.5955+03	.5076+03	.4095+03	.3137+03	.2304+03	.1643+03	.1139+03

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR .2500+03

H2S	.2460+03	.2453+03	.2447+03	.2442+03	.2438+03	.2433+03	.2429+03	.2425+03	.2421+03
SO2	.1673-05	.3593-05	.7724-05	.1817-04	.4823-04	.1446-03	.4792-03	.1693-02	.6404-02
CS2	.2297-04	.2407-04	.2501-04	.2600-04	.2716-04	.2856-04	.3021-04	.3206-04	.3408-04
COS	.3960+01	.4676+01	.5248+01	.5752+01	.6218+01	.6667+01	.7104+01	.7521+01	.7918+01
S2	.2754-05	.3860-05	.5723-05	.9313-05	.1684-04	.3369-04	.7325-04	.1684-03	.4050-03
H2/H2S	.5801+03	.5339+03	.4767+03	.4061+03	.3276+03	.2509+03	.1843+03	.1314+03	.9112+02

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR .5000+03

H2S	.4921+03	.4906+03	.4895+03	.4885+03	.4875+03	.4866+03	.4856+03	.4845+03	.4841+03
SO2	.3347-05	.7185-05	.1545-04	.3634-04	.9646-04	.2892-03	.9584-03	.3386-02	.1281-01
CS2	.9186-04	.9629-04	.1000-03	.1040-03	.1086-03	.1142-03	.1208-03	.1282-03	.1363-03
COS	.7915+01	.9351+01	.1050+02	.1150+02	.1244+02	.1333+02	.1421+02	.1504+02	.1584+02
S2	.1102-04	.1544-04	.2285-04	.3725-04	.6736-04	.1348-03	.2930-03	.6734-03	.1636-02
H2/H2S	.2901+03	.2669+03	.2384+03	.2030+03	.1638+03	.1255+03	.9215+02	.6572+02	.4556+02

As the fuel gases enter the anode, Zn exists initially as volatile Zn in sulfur environments containing 0 to 500 ppm H_2S (Table 62). At H_2S concentrations higher than 250 ppm, Zn is projected to form zinc sulfide (ZnS), with the potential to deposit along the anode at distances of 15.3 to 45.8 cm from the inlet. Thereafter, Zn is projected once again to remain as gaseous Zn, independent of sulfur concentrations that are less than 500 ppm.

Table 62

Dwg. 7756A-6

PROJECTED ZINC SPECIES AS A FUNCTION OF LOCATION IN THE ROCKWELL
MOLTEN CARBONATE AIR-BLOWN MCFC

Distance From Anode Inlet, cm	Total Sulfur Concentration, ppm								
	1	5	10	50	100	150	200	250	500
0	←				Zn (g)				→
15.3	←				Zn (g)				ZnS (s) →
30.5	←				Zn (g)				ZnS (s) →
45.8	←				Zn (g)				ZnS (s) →
61.0	←				Zn (g)				→
76.2	←				Zn (g)				→
91.5	←				Zn (g)				→
106.7	←				Zn (g)				→
122.0	←				Zn (g)				→

The prime objective in using ZnO polishing is to desulfurize fuel gases before they enter the anode channel. Comparison of Figures 34 and 35 indicates that Rockwell molten carbonate fuel gas containing 132 ppm H_2S enhance nickel sulfidation after a distance of 75 cm from the anode inlet, while no sulfidation is projected to occur over the entire cell length when fuel gases are purified to levels of 66 ppm H_2S .

Rockwell Molten Carbonate Zinc Oxide Polished Air-Blown MCFC

Fuel Gas Velocity: 14.63 cm/sec

Oxidant Gas Velocity: 70.10 cm/sec

Anode Inlet Temperature: 923K

Anode Outlet Temperature: 977K

Cathode Inlet Temperature: 866K

Cathode Outlet Temperature: 977K

Cell Resistance: 0.4035-4 ohms

Total Electrode Impedance: 1.200 ohms·cm²Average Current Density: 0.2498 Amps/cm²

Terminal Voltage: 0.6540 Volts

Figure 35 -- Nickel Anode and Trace Element Sulfur Tolerance in the Rockwell Molten Carbonate Air-Blown ZnO Polished 0.250 A/cm² MCFC

3.3.4.2 Evaluation of the METC Gravitating-Bed Air-Blown Gas to MCFC

Iron oxide desulfurization of fuel gases from the METC gravitating-bed gasifier reduces sulfur to concentrations of 139.1 ppm. In addition to sulfur, the METC fuel gases entering the anode are estimated to contain 1.7 ppm Pb, 695.4 ppm HCl, 278.3 ppm carbon, and 5563.3 ppm tar. The MCFC performance with METC fuel gases for similar system operating conditions (fuel gas and oxidant gas velocities, anode and cathode temperature gradients, and total pressure), as previously discussed for the Rockwell molten carbonate fuel gas MCFC, is shown in Table 63 for a cell with an average current density of 0.160 A/cm^2 , and in Table 64 for a comparable cell of 0.250 A/cm^2 . With an average current density of 0.160 A/cm^2 , an exchange current is achieved at 96.1 cm from the anode inlet, with an overall utilization of only 24.4% H_2 and CO in the fuel gas, and 28.4% CO_2 and 25.8% O_2 utilization of the oxidant. Increasing the average current density to 0.250 A/cm^2 and cell resistance and total impedance to $0.4 \times 10^{-4} \text{ ohms}$ and $1.2 \text{ ohms}\cdot\text{cm}^2$, respectively, enhances utilization in both fuel gas (71.0% H_2 and CO) and oxidant gas (46.9% CO_2 , 42.6% O_2) streams. Although the METC gravitating-bed air-blown MCFC oxidant gas utilization is similar to that projected in the Rockwell molten carbonate air-blown cell, the METC fuel gas utilization is approximately 7% less than in the Rockwell system over the entire cell length.

The METC gravitating-bed system permits the presence of a higher level of sulfur in the fuel gas than does the Rockwell molten carbonate MCFC prior to sulfidation of the anode material. For MCFC operations with an average current density of 0.160 A/cm^2 , a Rockwell molten carbonate sulfur tolerance of 184 ppm is projected, while in the METC gravitating-bed system a sulfur tolerance of 208 ppm is estimated. Similarly, operations at 0.250 A/cm^2 in the Rockwell molten carbonate system permits 68 ppm sulfur to be present in the fuel gas at the anode outlet, while 82 ppm sulfur may exist in the METC anode outlet fuel gas prior to sulfidation (Figures 33, 34, 36). Even with FeO desulfurization, the METC gravitating-bed fuel gas, which initially contains

Table 63

FUEL AND OXIDANT GAS COMPOSITIONS AND UTILIZATIONS AS A FUNCTION
OF LOCATION IN THE METC 0.160 A/cm² GRAVITATING-BED
FeO AIR-BLOWN MCFC

TEST CASE WITH ANODE MATERIAL - METC/FEC AIR BLOWN MCFC										
VAPOR PRESSURE (ATM) DATA AT ELECTRODES (TERMINAL VOLTAGE : .92320+00 VOLTS)										
TOTAL GAS PRESSURE 10.00 ATMOSPHERE										
LENGTH (CM)	.0000	.1530+02	.3050+02	.4580+02	.6100+02	.7620+02	.9610+02	.1067+03	.1220+03	
FUEL CELL EMF (V)	.1115+01	.1069+01	.1032+01	.1000+01	.9726+00	.9487+00	.9232+00	.9232+00	.9232+00	
CATHODE :										
TEMPERATURE DEG. K	866.00	879.93	893.77	907.70	921.55	935.39	953.51	963.16	977.09	
CURRENT (AMP/CM2)	.4792+00	.3640+00	.2726+00	.1928+00	.1234+00	.6360-01	.0000	.0000	.0000	
VELOCITY (CM/SEC)	.7010+02	.6981+02	.6983+02	.7011+02	.7062+02	.7135+02	.7259+02	.7333+02	.7439+02	
H2O	.1458+01	.1518+01	.1542+01	.1580+01	.1572+01	.1579+01	.1582+01	.1582+01	.1582+01	
CO2	.1214+01	.1104+01	.1017+01	.9522+00	.9071+00	.8807+00	.8692+00	.8692+00	.8692+00	
N2	.6642+01	.6776+01	.6881+01	.6961+01	.7015+01	.7048+01	.7062+01	.7062+01	.7062+01	
O2	.6561+00	.6018+00	.5594+00	.5275+00	.5055+00	.4924+00	.4867+00	.4867+00	.4867+00	
TOTAL GAS MOLES	.4871+01	.4774+01	.4701+01	.4648+01	.4612+01	.4590+01	.4581+01	.4581+01	.4581+01	
X O2 CONSUMED	.0000	.8276+01	.1473+02	.1960+02	.2295+02	.2495+02	.2582+02	.2582+02	.2582+02	
X CO2 CONSUMED	.0000	.9108+01	.1621+02	.2157+02	.2526+02	.2746+02	.2841+02	.2841+02	.2841+02	
ANODE :										
TEMPERATURE DEG. K	923.00	929.78	936.51	943.29	950.02	956.78	965.57	970.27	977.04	
CURRENT (AMP/CM2)	.4792+00	.3640+00	.2726+00	.1928+00	.1234+00	.6360-01	.0000	.0000	.0000	
VELOCITY (CM/SEC)	.1463+02	.1573+02	.1660+02	.1728+02	.1779+02	.1814+02	.1841+02	.1849+02	.1862+02	
O2	.6047-22	.1470-21	.3975-21	.8819-21	.1866-20	.3372-20	.6535-20	.8869-20	.1375-19	
H2	.1477+01	.1347+01	.1213+01	.1093+01	.9960+00	.9312+00	.8007+00	.8888+00	.6975+00	
H2O	.1548+01	.1847+01	.2047+01	.2187+01	.2280+01	.2336+01	.2367+01	.2373+01	.2381+01	
CO	.6641+00	.7389+00	.7513+00	.7338+00	.7059+00	.6923+00	.6964+00	.7070+00	.7215+00	
CO2	.1456+01	.2058+01	.2482+01	.2781+01	.2977+01	.3088+01	.3126+01	.3118+01	.3106+01	
CH4	.4771+00	.2692+00	.1482+00	.8056-01	.4606-01	.2936-01	.2036-01	.1795-01	.1492-01	
NH3	.3690-02	.2934-02	.2343-02	.1875-02	.1535-02	.1313-02	.1170-02	.1130-02	.1074-02	
N2	.4363+01	.4086+01	.3901+01	.3774+01	.3694+01	.3648+01	.3629+01	.3629+01	.3629+01	
C(C)	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	
[H2O]/[H2]	.1065+01	.1777+01	.1687+01	.2000+01	.2299+01	.2508+01	.2628+01	.2637+01	.2653+01	
[CO2]/[CO]	.1379+01	.2767+01	.3282+01	.3766+01	.4173+01	.4560+01	.4860+01	.4982+01	.5078+01	
[SO2]/[H2S]	.5783-08	.1557-07	.2773-07	.5311-07	.9333-07	.1462-06	.2144-06	.2472-06	.3040-06	
[CS2]/[H2S]**2)	.3739-04	.3964-04	.4147-04	.4339-04	.4549-04	.4778-04	.5097-04	.5273-04	.5534-04	
[COS]/[H2S]	.1540-01	.1885-01	.2117-01	.2293-01	.2429-01	.2536-01	.2636-01	.2678-01	.2738-01	
TOTAL GAS MOLES	.9538+00	.1018+01	.1067+01	.1103+01	.1127+01	.1141+01	.1147+01	.1147+01	.1147+01	
X GRAPHITE IN MIX	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	
X H2 CONSUMED	.0000	.9187+01	.1787+02	.2599+02	.3257+02	.3696+02	.3903+02	.3909+02	.3925+02	
X CO CONSUMED	.0000	.1127+02	.1313+02	.1050+02	.6737+01	.4245+01	.4865+01	.6461+01	.8645+01	
X CO+H2 CONSUMED	.0000	.2843+01	.8256+01	.1467+02	.2038+02	.2418+02	.2542+02	.2496+02	.2439+02	
TOTAL CELL CURRENT (AMPS) :	.2337+04									
AVERAGE CURRENT DENSITY :	.1572+00 AMPS/CM2									
FUEL CELL PLATE DIMENSIONS (CM) : WIDTH	.1219+03				LENGTH		.1219+03		THICKNESS	
CELL RESISTANCE :	.13450-04 OHMS									
TOTAL ELECTRODE (2A+2C) IMPEDANCE :	.40000+00 OHMS.CM2									

Table 63 (Continued)

HEAT OF C. (KCAL/MOLE)	-.2235*02	-.1808*02	-.1509*02	-.1297*02	-.1156*02	-.1075*02	-.1043*02	-.1045*02	-.1047*02
THE FOLLOWING EFFICIENCIES ARE IN FRACTIONAL UNITS									
VOLTAGE EFFICIENCY	.8280+00	.8637+00	.8943+00	.9229+00	.9492+00	.9732+00	.1000+01	.1000+01	.1000+01
THERMODYNAMIC EFFICIENCY	.8236+00	.7881+00	.7596+00	.7347+00	.7129+00	.6941+00	.6737+00	.6728+00	.6715+00
ELECTROCHEMICAL EFF.	.6820+00	.6807+00	.6794+00	.6780+00	.6767+00	.6754+00	.6737+00	.6728+00	.6715+00
HEATING VALUE EFFICIENCY	.3908+00	.4388+00	.4755+00	.4987+00	.5095+00	.5126+00	.5113+00	.5098+00	.5073+00
FUEL CELL EFFICIENCY	.2665+00	.2987+00	.3231+00	.3381+00	.3448+00	.3462+00	.3445+00	.3430+00	.3406+00

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+01								
H ₂ S	.9849+00	.9816+00	.9794+00	.9777+00	.9764+00	.9754+00	.9744+00	.9740+00	.9735+00
SO ₂	.5696-08	.5132-07	.2716-07	.5192-07	.9113-07	.1426-06	.2089-06	.2408-06	.2959-06
CS ₂	.3605-09	.7795-09	.3952-09	.4171-09	.4310-09	.4517-09	.4809-09	.4971-09	.5211-09
CO ₂	.1507-01	.1839-01	.2061-01	.2228-01	.2357-01	.2458-01	.2552-01	.2592-01	.2649-01
S ₂	.4123-10	.5891-10	.8476-10	.1228-09	.1737-09	.2327-09	.3054-09	.3408-09	.3995-09
H ₂ /H ₂ S	.1500+06	.1367+06	.1239+06	.1118+06	.1020+06	.9548+05	.9243+05	.9238+05	.9219+05

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+01								
H ₂ S	.4925+01	.4908+01	.4897+01	.4898+01	.4882+01	.4877+01	.4872+01	.4870+01	.4867+01
SO ₂	.2848-07	.6662-07	.1358-08	.2596-06	.4556-06	.7132-06	.1045-05	.1504-05	.1679-05
CS ₂	.9011-08	.9488-08	.9881-08	.1030-07	.1077-07	.1126-07	.1202-07	.1243-07	.1303-07
CO ₂	.7535-01	.9193-01	.1030+00	.1114+00	.1179+00	.1229+00	.1276+00	.1296+00	.1324+00
S ₂	.1031-08	.1473-08	.2119-08	.3070-08	.4341-08	.5819-08	.7634-08	.8520-08	.9988-08
H ₂ /H ₂ S	.3000+05	.2733+05	.2478+05	.2236+05	.2040+05	.1910+05	.1849+05	.1848+05	.1844+05

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+02								
H ₂ S	.9849+01	.9816+01	.9794+01	.9777+01	.9764+01	.9754+01	.9744+01	.9740+01	.9735+01
SO ₂	.5696-07	.5132-06	.2716-06	.5192-06	.9113-06	.1426-05	.2089-05	.2408-05	.2959-05
CS ₂	.3605-07	.7795-07	.3952-07	.4172-07	.4310-07	.4517-07	.4809-07	.4971-07	.5211-07
CO ₂	.1507+00	.1839+00	.2061+00	.2228+00	.2357+00	.2458+00	.2552+00	.2592+00	.2649+00
S ₂	.4123-08	.5891-08	.8476-08	.1228-07	.1737-07	.2327-07	.3054-07	.3408-07	.3995-07
H ₂ /H ₂ S	.1500+05	.1367+05	.1239+05	.1118+05	.1020+05	.9548+04	.9243+04	.9238+04	.9219+04

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+02								
H ₂ S	.4925+02	.4908+02	.4897+02	.4898+02	.4882+02	.4877+02	.4872+02	.4870+02	.4867+02
SO ₂	.2848-06	.6662-06	.1358-05	.2596-05	.4556-05	.7132-05	.1045-04	.1504-04	.1679-04
CS ₂	.9011-06	.9488-06	.9881-06	.1030-05	.1077-05	.1129-05	.1202-05	.1243-05	.1303-05
CO ₂	.7535+00	.9193+00	.1030+01	.1114+01	.1179+01	.1229+01	.1276+01	.1296+01	.1324+01
S ₂	.1031-06	.1473-06	.2119-06	.3070-06	.4341-06	.5819-06	.7635-06	.8521-06	.9988-06
H ₂ /H ₂ S	.3000+04	.2733+04	.2477+04	.2236+04	.2040+04	.1909+04	.1849+04	.1848+04	.1844+04

Table 63 (Continued)

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+03									
H2S	.9849+02	.9816+02	.9794+02	.9777+02	.9764+02	.9754+02	.9744+02	.9740+02	.9735+02	.9735+02
SO2	.5696-06	.1332-05	.2716-05	.5192-05	.6113-05	.1426-04	.2682-04	.2408-04	.2959-04	.2959-04
CS2	.3604-05	.3795-05	.3952-05	.4122-05	.4310-05	.4517-05	.4809-05	.4971-05	.5211-05	.5211-05
COS	.1507+01	.1839+01	.2061+01	.2228+01	.2357+01	.2458+01	.2552+01	.2592+01	.2649+01	.2649+01
S2	.4123-06	.5891-06	.8477-06	.1228-05	.1737-05	.2327-05	.3054-05	.3408-05	.3995-05	.3995-05
H2/H2S	.1500+04	.1367+04	.1239+04	.1118+04	.1020+04	.9547+03	.9243+03	.9238+03	.9219+03	.9219+03

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1500+03									
H2S	.1477+03	.1472+03	.1469+03	.1467+03	.1465+03	.1463+03	.1462+03	.1461+03	.1460+03	.1460+03
SO2	.8544-06	.1998-05	.4074-05	.7789-05	.1367-04	.2140-04	.3134-04	.3611-04	.4298-04	.4298-04
CS2	.8110-05	.8539-05	.8893-05	.9273-05	.9697-05	.1016-04	.1082-04	.1119-04	.1172-04	.1172-04
COS	.2261+01	.2758+01	.3091+01	.3341+01	.3536+01	.3687+01	.3828+01	.3887+01	.3973+01	.3973+01
S2	.9277-06	.1325-05	.1907-05	.2763-05	.3907-05	.5237-05	.6871-05	.7669-05	.8990-05	.8990-05
H2/H2S	.9999+03	.9111+03	.8258+03	.7455+03	.6801+03	.6365+03	.6162+03	.6158+03	.6146+03	.6146+03

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.2000+03									
H2S	.1976+03	.1963+03	.1959+03	.1955+03	.1953+03	.1951+03	.1949+03	.1948+03	.1947+03	.1947+03
SO2	.1139-05	.2863-05	.5253-05	.1018-04	.1724-04	.2853-04	.4198-04	.5618-04	.7198-04	.7198-04
CS2	.1442-04	.1516-04	.1581-04	.1649-04	.1724-04	.1807-04	.1924-04	.1989-04	.2084-04	.2084-04
COS	.3014+01	.3677+01	.4121+01	.4455+01	.4714+01	.4916+01	.5104+01	.5183+01	.5297+01	.5297+01
S2	.1649-05	.2356-05	.3391-05	.4913-05	.6946-05	.9310-05	.1222-04	.1363-04	.1598-04	.1598-04
H2/H2S	.7499+03	.6833+03	.6194+03	.5591+03	.5101+03	.4774+03	.4621+03	.4619+03	.4610+03	.4610+03

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.2500+03									
H2S	.2462+03	.2454+03	.2448+03	.2444+03	.2441+03	.2438+03	.2436+03	.2435+03	.2434+03	.2434+03
SO2	.1424-05	.3331-05	.6791-05	.1298-04	.2278-04	.3566-04	.5223-04	.6019-04	.7397-04	.7397-04
CS2	.2253-04	.2372-04	.2470-04	.2576-04	.2694-04	.2823-04	.3006-04	.3107-04	.3257-04	.3257-04
COS	.3768+01	.4596+01	.5151+01	.5589+01	.5893+01	.6145+01	.6380+01	.6479+01	.6622+01	.6622+01
S2	.2577-05	.3682-05	.5298-05	.7676-05	.1085-04	.1455-04	.1909-04	.2150-04	.2497-04	.2497-04
H2/H2S	.5999+03	.5467+03	.4955+03	.4473+03	.4080+03	.3819+03	.3697+03	.3695+03	.3688+03	.3688+03

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+03									
H2S	.4923+03	.4908+03	.4897+03	.4889+03	.4882+03	.4877+03	.4872+03	.4870+03	.4867+03	.4867+03
SO2	.2848-05	.6662-05	.1358-04	.2596-04	.4556-04	.7132-04	.1045-03	.1204-03	.1479-03	.1479-03
CS2	.9011-04	.9488-04	.9881-04	.1030-03	.1077-03	.1129-03	.1179-03	.1229-03	.1276-03	.1276-03
COS	.7533+01	.9193+01	.1030+02	.1114+02	.1179+02	.1259+02	.1341+02	.1426+02	.1514+02	.1514+02
S2	.1031-04	.1473-04	.2119-04	.3070-04	.4341-04	.5815-04	.7635-04	.9821-04	.1264-03	.1264-03
H2/H2S	.3000+03	.2733+03	.2477+03	.2276+03	.2040+03	.1909+03	.1849+03	.1847+03	.1844+03	.1844+03

Table 64

FUEL AND OXIDANT GAS COMPOSITIONS AND UTILIZATIONS AS A
FUNCTION OF LOCATION IN THE METC 0.250 A/cm² GRAVITATING-BED
FeO AIR-BLOWN MCFC

TEST CASE WITH ANODE MATERIAL - METC/FeO/AIR BLOWN MCFC

VAPOR PRESSURE (ATM) DATA AT ELECTRODES (TERMINAL VOLTAGE = .66314+00 VOLTS)

TOTAL GAS PRESSURE 10.00 ATMOSPHERE

LENGTH (CM)	.0000	.1530+02	.3050+02	.4580+02	.6100+02	.7620+02	.9150+02	.1067+03	.1220+03
FUEL CELL EMF (V)	.1115+01	.1073+01	.1036+01	.9995+00	.9633+00	.9265+00	.8892+00	.8523+00	.8156+00

CATHODE :

TEMPERATURE DEG. K	866.00	879.93	893.77	907.70	921.55	935.39	949.32	963.16	977.09
CURRENT (AMP/CM ²)	.3764+00	.3415+00	.3104+00	.2802+00	.2500+00	.2194+00	.1883+00	.1575+00	.1270+00
VELOCITY (CM/SEC)	.7010+02	.7002+02	.7001+02	.7007+02	.7020+02	.7042+02	.7072+02	.7112+02	.7161+02
H ₂ O	.1486+01	.1516+01	.1538+01	.1561+01	.1581+01	.1600+01	.1617+01	.1631+01	.1644+01
CO ₂	.1212+01	.1120+01	.1032+01	.0948+01	.0872+01	.0808+01	.0742+01	.0682+01	.0628+01
N ₂	.6642+01	.6757+01	.6864+01	.6965+01	.7057+01	.7141+01	.7217+01	.7281+01	.7335+01
O ₂	.6561+00	.6097+00	.5665+00	.5258+00	.4885+00	.4546+00	.4243+00	.3983+00	.3764+00
TOTAL GAS MOLES	.4871+01	.4788+01	.4713+01	.4645+01	.4584+01	.4530+01	.4483+01	.4443+01	.4410+01
% O ₂ CONSUMED	.0000	.7065+01	.1366+02	.1986+02	.2554+02	.3071+02	.3532+02	.3929+02	.4262+02
% CO ₂ CONSUMED	.0000	.7775+01	.1503+02	.2185+02	.2811+02	.3379+02	.3887+02	.4323+02	.4691+02

ANODE :

TEMPERATURE DEG. K	923.00	929.78	936.51	943.29	950.02	956.76	963.53	970.27	977.04
CURRENT (AMP/CM ²)	.3764+00	.3415+00	.3104+00	.2802+00	.2500+00	.2194+00	.1883+00	.1575+00	.1270+00
VELOCITY (CM/SEC)	.1463+02	.1559+02	.1648+02	.1731+02	.1808+02	.1878+02	.1941+02	.1998+02	.2047+02
O ₂	.6047+22	.1533+21	.3680+21	.9001+21	.2294+20	.6154+20	.1723+19	.4863+19	.1360+18
H ₂	.1477+01	.1369+01	.1242+01	.1085+01	.9081+00	.7270+00	.5622+00	.4266+00	.3198+00
H ₂ O	.1548+01	.1806+01	.2016+01	.2194+01	.2342+01	.2464+01	.2561+01	.2634+01	.2689+01
CO	.6641+00	.7386+00	.7584+00	.7306+00	.6629+00	.5705+00	.4712+00	.3795+00	.3004+00
CO ₂	.1456+01	.1971+01	.2410+01	.2797+01	.3138+01	.3438+01	.3700+01	.3918+01	.4097+01
CH ₄	.4771+00	.2927+00	.1629+00	.7825+01	.3177+01	.1091+01	.3286+02	.9246+03	.2490+03
NH ₃	.3690+02	.3040+02	.2436+02	.1853+02	.1325+02	.8903+03	.5692+03	.3549+03	.2179+03
N ₂	.4363+01	.4124+01	.3930+01	.3768+01	.3635+01	.3524+01	.3433+01	.3360+01	.3301+01
C(C)	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
[H ₂ O]/[H ₂]	.1048+01	.1739+01	.1624+01	.3021+01	.2579+01	.2389+01	.2555+01	.6175+01	.8406+01
[CO ₂]/[CO]	.2179+01	.2652+01	.3158+01	.3805+01	.4703+01	.5989+01	.7803+01	.1026+02	.1355+02
[CO ₂]/[CH ₂ S]	.5783+08	.1221+07	.2508+07	.5460+07	.1300+06	.3420+06	.9730+06	.2839+05	.8582+05
[CS ₂]/[H ₂ S]**2)	.3739+04	.3968+04	.4133+04	.4338+04	.4542+04	.4782+04	.5063+04	.5378+04	.5722+04
[COS]/[H ₂ S]	.1540+01	.1846+01	.2088+01	.2299+01	.2492+01	.2677+01	.2858+01	.3031+01	.3159+01

TOTAL GAS MOLES	.9538+00	.1009+01	.1059+01	.1105+01	.1145+01	.1181+01	.1213+01	.1239+01	.1261+01
% GRAPHITE IN MIX	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
% H ₂ CONSUMED	.0000	.7297+01	.1594+02	.2652+02	.3853+02	.5078+02	.6194+02	.7112+02	.7835+02
% CO CONSUMED	.0000	.1122+02	.1420+02	.1001+02	.1786+00	.1409+02	.2905+02	.4286+02	.5477+02
% CO+H ₂ CONSUMED	.0000	.1554+01	.6591+01	.1519+02	.2663+02	.3941+02	.5174+02	.6236+02	.7104+02
TOTAL CELL CURRENT (AMPS) :	.3715+04								
AVERAGE CURRENT DENSITY :	.2498+00 AMPS/CM ²								
FUEL CELL PLATE DIMENSIONS (CM) : WIDTH	.1219+03								
CELL RESISTANCE 40350-02 OHMS	.1219+03								
TOTAL ELECTRODE (2A+2C) IMPEDANCE :	.12000+01 OHMS/CM ²								

Table 64 (Continued)

HEAT OF C. (KCAL/MOLE)	-.2235+02	-.1869+02	-.1559+02	-.1286+02	-.1046+02	-.8366+01	-.6574+01	-.5107+01	-.3928+01
THE FOLLOWING EFFICIENCIES ARE IN FRACTIONAL UNITS									
VOLTAGE EFFICIENCY	.5948+00	.6180+00	.6402+00	.6635+00	.6884+00	.7157+00	.7458+00	.7781+00	.8131+00
THERMODYNAMIC EFFICIENCY	.8236+00	.7912+00	.7622+00	.7341+00	.7061+00	.6779+00	.6493+00	.6211+00	.5932+00
ELECTROCHEMICAL EFF.	.4899+00	.4889+00	.4880+00	.4870+00	.4861+00	.4852+00	.4842+00	.4833+00	.4823+00
HEATING VALUE EFFICIENCY	.3908+00	.4333+00	.4712+00	.4994+00	.5136+00	.5142+00	.5061+00	.4944+00	.4821+00
FUEL CELL EFFICIENCY	.1914+00	.2118+00	.2299+00	.2433+00	.2497+00	.2495+00	.2451+00	.2389+00	.2325+00

139.1 ppm sulfur, does not achieve an adequate sulfur tolerance in the 0.250 A/cm^2 cell, but is sufficient for operations at 0.160 A/cm^2 .

Trace constituents such as Pb in the METC gravitating-bed fuel gas containing chlorine are projected to remain as volatile chlorides throughout the entire length of the anode channel (Table 65). Deposition of Fe solids along the anode will not occur when chlorine is present in the fuel gas.

In order to achieve a sulfur concentration below the nickel anode material tolerance, the METC fuel gases are desulfurized with FeO followed by ZnO polishing. This technique is estimated to reduce sulfur within the fuel gases to levels of 69.5 ppb. Traces of ZnO (139.1 ppb), however, are projected to remain within the fuel gas after desulfurization. The METC gravitating-bed air-blown MCFC performance using FeO/ZnO desulfurization shown in Tables 66 and 67 are virtually identical to the FeO desulfurization system. Referring to Figure 36, therefore, we can see that the residual 69.5 ppb sulfur in the METC fuel gas is not projected to enhance sulfidation of the anode in either the 0.160 or 0.250 A/cm^2 MCFC. Trace contaminants of Pb and Zn in the chlorine-laden fuel gas exist as volatile chlorides throughout the length of the cell (Table 68). Deposition of these constituents is not projected under these conditions.

The METC gravitating-bed fuel gas has been humidified to the extent of preventing solid carbon deposition at the anode inlet through either the Boudouard or the water gas shift reaction in the bulk fuel gas stream. Table 63 indicates that this humidification is sufficient to prevent carbon deposition throughout the entire length of the anode channel. Solid carbon (4.2 ppm) and tar (5563.3 ppm) entrained as trace constituents in the fuel gas have the potential to deposit along the anode, react with, or volatilize into the bulk gas stream. As a trace constituent under the defined humidification conditions, 66.21% of the incoming carbon is projected to form solids within the anode channel,

Curve 731008-8

METC Gravitating-Bed FeO Air-Blown MCFC

Fuel Gas Velocity: 14.63 cm/sec

Oxidant Gas Velocity: 70.10 cm/sec

Anode Inlet Temperature: 923K

Anode Outlet Temperature: 977K

Cathode Inlet Temperature: 866K

Cathode Outlet Temperature: 977K

Cell Resistance: 0.1345-4 ohms (0.4035-4 ohms)

Total Electrode Impedance: 0.4 ohms·cm² (1.200 ohms·cm²)

Average Current Density: 0.160 Amps/cm² (0.250 Amps/cm²)

Terminal Voltage: 0.9230 Volts (0.6631 Volts)

Figure 36 - Nickel Anode Sulfur Tolerance in the METC Gravitating-Bed FeO Air-Blown MCFC

Table 65

Dwg. 7756A78

VOLATILE CHLORINE COMPLEXES IN THE METC GRAVITATING-BED
FeO AIR-BLOWN MCFC

Distance From Anode Inlet, cm	0.160 Amps/cm ² MCFC	0.250 Amps/cm ² MCFC
0	HCl, PbCl ₂	HCl, PbCl ₂
15.3	HCl, PbCl	HCl, PbCl ₂
30.5	HCl, PbCl	HCl, PbCl
45.8	HCl, PbCl	HCl, PbCl
61.0	HCl, PbCl	HCl, PbCl
76.2	HCl, PbCl	HCl, PbCl
91.5	HCl, PbCl	HCl, PbCl
106.7	HCl, PbCl	HCl, PbCl
122.0	HCl, PbCl	HCl, PbCl

while 33.79% volatilizes. Deposition of the solid carbon or tar, therefore, may occur at the anode surface, plugging pores that are essential for electrolysis.

3.3.4.3 Evaluation of the Westinghouse Fluidized-bed Oxygen-Blown
Gas to MCFC

After being subjected to desulfurization with dolomite and ZnO polishing with regenerative heat exchange, the Westinghouse fluidized-bed fuel gas containing as little as 51.9 ppb sulfur enters the MCFC at a gas stream velocity and at cell conditions similar to those previously discussed for the Rockwell molten carbonate and METC gravitating-bed cells. The oxidant under these conditions has been modified to contain 13% CO₂, 17 percent H₂O, 63% N₂, and 7% O₂ on a mole basis, representing an oxygen-blown gasifier effluent, with additional oxygen being supplied into the recycle anode exhaust gases prior to entering the cathode chamber. As shown in Table 69, utilization of both fuel and oxidant gases for the 0.160 A/cm² MCFC is considerably less in the Westinghouse MCFC than in either the Rockwell molten carbonate or METC

Table 66

FUEL AND OXIDANT GAS COMPOSITIONS AND UTILIZATIONS AS A FUNCTION
OF LOCATION IN THE METC 0.160 A/cm² GRAVITATING-BED
FeO/ZnO AIR-BLOWN MCFC

TEST CASE WITH ANODE MATERIAL - METC/AIR BLOWN MCFC										
VAPOR PRESSURE (ATM) DATA AT ELECTRODES (TERMINAL VOLTAGE : .92320+00 VOLTS)										
TOTAL GAS PRESSURE 10.00 ATMOSPHERE										
LENGTH (CM)	.0000	.1530+02	.3050+02	.4580+02	.6100+02	.7620+02	.9610+02	.1067+03	.1220+03	
FUEL CELL EMF (V)	.1115+01	.1069+01	.1032+01	.1000+01	.9726+00	.9487+00	.9232+00	.9232+00	.9232+00	
CATHODE :										
TEMPERATURE DEG. K	866.00	879.93	893.77	907.70	921.55	935.39	953.51	963.16	977.09	
CURRENT (AMP/CM2)	.4792+00	.3640+00	.2726+00	.1928+00	.1234+00	.6360-01	.0000	.0000	.0000	
VELOCITY (CM/SEC)	.7010+02	.6981+02	.6983+02	.7011+02	.7062+02	.7135+02	.7259+02	.7333+02	.7439+02	
H2O	.1488+01	.1318+01	.1144+01	.1060+01	.1072+01	.1079+01	.1082+01	.1082+01	.1082+01	
CO2	.1214+01	.1104+01	.1017+01	.9522+00	.9078+00	.8807+00	.8892+00	.8892+00	.8892+00	
N2	.6642+01	.6776+01	.6881+01	.6961+01	.7015+01	.7048+01	.7062+01	.7062+01	.7062+01	
O2	.6561+00	.6018+00	.5594+00	.5275+00	.5055+00	.4924+00	.4867+00	.4867+00	.4867+00	
TOTAL GAS MOLES	.4871+01	.4774+01	.4701+01	.4648+01	.4612+01	.4590+01	.4561+01	.4581+01	.4581+01	
X O2 CONSUMED	.0000	.6276+01	.1473+02	.1960+02	.2295+02	.2495+02	.2582+02	.2582+02	.2582+02	
X CO2 CONSUMED	.0000	.9108+01	.1621+02	.2157+02	.2526+02	.2746+02	.2841+02	.2841+02	.2841+02	
ANODE :										
TEMPERATURE DEG. K	923.00	929.78	936.51	943.29	950.02	956.76	965.57	970.27	977.04	
CURRENT (AMP/CM2)	.4792+00	.3640+00	.2726+00	.1928+00	.1234+00	.6360-01	.0000	.0000	.0000	
VELOCITY (CM/SEC)	.7463+02	.1573+02	.1660+02	.1728+02	.1779+02	.1814+02	.1841+02	.1849+02	.1862+02	
O2	.6047-22	.1670-21	.3975-21	.8819-21	.1806-20	.3372-20	.6535-20	.8869-20	.1375-19	
H2	.1477+01	.1341+01	.1215+01	.1093+01	.9960+00	.9512+00	.9007+00	.8998+00	.8975+00	
H2O	.1548+01	.1847+01	.2047+01	.2187+01	.2280+01	.2336+01	.2367+01	.2373+01	.2381+01	
CO	.6641+00	.7389+00	.7513+00	.7338+00	.7088+00	.6923+00	.6964+00	.7070+00	.7215+00	
CO2	.1456+01	.2058+01	.2482+01	.2781+01	.2977+01	.3088+01	.3126+01	.3118+01	.3106+01	
CH4	.4771+00	.2692+00	.1482+00	.8056-01	.4606-01	.2936-01	.2036-01	.1793-01	.1492-01	
NH3	.3690-02	.2934-02	.2343-02	.1875-02	.1535-02	.1313-02	.1170-02	.1130-02	.1074-02	
N2	.4363+01	.4086+01	.3901+01	.3774+01	.3694+01	.3648+01	.3629+01	.3629+01	.3629+01	
(C)	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	
[H2O]/[H2]	.1048+01	.1377+01	.1687+01	.2000+01	.2299+01	.2509+01	.2628+01	.2637+01	.2653+01	
[CO2]/[CO]	.2179+01	.2767+01	.3282+01	.3711+01	.4177+01	.4622+01	.5077+01	.5472+01	.5828+01	
[SO2]/[H2S]	.5783-08	.1837-07	.2773-07	.3511-07	.4133-07	.4662-06	.5144-06	.5672-06	.6204-06	
[CS2]/[CH2S]**2)	.3739-04	.3984-04	.4147-04	.4339-04	.4549-04	.4778-04	.5097-04	.5273-04	.5534-04	
[CO2]/[H2S]	.1540-01	.1885-01	.2117-01	.2293-01	.2429-01	.2536-01	.2636-01	.2678-01	.2738-01	
TOTAL GAS MOLES	.9538+00	.1018+01	.1067+01	.1103+01	.1127+01	.1141+01	.1147+01	.1147+01	.1147+01	
X GRAPHITE IN MIX	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	
X H2 CONSUMED	.0000	.9187+01	.1787+02	.2599+02	.3257+02	.3696+02	.3903+02	.3909+02	.3925+02	
X CO CONSUMED	.0000	.1127+02	.1313+02	.1050+02	.6737+01	.4245+01	.4865+01	.6461+01	.8645+01	
X CO+H2 CONSUMED	.0000	.2843+01	.8256+01	.1467+02	.2038+02	.2418+02	.2542+02	.2496+02	.2439+02	
TOTAL CELL CURRENT (AMPS) :	.2337+04									
AVERAGE CURRENT DENSITY :	.1572+00 AMPS/CM2									
FUEL CELL PLATE DIMENSIONS (CM) : WIDTH	.1219+03									
CELL RESISTANCE : .13450-04 OHMS										
TOTAL ELECTRODE (2A+2C) IMPEDANCE :	.40000+00 OHMS/CM2									

Table 66 (Continued)

HEAT OF C. (KCAL/MOLE)	-.2235+02	-.1808+02	-.1509+02	-.1297+02	-.1156+02	-.1075+02	-.1043+02	-.1045+02	-.1047+02
THE FOLLOWING EFFICIENCIES ARE IN FRACTIONAL UNITS									
VOLTAGE EFFICIENCY	.8280+00	.8637+00	.8943+00	.9229+00	.9492+00	.9732+00	.1000+01	.1000+01	.1000+01
THERMODYNAMIC EFFICIENCY	.8236+00	.7881+00	.7596+00	.7347+00	.7129+00	.6941+00	.6737+00	.6728+00	.6715+00
ELECTROCHEMICAL EFF.	.6820+00	.6807+00	.6794+00	.6780+00	.6767+00	.6754+00	.6737+00	.6728+00	.6715+00
HEATING VALUE EFFICIENCY	.3908+00	.4388+00	.4755+00	.4987+00	.5095+00	.5126+00	.5113+00	.5098+00	.5073+00
FUEL CELL EFFICIENCY	.2665+00	.2987+00	.3231+00	.3381+00	.3448+00	.3462+00	.3445+00	.3430+00	.3406+00

Table 67

FUEL AND OXIDANT GAS COMPOSITIONS AND UTILIZATIONS AS A FUNCTION
OF LOCATION IN THE METC 0.250 A/cm² GRAVITATING-BED
FeO/ZnO AIR-BLOWN MCFC

TEST CASE WITH ANODE MATERIAL - METC/ZNO-FeO/AIR BLOWN MCFC

VAPOR PRESSURE (ATM) DATA AT ELECTRODES (TERMINAL VOLTAGE : .66314+00 VOLTS)

TOTAL GAS PRESSURE 10.00 ATMOSPHERE

LENGTH (CM)	.0000	.1530+02	.3050+02	.4580+02	.6100+02	.7620+02	.9150+02	.1067+03	.1220+03
FUEL CELL EMF (V)	.1115+01	.1073+01	.1036+01	.9995+00	.9633+00	.9265+00	.8892+00	.8523+00	.8156+00

CATHODE :

TEMPERATURE DEG. K	866.00	879.93	893.77	907.70	921.55	935.39	949.32	963.16	977.09
CURRENT(AMP/CM2)	.3764+00	.3415+00	.3104+00	.2802+00	.2500+00	.2194+00	.1883+00	.1575+00	.1270+00
VELOCITY (CM/SEC)	.7010+02	.7002+02	.7001+02	.7007+02	.7020+02	.7042+02	.7072+02	.7112+02	.7161+02
H2O	.1488+01	.1514+01	.1538+01	.1561+01	.1581+01	.1600+01	.1617+01	.1631+01	.1644+01
CO2	.1214+01	.1120+01	.1032+01	.9488+00	.8728+00	.8038+00	.7422+00	.6892+00	.6446+00
N2	.6642+01	.6757+01	.6864+01	.6965+01	.7057+01	.7141+01	.7217+01	.7281+01	.7335+01
O2	.6561+00	.6097+00	.5665+00	.5258+00	.4865+00	.4546+00	.4243+00	.3983+00	.3764+00
TOTAL GAS MOLES	.4871+01	.4788+01	.4713+01	.4645+01	.4584+01	.4530+01	.4483+01	.4443+01	.4410+01
% O2 CONSUMED	.0000	.7065+01	.1366+02	.1986+02	.2554+02	.3071+02	.3532+02	.3929+02	.4262+02
% CO2 CONSUMED	.0000	.7775+01	.1503+02	.2185+02	.2811+02	.3379+02	.3887+02	.4323+02	.4691+02

ANODE :

TEMPERATURE DEG. K	923.00	929.78	936.51	943.29	950.02	956.76	963.53	970.27	977.04
CURRENT(AMP/CM2)	.3764+00	.3415+00	.3104+00	.2802+00	.2500+00	.2194+00	.1883+00	.1575+00	.1270+00
VELOCITY (CM/SEC)	.1463+02	.1559+02	.1648+02	.1731+02	.1808+02	.1878+02	.1941+02	.1998+02	.2047+02

O2	.6047-22	.1533-21	.3680-21	.9001-21	.2294-20	.6156-20	.1723-19	.4863-19	.1380-18
H2O	.1477+01	.1369+01	.1242+01	.1085+01	.9081+00	.7270+00	.5622+00	.4266+00	.3198+00
CO2	.1548+01	.1806+01	.2016+01	.2194+01	.2342+01	.2464+01	.2561+01	.2634+01	.2689+01
CO	.6641+00	.7366+00	.7584+00	.7306+00	.6629+00	.5705+00	.4712+00	.3795+00	.3004+00
CH4	.1456+01	.1971+01	.2410+01	.2797+01	.3138+01	.3438+01	.3700+01	.3918+01	.4097+01
NH3	.4771+00	.2927+00	.1629+00	.7825-01	.3177-01	.1091-01	.3286-02	.9246-03	.2490-03
N2	.3690-02	.3040-02	.2436-02	.1853-02	.1325-02	.8903-03	.5692-03	.3549-03	.2179-03
	.4363+01	.4124+01	.3930+01	.3768+01	.3635+01	.3524+01	.3433+01	.3360+01	.3301+01

CO	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
[H2O]/[H2]	.1045+01	.1719+01	.1624+01	.2021+01	.2579+01	.3389+01	.4555+01	.6175+01	.8406+01
[CO2]/[CO]	.2179+01	.2652+01	.3158+01	.3805+01	.4703+01	.5989+01	.7803+01	.1026+02	.1355+02
[SC2]/[H2S]	.5783-02	.1221-07	.2508-07	.5460-07	.1300-06	.3420-06	.9730-06	.2859-05	.8562-05
[S2]/[H2S]**2)	.3759-04	.3968-04	.4153-04	.4338-04	.4542-04	.4782-04	.5063-04	.5378-04	.5725-04
[CO2]/[H2S]	.1540-01	.1846-01	.2088-01	.2299-01	.2492-01	.2677-01	.2858-01	.3031-01	.3199-01

TOTAL GAS MOLES	.9538+00	.1009+01	.1059+01	.1105+01	.1145+01	.1181+01	.1213+01	.1239+01	.1261+01
% GRAPHITE IN MIX	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
% H2 CONSUMED	.0000	.7297+01	.1594+02	.2652+02	.3853+02	.5078+02	.6194+02	.7112+02	.7835+02
% CO CONSUMED	.0000	.1122+02	.1420+02	.1100+02	.1766+00	.1409+02	.2905+02	.4286+02	.5477+02
% CO+H2 CONSUMED	.0000	.1554+01	.6591+01	.1519+02	.2663+02	.3941+02	.5174+02	.6236+02	.7104+02
TOTAL CELL CURRENT (AMPS) :		.3715+04							

AVERAGE CURRENT DENSITY : .2498+00 AMPS/CM2

FUEL CELL PLATE DIMENSIONS (CM) : WIDTH	.1219+03	LENGTH	.1219+03	THICKNESS	.2540+00
CELL RESISTANCE : .10380-04 OHMS					
TOTAL ELECTRODE (2A+2C) IMPEDANCE : .12000+01 OHMS.CM2					

Table 67 (Continued)

HEAT OF C. (KCAL/MOLE)	-.2235+02	-.1869+02	-.1559+02	-.1286+02	-.1046+02	-.8366+01	-.6574+01	-.5107+01	-.3928+01
THE FOLLOWING EFFICIENCIES ARE IN FRACTIONAL UNITS									
VOLTAGE EFFICIENCY	.5948+00	.6180+00	.6402+00	.6635+00	.6884+00	.7157+00	.7458+00	.7781+00	.8131+00
THERMODYNAMIC EFFICIENCY	.8236+00	.7912+00	.7622+00	.7341+00	.7061+00	.6779+00	.6493+00	.6211+00	.5932+00
ELECTROCHEMICAL EFF.	.4899+00	.4889+00	.4880+00	.4870+00	.4861+00	.4852+00	.4842+00	.4833+00	.4823+00
HEATING VALUE EFFICIENCY	.3908+00	.4333+00	.4712+00	.4994+00	.5136+00	.5142+00	.5061+00	.4944+00	.4821+00
FUEL CELL EFFICIENCY	.1914+00	.2118+00	.2299+00	.2433+00	.2497+00	.2495+00	.2451+00	.2389+00	.2325+00

Table 68

VOLATILE CHLORINE COMPLEXES IN THE METC GRAVITATING-BED
FeO/ZnO AIR-BLOWN MCFC

Distance From Anode Inlet, cm	0.160 Amps/cm ² MCFC	0.250 Amps/cm ² MCFC
0	HCl, PbCl ₂ , ZnCl ₂	HCl, PbCl ₂ , ZnCl ₂
15.3	HCl, PbCl, ZnCl ₂	HCl, PbCl, ZnCl ₂
30.5	HCl, PbCl, ZnCl ₂	HCl, PbCl, ZnCl ₂
45.8	HCl, PbCl, ZnCl ₂	HCl, PbCl, ZnCl ₂
61.0	HCl, PbCl, ZnCl ₂	HCl, PbCl, ZnCl ₂
76.2	HCl, PbCl, ZnCl ₂	HCl, PbCl, ZnCl ₂
91.5	HCl, PbCl, ZnCl ₂	HCl, PbCl, ZnCl ₂
106.7	HCl, PbCl, ZnCl ₂	HCl, PbCl, ZnCl ₂
122.0	HCl, PbCl, ZnCl ₂	HCl, PbCl, ZnCl ₂

gravitating-bed cell. Although hydrogen is continuously being consumed in the initial 108.6 cm of the anode channel, the electrolytic reaction product CO₂ is simultaneously decomposing to yield an increase in the CO content of the fuel gas stream. The CO dissociation reaction is also apparent in the 0.250 A/cm² Westinghouse fluidized-bed cell (Table 70) but far less than in the 0.160 A/cm² cell. Utilization of 36.21 % H₂ or a net of 21.28% H₂ and CO in the fuel gas and 30.52% CO₂ and O₂ in the oxidant gases is projected in the 0.250 A/cm² Westinghouse fluidized-bed MCFC.

Figure 37 illustrates the nickel anode material sulfur tolerance for both Westinghouse cells. The general increase in sulfur throughout the 0.160 A/cm² cell is attributed to the relatively high hydrogen content of the fuel gases, which establishes a larger allowable concentration ratio and, therefore, a larger sulfur concentration than can be present to promote sulfidation of the anode material. Sulfur tolerances of 364 ppm in the 0.160 A/cm² cell and 334 ppm in the 0.250 A/cm² cell under these operating conditions are significantly higher than in the incoming 51.9 ppb sulfur-containing fuel gases. Under these

Table 69

FUEL AND OXIDANT GAS COMPOSITIONS AND UTILIZATIONS AS A FUNCTION
OF LOCATION IN THE WESTINGHOUSE 0.160 A/cm² FLUIDIZED-BED
DOLOMITE/ZnO OXYGEN-BLOWN MCFC

TEST CASE WITH ANODE MATERIAL - WESTINGHOUSE/DOLOMITE/ZnO/OXYGEN BLOWN MCFC									
VAPOR PRESSURE (ATM) DATA AT ELECTRODES (TERMINAL VOLTAGE : .92964+00 VOLTS)									
TOTAL GAS PRESSURE 10.00 ATMOSPHERE									
LENGTH (CM)	.0000	.1530+02	.1050+02	.4580+02	.6100+02	.7620+02	.9150+02	.1086+02	.1120+02
FUEL CELL EMF (V)	.1086+01	.1058+01	.1033+01	.1009+01	.9874+00	.9672+00	.9485+00	.9296+00	.9196+00
CATHODE :									
TEMPERATURE DEG. K	866.00	879.93	893.77	907.70	921.55	935.39	949.32	964.89	977.11
CURRENT (AMP/CM ²)	.3912+00	.3206+00	.2573+00	.1985+00	.1443+00	.9396-01	.4725-01	.0000	.0000
VELOCITY (CM/SEC)	.7010+02	.7003+02	.7014+02	.7044+02	.7092+02	.7156+02	.7237+02	.7346+02	.7439+02
H ₂ O	.1360+01	.1322+01	.1321+01	.1286+01	.1297+01	.1276+01	.1280+01	.1282+01	.1282+01
CO ₂	.1700+01	.1648+01	.1648+01	.1648+01	.1648+01	.1648+01	.1648+01	.1648+01	.1648+01
N ₂	.6300+01	.6408+01	.6498+01	.6571+01	.6627+01	.6666+01	.6690+01	.6699+01	.6699+01
O ₂	.7000+00	.6548+00	.6172+00	.5866+00	.5633+00	.5469+00	.5370+00	.5334+00	.5334+00
TOTAL GAS MOLES	.4570+01	.4493+01	.4431+01	.4381+01	.4344+01	.4319+01	.4304+01	.4218+01	.4298+01
X O ₂ CONSUMED	.0000	.6452+01	.1182+02	.1619+02	.1952+02	.2187+02	.2328+02	.2380+02	.2380+02
X CO ₂ CONSUMED	.0000	.5011+01	.9181+01	.1258+02	.1516+02	.1698+02	.1808+02	.1848+02	.1848+02
ANODE :									
TEMPERATURE DEG. K	923.00	929.78	936.51	943.29	950.02	956.76	963.53	971.11	977.04
CURRENT (AMP/CM ²)	.3912+00	.3206+00	.2573+00	.1985+00	.1443+00	.9396-01	.4725-01	.0000	.0000
VELOCITY (CM/SEC)	.1463+02	.1558+02	.1638+02	.1705+02	.1759+02	.1800+02	.1830+02	.1851+02	.1862+02
O ₂	.1264-21	.2400-21	.4335-21	.7590-21	.1283-20	.2101-20	.3335-20	.5346-20	.7591-20
H ₂	.2062+01	.1984+01	.1922+01	.1871+01	.1833+01	.1810+01	.1804+01	.1823+01	.1847+01
H ₂ O	.3124+01	.3275+01	.3387+01	.3473+01	.3537+01	.3584+01	.3615+01	.3633+01	.3642+01
CO	.9264+00	.1008+01	.1067+01	.1111+01	.1148+01	.1182+01	.1218+01	.1266+01	.1306+01
CO ₂	.2937+01	.3366+01	.3679+01	.3907+01	.4063+01	.4161+01	.4207+01	.4203+01	.4179+01
CH ₄	.8968+00	.6698+00	.5054+00	.3852+00	.2997+00	.2397+00	.1988+00	.1702+00	.1540+00
NH ₃	.5313-03	.4631-03	.4109-03	.3693-03	.3369-03	.3122-03	.2946-03	.2832-03	.2772-03
N ₂	.3326-01	.3147-01	.3017-01	.2921-01	.2854-01	.2809-01	.2783-01	.2774-01	.2774-01
C(C)	.0000	.0000	.0000	.0100	.0000	.0000	.0000	.0000	.0000
[H ₂ O]/[H ₂]	.1515+01	.1651+01	.1762+01	.1856+01	.1929+01	.1980+01	.2004+01	.1993+01	.1972+01
[CO ₂]/[CO]	.3150+01	.3275+01	.3387+01	.3473+01	.3537+01	.3584+01	.3615+01	.3633+01	.3642+01
[SO ₂]/[H ₂ S]	.8680-08	.1319-07	.1909-07	.2671-07	.3603-07	.4689-07	.5867-07	.7143-07	.8155-07
[CS ₂]/[CH ₂ S]**2)	.1852-04	.2062-04	.2246-04	.2417-04	.2579-04	.2735-04	.2888-04	.3054-04	.3183-04
[COS]/[H ₂ S]	.1539-01	.1739-01	.1897-01	.2029-01	.2137-01	.2227-01	.2302-01	.2366-01	.2409-01
TOTAL GAS MOLES	.8948+00	.9462+00	.9877+00	.1021+01	.1045+01	.1062+01	.1072+01	.1076+01	.1076+01
X GRAPHITE IN MIX	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
X H ₂ CONSUMED	.0000	.3778+01	.6784+01	.9237+01	.1108+02	.1222+02	.1249+02	.1159+02	.1041+02
X CO CONSUMED	.0000	.8803+01	.1512+02	.1995+02	.2319+02	.2756+02	.3148+02	.3662+02	.4101+02
X CO+H ₂ CONSUMED	.0000	.1227+00	.2717-02	.1893+00	.3318+00	.4135+00	.4139+01	.4335+01	.4553+01
TOTAL CELL CURRENT (AMPS) :		.2338+04							
AVERAGE CURRENT DENSITY :		.1572+00 AMPS/CM ²							
FUEL CELL PLATE DIMENSIONS (CM) : WIDTH			.1219+03	LENGTH	1219+03	HEIGHT	25.0+00		
CELL RESISTANCE :		.13450-04 OHMS							
TOTAL ELECTRODE (2A+2C) IMPEDANCE :		.40000+00 OHMS CM ²							

Table 69 (Continued)

HEAT OF C. (KCAL/MOLE)	-.3560+02	-.3135+02	-.2824+02	-.2595+02	-.2434+02	-.2328+02	-.2271+02	-.2260+02	-.2271+02
THE FOLLOWING EFFICIENCIES ARE IN FRACTIONAL UNITS									
VOLTAGE EFFICIENCY	.8559+00	.8787+00	.9003+00	.9213+00	.9415+00	.9611+00	.9801+00	.1000+01	.1000+01
THERMODYNAMIC EFFICIENCY	.8024+00	.7800+00	.7599+00	.7411+00	.7238+00	.7077+00	.6926+00	.6773+00	.6762+00
ELECTROCHEMICAL EFF.	.6867+00	.6854+00	.6841+00	.6828+00	.6815+00	.6801+00	.6788+00	.6773+00	.6762+00
HEATING VALUE EFFICIENCY	.3423+00	.3741+00	.4024+00	.4266+00	.4457+00	.4600+00	.4701+00	.4774+00	.4816+00
FUEL CELL EFFICIENCY	.2351+00	.2564+00	.2753+00	.2913+00	.3037+00	.3129+00	.3191+00	.3234+00	.3256+00

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+01								
H2S	.9849+00	.9830+00	.9815+00	.9802+00	.9792+00	.9783+00	.9776+00	.9770+00	.9766+00
SO2	.8530+00	.8519+00	.8510+00	.8502+00	.8496+00	.8492+00	.8488+00	.8485+00	.8483+00
CS2	.1785+00	.1780+00	.1777+00	.1771+00	.1764+00	.1758+00	.1754+00	.1750+00	.1748+00
COS	.1506+01	.1498+01	.1490+01	.1482+01	.1476+01	.1470+01	.1466+01	.1462+01	.1460+01
S2	.2117+10	.2101+10	.2092+10	.2080+10	.2068+10	.2058+10	.2050+10	.2042+10	.2036+10
H2/H2S	.2093+06	.2018+06	.1958+06	.1909+06	.1872+06	.1850+06	.1845+06	.1866+06	.1891+06

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+01								
H2S	.4925+01	.4915+01	.4907+01	.4901+01	.4896+01	.4892+01	.4888+01	.4885+01	.4883+01
SO2	.4263+07	.4263+07	.4263+07	.4263+07	.4263+07	.4263+07	.4263+07	.4263+07	.4263+07
CS2	.4464+08	.4450+08	.4437+08	.4424+08	.4414+08	.4404+08	.4395+08	.4386+08	.4378+08
COS	.7532+01	.7492+01	.7452+01	.7412+01	.7372+01	.7332+01	.7292+01	.7252+01	.7212+01
S2	.5291+09	.5254+09	.5217+09	.5180+09	.5143+09	.5106+09	.5069+09	.5032+09	.5000+09
H2/H2S	.4187+05	.4036+05	.3916+05	.3818+05	.3744+05	.3700+05	.3691+05	.3731+05	.3783+05

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+02								
H2S	.9849+01	.9830+01	.9815+01	.9802+01	.9792+01	.9783+01	.9776+01	.9770+01	.9766+01
SO2	.8530+00	.8519+00	.8510+00	.8502+00	.8496+00	.8492+00	.8488+00	.8485+00	.8483+00
CS2	.1785+07	.1780+07	.1777+07	.1771+07	.1764+07	.1758+07	.1754+07	.1750+07	.1748+07
COS	.1506+00	.1498+00	.1490+00	.1482+00	.1476+00	.1470+00	.1466+00	.1462+00	.1460+00
S2	.2117+08	.2101+08	.2092+08	.2080+08	.2068+08	.2058+08	.2050+08	.2042+08	.2036+08
H2/H2S	.2093+05	.2018+05	.1958+05	.1909+05	.1872+05	.1850+05	.1845+05	.1866+05	.1891+05

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+02								
H2S	.4925+02	.4915+02	.4907+02	.4901+02	.4896+02	.4892+02	.4888+02	.4885+02	.4883+02
SO2	.4263+06	.4263+06	.4263+06	.4263+06	.4263+06	.4263+06	.4263+06	.4263+06	.4263+06
CS2	.4464+06	.4450+06	.4437+06	.4424+06	.4414+06	.4404+06	.4395+06	.4386+06	.4378+06
COS	.7532+00	.7492+00	.7452+00	.7412+00	.7372+00	.7332+00	.7292+00	.7252+00	.7212+00
S2	.5291+07	.5254+07	.5217+07	.5180+07	.5143+07	.5106+07	.5069+07	.5032+07	.5000+07
H2/H2S	.4187+04	.4036+04	.3916+04	.3818+04	.3744+04	.3700+04	.3691+04	.3731+04	.3783+04

Table 69 (Continued)

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+03									
H ₂ S	.9549+02	.9839+02	.9812+02	.9802+02	.9726+02	.9783+02	.9776+02	.9778+02	.9766+02	
SO ₂	.8510-02	.1989+02	.2812+02	.2818+02	.2458+02	.2482+02	.2476+02	.2478+02	.2464+02	
CS ₂	.1785-05	.1980-05	.2150-05	.2308-05	.2458-05	.2402-05	.2743-05	.2897-05	.3017-05	
COS	.1506+01	.1698+01	.1850+01	.1976+01	.2080+01	.2166+01	.2236+01	.2297+01	.2338+01	
S ₂	.2117-06	.2701-06	.3392-06	.4214-06	.5155-06	.6200-06	.7305-06	.8520-06	.9893-06	
H ₂ /H ₂ S	.2093+04	.2018+04	.1958+04	.1909+04	.1872+04	.1850+04	.1845+04	.1866+04	.1891+04	

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1500+03									
H ₂ S	.1477+03	.1475+03	.1472+03	.1470+03	.1469+03	.1467+03	.1466+03	.1466+03	.1465+03	
SO ₂	.1279-05	.1946-05	.2811-05	.3727-05	.4293-05	.6882-05	.8604-05	.1047-04	.1195-04	
CS ₂	.4017-05	.4455-05	.4818-05	.5194-05	.5530-05	.5854-05	.6172-05	.6518-05	.6788-05	
COS	.2259+01	.2547+01	.2776+01	.2944+01	.3119+01	.3248+01	.3354+01	.3446+01	.3507+01	
S ₂	.4762-06	.6078-06	.7633-06	.9481-06	.1160-05	.1355-05	.1644-05	.1917-05	.2136-05	
H ₂ /H ₂ S	.1396+04	.1345+04	.1305+04	.1273+04	.1248+04	.1233+04	.1230+04	.1244+04	.1261+04	

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.2000+03									
H ₂ S	.1970+03	.1966+03	.1963+03	.1960+03	.1958+03	.1957+03	.1955+03	.1954+03	.1953+03	
SO ₂	.1706-05	.2594-05	.3748-05	.5238-05	.7057-05	.9175-05	.1147-04	.1396-04	.1593-04	
CS ₂	.7142-05	.7920-05	.8601-05	.9233-05	.9830-05	.1041-04	.1097-04	.1159-04	.1207-04	
COS	.3013+01	.3397+01	.3701+01	.3982+01	.4159+01	.4331+01	.4472+01	.4594+01	.4675+01	
S ₂	.8466-06	.1081-05	.1357-05	.1686-05	.2062-05	.2480-05	.2922-05	.3408-05	.3797-05	
H ₂ /H ₂ S	.1047+04	.1009+04	.9791+03	.9545+03	.9361+03	.9250+03	.9227+03	.9328+03	.9457+03	

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.2500+03									
H ₂ S	.2462+03	.2455+03	.2454+03	.2451+03	.2448+03	.2446+03	.2444+03	.2443+03	.2441+03	
SO ₂	.2132-05	.3243-05	.4685-05	.6544-05	.8821-05	.1147-04	.1434-04	.1745-04	.1991-04	
CS ₂	.1116-04	.1238-04	.1344-04	.1443-04	.1536-04	.1626-04	.1714-04	.1811-04	.1885-04	
COS	.3766+01	.4246+01	.4626+01	.4940+01	.5199+01	.5414+01	.5590+01	.5743+01	.5844+01	
S ₂	.1323-05	.1688-05	.2120-05	.2634-05	.3222-05	.3875-05	.4566-05	.5325-05	.5933-05	
H ₂ /H ₂ S	.8373+03	.8073+03	.7832+03	.7636+03	.7489+03	.7400+03	.7382+03	.7462+03	.7565+03	

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+03									
H ₂ S	.4925+03	.4915+03	.4907+03	.4901+03	.4896+03	.4892+03	.4888+03	.4885+03	.4883+03	
SO ₂	.4265-05	.6485-05	.9370-05	.1309-04	.1764-04	.2294-04	.2868-04	.3489-04	.3982-04	
CS ₂	.4464-04	.4950-04	.5376-04	.5771-04	.6144-04	.6504-04	.6858-04	.7242-04	.7542-04	
COS	.7532+01	.8492+01	.9252+01	.9680+01	.1040+02	.1083+02	.1118+02	.1149+02	.1169+02	
S ₂	.5292-05	.6754-05	.8481-05	.1053-04	.1289-04	.1550-04	.1826-04	.2130-04	.2373-04	
H ₂ /H ₂ S	.4187+03	.4036+03	.3916+03	.3818+03	.3744+03	.3700+03	.3691+03	.3731+03	.3783+03	

Table 70

FUEL AND OXIDANT GAS COMPOSITIONS AND UTILIZATIONS AS A FUNCTION
OF LOCATION IN THE WESTINGHOUSE 0.250 A/cm² FLUIDIZED-BED
DOLOMITE/ZnO OXYGEN-BLOWN MCFC

TEST CASE WITH ANODE MATERIAL - WESTINGHOUSE/DOLOMITE/ZnO/OXYGEN BLOWN MCFC

VAPOR PRESSURE (ATM) DATA AT ELECTRODES (TERMINAL VOLTAGE : .66256+00 VOLTS)

TOTAL GAS PRESSURE 10.00 ATMOSPHERE

LENGTH (CM)	.0000	.1530+02	.3050+02	.4560+02	.6100+02	.7620+02	.9150+02	.1067+03	.1220+03
FUEL CELL EMF (V)	.1066+01	.1059+01	.1033+01	.1008+01	.9824+00	.9571+00	.9315+00	.9058+00	.8799+00

CATHODE :

TEMPERATURE DEG. K	866.00	879.93	893.77	907.70	921.55	935.39	949.32	963.16	977.09
CURRENT (AMP/CM ²)	.3362+00	.3136+00	.2921+00	.2708+00	.2498+00	.2287+00	.2074+00	.1860+00	.1644+00
VELOCITY (CM/SEC)	.7010+02	.7013+02	.7020+02	.7031+02	.7047+02	.7067+02	.7093+02	.7124+02	.7161+02

H ₂ O	.1308+01	.1320+01	.1348+01	.1359+01	.1376+01	.1393+01	.1408+01	.1423+01	.1436+01
CO ₂	.6300+01	.6399+01	.6493+01	.6584+01	.6669+01	.6750+01	.6825+01	.6895+01	.6958+01
N ₂	.7000+00	.6588+00	.6194+00	.5815+00	.5457+00	.5120+00	.4804+00	.4514+00	.4249+00

TOTAL GAS MOLES	.4570+01	.4499+01	.4434+01	.4373+01	.4317+01	.4265+01	.4218+01	.4176+01	.4138+01
% O ₂ CONSUMED	.0000	.5892+01	.1152+02	.1693+02	.2204+02	.2665+02	.3137+02	.3551+02	.3929+02
% CO ₂ CONSUMED	.0000	.4576+01	.8944+01	.1315+02	.1712+02	.2086+02	.2437+02	.2758+02	.3052+02

ANODE :

TEMPERATURE DEG. K	923.00	929.78	936.51	943.29	950.02	956.76	963.53	970.27	977.04
CURRENT (AMP/CM ²)	.3362+00	.3136+00	.2921+00	.2708+00	.2498+00	.2287+00	.2074+00	.1860+00	.1644+00
VELOCITY (CM/SEC)	.1463+02	.1551+02	.1635+02	.1714+02	.1790+02	.1861+02	.1928+02	.1990+02	.2047+02

O ₂	.1264-21	.2351-21	.4267-21	.7803-21	.1418-20	.2504-20	.4814-20	.6984-20	.1492-19
H ₂	.2062+01	.1997+01	.1929+01	.1853+01	.1776+01	.1686+01	.1584+01	.1473+01	.1351+01
H ₂ O	.3124+01	.3262+01	.3381+01	.3484+01	.3580+01	.3665+01	.3742+01	.3811+01	.3871+01
CO	.9264+00	.1007+01	.1067+01	.1108+01	.1129+01	.1140+01	.1153+01	.1168+01	.1183+01
CO ₂	.2937+01	.3328+01	.3660+01	.3948+01	.4199+01	.4420+01	.4619+01	.4795+01	.4953+01
CH ₄	.8968+00	.6851+00	.5123+00	.3712+00	.2601+00	.1749+00	.1122+00	.6941-01	.4151-01
NH ₃	.5313-03	.4668-03	.4137-03	.3629-03	.3157-03	.2713-03	.2297-03	.1922-03	.1590-03
N ₂	.3326-01	.3162-01	.3024-01	.2906-01	.2805-01	.2719-01	.2645-01	.2582-01	.2528-01

C (C)	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
[H ₂ O]/[H ₂]	.1515+01	.1634+01	.1752+01	.1882+01	.2028+01	.2200+01	.2408+01	.2654+01	.2943+01
[CO ₂]/[CO]	.3150+01	.3284+01	.3406+01	.3518+01	.3628+01	.3736+01	.3842+01	.3946+01	.4048+01
[CO ₂]/[H ₂ S]	.8660-06	.1264-07	.1881-07	.2773-07	.4133-07	.6268-07	.9831-07	.1569-06	.2553-06
[CO ₂]/[H ₂ S]**2)	.1852-04	.2055-04	.2243-04	.2424-04	.2601-04	.2778-04	.2958-04	.3144-04	.3338-04
[CO ₂]/[H ₂ S]	.1539-01	.1726-01	.1891-01	.2042-01	.2182-01	.2313-01	.2441-01	.2564-01	.2685-01

TOTAL GAS MOLES	.8948+00	.9418+00	.9853+00	.1026+01	.1063+01	.1099+01	.1129+01	.1158+01	.1183+01
% GRAPHITE IN MIX	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
% H ₂ CONSUMED	.0000	.3149+01	.6432+01	.1013+02	.1436+02	.1919+02	.2461+02	.3035+02	.3621+02
% CO CONSUMED	.0000	-.8714+01	-.1518+02	-.1957+02	-.2181+02	-.2197+02	-.2013+02	-.1663+02	-.1194+02
% CO+H ₂ CONSUMED	.0000	-.5291+00	-.2687+00	.9265+00	.3145+01	.6430+01	.1074+02	.1579+02	.2128+02
TOTAL CELL CURRENT (AMPS) :		.3715+04							

AVERAGE CURRENT DENSITY : .2498+00 AMPS/CM²

FUEL CELL PLATE DIMENSIONS (CM) : WIDTH .1219+03 LENGTH .1219+03 THICKNESS .2540+00
CELL RESISTANCE : .40350-04 OHMS
TOTAL ELECTRODE (2A+2C) IMPEDANCE : .12000+01 OHMS/CM²

Table 70 (Continued)

HEAT OF C. (KCAL/MOLE)	-.3560+02	-.3172+02	-.2842+02	-.2555+02	-.2305+02	-.2084+02	-.1867+02	-.1713+02	-.1559+02
THE FOLLOWING EFFICIENCIES ARE IN FRACTIONAL UNITS									
VOLTAGE EFFICIENCY	.6284+00	.6445+00	.6606+00	.6774+00	.6948+00	.7131+00	.7328+00	.7535+00	.7757+00
THERMODYNAMIC EFFICIENCY	.8024+00	.7808+00	.7603+00	.7401+00	.7202+00	.7003+00	.6802+00	.6601+00	.6400+00
ELECTROCHEMICAL EFF.	.5042+00	.5032+00	.5023+00	.5013+00	.5003+00	.4994+00	.4984+00	.4974+00	.4965+00
HEATING VALUE EFFICIENCY	.3423+00	.3722+00	.4014+00	.4290+00	.4532+00	.4731+00	.4876+00	.4962+00	.4995+00
FUEL CELL EFFICIENCY	.1726+00	.1873+00	.2016+00	.2151+00	.2268+00	.2362+00	.2430+00	.2468+00	.2480+00

Westinghouse Fluidized-Bed Dolomite/ZnO Oxygen-Blown MCFC

Fuel Gas Velocity: 14.63 cm/sec

Oxidant Gas Velocity: 70.10 cm/sec

Anode Inlet Temperature: 923K

Anode Outlet Temperature: 977K

Cathode Inlet Temperature: 866K

Cathode Outlet Temperature: 977K

Cell Resistance: 0.1345-4 ohms (0.4035-4 ohms)

Total Electrode Impedance: 0.4 ohms·cm² (1.200 ohms·cm²)Average Current Density: 0.160 Amps/cm² (0.250 Amps/cm²)

Terminal Voltage: 0.9296 Volts (0.6826 Volts)

Figure 37 -- Nickel Anode Sulfur Tolerance in the Westinghouse Fluidized-Bed Dolomite/ZnO Oxygen-Blown MCFC

conditions, therefore, the anode material is not projected to experience sulfidation when Westinghouse fluidized-bed fuel gas is used.

Trace contaminants of Pb and As in the chlorine-laden fuel gas are projected to exist as PbCl and AsCl in equilibrium with HCl (Table 71). The formation of trace contaminant solids is unlikely when volatile chlorine is present in the anode channel.

Selextol desulfurization of the Westinghouse fluidized-bed fuel gas followed by ZnO treatment is projected to achieve residual sulfur concentrations of 51.9 ppb within the fuel gas. The principal

Table 71

Dwg. 7756A79

VOLATILE CHLORINE COMPLEXES IN THE WESTINGHOUSE FLUIDIZED-BED
DOLOMITE/ZnO OXYGEN-BLOWN MCFC

Distance From Anode Inlet, cm	0.160 Amps/cm ² MCFC	0.250 Amps/cm ² MCFC
0	HCl, PbCl, AsCl	HCl, PbCl, AsCl
15.3	HCl, PbCl, AsCl	HCl, PbCl, AsCl
30.5	HCl, PbCl, AsCl	HCl, PbCl, AsCl
45.8	HCl, PbCl, AsCl	HCl, PbCl, AsCl
61.0	HCl, PbCl, AsCl	HCl, PbCl, AsCl
76.2	HCl, PbCl, AsCl	HCl, PbCl, AsCl
91.5	HCl, PbCl, AsCl	HCl, PbCl, AsCl
106.7	HCl, PbCl, AsCl	HCl, PbCl, AsCl
122.0	HCl, PbCl, AsCl	HCl, PbCl, AsCl

differences between the Selexol/ZnO desulfurized fuel gas and the dolomite/ZnO treated gas are that both Pb and As are reduced to concentrations of 104 ppb, and that NH_3 and HCl are virtually nonexistent in the incoming Selexol purified fuel gas stream. Although the fuel gas utilizations for the 0.160 and 0.250 A/cm^2 MCFC (Tables 72 and 73) are similar to the dolomite desulfurized fuel gas utilization and the anode sulfur tolerances are identical, the trace constituent phases are modified in the absence of chlorine. As shown in Table 74, the Selexol desulfurized fuel gases contain As as volatile arsenic hydride (AsH_3) and Pb as gaseous Pb when less than 200 ppm sulfur are present at the anode inlet and as PbS in higher fuel gas sulfur concentrations. As the gas progresses along the anode channel, AsH_3 exists predominantly as the stable arsenic phase, while the transition of gaseous Pb to PbS occurs when the fuel gas contains 250 ppm sulfur.

Under the cell parameters defined by the air-blown Rockwell molten carbonate and METC gravitating-bed fuel gas MCFC, utilization within the Westinghouse fluidized-bed MCFC does not exceed 25% of the initial fuel gas constituents. Reducing the velocity of the fuel gas passing through the anode channel from 14.63 to 8.63 cm/s is shown in Figure 38 to increase fuel gas utilization in the Westinghouse oxygen-blown cell to 76.8%. While fuel gas utilization is increased, sulfur tolerances for the system become more stringent. In the MCFC operating with a fuel gas velocity of 14.63 cm/s, 335 ppm total sulfur can be present within the anode channel prior to sulfidation, as compared with 91 ppm total sulfur for a cell operating with a fuel gas velocity of 8.63 cm/s. No variation is apparent in the trace constituent volatile chloride composition as the fuel gas velocity in the Westinghouse cell is reduced.

Trace concentrations of 3.1 ppm carbon in the dolomite/ZnO treated or 18.7 ppm carbon remaining in the Selexol/ZnO treated, humidified, Westinghouse fluidized-bed fuel gases are projected to remain as solid carbon particles throughout the anode channel.

Table 72

FUEL AND OXIDANT GAS COMPOSITIONS AND UTILIZATIONS AS A FUNCTION
OF LOCATION IN THE WESTINGHOUSE 0.160 A/cm² FLUIDIZED-BED
SELEXOL/ZnO OXYGEN-BLOWN MCFC

TEST CASE WITH ANODE MATERIAL - WESTINGHOUSE/SELEXOL/ZNO/OXYGEN BLOWN MCFC									
VAPOR PRESSURE (ATM) DATA AT ELECTRODES (TERMINAL VOLTAGE : .92964+00 VOLTS)									
TOTAL GAS PRESSURE 10.00 ATMOSPHERE									
LENGTH (CM)	.0000	.1530+02	.3050+02	.4580+02	.6100+02	.7620+02	.9150+02	.1086+03	.1220+03
FUEL CELL EMF (V)	.1086+01	.1058+01	.1033+01	.1009+01	.9874+00	.9672+00	.9485+00	.9296+00	.9296+00
CATHODE :									
TEMPERATURE DEG. K	866.00	879.93	893.77	907.70	921.55	935.39	949.32	964.89	977.09
CURRENT (AMP/CM2)	.3912+00	.3206+00	.2573+00	.1985+00	.1443+00	.9396-01	.4725-01	.0000	.0000
VELOCITY (CM/SEC)	.7010+02	.7003+02	.7014+02	.7044+02	.7092+02	.7156+02	.7237+02	.7346+02	.7439+02
H2O	.1300+01	.1322+01	.1341+01	.1356+01	.1367+01	.1376+01	.1380+01	.1382+01	.1382+01
CO2	.1700+01	.1615+01	.1544+01	.1426+01	.1422+01	.1411+01	.1393+01	.1386+01	.1386+01
N2	.6300+01	.6408+01	.6498+01	.6571+01	.6627+01	.6666+01	.6690+01	.6699+01	.6699+01
O2	.7000+00	.6548+00	.6173+00	.5866+00	.5633+00	.5469+00	.5370+00	.5334+00	.5334+00
TOTAL GAS MOLES	.4570+01	.4493+01	.4430+01	.4381+01	.4344+01	.4319+01	.4303+01	.4298+01	.4298+01
% O2 CONSUMED	.0000	.6452+01	.1182+02	.1619+02	.1952+02	.2187+02	.2328+02	.2380+02	.2380+02
% CO2 CONSUMED	.0000	.5011+01	.9181+01	.1258+02	.1516+02	.1698+02	.1808+02	.1848+02	.1848+02
ANODE :									
TEMPERATURE DEG. K	923.00	929.78	936.51	943.29	950.02	956.76	963.53	971.11	977.04
CURRENT (AMP/CM2)	.3912+00	.3206+00	.2573+00	.1985+00	.1443+00	.9396-01	.4725-01	.0000	.0000
VELOCITY (CM/SEC)	.1463+02	.1558+02	.1638+02	.1705+02	.1759+02	.1800+02	.1830+02	.1851+02	.1862+02
O2	.1264-21	.2400-21	.4335-21	.7590-21	.1283-20	.2101-20	.3334-20	.5345-20	.7591-20
H2	.7062+01	.1984+01	.1922+01	.1871+01	.1833+01	.1810+01	.1804+01	.1823+01	.1847+01
H2O	.3124+01	.3275+01	.3387+01	.3473+01	.3537+01	.3584+01	.3615+01	.3634+01	.3642+01
CO	.9265+00	.1008+01	.1067+01	.1111+01	.1148+01	.1182+01	.1218+01	.1266+01	.1306+01
CO2	.2937+01	.3366+01	.3679+01	.3907+01	.4063+01	.4161+01	.4207+01	.4203+01	.4179+01
CH4	.8969+00	.6699+00	.5055+00	.3853+00	.2998+00	.2398+00	.1989+00	.1703+00	.1540+00
NH3	.5313-05	.4630-05	.4107-05	.3691-05	.3366-05	.3119-05	.2943-05	.2828-05	.2768-05
N2	.3326-01	.3146-01	.3014-01	.2916-01	.2848-01	.2802-01	.2776-01	.2766-01	.2766-01
CCC	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
[H2O]/[H2]	.1515+01	.1651+01	.1762+01	.1856+01	.1929+01	.1980+01	.2004+01	.1993+01	.1971+01
[CO2]/[CO]	.3150+01	.3318+01	.3428+01	.3528+01	.3518+01	.3499+01	.3432+01	.3300+01	.3179+01
[SO2]/[H2S]	.8660-08	.1719-07	.1909-07	.2670-07	.3603-07	.4689-07	.5866-07	.7141-07	.8154-07
[CS2]/[H2S]**2)	.1852-04	.2062-04	.2246-04	.2417-04	.2579-04	.2735-04	.2888-04	.3054-04	.3183-04
[COS]/[H2S]	.1539-01	.1739-01	.1897-01	.2029-01	.2137-01	.2227-01	.2302-01	.2366-01	.2409-01
TOTAL GAS MOLES	.8948+00	.9462+00	.9876+00	.1021+01	.1045+01	.1062+01	.1072+01	.1076+01	.1076+01
% GRAPHITE IN MIX	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
% H2 CONSUMED	.0000	.3777+01	.6784+01	.9237+01	.1108+02	.1222+02	.1249+02	.1159+02	.1041+02
% CO CONSUMED	.0000	.8803+01	.1512+02	.1995+02	.2389+02	.2756+02	.3148+02	.3663+02	.4102+02
% CO+H2 CONSUMED	.0000	.1230+00	.7883-02	.1880+00	.2381+00	.1155+00	.1141+01	.3357+01	.5534+01
TOTAL CELL CURRENT (AMPS) :	.2338+04								
AVERAGE CURRENT DENSITY :	.1572+00 AMPS/CM2								
FUEL CELL PLATE DIMENSIONS (CM) : WIDTH	.1219+03			LENGTH	.1219+03		THICKNESS	.2540+00	
CELL RESISTANCE :	.13450-04 OHMS								
TOTAL ELECTRODE (2A+2C) IMPEDANCE :	.40000+00 OHMS.CM2								

Table 72 (Continued)

HEAT OF C. (KCAL/MOLE)	-.3561+02	-.3136+02	-.2824+02	-.2595+02	-.2434+02	-.2328+02	-.2271+02	-.2260+02	-.2271+02
THE FOLLOWING EFFICIENCIES ARE IN FRACTIONAL UNITS									
VOLTAGE EFFICIENCY	.8559+00	.8787+00	.9003+00	.9213+00	.9415+00	.9611+00	.9801+00	.1000+01	.1000+01
THERMODYNAMIC EFFICIENCY	.8024+00	.7800+00	.7599+00	.7411+00	.7238+00	.7077+00	.6926+00	.6773+00	.6762+00
ELECTROCHEMICAL EFF.	.6867+00	.6854+00	.6841+00	.6828+00	.6815+00	.6801+00	.6788+00	.6773+00	.6762+00
HEATING VALUE EFFICIENCY	.3423+00	.3741+00	.4024+00	.4266+00	.4457+00	.4600+00	.4701+00	.4774+00	.4816+00
FUEL CELL EFFICIENCY	.2351+00	.2564+00	.2753+00	.2912+00	.3037+00	.3128+00	.3191+00	.3234+00	.3256+00

Table 73

FUEL AND OXIDANT GAS COMPOSITIONS AND UTILIZATIONS AS A FUNCTION
OF LOCATION IN THE WESTINGHOUSE 0.250 A/cm² FLUIDIZED-BED
SELEXOL/ZnO OXYGEN-BLOWN MCFC

TEST CASE WITH ANODE MATERIAL - WESTINGHOUSE/SELEXOL/ZnO/OXYGEN BLOWN MCFC										
VAPOR PRESSURE (ATM) DATA AT ELECTRODES (TERMINAL VOLTAGE : .68256+00 VOLTS)										
TOTAL GAS PRESSURE 10.00 ATMOSPHERE										
LENGTH (CM)	.0000	.1530+02	.3050+02	.4510+02	.6110+02	.7620+02	.9150+02	.1067+03	.1220+03	
FUEL CELL EMF (V)	.1086+01	.1059+01	.1033+01	.1018+01	.9814+00	.9572+00	.9315+00	.9018+00	.8799+00	
CATHODE										
TEMPERATURE DEG. K	866.00	879.93	893.77	907.70	921.55	935.39	949.32	963.16	977.09	
CURRENT (AMP/CM ²)	.3362+00	.3136+00	.2921+00	.2708+00	.2498+00	.2287+00	.2074+00	.1860+00	.1644+00	
VELOCITY (CM/SEC)	.7010+02	.7013+02	.7020+02	.7031+02	.7047+02	.7067+02	.7093+02	.7124+02	.7161+02	
H ₂	.1300+01	.1320+01	.1350+01	.1359+01	.1376+01	.1393+01	.1408+01	.1423+01	.1436+01	
CO ₂	.1700+01	.1622+01	.1548+01	.1476+01	.1406+01	.1345+01	.1288+01	.1231+01	.1181+01	
H ₂	.6300+01	.6399+01	.6493+01	.6584+01	.6669+01	.6750+01	.6825+01	.6895+01	.6958+01	
O ₂	.7000+00	.6588+00	.6194+00	.5815+00	.5457+00	.5120+00	.4804+00	.4514+00	.4249+00	
TOTAL GAS MOLES	.4570+01	.4499+01	.4434+01	.4373+01	.4317+01	.4265+01	.4218+01	.4175+01	.4137+01	
% O ₂ CONSUMED	.0000	.5892+01	.1152+02	.1693+02	.2204+02	.2685+02	.3137+02	.3551+02	.3929+02	
% CO ₂ CONSUMED	.0000	.4576+01	.8944+01	.1315+02	.1712+02	.2086+02	.2437+02	.2758+02	.3052+02	
ANODE :										
TEMPERATURE DEG. K	923.00	929.76	936.51	943.29	950.02	956.76	963.53	970.27	977.04	
CURRENT (AMP/CM ²)	.3362+00	.3136+00	.2921+00	.2708+00	.2498+00	.2287+00	.2074+00	.1860+00	.1644+00	
VELOCITY (CM/SEC)	.1463+02	.1551+02	.1635+02	.1714+02	.1790+02	.1861+02	.1928+02	.1990+02	.2047+02	
O ₂	.1264-21	.1251-21	.1286-21	.1301-21	.1317-20	.1334-20	.1351-20	.1368-20	.1385-19	
H ₂	.2082+01	.1997+01	.1929+01	.1851+01	.1766+01	.1686+01	.1613+01	.1538+01	.1461+01	
CO	.3124+01	.3262+01	.3381+01	.3486+01	.3580+01	.3665+01	.3743+01	.3811+01	.3871+01	
CO ₂	.9265+00	.1007+01	.1067+01	.1108+01	.1129+01	.1130+01	.1113+01	.1081+01	.1037+01	
CH ₄	.2937+01	.3328+01	.3660+01	.3949+01	.4199+01	.4420+01	.4619+01	.4795+01	.4953+01	
NH ₃	.8969+00	.6852+00	.5124+00	.3713+00	.2601+00	.1749+00	.1123+00	.6943-01	.4152-01	
N ₂	.5313-05	.4687-05	.4135-05	.3626-05	.3154-05	.2710-05	.2293-05	.1918-05	.1586-05	
	.3326-01	.3160-01	.3021-01	.2901-01	.2799-01	.2711-01	.2636-01	.2571-01	.2516-01	
C(C)	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	
[H ₂]/[H ₂]	.1515+01	.1634+01	.1752+01	.1882+01	.2028+01	.2200+01	.2407+01	.2634+01	.2942+01	
[CO ₂]/[CO]	.3150+01	.3284+01	.3408+01	.3541+01	.3677+01	.3808+01	.3934+01	.4056+01	.4173+01	
[O ₂]/[H ₂ S]	.8660-08	.1284-07	.1881-07	.2775-07	.4132-07	.6286-07	.9829-07	.1568-06	.2532-06	
[CS ₂]/[H ₂ S]*2)	.1852-04	.2055-04	.2243-04	.2424-04	.2601-04	.2778-04	.2958-04	.3144-04	.3328-04	
[COS]/[H ₂ S]	.1539-01	.1726-01	.1891-01	.2042-01	.2182-01	.2313-01	.2441-01	.2564-01	.2685-01	
TOTAL GAS MOLES	.8948+00	.9418+00	.9853+00	.1026+01	.1063+01	.1098+01	.1129+01	.1158+01	.1183+01	
% GRAPHITE IN MIX	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	
% H ₂ CONSUMED	.0000	.3149+01	.6431+01	.1013+02	.1436+02	.1919+02	.2460+02	.3035+02	.3621+02	
% CO CONSUMED	.0000	.8715+01	.1518+02	.1957+02	.2182+02	.2197+02	.2013+02	.1664+02	.1195+02	
% CO+H ₂ CONSUMED	.0000	.5293+00	.2694+00	.9252+00	.3143+01	.6427+01	.1073+02	.1578+02	.2128+02	
TOTAL CELL CURRENT (AMPS) :		.3715+04								
AVERAGE CURRENT DENSITY :		.1498+00	AMPS/CM ²							
FUEL CELL PLATE DIMENSIONS (CM) : WIDTH			.1219+03	LENGTH	1219+03	HICKNESS	2540+00			
CELL RESISTANCE :		.4030-04	OHMS							
TOTAL ELECTRODE (2A+2C) IMPEDANCE :			.12000+01	OHMS CM ²						

Table 73 (Continued)

HEAT OF C. (KCAL/MOLE)	-.3561+02	-.3172+02	-.2842+02	-.2555+02	-.2305+02	-.2084+02	-.1887+02	-.1713+02	-.1559+02
THE FOLLOWING EFFICIENCIES ARE IN FRACTIONAL UNITS									
VOLTAGE EFFICIENCY	.6284+00	.6445+00	.6606+00	.6774+00	.6948+00	.7131+00	.7328+00	.7535+00	.7757+00
THERMODYNAMIC EFFICIENCY	.8024+00	.7803+00	.7603+00	.7401+00	.7202+00	.7003+00	.6802+00	.6601+00	.6400+00
ELECTROCHEMICAL EFF.	.5042+00	.5032+00	.5023+00	.5013+00	.5003+00	.4994+00	.4984+00	.4974+00	.4965+00
HEATING VALUE EFFICIENCY	.3423+00	.3722+00	.4014+00	.4290+00	.4532+00	.4730+00	.4876+00	.4962+00	.4995+00
FUEL CELL EFFICIENCY	.1726+00	.1873+00	.2016+00	.2150+00	.2268+00	.2362+00	.2430+00	.2468+00	.2480+00

Table 74

VOLATILE TRACE COMPLEXES IN THE WESTINGHOUSE FLUIDIZED-BED
SELEXOL/ZnO OXYGEN-BLOWN MCFC

Distance From Anode Inlet, cm	0.160 Amps/cm ² or 0.250 Amps/cm ² MCFC								
	Total Sulfur Concentration, ppm								
	1	5	10	50	100	150	200	250	500
0				AsH ₃					
			Pb					PbS	
15.3				AsH ₃					
			Pb						PbS
30.5				AsH ₃					
			Pb						PbS
45.8				AsH ₃					
			Pb						PbS
61.0				AsH ₃					
			Pb						PbS
76.2				AsH ₃					
			Pb						PbS
91.5				AsH ₃					
			Pb						PbS
106.7				AsH ₃					
			Pb						PbS
122.0				AsH ₃					
			Pb						PbS

Polyethylene glycol in ether, present at concentrations of 103.9 ppb from the Selexol desulfurization process, immediately volatilizes in the 923 K (1202°F) MCFC reaction temperatures. Provided that solid carbon particles are deposited along the anode surface, utilization of the fuel gas hydrogen and CO may be reduced at the gas/electrolyte interface.

3.3.4.4 Evaluation of the Texaco Entrained Oxygen-Blown Gas to MCFC

The Texaco entrained fuel gas is desulfurized prior to entering the anode channel, using a Benfield/ZnO combination to reduce the sulfur concentration to levels of 56.3 ppb. With the same operating MCFC conditions as those described for the Rockwell molten carbonate and METC gravitating-bed cells, performance of the Texaco entrained fuel gas is similar to that projected with the Westinghouse fluidized-bed fuel gas. For the 0.160 A/cm² cell, a maximum fuel gas utilization of 11.53%

Westinghouse Fluidized-Bed Dolomite/ZnO Oxygen-Blown MCFC

Anode Inlet Temperature: 923K

Anode Outlet Temperature: 977K

Cathode Inlet Temperature: 866K

Cathode Outlet Temperature: 977K

Cell Resistance: 0.4035-4 ohms

Total Electrode Impedance: 1.2000 ohms-cm²

Oxidant Gas Velocity: 70.10 cm/sec

Sulfur Tolerance: 1-500 ppm

Fuel Gas Velocity, cm/sec	Utilization			Location From Anode Inlet, cm	Average Current Density, Amps/cm ²	Estimated Terminal Voltage, Volts	Projected Trace Constituent Phases as a Function of Distance From Anode Inlet, cm								
	Fuel Gas % (H ₂ + CO)	Oxidant Gas % CO ₂	Oxidant Gas % O ₂				0	15.30	30.50	45.80	61.00	76.20	91.50	106.70	122.20
14.63	21.28	30.52	39.29	122.0	0.2498	0.6826									
12.63	33.98	30.51	39.39	122.0	0.2498	0.6770									
10.63	51.81	30.51	39.29	122.0	0.2498	0.6685									
8.63	76.81	30.51	39.29	122.0	0.2498	0.6533

Figure 38 -- Nickel Anode Sulfur Tolerance in the Westinghouse Fluidized-Bed Dolomite/ZnO Oxygen-Blown MCFC as a Function of Fuel Gas Velocity

occurs at 91.5 cm from the anode inlet (Table 75). Once again, the fuel gas CO reacts with the electrolyte, forming CO_2 , which immediately dissociates, reforming CO. In the 0.250 A/cm^2 cell a maximum H_2 and CO utilization of 19.57% is achieved through reactions that have consumed 34.73% of the fuel gas hydrogen but in which CO has been replenished through the CO_2 dissociation reaction (Table 76).

The stability of the anode material and the potential formation of trace constituent solids or condensed phases are shown in Figure 39. A minimum sulfur tolerance of 362 ppm sulfur is permitted within the 0.160 A/cm^2 cell prior to sulfidation of the material. This level exceeds the 56.3 ppm sulfur remaining in the fuel gas after desulfurization with the Benfield/ ZnO scrub. For this system the region of greatest concern for sulfidation is at the anode inlet. In the 0.250 A/cm^2 cell sulfur tolerances are reduced to 341 ppm, with possible damage most likely at the anode outlet. Once again this tolerance exceeds the incoming sulfur content of the Texaco entrained fuel gas.

Fuel gases generated in the Texaco entrained gasifier under oxygen-blown conditions can be more efficiently utilized at the anode by decreasing the fuel gas velocity through the anode channel from 14.63 to 8.63 cm/s. Under these conditions 74.8% of the H_2 and CO present in the incoming fuel gas stream is consumed, while permissible sulfur tolerances decrease to 99.4 ppm.

Trace constituents of Pb, As, and K in the Texaco entrained fuel gas are projected to form both volatile and condensed phases along the anode channel. Initially, Pb and K exist as solid Pb and K_2CO_3 , while As exists predominantly as volatile As_4 throughout the anode channel. Between 30 and 61 cm from the anode inlet solid Pb volatilizes, forming gaseous PbS or Pb, depending on the local sulfur concentration (Table 77). The operation of the cell at either 0.160 or 0.250 A/cm^2 does not dramatically shift the stability of the trace constituent phases. (In Figure 39 the solid line is for the 0.160 A/cm^2 cell, the dashed line for the 0.250 A/cm^2 cell.)

Table 75

FUEL AND OXIDANT GAS COMPOSITIONS AND UTILIZATIONS AS A FUNCTION
OF LOCATION IN THE TEXACO 0.160 A/cm² ENTRAINED
BENFIELD/ZnO OXYGEN-BLOWN MCFC

TEST CASE WITH ANODE MATERIAL - TEXACO/BENFIELD/ZNO/OXYGEN BLOWN MCFC										
VAPOR PRESSURE (ATM) DATA AT ELECTRODES (TERMINAL VOLTAGE : .93039+00 VOLTS)										
TOTAL GAS PRESSURE 10.00 ATMOSPHERE										
LENGTH (CM)	.0000	.1530+02	.3050+02	.4580+02	.6100+02	.7620+02	.9150+02	.1087+03	.1220+03	
FUEL CELL EMF (V)	.1087+01	.1059+01	.1033+01	.1010+01	.9882+00	.9681+00	.9494+00	.9304+00	.9304+00	
CATHODE :										
TEMPERATURE DEG. K	866.00	879.93	893.77	907.70	921.55	935.39	949.32	964.98	977.09	
CURRENT (AMP/CM ²)	.3906+00	.3202+00	.2570+00	.1985+00	.1444+00	.9420-01	.4761-01	.0000	.0000	
VELOCITY (CM/SEC)	.7010+02	.7003+02	.7015+02	.7045+02	.7092+02	.7156+02	.7237+02	.7346+02	.7439+02	
H ₂ O	.1300+01	.1322+01	.1341+01	.1356+01	.1367+01	.1376+01	.1380+01	.1382+01	.1382+01	
CO ₂	.1700+01	.1615+01	.1544+01	.1486+01	.1442+01	.1411+01	.1393+01	.1386+01	.1386+01	
N ₂	.6300+01	.6408+01	.6498+01	.6571+01	.6627+01	.6666+01	.6690+01	.6699+01	.6699+01	
O ₂	.7000+00	.6549+00	.6174+00	.5868+00	.5635+00	.5470+00	.5371+00	.5334+00	.5334+00	
TOTAL GAS MOLES	.4307+01	.4234+01	.4176+01	.4129+01	.4094+01	.4070+01	.4056+01	.4050+01	.4050+01	
% O ₂ CONSUMED	.0000	.6443+01	.1181+02	.1618+02	.1951+02	.2186+02	.2327+02	.2380+02	.2380+02	
% CO ₂ CONSUMED	.0000	.5004+01	.9169+01	.1256+02	.1515+02	.1697+02	.1807+02	.1848+02	.1848+02	
ANODE :										
TEMPERATURE DEG. K	923.00	929.78	936.51	943.29	950.02	956.76	963.53	971.15	977.04	
CURRENT (AMP/CM ²)	.3906+00	.3202+00	.2570+00	.1985+00	.1444+00	.9420-01	.4761-01	.0000	.0000	
VELOCITY (CM/SEC)	.1463+02	.1558+02	.1638+02	.1705+02	.1759+02	.1800+02	.1830+02	.1851+02	.1862+02	
O ₂	.1221-21	.2317-21	.4178-21	.7300-21	.1232-20	.2012-20	.3188-20	.5118-20	.7241-20	
H ₂	.2048+01	.1975+01	.1918+01	.1871+01	.1836+01	.1816+01	.1812+01	.1832+01	.1858+01	
H ₂ O	.3050+01	.3204+01	.3318+01	.3405+01	.3471+01	.3518+01	.3550+01	.3589+01	.3627+01	
CO	.6463+00	.1029+01	.1089+01	.1195+01	.1173+01	.1209+01	.1247+01	.1297+01	.1359+01	
CO ₂	.2949+01	.3376+01	.3687+01	.3914+01	.4070+01	.4166+01	.4212+01	.4207+01	.4182+01	
CH ₄	.9197+00	.6900+00	.5294+00	.4011+00	.3158+00	.2529+00	.2101+00	.1802+00	.1534+00	
NH ₃	.7411-05	.6482-05	.5768-05	.5199-05	.4753-05	.4415-05	.4173-05	.4014-05	.3933-05	
N ₂	.6604-01	.6246-01	.5984-01	.5791-01	.5655-01	.5564-01	.5511-01	.5491-01	.5491-01	
C (C)	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	
[H ₂ O]/[H ₂]	.1489+01	.1622+01	.1730+01	.1820+01	.1890+01	.1938+01	.1959+01	.1948+01	.1926+01	
[CO ₂]/[CO]	.3096+01	.3260+01	.3365+01	.3426+01	.3466+01	.3476+01	.3466+01	.3424+01	.3356+01	
[SO ₂]/[H ₂ S]	.8423-08	.1279-07	.1844-07	.2569-07	.3452-07	.4476-07	.5584-07	.6791-07	.7734-07	
[CS ₂]/[CH ₂ S]**2	.1950-04	.2161-04	.2346-04	.2519-04	.2683-04	.2842-04	.2998-04	.3170-04	.3302-04	
[COS]/[CH ₂ S]	.1583-01	.1782-01	.1941-01	.2073-01	.2181-01	.2272-01	.2347-01	.2412-01	.2454-01	
TOTAL GAS MOLES	.8433+00	.8916+00	.9306+00	.9616+00	.9848+00	.1001+01	.1011+01	.1014+01	.1014+01	
% GRAPHITE IN MIX	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	
% H ₂ CONSUMED	.0000	.3548+01	.6363+01	.8646+01	.1034+02	.1135+02	.1153+02	.1053+02	.9294+01	
% CO CONSUMED	.0000	.8735+01	.1506+02	.1996+02	.2400+02	.2778+02	.3180+02	.3705+02	.4146+02	
% CO+H ₂ CONSUMED	.0000	.3337+00	.4087+00	.3936+00	.5111+00	.5101+01	.5216+01	.54507+01	.6747+01	
TOTAL CELL CURRENT (AMPS) :	.2338+04									
AVERAGE CURRENT DENSITY :	.1572+00 AMPS/CM ²									
FUEL CELL PLATE DIMENSIONS (CM) : WIDTH	.1219+03									
CELL RESISTANCE :	.13450-04 OHMS									
TOTAL ELECTRODE (2A+2C) IMPEDANCE :	.40000+00 OHMS.CM ²									

Table 75 (Continued)

HEAT OF C. (KCAL/MOLE)	-.3609+02	-.3183+02	-.2871+02	-.2641+02	-.2480+02	-.2374+02	-.2317+02	-.2306+02	-.2317+02
THE FOLLOWING EFFICIENCIES ARE IN FRACTIONAL UNITS									
VOLTAGE EFFICIENCY	.8562+00	.8790+00	.9004+00	.9214+00	.9415+00	.9611+00	.9799+00	.1000+01	.1000+01
THERMODYNAMIC EFFICIENCY	.8028+00	.7804+00	.7603+00	.7417+00	.7244+00	.7083+00	.6933+00	.6779+00	.6767+00
ELECTROCHEMICAL EFF.	.6873+00	.6860+00	.6847+00	.6833+00	.6820+00	.6807+00	.6794+00	.6779+00	.6767+00
HEATING VALUE EFFICIENCY	.3354+00	.3669+00	.3950+00	.4190+00	.4381+00	.4525+00	.4628+00	.4704+00	.4747+00
FUEL CELL EFFICIENCY	.2305+00	.2517+00	.2704+00	.2863+00	.2988+00	.3080+00	.3144+00	.3189+00	.3212+00

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+01								
H2S	.9845+00	.9826+00	.9811+00	.9798+00	.9788+00	.9779+00	.9772+00	.9766+00	.9762+00
SO2	.8292-08	.1257-07	.1809-07	.2517-07	.3379-07	.4377-07	.5457-07	.6632-07	.7550-06
CS2	.1879-09	.2073-09	.2244-09	.2403-09	.2554-09	.2701-09	.2845-09	.3004-09	.3126-09
COS	.1548-01	.1740-01	.1892-01	.2018-01	.2122-01	.2208-01	.2279-01	.2340-01	.2381-01
S2	.2143-10	.2722-10	.3404-10	.4212-10	.5134-10	.6155-10	.7235-10	.8431-10	.9376-10
H2/H2S	.2080+06	.2010+06	.1955+06	.1910+06	.1876+06	.1857+06	.1854+06	.1876+06	.1903+06

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+01								
H2S	.4923+01	.4913+01	.4905+01	.4899+01	.4894+01	.4889+01	.4886+01	.4883+01	.4881+01
SO2	.4146-07	.6284-07	.9046-07	.1259-06	.1690-06	.2189-06	.2728-06	.3316-06	.3772-06
CS2	.4697-08	.5183-08	.5610-08	.6008-08	.6386-08	.6752-08	.7113-08	.7510-08	.7816-08
COS	.7741-01	.8702-01	.9463-01	.1009+00	.1061+00	.1104+00	.1139+00	.1170+00	.1190+00
S2	.5358-09	.6806-09	.8510-09	.1053-08	.1284-08	.1539-08	.1809-08	.2108-08	.2344-08
H2/H2S	.4161+05	.4021+05	.3910+05	.3819+05	.3752+05	.3713+05	.3709+05	.3753+05	.3806+05

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+02								
H2S	.9845+01	.9826+01	.9811+01	.9798+01	.9788+01	.9779+01	.9772+01	.9766+01	.9762+01
SO2	.8292-07	.1257-06	.1809-06	.2517-06	.3379-06	.4377-06	.5457-06	.6632-06	.7550-06
CS2	.1879-07	.2073-07	.2244-07	.2403-07	.2554-07	.2701-07	.2845-07	.3004-07	.3126-07
COS	.1548+00	.1740+00	.1893+00	.2018+00	.2122+00	.2208+00	.2279+00	.2340+00	.2381+00
S2	.2143-08	.2722-08	.3404-08	.4212-08	.5134-08	.6155-08	.7236-08	.8431-08	.9376-08
H2/H2S	.2080+05	.2010+05	.1955+05	.1910+05	.1876+05	.1857+05	.1854+05	.1876+05	.1903+05

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+02								
H2S	.4923+02	.4913+02	.4905+02	.4899+02	.4894+02	.4889+02	.4886+02	.4883+02	.4881+02
SO2	.4146-06	.6284-06	.9046-06	.1259-05	.1690-05	.2189-05	.2728-05	.3316-05	.3772-05
CS2	.4697-07	.5183-07	.5610-07	.6008-07	.6386-07	.6752-07	.7113-07	.7510-07	.7816-07
COS	.7741+00	.8702+00	.9463+00	.1009+01	.1061+01	.1104+01	.1139+01	.1170+01	.1190+01
S2	.5358-07	.6806-07	.8510-07	.1053-06	.1284-06	.1539-06	.1809-06	.2108-06	.2344-06
H2/H2S	.4161+04	.4021+04	.3910+04	.3819+04	.3752+04	.3713+04	.3709+04	.3753+04	.3806+04

Table 75 (Continued)

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1000+03									
H ₂ S	.9845+02	.9826+02	.9811+02	.9798+02	.9788+02	.9779+02	.9772+02	.9766+02	.9762+02	
SO ₂	.8292-06	.1257-05	.1809-05	.2517-05	.3379-05	.4377-05	.5457-05	.6632-05	.7550-05	
CS ₂	.1879-05	.2073-05	.2244-05	.2403-05	.2554-05	.2701-05	.2845-05	.3004-05	.3126-05	
CO ₂	.1348+01	.1740+01	.1893+01	.2018+01	.2122+01	.2208+01	.2279+01	.2340+01	.2381+01	
S ₂	.2143-06	.272-06	.3404-06	.4212-06	.5154-06	.6155-06	.7236-06	.8431-06	.9376-06	
H ₂ /H ₂ S	.2080+04	.2010+04	.1955+04	.1910+04	.1876+04	.1857+04	.1824+04	.1876+04	.1903+04	

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.1500+03									
H ₂ S	.1477+03	.1474+03	.1472+03	.1470+03	.1468+03	.1467+03	.1466+03	.1465+03	.1464+03	
SO ₂	.1244-05	.1882-05	.2716-05	.3776-05	.5092-05	.6599-05	.8185-05	.9948-05	.1132-04	
CS ₂	.4227-05	.4665-05	.5049-05	.5407-05	.5747-05	.6079-05	.6402-05	.6759-05	.7032-05	
CO ₂	.2322+01	.2611+01	.2839+01	.3027+01	.3183+01	.3312+01	.3418+01	.3511+01	.3571+01	
S ₂	.4822-06	.6125-06	.7659-06	.9476-06	.1153-05	.1385-05	.1628-05	.1897-05	.2110-05	
H ₂ /H ₂ S	.1387+04	.1340+04	.1303+04	.1273+04	.1251+04	.1238+04	.1236+04	.1251+04	.1269+04	

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.2000+03									
H ₂ S	.1969+03	.1965+03	.1962+03	.1960+03	.1958+03	.1956+03	.1954+03	.1953+03	.1952+03	
SO ₂	.1658-05	.2514-05	.3619-05	.5034-05	.6758-05	.8755-05	.1091-04	.1326-04	.1510-04	
CS ₂	.7515-05	.8293-05	.8975-05	.9613-05	.1022-04	.1080-04	.1138-04	.1202-04	.1251-04	
CO ₂	.3097+01	.3481+01	.3785+01	.4036+01	.4243+01	.4416+01	.4557+01	.4681+01	.4762+01	
S ₂	.8572-06	.1089-05	.1362-05	.1685-05	.2054-05	.2462-05	.2894-05	.3372-05	.3751-05	
H ₂ /H ₂ S	.1040+04	.1005+04	.9724+03	.9548+03	.9381+03	.9283+03	.9272+03	.9382+03	.9515+03	

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.2500+03									
H ₂ S	.2461+03	.2456+03	.2453+03	.2450+03	.2447+03	.2445+03	.2443+03	.2441+03	.2440+03	
SO ₂	.2073-05	.3142-05	.4523-05	.6293-05	.8448-05	.1094-04	.1364-04	.1658-04	.1887-04	
CS ₂	.1174-04	.1296-04	.1402-04	.1502-04	.1596-04	.1688-04	.1778-04	.1878-04	.1954-04	
CO ₂	.3871+01	.4351+01	.4731+01	.5045+01	.5304+01	.5520+01	.5697+01	.5851+01	.5952+01	
S ₂	.1339-05	.1701-05	.2127-05	.2632-05	.3209-05	.3847-05	.4522-05	.5269-05	.5860-05	
H ₂ /H ₂ S	.8321+03	.8042+03	.7819+03	.7638+03	.7504+03	.7426+03	.7417+03	.7505+03	.7612+03	

MINORITY SULFUR CHEMICAL SPECIES IN PPM UNITS

PPM SULFUR	.5000+03									
H ₂ S	.4923+03	.4913+03	.4905+03	.4899+03	.4894+03	.4889+03	.4886+03	.4883+03	.4881+03	
SO ₂	.4199-05	.6284-05	.9046-05	.1259-04	.1690-04	.2189-04	.2728-04	.3316-04	.3775-04	
CS ₂	.4667-04	.5183-04	.5610-04	.6008-04	.6386-04	.6752-04	.7113-04	.7510-04	.7816-04	
CO ₂	.7741+01	.8702+01	.9463+01	.1009+02	.1061+02	.1104+02	.1139+02	.1170+02	.1170+02	
S ₂	.5558-05	.6806-05	.8510-05	.1053-04	.1284-04	.1539-04	.1809-04	.2108-04	.2420-04	
H ₂ /H ₂ S	.4161+03	.4021+03	.3910+03	.3819+03	.3752+03	.3713+03	.3709+03	.3753+03	.3806+03	

Table 76

FUEL AND OXIDANT GAS COMPOSITIONS AND UTILIZATIONS AS A FUNCTION
OF LOCATION IN THE TEXACO 0.250 A/cm² ENTRAINED
BENFIELD/ZnO OXYGEN-BLOWN MCFC

TEST CASE WITH ANODE MATERIAL - TEXACO/BENFIELD/ZNO/OXYGEN BLOWN MCFC									
VAPOR PRESSURE (ATM) DATA AT ELECTRODES (TERMINAL VOLTAGE : .68342+00 VOLTS)									
TOTAL GAS PRESSURE 10.00 ATMOSPHERE									
LENGTH (CM)	.0000	.1530+02	.3050+02	.4580+02	.6100+02	.7620+02	.9150+02	.1067+03	.1220+03
FUEL CELL EMF (V)	.1087+01	.1060+01	.1034+01	.1008+01	.9833+00	.9581+00	.9326+00	.9070+00	.8812+00
CATHODE :									
TEMPERATURE DEG. K	866.00	879.93	893.77	907.70	921.55	935.39	949.32	963.16	977.09
CURRENT (AMP/CM ²)	.3359+00	.3134+00	.2919+00	.2707+00	.2498+00	.2288+00	.2075+00	.1863+00	.1648+00
VELOCITY (CM/SEC)	.7010+02	.7013+02	.7020+02	.7031+02	.7047+02	.7067+02	.7093+02	.7124+02	.7161+02
H ₂ O	.1300+01	.1320+01	.1340+01	.1358+01	.1376+01	.1393+01	.1408+01	.1423+01	.1436+01
CO ₂	.6300+01	.6399+01	.6493+01	.6583+01	.6669+01	.6749+01	.6825+01	.6895+01	.6958+01
O ₂	.7000+00	.6588+00	.6194+00	.5816+00	.5458+00	.5121+00	.4805+00	.4515+00	.4249+00
TOTAL GAS MOLES	.4307+01	.4240+01	.4179+01	.4121+01	.4068+01	.4020+01	.3975+01	.3935+01	.3899+01
% O ₂ CONSUMED	.0000	.5887+01	.1151+02	.1692+02	.2202+02	.2684+02	.3136+02	.3550+02	.3929+02
% CO ₂ CONSUMED	.0000	.4572+01	.8937+01	.1314+02	.1710+02	.2084+02	.2436+02	.2757+02	.3052+02
ANODE :									
TEMPERATURE DEG. K	923.00	929.78	936.51	943.29	950.02	956.76	963.53	970.27	977.04
CURRENT (AMP/CM ²)	.3359+00	.3134+00	.2919+00	.2707+00	.2498+00	.2288+00	.2075+00	.1863+00	.1648+00
VELOCITY (CM/SEC)	.1463+02	.1551+02	.1634+02	.1714+02	.1789+02	.1860+02	.1927+02	.1989+02	.2047+02
O ₂	.1221-21	.2270-21	.4133-21	.7505-21	.1359-20	.2475-20	.4568-20	.8473-20	.1586-19
H ₂	.2028+01	.1688+01	.1025+01	.1853+01	.1770+01	.1272+01	.1298+01	.1272+01	.1339+01
H ₂ O	.3050+01	.3191+01	.3312+01	.3419+01	.3515+01	.3601+01	.3690+01	.3778+01	.3809+01
CO	.9463+00	.1028+01	.1089+01	.1132+01	.1154+01	.1158+01	.1143+01	.1113+01	.1072+01
CO ₂	.2949+01	.3338+01	.3669+01	.3956+01	.4205+01	.4425+01	.4623+01	.4798+01	.4955+01
CH ₄	.9197+00	.7055+00	.5303+00	.3868+00	.2732+00	.1856+00	.1205+00	.7552-01	.4578-01
NH ₃	.7411-05	.6559-05	.5806-05	.5109-05	.4461-05	.3850-05	.3275-05	.2754-05	.2290-05
N ₂	.6604-01	.6275-01	.5998-01	.5760-01	.5557-01	.5383-01	.5233-01	.5105-01	.4995-01
C (C)	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
[H ₂ O]/[H ₂]	.1489+01	.1605+01	.1721+01	.1845+01	.1985+01	.2149+01	.2335+01	.2577+01	.2869+01
[CO ₂]/[CO]	.3096+01	.3297+01	.3527+01	.3772+01	.4030+01	.4297+01	.4572+01	.4854+01	.5144+01
[H ₂ O]/[H ₂ O]	.8423-08	.1255-07	.1818-07	.2667-07	.3891-07	.5966-07	.9245-07	.1481-06	.2554-06
[CO ₂]/[H ₂ O]*2)	.1950-04	.2154-04	.2343-04	.2525-04	.2703-04	.2882-04	.3064-04	.3252-04	.3449-04
[CO ₂]/[H ₂ O]	.1583-01	.1770-01	.1935-01	.2086-01	.2226-01	.2358-01	.2485-01	.2609-01	.2730-01
TOTAL GAS MOLES	.8433+00	.8875+00	.9285+00	.9668+00	.1002+01	.1034+01	.1064+01	.1091+01	.1115+01
% GRAPHITE IN MIX	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
% H ₂ CONSUMED	.0000	.2939+01	.6025+01	.9532+01	.1356+02	.1819+02	.2341+02	.2900+02	.3473+02
% CO CONSUMED	.0000	-.8649+01	-.1512+02	-.1959+02	-.2199+02	-.2238+02	-.2083+02	-.1764+02	-.1325+02
% CO+H ₂ CONSUMED	.0000	-.7231+00	-.6573+00	.5293+00	.2323+01	.5368+01	.9431+01	.1426+02	.1957+02
TOTAL CELL CURRENT (AMPS) :	.3715+04								
AVERAGE CURRENT DENSITY :	.2498+00 AMPS/CM ²								
FUEL CELL PLATE DIMENSIONS (CM) : WIDTH	.1219+03								
CELL RESISTANCE : .40350-04 OHMS									
TOTAL ELECTRODE (ZA+ZC) IMPEDANCE :	.12000+01 OHMS/CM ²								

Table 76 (Continued)

HEAT OF C. (KCAL/MOLE)	-.3609+02	-.3220+02	-.2889+02	-.2601+02	-.2350+02	-.2129+02	-.1932+02	-.1758+02	-.1603+02
THE FOLLOWING EFFICIENCIES ARE IN FRACTIONAL UNITS.									
VOLTAGE EFFICIENCY	.6289+00	.6450+00	.6611+00	.6777+00	.6951+00	.7133+00	.7328+00	.7535+00	.7755+00
THERMODYNAMIC EFFICIENCY	.6028+00	.7813+00	.7608+00	.7406+00	.7208+00	.7009+00	.6810+00	.6610+00	.6410+00
ELECTROCHEMICAL EFF.	.5049+00	.5039+00	.5029+00	.5019+00	.5010+00	.5000+00	.4990+00	.4981+00	.4971+00
HEATING VALUE EFFICIENCY	.3354+00	.3651+00	.3940+00	.4214+00	.4456+00	.4657+00	.4806+00	.4898+00	.4937+00
FUEL CELL EFFICIENCY	.1693+00	.1839+00	.1982+00	.2115+00	.2233+00	.2328+00	.2398+00	.2439+00	.2454+00

Texaco Entrained Benfield/ZnO Oxygen-Blown MCFC

Fuel Gas Velocity: 14.63 cm/sec

Oxidant Gas Velocity: 70.10 cm/sec

Anode Inlet Temperature: 923K

Anode Outlet Temperature: 977K

Cathode Inlet Temperature: 866K

Cathode Outlet Temperature: 977K

Cell Resistance: 0.1345-4 ohms (0.4035-4 ohms)

Total Electrode Impedance: 0.40 ohms·cm² (1.200 ohms·cm²)Average Current Density: 0.160 Amps / cm² (0.250 Amps/cm²)

Terminal Voltage: 0.9309 Volts (0.6834 Volts)

Figure 39 -- Nickel Anode and Trace Element Sulfur Tolerance in the Texaco Entrained Benfield/ZnO Oxygen-Blown MCFC

Table 77

Dwg. 7756A80

VOLATILE TRACE COMPLEXES IN THE TEXACO ENTRAINED BENFIELD/ZnO
OXYGEN-BLOWN MCFC

Distance From Anode Inlet, cm	Total Sulfur Concentration, ppm								
	1	5	10	50	100	150	200	250	500
0					Pb (s)				
15.3					Pb (s)				
30.5					Pb (s)				PbS (g)
45.8					Pb (s)				PbS (g)
61.0				Pb (g)					PbS (g)
76.2				Pb (g)					PbS (g)
91.5				Pb (g)					PbS (g)
106.7				Pb (g)					PbS (g)
122.0				Pb (g)					PbS (g)

In contrast to desulfurization using the Benfield/ZnO scrub, the molten carbonate/ZnO desulfurization increases the NH_3 and Na_2CO_3 content of the fuel gas. Both systems effectively reduce sulfur to levels of 56.3 ppb. MCFC performances using the Texaco molten carbonate/ZnO desulfurized fuel gas are shown in Tables 78 and 79. These are similar to the Benfield/ZnO system discussed previously.

Figure 40 illustrates the stability of the nickel anode material and trace constituent phases within the anode channel when the Texaco molten carbonate/ZnO fuel gas is used. Sulfur tolerances of the anode material, and the behavior of Pb and As in this system are identical to those in the Benfield/ZnO scrubbed Texaco cell. The presence of 338 ppm Na_2CO_3 in the incoming molten carbonate/ZnO fuel gas remains as Na_2CO_3 throughout the length of the anode channel.

Table 78

FUEL AND OXIDANT GAS COMPOSITIONS AND UTILIZATIONS AS A FUNCTION
OF LOCATION IN THE TEXACO 0.160 A/cm² ENTRAINED
MOLTEN CARBONATE/ZnO OXYGEN-BLOWN MCFC

TEST CASE WITH ANODE MATERIAL - TEXACO/MOLTEN CARBONATE/ZNO/OXYGEN BLOWN										
VAPOR PRESSURE (ATM) DATA AT ELECTRODES (TERMINAL VOLTAGE : .93039+00 VOLTS)										
TOTAL GAS PRESSURE 10.00 ATMOSPHERE										
LENGTH (CM)	.0000	.1530+02	.3050+02	.4580+02	.6100+02	.7620+02	.9150+02	.1087+03	.1220+03	
FUEL CELL EMF (V)	.1087+01	.1059+01	.1033+01	.1010+01	.9882+00	.9681+00	.9494+00	.9304+00	.9304+00	
CATHODE :										
TEMPERATURE DEG. K	866.00	879.93	893.77	907.70	921.55	935.39	949.32	964.98	977.09	
CURRENT (AMP/CM2)	.2906+00	.3202+00	.2570+00	.1985+00	.1444+00	.9420-01	.4760-01	.0000	.0000	
VELOCITY (CM/SEC)	.7010+02	.7003+02	.7015+02	.7045+02	.7092+02	.7156+02	.7237+02	.7346+02	.7439+02	
H2O	.1300+01	.1322+01	.1341+01	.1356+01	.1367+01	.1376+01	.1380+01	.1382+01	.1392+01	
CO2	.1700+01	.1615+01	.1544+01	.1486+01	.1442+01	.1411+01	.1393+01	.1386+01	.1386+01	
N2	.6300+01	.6408+01	.6498+01	.6571+01	.6627+01	.6666+01	.6690+01	.6699+01	.6699+01	
O2	.7000+00	.6549+00	.6174+00	.5868+00	.5635+00	.5470+00	.5371+00	.5334+00	.5334+00	
TOTAL GAS MOLES	.4307+01	.4234+01	.4176+01	.4129+01	.4095+01	.4070+01	.4056+01	.4051+01	.4051+01	
% O2 CONSUMED	.0000	.6443+01	.1181+02	.1618+02	.1951+02	.2186+02	.2327+02	.2380+02	.2380+02	
% CO2 CONSUMED	.0000	.5004+01	.9169+01	.1256+02	.1515+02	.1697+02	.1807+02	.1848+02	.1848+02	
ANODE :										
TEMPERATURE DEG. K	923.00	929.78	936.51	943.29	950.02	956.76	963.53	971.15	977.04	
CURRENT (AMP/CM2)	.3906+00	.3202+00	.2570+00	.1985+00	.1444+00	.9420-01	.4760-01	.0000	.0000	
VELOCITY (CM/SEC)	.7463+02	.7558+02	.7638+02	.7705+02	.7759+02	.7800+02	.7830+02	.7851+02	.7862+02	
O2	.1221-21	.2317-21	.4178-21	.7301-21	.1232-20	.2013-20	.3188-20	.5118-20	.7242-20	
H2	.0446+01	.1975+01	.1918+01	.1871+01	.1836+01	.1815+01	.1812+01	.1832+01	.1858+01	
H2O	.3050+01	.3203+01	.3318+01	.3405+01	.3470+01	.3518+01	.3550+01	.3569+01	.3577+01	
CO	.5463+00	.1029+01	.1086+01	.1135+01	.1173+01	.1209+01	.1247+01	.1297+01	.1339+01	
CO2	.5948+01	.3375+01	.3687+01	.3914+01	.4069+01	.4166+01	.4212+01	.4207+01	.4182+01	
CH4	.5195+00	.6899+00	.5232+00	.4610+00	.3137+00	.2522+00	.2100+00	.1801+00	.1634+00	
NH3	.7411-03	.6483-03	.5770-03	.5201-03	.4756-03	.4418-03	.4176-03	.4018-03	.3937-03	
N2	.6603-01	.6248-01	.5988-01	.5797-01	.5662-01	.5572-01	.5520-01	.5502-01	.5502-01	
C (C)	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	
[H2O]/[H2]	.1489+01	.1622+01	.1730+01	.1820+01	.1890+01	.1938+01	.1959+01	.1948+01	.1926+01	
[CO2]/[CO]	.3096+01	.3260+01	.3365+01	.3426+01	.3447+01	.3424+01	.3356+01	.3224+01	.3105+01	
[SO2]/[H2S]	.6423-08	.1279-07	.1844-07	.2569-07	.3453-07	.4477-07	.5586-07	.6793-07	.7736-07	
[CS2]/[H2S]**2	.1951-04	.2161-04	.2346-04	.2519-04	.2683-04	.2842-04	.2998-04	.3170-04	.3302-04	
[CCS]/[H2S]	.1583-01	.1782-01	.1941-01	.2073-01	.2181-01	.2272-01	.2347-01	.2412-01	.2454-01	
TOTAL GAS MOLES	.6433+00	.8917+00	.9307+00	.9617+00	.9849+00	.1001+01	.1011+01	.1014+01	.1014+01	
% GRAPHITE IN MIX	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	
% H2 CONSUMED	.0000	.3549+01	.6364+01	.8647+01	.1034+02	.1135+02	.1153+02	.1053+02	.9296+01	
% CO CONSUMED	.0000	.8734+01	.1506+02	.1995+02	.2399+02	.2777+02	.3179+02	.3705+02	.4146+02	
% CO+H2 CONSUMED	.0000	.3333+00	.4076+00	.3918+00	.5066+00	.1011+01	.2162+01	.4503+01	.6743+01	
TOTAL CELL CURRENT (AMPS) :	.2338+04									
AVERAGE CURRENT DENSITY :	.1572+00 AMPS/CM2									
FUEL CELL PLATE DIMENSIONS (CM) : WIDTH	.1219+03			LENGTH	.1219+03			THICKNESS	.2540+00	
CELL RESISTANCE :	.13450-04 OHMS									
TOTAL ELECTRODE (2A+2C) IMPEDANCE :	.40000+00 OHMS.CM2									

Table 78 (Continued)

HEAT OF C. (KCAL/MOLE)	-.3609+02	-.3163+02	-.2871+02	-.2641+02	-.2479+02	-.2374+02	-.2317+02	-.2305+02	-.2317+02
THE FOLLOWING EFFICIENCIES ARE IN FRACTIONAL UNITS									
VOLTAGE EFFICIENCY	.8562+00	.8790+00	.9004+00	.9214+00	.9415+00	.9611+00	.9799+00	.1000+01	.1000+01
THERMODYNAMIC EFFICIENCY	.6028+00	.7804+00	.7603+00	.7417+00	.7244+00	.7083+00	.6933+00	.6779+00	.6767+00
ELECTROCHEMICAL EFF.	.6873+00	.6860+00	.6847+00	.6833+00	.6820+00	.6807+00	.6794+00	.6779+00	.6767+00
HEATING VALUE EFFICIENCY	.3355+00	.3669+00	.3950+00	.4190+00	.4381+00	.4525+00	.4628+00	.4704+00	.4747+00
FUEL CELL EFFICIENCY	.2306+00	.2517+00	.2705+00	.2863+00	.2988+00	.3080+00	.3144+00	.3169+00	.3212+00

Table 79

FUEL AND OXIDANT GAS COMPOSITIONS AND UTILIZATIONS AS A FUNCTION
OF LOCATION IN THE TEXACO 0.250 A/cm² ENTRAINED MOLTEN
CARBONATE/ZnO OXYGEN-BLOWN MCFC

TEST CASE WITH ANODE MATERIAL - TEXACO/MOLTEN CARBONATE/ZNO/OXYGEN BLOWN									
VAPOR PRESSURE (ATM) DATA AT ELECTRODES (TERMINAL VOLTAGE : .68342+00 VOLTS)									
TOTAL GAS PRESSURE 10.00 ATMOSPHERE									
LENGTH (CM)	.0000	.1530+02	.3050+02	.4580+02	.6100+02	.7620+02	.9150+02	.1067+03	.1220+03
FUEL CELL EMF (V)	.1087+01	.1060+01	.1034+01	.1008+01	.9833+00	.9581+00	.9326+00	.9070+00	.8812+00
CATHODE :									
TEMPERATURE DEG. K	866.00	879.93	893.77	907.70	921.55	935.39	949.32	963.16	977.09
CURRENT (AMP/CM2)	.3359+00	.3134+00	.2919+00	.2707+00	.2498+00	.2288+00	.2075+00	.1863+00	.1648+00
VELOCITY (CM/SEC)	.7010+02	.7013+02	.7020+02	.7031+02	.7047+02	.7067+02	.7093+02	.7124+02	.7161+02
H2O	.1308+01	.1369+01	.1368+01	.1355+01	.1308+01	.1323+01	.1308+01	.1233+01	.1136+01
CO2	.6300+01	.6399+01	.6493+01	.6583+01	.6669+01	.6749+01	.6823+01	.6895+01	.6958+01
N2	.7000+00	.6588+00	.6194+00	.5816+00	.5458+00	.5121+00	.4805+00	.4515+00	.4249+00
TOTAL GAS MOLES	.4307+01	.4240+01	.4179+01	.4122+01	.4069+01	.4020+01	.3975+01	.3935+01	.3900+01
X O2 CONSUMED	.0000	.5887+01	.1151+02	.1692+02	.2202+02	.2684+02	.3136+02	.3550+02	.3929+02
X CO2 CONSUMED	.0000	.4572+01	.8937+01	.1314+02	.1710+02	.2084+02	.2436+02	.2757+02	.3052+02
ANODE :									
TEMPERATURE DEG. K	923.00	929.78	936.51	943.29	950.02	956.76	963.53	970.27	977.04
CURRENT (AMP/CM2)	.3359+00	.3134+00	.2919+00	.2707+00	.2498+00	.2288+00	.2075+00	.1863+00	.1648+00
VELOCITY (CM/SEC)	.1463+02	.1551+02	.1634+02	.1714+02	.1789+02	.1860+02	.1927+02	.1989+02	.2047+02
O2	.1221-21	.2270-21	.5133-21	.7506-21	.1338-20	.2475-20	.4569-20	.8475-20	.1586-19
H2	.2068+01	.1988+01	.1923+01	.1853+01	.1770+01	.1675+01	.1568+01	.1454+01	.1339+01
H2O	.3050+01	.3191+01	.3312+01	.3419+01	.3515+01	.3601+01	.3679+01	.3748+01	.3809+01
CO	.9463+00	.1028+01	.1089+01	.1132+01	.1154+01	.1158+01	.1143+01	.1113+01	.1072+01
CO2	.2948+01	.3338+01	.3669+01	.3956+01	.4205+01	.4425+01	.4623+01	.4798+01	.4953+01
CH4	.9195+00	.7053+00	.5301+00	.3866+00	.2731+00	.1855+00	.1205+00	.7549-01	.4575-01
NH3	.7411-03	.6559-03	.5808-03	.5112-03	.4464-03	.3853-03	.3279-03	.2757-03	.2293-03
N2	.6603-01	.6277-01	.6002-01	.5766-01	.5566-01	.5394-01	.5245-01	.5119-01	.5012-01
C (C)	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
[H2O]/[H2]	.1689+01	.1605+01	.1721+01	.1895+01	.1985+01	.2168+01	.2318+01	.2528+01	.2850+01
[CO2]/[CO]	.6423-08	.1245-07	.1816-07	.2667-07	.3952-07	.5967-07	.9248-07	.1461-06	.2355-06
[CS2]/[CH2S]**2)	.1951-04	.2154-04	.2343-04	.2525-04	.2703-04	.2882-04	.3064-04	.3252-04	.3449-04
[COS]/[H2S]	.1583-01	.1770-01	.1935-01	.2086-01	.2226-01	.2358-01	.2485-01	.2608-01	.2730-01
TOTAL GAS MOLES	.8433+00	.8876+00	.9286+00	.9669+00	.1002+01	.1035+01	.1064+01	.1091+01	.1115+01
X GRAPHITE IN MIX	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
X H2 CONSUMED	.0000	.2939+01	.6026+01	.9533+01	.1356+02	.1819+02	.2342+02	.2900+02	.3473+02
X CO CONSUMED	.0000	.8648+01	.1512+02	.1958+02	.2199+02	.2237+02	.2082+02	.1763+02	.1324+02
X CO+H2 CONSUMED	.0000	.7227+00	.6563+00	.3311+00	.2326+01	.5372+01	.9436+01	.1426+02	.1957+02
TOTAL CELL CURRENT (AMPS) :	.3715+04								
AVERAGE CURRENT DENSITY :	.2498+00 AMPS/CM2								
FUEL CELL PLATE DIMENSIONS (CM) : WIDTH	.1219+03								
CELL RESISTANCE :	.10350-04 OHMS								
TOTAL ELECTRODE (2A+2C) IMPEDANCE :	.12000+01 OHMS.CM2								

Table 79 (Continued)

HEAT OF C. (KCAL/MOLE)	-.3609+02	-.3219+02	-.2888+02	-.2600+02	-.2350+02	-.2129+02	-.1931+02	-.1757+02	-.1603+02
THE FOLLOWING EFFICIENCIES ARE IN FRACTIONAL UNITS									
VOLTAGE EFFICIENCY	.6289+00	.6450+00	.6611+00	.6777+00	.6951+00	.7133+00	.7328+00	.7535+00	.7755+00
THERMODYNAMIC EFFICIENCY	.8028+00	.7813+00	.7608+00	.7406+00	.7208+00	.7009+00	.6809+00	.6610+00	.6410+00
ELECTROCHEMICAL EFF.	.5049+00	.5039+00	.5029+00	.5019+00	.5010+00	.5000+00	.4990+00	.4981+00	.4971+00
HEATING VALUE EFFICIENCY	.3355+00	.3651+00	.3940+00	.4214+00	.4457+00	.4657+00	.4806+00	.4898+00	.4937+00
FUEL CELL EFFICIENCY	.1694+00	.1840+00	.1982+00	.2115+00	.2233+00	.2329+00	.2398+00	.2439+00	.2454+00

Texaco Entrained Molten Carbonate/ZnO Oxygen-Blown MCFC

Fuel Gas Velocity: 14.63 cm/sec

Oxidant Gas Velocity: 70.10 cm/sec

Anode Inlet Temperature: 923K

Anode Outlet Temperature: 977K

Cathode Inlet Temperature: 866K

Cathode Outlet Temperature: 977K

Cell Resistance: 0.1345-4 ohms (0.4035-4 ohms)

Total Electrode Impedance: 0.40 ohms-cm² (1.20 ohms-cm²)Average Current Density: 0.160 Amps/cm² (0.250 Amps/cm²)

Terminal Voltage: 0.9304 Volts (0.6834 Volts)

Figure 40 -- Nickel Anode and Trace Element Sulfur Tolerance in the Texaco Entrained Molten Carbonate/ZnO Oxygen-Blown MCFC

As previously discussed for the METC gravitating bed and the Westinghouse fluidized-bed fuel gas MCFC systems, the Texaco entrained fuel gas that undergoes Benfield desulfurization or molten carbonate/ZnO desulfurization contains residual trace concentrations of carbon. The 3.4 ppm carbon level within the Texaco fuel gas is projected to exist as a solid, in equilibrium with the humidified fuel gas, throughout the anode channel. Deposition of solid carbon particles with either condensed Pb, Na_2CO_3 , or K_2CO_3 can occur along the anode surface, minimizing utilization of the fuel gas H_2 and CO in the electrolysis reaction.

3.3.4.5 Summary of the MCFC Sulfur Tolerance Projections

The anode sulfur tolerance is based on achieving 85% utilization of the fuel gas or 50% utilization of the oxidant gas in a current-producing cell. In the following discussion, the location within the cell where the gas utilizations have been achieved or where an exchange current is projected to occur is used as the base-line criterion for establishing the minimum sulfur tolerance for a given system. Tables 80 through 85 summarize the projected utilizations, location of termination along the anode, estimated average current density, and anode sulfur tolerances as a function of position for a MCFC operating with terminal voltages of 0.6, 0.7, 0.8, and 0.9 V for cell resistances of 0.1345×10^{-4} and 0.4035×10^{-4} ohms, and for total cell impedances of 0.4000 and 1.2000 ohms $\cdot\text{cm}^2$. Figures 41 and 42 illustrate the projected sulfur tolerance at the point of termination within the cell as a function of terminal voltage. As shown in these tables and figures, cells operating at a terminal voltage of 0.9 V permit a greater total concentration of sulfur in the incoming fuel gas prior to sulfidation of the anode surface. Similarly, increasing the cell resistance and total cell impedance also increases the concentration that must be present prior to sulfidation. Chemisorption of $\text{H}_2\text{S}/\text{COS}$ has not been included in the model, so MCFC sulfur tolerance will be significantly lower than the model predicts.

Table 80

SULFUR TOLERANCE SUMMARY FOR THE ROCKWELL 14.63 cm/s MOLTEN
CARBONATE FUEL GAS AIR-BLOWN MCFC

Dwg. 5600C03

MCFC Parameters

Fuel Gas Velocity: 14.63 cm/sec
 Oxidant Gas Velocity: 70.10 cm/sec
 Anode Inlet Temperature: 923K
 Anode Outlet Temperature: 977K
 Cathode Inlet Temperature: 866K
 Cathode Outlet Temperature: 977K

Rockwell Air-Blown MCFC

Cell Resistance: 0.1345-4 ohms
 Total Electrode Impedance: 0.4000 ohms-cm²

Terminal Voltage, Volts	Utilization			Location From Anode Inlet, cm	Estimated Average Current Density, Amps/cm ²	Anode Sulfur Tolerance, ppm								
	Fuel Gas	Oxidant Gas				Distance From Anode Inlet, cm								
	% (H ₂ + CO)	% CO ₂	% O ₂			0	15.30	30.50	45.80	61.00	76.20	91.50	106.70	122.20
0.6	85.19	49.44	44.92	31.40*	1.018	252.8	161.5	39.6	(33.7)					
0.7	85.09	49.39	44.88	43.00*	0.7426	252.8	188.7	97.9	(34.8)					
0.8	85.03	49.37	44.86	79.80*	0.3999	252.8	213.2	159.2	102.7	62.5	40.5	(37.6)		
0.9	41.31	31.94	29.03	97.80**	0.1754	252.8	235.2	214.1	191.4	172.6	161.4	160.8	(164.2)	(169.9)

Rockwell Air-Blown MCFC

Cell Resistance: 0.4035-4 ohms
 Total Electrode Impedance: 1.2000 ohms-cm²

Terminal Voltage, Volts	Utilization			Location From Anode Inlet, cm	Estimated Average Current Density, Amps/cm ²	Anode Sulfur Tolerance, ppm								
	Fuel Gas % (H ₂ + CO)	Oxidant Gas				Distance From Anode Inlet, cm								
		% CO ₂	% O ₂			0	15.30	30.50	45.80	61.00	76.20	91.50	106.70	122.20
0.6	85.04	49.37	44.86	106.6*	0.2994	252.8	240.1	218.4	185.5	144.9	104.1	68.2	(39.6)	
0.7	65.70	41.26	37.49	122.0	0.2222	252.8	247.3	236.2	218.1	193.9	166.4	139.3	115.6	95.9
0.8	32.75	28.81	26.18	122.0	0.1593	252.8	254.2	252.8	248.0	239.9	229.2	217.5	206.4	197.2
0.9	11.49	16.64	15.12	122.0	0.0944	252.8	260.9	268.5	275.3	281.4	287.2	293.4	300.3	308.9

* Termination Due to Attainment of Fuel or Oxidant Gas Utilization

** Termination Due to Exchange Current Density Achieved Within the Cell

Table 81

Dwg. 5600C05

SULFUR TOLERANCE SUMMARY FOR THE METC 14.63 cm/s GRAVITATING-
BED FUEL GAS AIR-BLOWN MCFC

MCFC Parameters

Fuel Gas Velocity: 14.63 cm/sec
Oxidant Gas Velocity: 70.10 cm/sec
Anode Inlet Temperature: 923K
Anode Outlet Temperature: 977K
Cathode Inlet Temperature: 866K
Cathode Outlet Temperature: 977K

METC/FeO/ZnO Air-Blown MCFC

Cell Resistance: 0.1345-4 ohms

Total Electrode Impedance: 0.4000 ohms·cm²

Terminal Voltage, Volts	Utilization			Location From Anode Inlet, cm	Estimated Average Current Density, Amps/cm ²	Anode Sulfur Tolerance, ppm								
	Fuel Gas %(H ₂ + CO)	Oxidant Gas				Distance From Anode Inlet, cm								
		% CO ₂	% O ₂			0	15.30	30.50	45.80	61.00	76.20	91.50	106.70	122.20
0.6	78.33	50.08	45.51	31.20*	1.0360	261.5	176.0	55.5	(50.60)					
0.7	78.19	50.03	45.46	42.30*	0.7636	261.5	201.5	114.8	(52.2)					
0.8	78.16	50.02	45.45	72.90*	0.4430	261.5	224.5	174.4	118.8	76.5	(55.7)			
0.9	37.70	33.49	30.43	100.3**	0.1833	261.5	245.2	226.8	205.6	187.7	176.3	175.8	(175.6)	(185.0)

METC/FeO/ZnO Air-Blown MCFC

Cell Resistance: 0.4035-4 ohms

Total Electrode Impedance: 1.2000 ohms·cm²

Terminal Voltage, Volts	Utilization			Location From Anode Inlet, cm	Estimated Average Current Density, Amps/cm ²	Anode Sulfur Tolerance, ppm								
	Fuel Gas % (H ₂ + CO)	Oxidant Gas				Distance From Anode Inlet, cm								
		% CO ₂	% O ₂			0	15.30	30.50	45.80	61.00	76.20	91.50	106.70	122.20
0.6	78.10	50.00	45.43	105.1*	0.3072	261.5	250.6	231.9	202.7	164.7	124.2	87.2	(59.4)	
0.7	59.91	42.24	38.38	122.0	0.2271	261.5	257.4	248.7	233.6	212.1	186.5	159.9	135.8	115.3
0.8	27.51	29.60	26.90	122.0	0.1633	261.5	264.0	264.4	261.8	255.9	247.4	237.3	227.3	218.6
0.9	-3.35***	17.34	15.75	122.0	0.0982	261.5	270.6	279.3	287.6	295.3	302.8	310.5	318.9	328.8

* Termination Due to Attainment of Fuel or Oxidant Gas Utilization

** Termination Due to Exchange Current Density Achieved Within the Cell

*** % H₂ Utilization = 12.54, % CO Utilization = -38.66

Table 82

Dwg. 5600C06

SULFUR TOLERANCE SUMMARY FOR THE WESTINGHOUSE 14.63 cm/s FLUIDIZED-
BED FUEL GAS OXYGEN-BLOWN MCFC

MCFC Parameters

Fuel Gas Velocity: 14.63 cm/sec
Oxidant Gas Velocity: 70.10 cm/sec
Anode Inlet Temperature: 923K
Anode Outlet Temperature: 977K
Cathode Inlet Temperature: 866K
Cathode Outlet Temperature: 977K

Westinghouse/Dolomite/ZnO Oxygen-Blown MCFC

Cell Resistance: 0.1345-4 ohms
Total Electrode Impedance: 0.4000 ohms·cm²

Terminal Voltage, Volts	Utilization			Location From Anode Inlet, cm	Estimated Average Current Density, Amps/cm ²	Anode Sulfur Tolerance, ppm								
	Fuel Gas % (H ₂ + CO)	Oxidant Gas				Distance From Anode Inlet, cm								
		% CO ₂	% O ₂			0	15.30	30.50	45.80	61.00	76.20	91.50	106.70	122.20
0.6	43.92	38.93	50.13	36.20*	1.0470	364.9	306.9	229.9	(193.8)					
0.7	43.23	38.90	50.08	48.70*	0.7775	364.9	326.1	278.5	215.0	(201.8)				
0.8	41.91	38.85	50.02	79.30*	0.4770	364.9	344.9	322.3	293.8	260.6	227.1	(220.8)		
0.9	77.90	24.64	31.72	119.9**	0.2054	364.9	363.4	363.1	363.3	364.2	366.9	372.9	398.4	401.1

Westinghouse/Dolomite/ZnO Oxygen-Blown MCFC

Cell Resistance: 0.4035-4 ohms
Total Electrode Impedance: 1.2000 ohms·cm²

Terminal Voltage, Volts	Utilization			Location From Anode Inlet, cm	Estimated Average Current Density, Amps/cm ²	Anode Sulfur Tolerance, ppm								
	Fuel Gas % (H ₂ + CO)	Oxidant Gas				Distance From Anode Inlet, cm								
		% CO ₂	% O ₂			0	15.30	30.50	45.80	61.00	76.20	91.50	106.70	122.20
0.6	40.41	38.70	49.84	122.0	0.3090	364.9	366.0	364.7	359.2	347.9	330.2	305.9	277.6	247.5
0.7	17.35	28.83	37.12	122.0	0.2372	364.9	372.4	378.7	382.9	384.2	381.8	375.7	366.3	354.3
0.8	-3.99**	19.41	24.99	122.0	0.1645	364.9	378.8	392.6	406.1	418.7	430.4	441.0	450.7	459.7
0.9	-21.11**	10.45	13.51	122.0	0.0916	364.9	385.3	406.6	428.9	452.3	476.8	+500	+500	+500

* Termination Due to Attainment of Fuel or Oxidant Gas Utilization

** Termination Due to Exchange Current Density Achieved Within the Cell

*** For 0.8 Volts: % H₂ Utilization = 12.40, % CO Utilization = -39.2; for 0.9 Volts: % H₂ Utilization = -6.76, % CO Utilization = -53.05

Table 83

Dwg. 5600C07

SULFUR TOLERANCE SUMMARY FOR THE WESTINGHOUSE 8.63 cm/s FLUIDIZED-BED FUEL GAS OXYGEN-BLOWN MCFC

MCFC Parameters

Fuel Gas Velocity: 8.63 cm/sec
 Oxidant Gas Velocity: 70.10 cm/sec
 Anode Inlet Temperature: 923K
 Anode Outlet Temperature: 977K
 Cathode Inlet Temperature: 866K
 Cathode Outlet Temperature: 977K

Westinghouse/Dolomite/ZnO Oxygen-Blown MCFC

Cell Resistance: 0.1345-4 ohms

Total Electrode Impedance: 0.4000 ohms-cm²

Terminal Voltage, Volts	Utilization			Location From Anode Inlet, cm	Estimated Average Current Density, Amps/cm ²	Anode Sulfur Tolerance, ppm								
	Fuel Gas % (H ₂ + CO)	Oxidant Gas				Distance From Anode Inlet, cm								
		% CO ₂	% O ₂			0	15.30	30.50	45.80	61.00	76.20	91.50	106.70	122.20
0.6	85.20	32.81	42.24	32.40*	1.0040	364.9	240.9	67.8	(48.5)					
0.7	85.14	32.79	42.22	44.50*	0.7308	364.9	277.1	158.2	(50.0)					
0.8	85.00	32.75	42.17	81.40*	0.3991	364.9	310.3	245.5	167.9	102.3	62.5	(54.4)		
0.9	34.09	20.21	26.02	102.7**	0.1709	364.9	341.7	319.9	297.1	276.5	261.2	262.6	265.4	276.1

Westinghouse/Dolomite/ZnO Oxygen-Blown MCFC

Cell Resistance: 0.4035-4 ohms

Total Electrode Impedance: 1.2000 ohms-cm²

Terminal Voltage, Volts	Utilization			Location From Anode Inlet, cm	Estimated Average Current Density, Amps/cm ²	Anode Sulfur Tolerance, ppm								
	Fuel Gas %(H ₂ + CO)	Oxidant Gas				Distance From Anode Inlet, cm								
		% CO ₂	% O ₂			0	15.30	30.50	45.80	61.00	76.20	91.50	106.70	122.20
0.6	85.04	32.76	42.19	110.1*	0.2952	364.9	345.2	319.1	280.7	228.6	169.1	112.7	66.3	57.4
0.7	61.27	26.56	34.20	122.0	0.2201	364.9	355.9	343.6	324.8	297.9	263.7	225.4	188.7	156.6
0.8	24.59***	18.03	23.21	122.0	0.1535	364.9	366.7	367.4	365.7	360.9	353.1	342.6	330.9	319.9
0.9	-8.88***	9.71	12.51	122.0	0.1264	364.9	377.4	390.6	404.5	418.8	433.8	450.0	467.8	488.1

Termination Due to Attainment of Fuel or Oxidant Gas Utilization

* Termination Due to Exchange Current Density Achieved Within the Cell

** For 0.8 Volts: % H₂ Utilization = 39.19, % CO Utilization = - 7.91; for 0.9 Volts: % H₂ Utilization = 6.91, % CO Utilization = - 44.02

Table 84

Dwg. 5600C08

SULFUR TOLERANCE SUMMARY FOR THE TEXACO 14.63 cm/s ENTRAINED
FUEL GAS OXYGEN-BLOWN MCFC

MCFC Parameters

Fuel Gas Velocity: 14.63 cm/sec
Oxidant Gas Velocity: 70.10 cm/sec
Anode Inlet Temperature: 923K
Anode Outlet Temperature: 977K
Cathode Inlet Temperature: 866K
Cathode Outlet Temperature: 977K

Texaco/Benfield/ZnO Oxygen-Blown MCFC

Cell Resistance: 0.1345-4 ohms

Total Electrode Impedance: 0.4000 ohms·cm²

Terminal Voltage, Volts	Utilization			Location From Anode Inlet, cm	Estimated Average Current Density, Amps/cm ²	Anode Sulfur Tolerance, ppm								
	Fuel Gas % (H ₂ + CO)	Oxidant Gas				Distance From Anode Inlet, cm								
		% CO ₂	% O ₂			0	15.30	30.50	45.80	61.00	76.20	91.50	106.70	122.20
0.6	42.30	38.91	50.10	36.10*	1.0490	362.7	307.2	232.9	(198.5)					
0.7	41.54	38.86	50.04	48.50*	0.7801	362.7	325.8	280.2	218.8	(206.8)				
0.8	40.13	38.84	50.04	78.70*	0.4805	362.7	344.0	322.9	295.8	263.8	231.3	(226.3)		
0.9	6.72***	24.82	31.96	120.5**	0.2068	362.7	362.1	362.6	363.4	365.0	368.3	374.8	401.5	403.5

Texaco/Benfield/ZnO Oxygen-Blown MCFC

Cell Resistance: 0.4035-4 ohms

Total Electrode Impedance: 1.2000 ohms·cm²

Terminal Voltage, Volts	Utilization			Location From Anode Inlet, cm	Estimated Average Current Density, Amps/cm ²	Anode Sulfur Tolerance, ppm								
	Fuel Gas %(H ₂ + CO)	Oxidant Gas				Distance From Anode Inlet, cm								
		% CO ₂	% O ₂			0	15.30	30.50	45.80	61.00	76.20	91.50	106.70	122.20
0.6	38.71	38.80	49.97	122.20	0.3097	362.7	364.6	364.2	359.7	349.6	333.0	310.1	282.7	253.3
0.7	15.88	28.91	37.22	122.20	0.2378	362.7	370.8	377.9	382.8	384.9	383.5	378.4	369.8	358.7
0.8	-4.72 (*)	19.47	25.08	122.20	0.1651	362.7	377.0	391.3	405.3	418.6	430.8	442.1	452.4	462.1

* Termination Due to Attainment of Fuel or Oxidant Gas Utilization

** Termination Due to Exchange Current Density Achieved Within the Cell

*** For 0.9 Volts: % H₂ Utilization = 22.72, % CO Utilization = - 27.92

(*) For 0.8 Volts: % H₂ Utilization = 11.39, % CO Utilization = - 39.57

Table 85

SULFUR TOLERANCE SUMMARY FOR THE TEXACO 8.63 cm/s ENTRAINED
FUEL GAS OXYGEN-BLOWN MCFC

MCFC Parameters

Fuel Gas Velocity: 8.63 cm/sec
 Oxidant Gas Velocity: 70.10 cm/sec
 Anode Inlet Temperature: 923K
 Anode Outlet Temperature: 977K
 Cathode Inlet Temperature: 866K
 Cathode Outlet Temperature: 977K

Texaco/Benfield/ZnO Oxygen-Blown MCFC

Cell Resistance: 0.1345-4 ohms

Total Electrode Impedance: 0.4000 ohms-cm²

Terminal Voltage, Volts	Utilization			Location From Anode Inlet, cm	Estimated Average Current Density, Amps/cm ²	Anode Sulfur Tolerance, ppm								
	Fuel Gas % (H ₂ + CO)	Oxidant Gas				Distance From Anode Inlet, cm								
		% CO ₂	% O ₂			0	15.30	30.50	45.80	61.00	76.80	91.50	106.20	122.20
0.6	85.11	33.35	42.94	32.90*	1.0030	362.7	242.9	72.8	(48.6)					
0.7	85.01	33.32	42.90	45.20*	0.7298	362.7	278.1	162.5	(50.3)					
0.8	85.00	33.32	42.90	83.90*	0.5932	362.7	310.4	247.9	172.0	106.5	65.9	(54.3)		
0.9	33.00	20.39	26.25	103.3**	0.1723	362.7	340.9	320.3	298.7	278.8	264.9	265.7	268.2	279.0

Texaco/Benfield/ZnO Oxygen-Blown MCFC

Cell Resistance: 0.4035-4 ohms

Total Electrode Impedance: 1.2000 ohms-cm²

Terminal Voltage, Volts	Utilization			Location From Anode Inlet, cm	Estimated Average Current Density, Amps/cm ²	Anode Sulfur Tolerance, ppm								
	Fuel Gas % (H ₂ + CO)	Oxidant Gas				Distance From Anode Inlet, cm								
		% CO ₂	% O ₂			0	15.30	30.50	45.80	61.00	76.80	91.50	106.20	122.20
0.6	85.06	33.33	42.92	112.3*	0.2939	362.7	344.4	319.8	283.1	232.9	174.5	118.4	71.7	(57.1)
0.7	59.71	26.67	34.35	122.0	0.2210	362.7	354.8	343.7	326.1	300.7	267.7	230.4	194.2	162.1
0.8	23.16	18.11	23.31	122.0	0.1541	362.7	365.2	366.8	365.9	362.1	355.2	345.6	334.7	324.3
0.9	-9.81***	9.77	12.58	122.0	0.0855	362.7	375.7	389.3	403.7	418.5	433.9	450.6	468.8	489.5

- Termination Due to Attainment of Fuel or Oxidant Gas Utilization
- ** Termination Due to Exchange Current Achieved Within the Cell
- *** For 0.9 Volts: % H₂ Utilization = 6.07; % CO Utilization = -44.20

Figure 41 -- Projected Sulfur Tolerance as a Function of Terminal Voltage in the Low-Resistance MCFC

Figure 42 -- Projected Sulfur Tolerance as a Function of Terminal Voltage in the High-Resistance MCFC

For the MCFC operating with an incoming fuel gas velocity of 14.63 cm/s, it is apparent in Figures 41 and 42 that in the Westinghouse oxygen-blown fluidized-bed and the Texaco entrained fuel gases a higher sulfur tolerance is permitted within the anode gas channel prior to sulfidation than in the Rockwell air-blown molten carbonate and METC gravitating-bed fuel gases. When the Westinghouse fluidized-bed and Texaco entrained fuel gas inlet velocity is decreased from 14.63 to 8.63 cm/s, utilization is enhanced, while the anode sulfur tolerance is substantially reduced. As indicated by the sulfur tolerance projections, under similar cell operating conditions anode sulfidation is less likely to occur within the cell using Texaco entrained or Westinghouse fluidized-bed fuel gases and more likely to occur in a cell using METC gravitating-bed or Rockwell molten carbonate fuel gases.

Without developing a parametric series of calculations that details the effect of cell total pressure on cell performance and reactions, we shall compare the Texaco entrained Benfield/ZnO oxygen-blown system operating at 10 and at 1 atm with a terminal voltage of 0.8 V. Cell resistances of 0.4035×10^{-4} ohms and total electrode impedances of $1.2000 \text{ ohms} \cdot \text{cm}^2$ are maintained for each pressure. In the 10 atm system fuel gas utilization was projected at -4.72%, so hydrogen was being utilized in the electrolysis reaction. Converted CO_2 , however, immediately dissociated into CO and $\frac{1}{2}\text{O}_2$. In the 1 atm fuel cell, operating at the same fuel gas velocities as the 10 atm system (14.63 cm/s), 85% of the fuel gas was utilized in the first 24.6 cm from the anode inlet. A drastic sulfur tolerance reduction is evident in this region: from an initial tolerance of 477.6 ppm sulfur at the anode inlet to 67.5 ppm sulfur at 24.6 cm. At 10 atm total pressure a minimum sulfur tolerance of 362.7 ppm was obtained. An estimated average current density of 0.1651 A/cm^2 is projected for the 10 atm system, while 0.1439 A/cm^2 results in the 1 atm system after 85% of the fuel gas has been utilized.

3.3.4.6 Electrolyte Stability

Thermodynamic data are readily available for simple complexes such as LiAlO_2 , Li_2CO_3 , and K_2CO_3 , which are present in the electrolyte matrix of the MCFC. Data are unavailable, however, for electrolyte melts of the pure carbonates or of the carbonate in association with LiAlO_2 . In order to assess the stability of the 37% LiAlO_2 /63% Li_2CO_3 - K_2CO_3 matrix in the various fuel gases containing sulfur and trace constituents, molecular constants and estimates of the heat capacity as a function of temperature for 37% LiAlO_2 ·39.06% Li_2CO_3 ·23.94% K_2CO_3 and 62% Li_2CO_3 ·38% K_2CO_3 were generated from reaction of the various constituents in their standard state.

Similarly, solubility measurements of soluble salts within these mixed electrolyte complexes are also unavailable. Since gas and condensed phase solubility data have not been incorporated into the thermodynamic equilibrium model, only a cursory review of the electrolyte stability will be made at this time.

Figure 43 illustrates the stability of the LiAlO_2 , LiCO_3 , and K_2CO_3 electrolyte matrix in contact with the nickel anode in a MCFC using Rockwell molten carbonate fuel gas. At the anode inlet 62% Li_2CO_3 ·38% K_2CO_3 is projected to exist as a stable equilibrium solid phase in association with Li_2CO_3 and metallic Al and Ni. Progression along the anode to approximately 25 cm from the inlet indicates that LiAlO_2 exists in equilibrium with the 62% Li_2CO_3 ·38% K_2CO_3 . The conversion of Al to LiAlO_2 results primarily from the slightly higher oxygen partial pressure within the channel caused by carbonate ion reactions with the fuel gas H_2 and CO. The presence of 1 to 500 ppm total sulfur in the fuel gas is not projected to convert the carbonate fraction of the electrolyte into the corresponding condensed sulfates, and, therefore, the electrolyte stability appears to remain intact throughout the cell. Sulfur is removed, however, through the catalytic reactions at the anode surface, and shifts of the $\text{Ni} \rightarrow \text{Ni}_3\text{S}_2$ phase boundary reflect fuel gas compositions and cell operating parameters.

Rockwell Molten Carbonate Air-Blown MCFC

Fuel Gas Velocity: 14.63 cm/sec

Oxidant Gas Velocity: 70.10 cm/sec

Anode Inlet Temperature: 923K

Anode Outlet Temperature: 977K

Cathode Inlet Temperature: 866K

Cathode Outlet Temperature: 977K

Cell Resistance: 0.1345-4 ohms

Total Electrode Impedance: 0.4000 ohms·cm²Average Current Density: 0.1600 Amps/cm²

Terminal Voltage: 0.9167 Volts

Figure 43 -- Electrolyte Stability in MCFC

The electrolyte phase stability diagram, however, does not vary when fuel gas compositions are changed.

3.3.5 Discussion and Conclusions

Throughout this study it has become apparent that variation in the fuel or oxidant stream velocities through the electrode channels, temperature gradients within the cell, cell resistance, and electrode impedances directly affect either the resulting current density or the terminal voltage for a given system. Alternatively, trace contaminants within a specified fuel gas exist as defined groups of species in the various fuel gas environments but reflect virtually no changes in the phase stabilities when cell operating parameters such as stream velocity, cell dimensions, cell resistance, and electrode impedances are modified. Variation in the temperature gradient along the electrode, however, reflects the equilibrium stability of each phase in the specified multiphase fuel gas stream. Although this study has not extensively covered all parameters of the MCFC, the selection of two system models has identified in a limited fashion the chemical reaction trends and cell performances that would be likely to result within the MCFC if equilibrium were to be achieved.

We have devoted extensive effort in this study to the development and initial use of the computer MCFC model. The projections obtained should be viewed as a first-level approximation to the chemical environment of the anode channel without chemisorption. Our initial approach has been to humidify the incoming fuel gases enough to prevent formation of solid carbon at the anode inlet. In the equilibrated, humidified, reducing environment of CO, CH₄, CO₂, H₂, H₂O, NH₃, and N₂, sulfur contaminants were shown to exist primarily as volatile H₂S, with COS occurring as a secondary volatile phase and with traces of volatile SO₂, CS, and S₂.

We have shown that nickel reacts with the sulfur-containing fuel gas environment, forming Ni₃S₂. Although solid at MCFC operating

temperatures, its formation is known to effectively reduce the electrolytic reaction. In the MCFC system that has achieved 85% utilization of the fuel gas H_2 and CO and 50% utilization of the oxidant gas O_2 and/or CO_2 , sulfidation was shown to occur at a dramatically lower sulfur tolerance at the anode outlet than at the inlet. This is a direct result of the reduced H_2 content of the fuel gas stream after the electrolytic reaction. In the anode channel for the various systems studied, trace constituents of Na or K, which may generally be considered as active species in the sulfur environment, do not compete with nickel to form an equilibrium between Ni_2S_3 and the alkali sulfide reaction products. The alkalis exist, however, as solid carbonate phases.

A review of the sulfur tolerance projections ignoring chemisorption, indicates that bulk sulfidation of the nickel anode will occur in the Rockwell molten carbonate and METC iron oxide desulfurized fuel gases containing 132 and 139.3 ppm sulfur, respectively, while nickel remains virtually stable in the Westinghouse fluidized-bed or Texaco entrained fuel gases. Sulfidation is more likely to occur in the 0.160 A/cm^2 average current density cell at terminal voltages of 0.8 to 0.9 V, while in the 0.250 A/cm^2 cell, sulfidation is enhanced between 0.7 and 0.75 V. Reducing the fuel gas stream velocity of the Westinghouse fluidized-bed and Texaco entrained systems in order to obtain fuel and oxidant utilizations comparable to the Rockwell molten carbonate and METC gravitating-bed systems invariably reduces the sulfur tolerance to that established in the Rockwell and METC systems. In the initial incoming 51.9 and 56.3 ppb sulfur-containing Westinghouse and Texaco systems, however, sulfidation of the anode is not projected to occur.

The projected phase and phase stabilities of the trace constituents Pb, As, Zn, K, and Na in the fuel gases were shown to vary as a function of location within the cell and were directly dependent on the bulk fuel gas composition. In the fuel gases Pb was projected initially to form stable solids within the first third of the anode channel, while

volatilization occurred throughout the remainder of the anode channel because of the temperature increase. In the presence of chlorine, Pb exists as volatile $PbCl$ throughout the entire anode channel. Although conversion of the volatile Pb phase into PbS is projected in high-sulfur-containing environments, the concentration of sulfur required to promote this transition exceeds the estimated desulfurized fuel gas content.

Arsenic is projected to exist throughout the cell as either the volatile As_4 , AsH_3 , or $AsCl$ phase, depending on the initial fuel gas composition. Zinc remains predominantly as volatile Zn or $ZnCl$ in these low-sulfur environments but can react with sulfur at concentrations greater than 250 ppm in the fuel gas stream, forming solid ZnS . As a trace contaminant from either the feedstock source or the desulfurization process, both Na and K exist as stable alkali carbonates throughout the length of the cell.

The presence of carbon particulates as either graphitic carbon or tar substances in the humidified fuel gases were shown to remain as intact solids. Note that humidification was based on limiting the reverse Boudouard and water gas shift reactions in the fuel streams and does not compensate for traces of carbon or tars retained in the bulk gas phase. Contaminants such as polyethylene glycol in ether are projected to volatilize at the MCFC reaction temperature, contributing minutely to the bulk gas stream composition.

In order to account for deposition of the projected solid phases within the MCFC, an integration of the contaminant arrival rate as a function of particle size, stream velocity, and so forth, should be incorporated into the program. Also, the reduction in the electrolyte activity due to pore blockage and solids formation at the anode surface and electrolyte interface should be defined and incorporated into the thermodynamic chemical equilibrium model.

The program has defined the stability of the electrolyte matrix at the anode interface to sulfur in the fuel gas stream.

Conversion of K_2CO_3 or Li_2CO_3 in the $LiAlO_2$ melt into sulfides or sulfates is not projected to result from contact of the fuel gases with the electrolyte filled pores at the anode. These reactions are considered to result only when sulfur has been transported into the oxidizing cathode channel and subsequently diffused through the electrolyte matrix.

Reviewing the tabulated fuel cell efficiencies in which comparable utilization of 85% of the fuel gas H_2 and CO , and 50% of the oxidant has been achieved, we can rank the 0.250 A/cm^2 systems in the following order: 14.63 cm/s Rockwell molten carbonate fuel gas < 8.63 cm/s Texaco entrained fuel gas < 8.63 cm/s Westinghouse fluidized-bed fuel gas < 14.63 cm/s METC gravitating-bed fuel gas. There is less than a 1% difference in the overall fuel cell efficiency results of the Rockwell and the METC cells. On the other hand, in the 0.160 A/cm^2 systems, a limiting current density is achieved at various locations along the anode, depending on the fuel gas composition. Within the Westinghouse and Texaco systems, with stream velocities of 14.63 cm/s, relatively poor fuel gas utilization was obtained, but the gas traveled 108.6 cm prior to attaining the limiting current in the cell. On an overall fuel cell efficiency basis, these cells rank lower than the Rockwell and METC 14.63 cm/s that attained a higher fuel gas utilization, yet achieved a limiting current density at approximately 95 cm from the anode inlet. The model indicates that by increasing the average current density of the cell or reducing the terminal voltage, utilization of the fuel gas increases and effective utilization of the entire cell length increases, but cell performance decreases.

This study has demonstrated the complex interactions in the physical and chemical parameters of the MCFC. Although all cell parameters have not been considered in detail, the two models that have been identified indicate the general cell performance and chemical reaction trends that occur within the MCFC.

In conclusion, the thermodynamic equilibrium MCFC model has indicated the general magnitude of sulfur contaminant gas species in various fuel gases, and has projected the stability of trace constituent phases of Pb, As, Zn, K and Na. The significant results of this study are that:

- Sulfur tolerance of the nickel anode material near the outlet is significantly lower than that projected near the inlet.
- In air-blown fuel gas systems lower sulfur tolerances for bulk sulfidation of the anode material are projected than in oxygen-blown fuel gas systems.
- Chemisorption of H_2S has not been included in the model, so actual MCFC sulfur tolerances will be significantly lower than those projected by the equilibrium model. At equilibrium, however, extensive sulfidation of the nickel anode is projected to occur in the 0.160 A/cm^2 MCFC operating with the Rockwell molten carbonate desulfurized gases containing 132 ppm sulfur and the METC iron oxide desulfurized gases containing 139.3 ppm. Increasing the average current density reduces fuel and oxidant gas utilization while increasing the sulfur tolerance for the $Ni \rightarrow Ni_3S_2$ conversion.
- With rigorous desulfurization techniques considered in the Westinghouse fluidized-bed and Texaco entrained systems, and the zinc oxide polished Rockwell molten carbonate and METC iron oxide systems sulfur levels of 52 to 70 ppb will not promote sulfidation at any location along the anode.
- Traces of Pb are projected to form stable solids within the initial third of the anode channel prior to volatilizing. In the presence of chlorine volatile $PbCl$ forms throughout the entire cell. Arsenic and Zn remain predominantly as volatile phases of As_4 , AsH_3 , $AsCl$, Zn, or $ZnCl$, depending on the local fuel gas environment. Traces of alkali present in the fuel form stable solid carbonates throughout the entire cell length. Carbon as graphitic particles or as tars exists as condensed phases in the humidified fuel gas stream.
- The electrolyte matrix has been projected to maintain its stability in contact with the reducing fuel gases. The model does not have adequate solubility data available for us to be able to thoroughly evaluate the interactions of trace contaminants within the Li_2CO_3 - K_2CO_3 or Li_2CO_3 - K_2CO_3 - $LiAlO_2$ matrix.
- Reduction in total cell pressure lowers the minimum allowable sulfur tolerances of the nickel anode material.

3.3.6 Recommendations for Future Study

Five areas have been identified for future study. These include:

- Inclusion of experimentally determined effects of H_2S/COS chemisorption on the anode for pressurized cell operations.
- Extending the cocurrent modeling capabilities so that alternative cross-flow and counterflow MCFC designs can be considered.
- Demonstrating the interaction of sulfur and trace constituents in the oxidant gas streams with the cathode surface and electrolyte matrix.
- Defining the trace constituent solubilities in the electrolyte matrix and evaluating their possible detrimental effect on the electrolysis reaction.
- Integrating the contaminant arrival rate as a function of particle composition and size, stream velocity, and so on, into the equilibrium MCFC model, and defining the reduction in the electrolytic and current-generating capacity of the cell caused by blockage of pores by solid deposition products formed at the anode and cathode surface and at the electrolyte interface.

Section 4

DEFINITION OF PROCESS CONFIGURATION

4.1 INTRODUCTION

Section 4 defines process configurations and selects those suitable for detailed evaluation of their ability to supply fuel to molten carbonate fuel cells in industrial and utility power plants. The information and data necessary for this process configuration definition were extracted from sources in the public domain, including reports from DOE, EPRI, and EPA; work sponsored in whole or in part by Federal agencies; and from trade journals, MCFC developers, and manufacturers. The configurations considered for detailed evaluation include entrained, fluidized-bed, gravitating-bed, and molten salt gasifiers, both air and oxygen blown. Desulfurization systems utilizing wet scrubbing processes, such as Selexol and Rectisol II, and dry sorbents, such as iron oxide and dolomite, were also considered. The method used to select systems for detailed evaluation includes a review of process and plant parameters, a listing of major evaluation criteria, flow diagrams with material and energy balances, selection of a reference wet cleanup system, and a matrix evaluation leading to recommendations of systems for detailed study in Sections 5 and 6 of this report. Major criteria for defining process configurations are established in Section 4.2. Process and plant parameters, including plant size, oxidant used, utility and industrial options, and coal selection are reviewed, along with environmental characteristics, cost of electricity, and reliability. A decision matrix has been established and weighting factors derived to use in evaluating processes to recommend for detailed study.

Section 4.3 provides flow diagrams with material and energy balances for the 17 proposed configurations. Section 4.4 selects a

reference wet cleanup system in accordance with contract requirements. Section 4.5 develops the matrix evaluation based on criteria and weighting factors from Section 4.2 and recommends configurations for detailed study.

4.2 DEFINITION OF PROCESS CONFIGURATION CRITERIA

In this section, we shall define those processes and plant parameters that affect process system design. The process parameters include size of facilities, oxidant to be employed in the gasifier, coal to be employed, gasifier types, and cleanup system types. Some process parameters have been assigned numerical values. The most suitable fuel processing equipment (gasifier types, gas cleanup system types) have been defined. The gas cleanup systems have been characterized by their principal duty: desulfurization. Ancillary gas cleanup equipment for control of particulates and such trace elements as chlorine and heavy metals will be added to the most suitable desulfurization systems, as required.

Since there are alternative MCFC power plant applications for both the utility-size and the industrial-size power plant, numerous configurations of gasifiers and cold gas cleanup systems can be postulated. These configurations require a process of evaluation and rating against certain selection criteria to reduce their number to a maximum of 12, as DOE has specified for this study.

Westinghouse has developed a process for making such a selection. The three basic steps involved are:

- 1) Determination of the relative importance of each performance or evaluation criterion
- 2) Rating of each feasible design concept against each performance or evaluation criterion, one concept against another
- 3) Calculation of figures of merit for each design concept and determination of the preferred concept.

For the first two steps, evaluations are arranged so that only two alternatives are considered at a time, employing every possible combination. Subjective judgment is reduced to a simple yes or no decision for each evaluation. In this manner the relative ranking for each aspect of the decision is derived rather than assigned.

The third step then produces a mathematically derived set of figures of merit for each configuration and each evaluation criterion. After summation, the largest figure of merit identifies the configuration that best satisfies the evaluation criteria, and so on. The first step, which is the derivation of a decision matrix to determine the relative importance of each evaluation criterion set, will be performed in this section. The second and third steps will be performed in Section 4.5, after flow diagrams and material and energy balances have provided a basis for ranking efficiency and complexity and after a reference wet cleanup system has been selected.

4.2.1 Criteria for Evaluation

4.2.1.1 Size of Facility

Two plant sizes, one for an electric utility and another for industrial applications, were selected as appropriate for consideration. The industrial electric plant size was determined from a study Westinghouse performed after surveying several industries suitable for cogeneration and investigating and comparing their power demands.⁷¹ They found an electric energy demand of 50 MW to be representative of many industrial power plants. The utility facility was based on the availability of utility size steam turbines and hot gas expansion turbines to be used in the power-producing "bottoming" cycles appropriate for MCFC power plants, and on the recent trends in utility power plant size. The average U.S. fossil-fueled utility power plant commissioned in 1982 is smaller than 400 MW, and the availability of utility-type generating equipment dictates that the total output of the

utility size MCFC system be at least 250 MW. Accordingly, the utility size facility to be evaluated will be in the 250/300 MW size range.

4.2.1.2 Type of Oxidant

In the ECAS Phase II Final Report⁷² the efficiency and cost of the fuel cell were found to differ only minimally when oxygen- and air-blown gasification were considered. Actually, the air-blown system was found to result in a simpler design, with more flexible operating characteristics for part-load operation.

Internally, Westinghouse has made an overall performance evaluation, comparing air- and oxygen-blown gasifiers for an integrated gasification/ combined-cycle (gas turbine/steam turbine) utility power generating system. A summary study evaluation comparing these two alternatives using Illinois No. 6 coal is shown in Table 86.

Table 86
COMPARISON OF OXYGEN-BLOWN/AIR-BLOWN GASIFIER, 1000 MW SIZE

	<u>Oxygen Blown</u>	<u>Air Blown</u>
Total Plant Investment, \$/kW	577	532
Total Capital Requirements, \$/kW	728	672
Overall Efficiency, %	38.5	40.5

While both the ECAS II⁷² study and the internal Westinghouse combined-cycle study rank air-blown gasifiers above oxygen-blown gasifiers, the differences between the two are not great. When the size of the system is reduced to that appropriate for industry, however, the high cost per unit of output obtained in the small oxygen plant required for the industrial application increases the attractiveness of the air-blown system.

An economic comparison, EPRI Report AP-1543,⁷³ ranked the oxygen-blown gasifier concept above the air-blown for application in a utility size, molten carbonate fuel cell. In the present study, both oxygen-blown and air-blown gasifiers will be integrated with the molten carbonate fuel cell for the utility system. For the industrial size concept, however, the air-blown case alone is attractive because of the simpler design and flexible operating characteristics provided by a system that does not require integration with an oxygen plant.

4.2.1.3 Type of Coal

Illinois No. 6 was selected as the primary coal for this study because its properties are well known, and much has been published on its use in pilot and demonstration plants, particularly by EPRI. For the air-blown Westinghouse cases, Ohio No. 9 coal will be used in place of Illinois No. 6 because that is the basis for information in the public domain on the Westinghouse air gasification tests.

4.2.1.4 Gasifier Types

A number of coal gasification processes are available with varying degrees of energy efficiency and overall cost effectiveness. In order to select a particular gasification process, one is required to evaluate its characteristics in the framework of the following decision factors.

The coal-derived fuel gas must be compatible with the fuel cell so as to maximize cycle efficiency. The projected methane content must be considered, since methane is an electrochemically inert species and must be consumed in the less efficient bottoming cycle. IGT states that, although data are unavailable, "tolerance is expected to be low" for hydrocarbons of higher molecular weight than ethane.⁷⁴ The gas, therefore, should not contain light oils and tars, which could hinder system performance efficiency, nor should the raw coal gas contain a high water vapor content, which could also hinder gasification efficiency.

Cold gas efficiency is defined as the ratio of the heating value of the product gas to the heating value of the coal. Even more helpful for this work would be the heating ratio of the value of the potential hydrogen ($H_2S + CO$) to the heating value of the coal, which eliminates methane and heavier hydrocarbons. This cold gas efficiency, if high, would not only lower equipment cost (higher throughput per unit capacity), but would also contribute to a lower heat rate for the integrated power plant.

The reliability of a coal gasifier would be judged by its ability to withstand off-design operating conditions, such as interruptions in coal feed, loss of oxidant and/or steam flow, and blockage in the ash withdrawal port. The controllability would determine its turndown ratio and the speed of its response to load changes in the downstream end of the power plant.

Economics strongly favors operation of the molten carbonate fuel cell under pressure. The capacity of the cells increases much more rapidly than the cost in the pressure range of up to at least 1013 kPa (10 atm), thus strongly favoring gasifiers that operate under pressure.⁷⁵

The fuel cell commercialization effort would realize maximum benefit by applying the most cost-effective coal gasification technology. The technical feasibility of the gasifier should have been demonstrated in a facility capable of direct scale-up to a commercial plant. Process know-how and, more importantly, information on the reliability of various hardware components and materials of construction must be available for scale-up purposes within the time frame of the proposed program.

In the final analysis the success of an integrated fuel cell power plant would be dictated by costs, both capital and operating. Table 87 presents the minimum characteristics judged to be most desirable in terms of gasification economics, along with the economic effects of these characteristics and the necessary operating conditions.

Table 87

Dwg. 4251B98

DESIRABLE CHARACTERISTICS OF ADVANCED GASIFICATION PROCESSES
FOR PRODUCING COAL GAS

Desirable Characteristics	Economic Effects	Process Conditions Leading to Desirable Characteristics		
		Temperature	Pressure	Other Conditions
1. High specific gasification rate	Fewer gasifiers, decreased investment*	High	High	High heat and mass transfer rates
2. Minimum gasification by-products	Decreased investment in recovery facilities possibly increased gasification efficiency [†]	About 816°C (1500°F) or greater	Little effect	—
3. Maximum flexibility in coal size	Decreased investment for coal grinding, no loss of fines	No effect	No effect	Minimum carry-over of fines, high heat and mass transfer rates
4. Ability to process caking coals	Reduced coal pretreatment losses, decreased investment, increased gasification efficiency	High, to prevent caking	Little effect	Stirring of fixed beds and jet injection into fluidized beds
5. Minimum oxygen or air requirements	Decreased investment, increased gasification efficiency, increased methane content in product gas	Low	High	Countercurrent flow of coal and oxygen (air)
6. Minimum gasifier steam requirements	Decreased investment in waste heat or auxiliary boilers	High	Depends on process	—
7. Minimum loss of unreacted carbon	Increased gasification efficiency	High	High	Molten bath advantageous
8. Minimum compression power	Decreased investment, possibly increased gasification efficiency	Low	Slightly higher than that desired for product gas	Use of oxygen rather than air if gasification pressure greatly exceeds 690 kPa (100 psia)

*Decreased investment resulting from desired characteristic alone. Method of achieving the particular characteristic may add enough investment to result in a net increase in investment.

[†]Increased gasification efficiency will usually result in decreased investment because of the reduced amount of coal being handled and gasified.

All gasifier types -- fixed bed, fluidized bed, entrained bed, and miscellaneous types such as the molten salt reactor -- are applicable for the molten carbonate fuel cell.

The molten carbonate fuel cell operates at an elevated pressure of at least 931 kPa (135 psig). It would be advantageous, therefore, to operate the gasifier at least from 931 kPa (135 psig) to 6895 kPa (1000 psig). The wet gas cleanup system would also benefit from high pressure [6895 kPa (1000 psig) is about the limit for economical absorption].

4.2.1.5 Gas Cleanup System Types

Hot, raw, product gas leaving the gasifier can contain tars, char, particulate matter, and small quantities of sulfur compounds and ammonia. Other elements, such as alkali and heavy metals, hydrogen cyanide, and halogen compounds, appear in trace amounts, although there is little information on their effect on the molten carbonate fuel cell.

There is also little information on the removal of particulates in the cold gas cleanup system; and the same is true of trace elements. Section 3.3 discusses some possibilities for particulate and trace element removal in water scrubbers before the gas reaches the cold gas cleanup system.

Sulfur compounds have been identified as critical contaminants of the fuel cell. These compounds adversely affect fuel cell performance and life expectancy. Of the sulfur compounds found in coal gas, H_2S is the primary compound. As much as 95% of the total sulfur compounds have been identified as H_2S . The sulfur compound found in the next largest quantity in the raw gas stream is COS, which is generally found in concentrations equal to about 10% of the H_2S . Even though initially less than 1 vol %, both COS and H_2S must be removed to still lower concentrations, probably 1 ppm or less.

The cold gas cleanup system types are amine-chemical absorbent, alkali salt chemical absorbent, physical absorbent, combined

physical-and-amine absorbent, and direct liquid phase oxidation absorbent. The constraint of total sulfur removal (which includes COS and H₂S) allows all except direct liquid phase oxidation absorbents, which cannot remove COS, to be considered for further study.

The hot gas cleanup system types are metal oxide adsorbents, naturally occurring chemical adsorbents (limestone, dolomite), or molten materials (salts, metals). The low sulfur levels required in the clean gas require multiple system cleanups.

The criteria discussed previously are summarized below. The gasifiers were selected from each category of gasifier type. These were the criteria used:

- 1) The fuel gas should have a low methane content.
- 2) The coal gas must be free of oils and tars.
- 3) The gasifier must have a good (H₂ + CO) efficiency.
- 4) The gasifier must be able to handle upsets in coal and oxidant feed.
- 5) Load-following capabilities must be met by the gasifier's turndown ability.
- 6) The gasifier must operate at at least 931 kPa (135 psig) but no higher than 6895 kPa (1000 psig).
- 7) The gasifier must handle all types of coal.
- 8) The gasifier must at least be demonstrated at a size where scale-up information (to commercial size) is known and available.

Prior to the listing of the gasifiers in Section 2.2, the high-methane-producing gasifiers were identified and omitted, so all the gasifiers listed meet condition 1, low methane content in fuel gas. Condition 3 specifies good efficiency. A numerical value has been derived for each gasifier in Section 4.3.

Both industrial- and utility-sized facilities are considered in this study, with an oxygen-blown gasifier to be used for the utility facility and an air-blown gasifier to be used for the industrial

facility. Selection of gasifiers, therefore, must be specified for each facility. Table 88 lists the gasifier selections.

Gas cleanup systems were selected for further consideration by reference to the salient points discussed in Section 2.2. They are summarized below:

- The total sulfur concentration in the feed gas to the fuel cell must be below 1 ppm.
- Halogens in the feed gas to the fuel cell must be limited to 10 ppm.
- Sulfur compounds from sorbent regeneration must be in a form suitable for sulfur production in Claus or Resox plants.
- The system should not produce dangerous compounds and should be environmentally acceptable.
- System sorbents must be compatible with constituents in the feed gas.
- Experimental data must be in the public domain to provide a basis for design of equipment for sorption and desorption, and of sorbent life.

Table 89 lists the cold gas cleanup selections and Table 90 the hot gas cleanup selections.

Those plant parameters considered important for selecting plant configurations were considered for this subtask: plant sizes, oxidant to be employed, coal to be used, gasifiers to be employed, and cold gas cleanup systems to be employed. They are listed in Table 91.

4.2.2 Major Evaluation Criteria

The five gasifiers identified in the Process and Plant Parameters Review, plus the four desulfurization systems, provide a large number of combinations of gas supply and gas cleaning. Evaluation criteria will be used to rank those combinations to choose the most suitable systems for detailed study. Each contains elements that require environmental, cost, efficiency, and reliability assessment. This section of the report will list the pertinent factors to be

Table 88
GASIFIER SELECTIONS

Dwg. 5600C34

	Footnote	Does Not Produce Tars & Oils	Can Use All Types of Coals	Can Use Both Oxygen & Air	Has Operated at 1013 kPa (10 atm) to 6888 kPa (66 atm)	Has Turndown Capability	Demonstrated
<u>Fixed-Bed Gasifiers</u>							
Lurgi		No	No	Yes	Yes	Yes	Yes
BGC/Lurgi Slagging	X	Yes (1)	Yes	Yes (1)	Yes	Yes	Yes
METC Stirred Bed		No	Yes	No	Yes	Yes	No
Wellman-Galusha		No	No	Yes	No	Yes	Yes
Foster Wheeler Sluic		No	No	No	No	Yes	Yes
Woodall Duckham/Gas Inbagrade		No	No	Yes	No	Yes	Yes
Wellman Incandescent		No	No	No	No	Yes	Yes
Slagging Fixed Bed (DOE)		No	No	Oxygen Only	Yes	Unknown	No
Riley Margin		No	Yes	No	No	Yes	Yes
Wilputte		No	No	No	No	Yes	Yes
<u>Fluidized-Bed Gasifiers</u>							
Winkler		Yes	No	Yes	No	Yes	Yes
Rheinbraun High-Temperature Winkler		Yes	No	Yes	Yes	Yes	Yes
Westinghouse Pressurized	X	Yes	Yes	Yes	Yes	Yes	Yes
Carbon-Dioxide Acceptor		Yes	No	NA	Yes	Unknown	No
Synthane		No	Yes	Yes	Yes	Yes	No
Tri-Gas		Yes	Yes	Yes	Unknown	Unknown	No
U-Gas	X	Yes	Yes	Yes	Yes	Yes	Yes
BCR Low Btu		Yes	Yes	Air Only	Yes	Unknown	No
Battelle/Carbide	+	Yes	Unknown	Unknown	Yes	Unknown	No
<u>Entrained-Bed Gasifier</u>							
Texaco	X	Yes	Yes	Yes (2)	Yes	Yes	Yes
Koppers Totzek		Yes	Yes	Yes	No	Yes	Yes
Foster Wheeler		Yes	Yes	No	Yes	Unknown	No
Combustion Engineering		Yes	Yes	No	No	Unknown	Yes
Bi-Gas	+	Yes	Yes	Yes	Yes	Unknown	No
Babcock and Wilcox	+	Yes	Yes	Yes	Yes	Yes	Yes
Shell-Koppers	•	Yes	Yes	Yes	Yes	Unknown	Yes
<u>Miscellaneous</u>							
Atomics International/Rockwell Molten Salt	X	Yes	Yes	No	Yes	Yes	Yes
Pullman-Kellogg Molten Salt	+	Yes	Yes	No	Yes	Unknown	No
Otto-Rummel		Yes	Yes	Yes	No	Yes	No
ATGAS	+	Yes	Yes	Yes	No	Unknown	No
Saarberg/Otto	+	Yes	Yes	Yes	Yes	Unknown	No
Kiln Gas		No	Yes	No	No	Yes	No

X - Denotes chosen for further consideration

+ - Not fully developed or limited information

(1) - Limited information on air-blown operation; recycles all tar and oil to the slagging zone.

(2) - Air-blown information limited.

Table 89
WET CLEANUP PROCESS SELECTIONS*

Process	Limit H ₂ S and COS to 1 ppm	Economical Sulfur Recovery	Compatible with Constituents in Feed	Environmentally Acceptable
MEA	Yes	Unknown	No	Unknown
DEA	No	Unknown	No	Unknown
SNPA-DEA	No	Unknown	No	Unknown
ADIP	No	Unknown	No	Unknown
MDEA	No	Unknown	No	Unknown
Fluor Econamine	No	Unknown	No	Unknown
Alkazid "DIK"	No	Yes	No	Unknown
Benfield HiPure	Yes	Unknown	Yes	Yes
Catacarb	No	Unknown	Yes	Unknown
Hot Pot	No	No	Yes	Unknown
Amisol	Yes	Unknown	No	Unknown
Sulfinol	Yes	Yes	No	Unknown
Estasolván	No	Unknown	Yes	Yes
Fluor Solvent	No	Unknown	Yes	Yes
Purisol	No	Unknown	Yes	Yes
Rectisol II X	Yes	Yes	Yes	Yes
Selexol X	Yes	Yes	Yes	Yes

*All processes listed have been adequately demonstrated are able to remove HCN, NH₃, and HCl via an aqueous prewash and require zinc oxide backup desulfurizer.

X - Selected for further study.

Table 90
HOT GAS CLEANUP PROCESS SELECTIONS*

Process	H ₂ S/COS Effluent Level ppmv	Demonstrated to Remove Halogens	Environmentally Acceptable	Demonstrated Adequately for Scale-up
X METC Iron Oxide	200 to 800	No	Yes	Yes
Appleby-Frodingham	< 150	No	Yes	No
Air Products Dolomite	~ 600	No	Yes	No
Conoco Half-Calcined Dolomite	200 to 300	No	Yes	Yes
X Westinghouse Dolomite	< 600	No	Yes	Yes
U.S. Steel Dolomite	< 65	No	Unknown	No
Battelle Molten Salt	< 40	Yes	Unknown	No
IFP Zinc Oxide	< 500	Unknown	Yes	No
METC Zinc Ferrite/Zinc Oxide	< 10	Unknown	Yes	No

• All Processes Listed Require Zinc Oxide Backup Desulfurizer.

X Denotes Selected for Further Study.

Table 91
PLANT PARAMETERS

Plant Size		
Utility application		250 to 300 MW
Industrial application		50 MW
Oxidant to Be Employed		
Utility application		Oxygen or air
Industrial application		Air
Coal to be Used		Illinois No. 6 or Ohio No. 9
Gasifier Type*	Utility application	Industrial application
	Fixed bed	BGC/Lurgi slagging --
	Fluidized bed	Westinghouse Westinghouse
	Entrained bed	Texaco --
	Molten salt	-- Rockwell
Pressure Level		931 to 6895 kPa (135 to 1000 psig)
Gas Cleanup Systems (both applications)		
Selexol	Iron oxide + zinc oxide	
Rectisol II	Molten carbonate + zinc oxide	

*Because of the similarity of the fluidized-bed coal gasification systems under development by Westinghouse and by U-Gas (IGT) and of the much more extensive amount of operating data available for the Westinghouse system in the pressure range suitable for MCFC operation [931 kPa (135 psig) and higher], the Westinghouse process will be used in subsequent evaluations to represent either system, U-Gas or Westinghouse.

considered in each of those four categories of criteria. The listing will then be used to derive a decision matrix.

Environmental characteristics of polluting equipment are included in the following list:

- Coal Storage
 - Particulate and fugitive dust
 - Coal pile runoff
- Coal Preparation
 - Particulate and fugitive dust
 - Wastewater from drains, dust control, cooling
 - Solid waste (undersize coal)
- Fuel (coal) Conversion
 - Combustion gases from start-up boiler
 - Wastewater such as sluice water
 - Solid waster (ash)
- Waste heat Recovery, COS Hydrolysis, Gas Scrubbing, and Sorption
 - Solid waste (entrained ash and unreacted coal)
 - Spent catalyst from COS hydrolysis
 - Wastewater from scrubbers and boiler blowdown.
- Gas Cleanup
 - Claus tail gas cleanup off-gas
 - Off-gases from start-up boiler
 - Off-gases from start-up ZnO polishers, reheaters
 - Cooling tower blowdown
 - Wastewater from absorber knock-out drum
 - Boiler blowdown from Claus plant
 - Sulfur from Claus plant
 - Spent catalyst from ZnO converters

The Clean Water Act and the Clean Air Act and their amendments will be satisfied by the use of proper pollution control techniques or equipment.

Comparisons of configurations will be based on such factors as size of coal required, amount of ash entrained in the raw gas, and the cleanup system's sulfur concentration in the gas stream to the Claus plant. these factors will increase or decrease facilities required to treat their respective pollutants.

4.2.2.1 Cost of Electricity

The cost of electricity depends on three categories of information: description of firm, general economic conditions, and description of power plant. The first two categories, although important, are not considered here since they are common to all the power plant configurations. Only the power plant description is applicable. The pertinent information for evaluations is:

- Cash Flow
 - Capital investment
 - Operating costs
 - Maintenance costs
- Lifetime of Plant
- Plant Capacity
- Capacity Factor.

The last three points outlined above are assumed to be common to all configurations and are excluded from further discussion. Estimated costs will then be placed on the major pieces of equipment to provide a means to compare configurations.

4.2.2.2 Conversion Efficiency

Conversion efficiency is the ratio of the energy that leaves the fuel conversion plant to that entering the plant. The fuel conversion plant is comprised of the coal gasification process, waste

heat recovery, and gas cleanup system. Each of these subsections has its own efficiency and was discussed in Section 2. Here it is integrated and must also show compatibility with other equipment, along with its inherent efficiency. An estimate of the coal to clean fuel gas efficiency will be sufficient to compare configurations and will be based on the data in Section 4.3 of this report.

4.2.2.3 Reliability

The development of evaluation criteria related to reliability will be composed of two separate concepts, one to identify a number of components as criteria and the other to identify the state of development as its criterion. Each concept will then be assigned, following certain guidelines, a high, low, or medium rating.

For the former concept, each major component part is considered as one block, and each block is considered equal in importance. The number of blocks, therefore, will influence the rating of reliability: the greater the number of blocks, the less reliable the system. For the latter concept, such factors as state of development (pilot, demonstration, or commercial phase) and duration of operation of the plant will influence the rating for reliability.

Selection criteria that needed to be identified to prepare the decision matrix, have been discussed. Since it was our intent to develop only selection criteria here, numerical values or ratings will be assigned in Section 4.4. The following lists the selection criteria developed:

1. Environmental Characteristics
 - a. Coal storage
 - b. Coal preparation
 - c. Fuel conversion
 - d. Waste heat recovery, COS hydrolysis, gas scrubbing, and sorption
 - e. Gas cleanup

2. Cost of Electricity
 - a. Capital investment
 - b. Operating costs
 - c. Maintenance costs
3. Conversion Efficiency
 - a. Heat rate
4. Reliability
 - a. Number of components
 - b. State of development of system.

4.2.3 Decision Matrix

All eleven decision criteria listed above are rated relative to each other. For example, 1a, coal storage environmental characteristics, is judged relative to 1b, coal preparation environmental characteristics. The judgment is based on the importance of each element in achieving an environmentally acceptable installation. Since coal storage requires a large land area, can produce undesirable runoff from rain, and involves both setting coal in place and removing it for processing, we judged it to be a more important factor in an environmental sense than coal preparation, which is compact and relatively easily controlled by bag filters, or noise reduction from either dust or noise pollution. Further on in the matrix evaluation, 1a, coal storage environmental characteristics are judged to be less important than 1e, gas cleanup, or 2a, capital investment for the overall facility. In this way each of the criteria is judged on a yes/no or greater/lesser importance basis, and a set of weighting factors is then derived.

The decision matrix, Table 92, shows that the five environmental criteria received a total of 10 yes decisions out of 55 decisions to be made. Thus, $10/55 = 0.182$ is the weighting factor for environmental characteristics compared to cost of electricity, efficiency, and reliability.

- a) Selection Criteria
 - 1. Environmental Characteristics
 - a. Coal Storage
 - b. Coal Preparation
 - c. Fuel Conversion
 - d. Waste Heat Recovery, CoS Hydrolysis, & Scrubbing
 - e. Gas Cleanup
 - 2. Cost of Electricity
 - a. Capital Investment
 - b. Operating Costs
 - c. Maintenance Costs
 - 3. Conversion Efficiency
 - a. Heat Rate
 - 4. Reliability
 - a. Number of Components
 - b. State of Development of System

Note that, for the cost of electricity, operating costs involve coal consumption, which depends on efficiency. Thus, overall, efficiency will enter into the final matrix evaluation in Section 4.4 of this report to a greater extent than indicated by the 0.273 weight derived for it in the decision matrix.

4.3 PROPOSED CONFIGURATIONS

In Section 4.2 the most applicable gasifiers were identified along with the most applicable gas cleanup systems.

The British Gas Council (BGC)/Lurgi Slagging Gasifier can be used with all four of the gas cleanup systems, although it is configured to recover and recycle to extinction the tars and oils contained in the raw coal gas. This tar and oil recovery is a part of the BGC/Lurgi process. Gas containing tar and oil is not acceptable for MCFC systems and is difficult to pipe, expand, recover heat from, etc., and so the recycling of tar and oil to extinction in the gasifier is mandatory for the purpose of this study. That requires coal gas cooling to well below the fuel cell operating temperature, and part of the coal gas must be burned in a reheater to permit use of iron oxide or dolomite for desulfurization.

Texaco and Westinghouse gasifiers do not require tar and oil recycle, since coal gas from them contains essentially no tar/oil. The gas from those two gasifiers can be cooled by appropriate heat recovery apparatus to either wet desulfurization or dry desulfurization temperatures.

The Rockwell molten salt (molten carbonate) gasifier is unique. It produces a gas already bulk desulfurized, with sulfur compound levels of approximately 40 ppmv. Likewise, the gas is low in halogen content. For this study the Rockwell gas is assumed to require only conventional zinc oxide final desulfurization, but at MCFC temperature levels of $\sim 650^{\circ}\text{C}$ (1200°F).

The Rockwell gasifier has only been tested using air as an oxidant. The Westinghouse gasifier was originally developed as an air-blown system, but since 1977 has also had many thousands of hours of hot testing on oxygen. All of the data for those gasifiers is in the public domain.

The Texaco and BGC/Lurgi gasifiers are proprietary. A large amount of test data on the oxygen-blown BGC/Lurgi unit, however, are available from OCR-, ERDA-, DOE-, and EPRI- funded reports. This is also true to a lesser extent of the Texaco oxygen-blown gasifier. There are no test data on the air-blown BGC/Lurgi slagging, and only limited data on the air-blown Texaco gasifier at Montebello. Those air-blown Texaco data are described, in EPRI's report AP-1543⁷³ as "in a less advanced state of development than the oxygen-blown version." We have chosen, therefore, to use the Texaco and BGC/Lurgi gasifiers only in the oxygen-blown mode for this report.

The gasifier and desulfurization systems can then be summarized as:

- Texaco Oxygen-Blown Entrained Gasification with
 - Selexol
 - Rectisol II
 - METC Iron Oxide
 - Dolomitefor bulk desulfurization
- BGC/Lurgi Oxygen-Blown Gravitating Bed Gasification with
 - Selexol
 - Rectisol II
 - METC Iron Oxide
 - Dolomitebulk desulfurization

- Westinghouse Oxygen-Blown Fluidized-Bed Gasification with
 - Selexol
 - Rectisol II
 - METC Iron Oxide
 - Dolomite
 bulk desulfurization
- Rockwell Molten Salt Air-Blown Gasification with in-situ Bulk Desulfurization
- Westinghouse Air-Blown Fluidized-Bed Gasification with
 - Selexol
 - Rectisol II
 - METC Iron Oxide
 - Dolomite
 bulk desulfurization.

4.3.1 Flow Diagrams With Material and Energy Balances

These seventeen configurations are the subject of the flow diagrams and material and energy balances that follow.

4.4 REFERENCE WET CLEANUP SYSTEM

This section satisfies the contractual requirements for selection of a wet gas cleanup reference system.

Criteria for the selection of a wet gas cleanup system are divided into three areas: Area 1 defines the system's ability to control the level of acid gases in the purified gas stream and in the stream going to a Claus plant; Area 2 identifies feed gas diversities resulting from swings in gasifier operation; and Area 3 includes operational considerations.

Directly affecting gas cleanup selection criteria are fuel cell design constraints for sulfur and trace elements. As was intended for this effort, assumptions based on previous MCFC studies are used. The following briefly summarize these assumptions. Pressure is assumed

[illegible]

9 INCLUDES 200.00 LB./MR TACS/OILS

BASIS: 1 TON DRY COAL/H.R.

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PROCESS FLOW DIAGRAM
BGC-LURGI SLAGGING-OXYGEN
BLOWN GASIFIER w/RECTISOL II

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* INCLUDES 36.90 LB/HR TARS & OILS BASIS: 1 TON DRY COAL/HR

R 4

[illegible]

PROCESS FLOW DIAGRAM
BGC-LURGI SLAGGING-OXYGEN
BLOWN GASIFIER W/SELEXOL

STREAM NO.	IDENT.	OXYGEN TO GASIFIER	COAL TO GRINDING & SLURRY PUMP	GAS TO H ₂ S COS REMOVAL	CLEAN GAS	ACID GAS TO CLAMS PLANT	REJECT WATER	SLAG/ASH CAKE (DRY)	RAN WATER TO DEWATERING	WASTE WATER	H.P. B.F.W. TO N.H.B.	N.P. B.F.W.	H.P. STEAM	L.P. B.F.W. TO N.H.B.	L.P. STEAM	WATER TO AMMONIA ABSORBER	MAKE UP WATER TO AMMONIA ABSORBER	WASTE WATER FROM RECTISO	NITROGEN TO STRIPPER
1	CH ₄			0.18	0.17	0.01													
2	H ₂			63.07	68.06	0.01													
3	CO			98.74	98.25	0.38													
4	CO ₂			19.68	18.38	4.30													
5	H ₂ S			2.27	1.00	2.27													
6	CO ₂			0.14	—	—													
7	H ₂	0.83		1.80	1.80	0.0002													
8	A ₂	0.27		0.27	0.27	0.0002													2.47
9	O ₂	23.60		—	—	—													
10	H ₂ O(l)			0.39	—	—							177.36		30.86				
11	COAL (LB/HR)		2000																
12	TOTAL WASH MPH	34.70		88.22	177.87	4.7							177.36		30.86				2.47
13	H ₂ O(l)	1749.31	2027.00	2027.00	3335.6	361.68	128.62	167.0	267.08	97.44	6084.28	3600.66	177.36	469.7	355.97	97.44	335.7	5.78	69.05
14	PRESSURE (PSIA)	735	847	847	847	847	847	847	847	847	847	847	847	847	847	847	847	847	847
15	TEMPERATURE (°F)	300	300	300	300	300	300	300	300	300	300	300	300	300	300	300	300	300	300

STREAM NO.	IDENT.	OXYGEN TO GASIFIER	COAL TO GRINDING & SLURRY PUMP	GAS TO H ₂ S COS REMOVAL	CLEAN GAS	ACID GAS TO CLAMS PLANT	REJECT WATER	SLAG/ASH CAKE (DRY)	RAN WATER TO DEWATERING	WASTE WATER	H.P. B.F.W. TO N.H.B.	N.P. B.F.W.	H.P. STEAM	L.P. B.F.W. TO N.H.B.	L.P. STEAM	WATER TO AMMONIA ABSORBER	MAKE UP WATER TO AMMONIA ABSORBER	WASTE WATER FROM RECTISO	NITROGEN TO STRIPPER
1	CH ₄			0.17															
2	H ₂			63.07															
3	CO			98.74															
4	CO ₂			19.68															
5	H ₂ S			2.27															
6	CO ₂			0.14															
7	H ₂	0.83		1.80															
8	A ₂	0.27		0.27															
9	O ₂	23.60		—															
10	H ₂ O(l)			0.39									177.36		30.86				
11	COAL (LB/HR)		2000																
12	TOTAL WASH MPH	34.70		88.22									177.36		30.86				
13	H ₂ O(l)	1749.31	2027.00	2027.00	3335.6	361.68	128.62	167.0	267.08	97.44	6084.28	3600.66	177.36	469.7	355.97	97.44	335.7	5.78	69.05
14	PRESSURE (PSIA)	735	847	847	847	847	847	847	847	847	847	847	847	847	847	847	847	847	847
15	TEMPERATURE (°F)	300	300	300	300	300	300	300	300	300	300	300	300	300	300	300	300	300	300

MATERIAL BALANCE FOR TEXACO-OXYGEN BLOWN GASIFIER W/RECTISOL II (BASIS: 1.0 TON DRY COAL/HR)

STREAM NO.	IDENT.	OXYGEN TO GASIFIER	COAL TO GRINDING & SLURRY PUMP	GAS TO H ₂ S COS REMOVAL	CLEAN GAS	ACID GAS TO CLAMS PLANT	REJECT WATER	SLAG/ASH CAKE (DRY)	RAN WATER TO DEWATERING	WASTE WATER	H.P. B.F.W. TO N.H.B.	N.P. B.F.W.	H.P. STEAM	L.P. B.F.W. TO N.H.B.	L.P. STEAM	WATER TO AMMONIA ABSORBER	MAKE UP WATER TO AMMONIA ABSORBER	WASTE WATER FROM RECTISO	NITROGEN TO STRIPPER
1	CH ₄			0.18	0.17	0.01													
2	H ₂			63.07	64.78	0.32													
3	CO			98.74	98.73	1.06													
4	CO ₂			19.68	8.32	11.32													
5	H ₂ S			2.27	—	2.27													
6	CO ₂			0.14	—	—													
7	H ₂	0.83		1.80	1.80	0.0002													
8	A ₂	0.27		0.27	0.27	0.0002													
9	O ₂	23.60		—	—	—													
10	H ₂ O(l)			0.39	—	0.27							177.36		30.86				
11	COAL (LB/HR)		2000																
12	TOTAL WASH MPH	34.70		88.22	84.74	15.18							177.36		30.86				
13	H ₂ O(l)	1749.31	2027.00	2027.00	3335.6	440.34	128.62	167.0	267.08	97.44	6084.28	3600.66	177.36	469.7	355.97	97.44	335.7	5.78	69.05
14	PRESSURE (PSIA)	735	847	847	847	847	847	847	847	847	847	847	847	847	847	847	847	847	847
15	TEMPERATURE (°F)	300	300	300	300	300	300	300	300	300	300	300	300	300	300	300	300	300	300

MATERIAL BALANCE FOR TEXACO-OXYGEN BLOWN GASIFIER W/SELEXOL
(BASIS: 1.0 TON DRY COAL/HR)

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PROCESS FLOW DIAGRAM	TEXACO OXYGEN BLOWN	GASIFIER MATERIAL BALANCE
T 3		

STREAM No.	IDENT.	OXYGEN TO GASIFIER	COAL TO COAL SLURRY	WASTE WATER	REJECT WATER	SLAG/ASH CASE	FUEL GAS TO DESULFURIZATION	RAW WATER	FUEL GAS TO FUEL CELL	FUEL GAS TO SULFUR RECOVERY										
CH ₄							0.18		0.18	0.02										
H ₂							65.07		65.07	0.41										
H ₂ O							93.74		93.74	0.45										
CO ₂							17.48		17.48	0.18										
H ₂ S							2.23		2.23	0.02										
SO ₂							0.18		0.18	0.01										
N ₂		0.83					1.60		1.60	0.01										
AS		0.27					0.27		0.27	0.003										
O ₂		83.80																		
H ₂ O (V)							0.27		0.27	0.004										
COAL SLURRY			2000																	
WASTE WATER		84.30					106.28		230.43	1.73										
REJECT WATER			37.68	91.64	183.62			274.08												
TOTAL WATER		1729.81	2007.68	91.64	183.62	107.0	1827.90	274.08	474.81	35.75										
WASTE WATER							387		500											
TEMP °F		300					1800	70	1800	1800										

BASIS: 1 TON DRY COAL/HR

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PROCESS FLOW DIAGRAM
TEXACO-OXYGEN BLOWN
GASIFIER w/METC

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STREAM NO.	IDENT.	COAL TO GASIFIER	STEAM TO GASIFIER	GASIFIER OFF. GAS	AIR FROM GASIFIER	OXYGEN TO GASIFIER	GAS TO SCRUBBER	SCRUBBER GAS OUTLET	PARTICULATE FREE FUEL GAS	CLEANED FUEL GAS TO PREHEAT	RECYCLE GAS 1 FLY ASH	CHAR SLUDGE TO DISPOSAL	ACID GAS TO CLAU	WASTE WATER	STEAMING H ₂	FUEL GAS TO TURBO-CHARGER
1	COAL	100.00		9.81			9.81	9.81	7.27	7.27	1.54		0.32			1.14
2	H ₂ O		80.77	80.77			80.77	80.77	64.98	64.98	15.79		0.01			48.33
3	H ₂		80.77	80.77			80.77	80.77	64.98	64.98	15.79		0.18			63.81
4	CO ₂		1.46	1.46			1.46	1.46	1.58	1.58	0.30		4.92			10.24
5	N ₂		0.82	0.82	0.18	0.82	0.82	0.82	0.18	0.18	0.04		2.38		2.38	0.18
6	H ₂ O (V)		52.1	52.1	38.42		52.1	52.1	0.98		0.22					47.23
7	COAL (H ₂ O)	100.00		1.46			1.46									
8	STEAM (H ₂ O)		52.1	52.1	188.74		52.1	52.1	146.77	146.77	62.0	2.16	9.59		2.38	183.03
9	COAL (H ₂ O)	100.00		1.46			1.46									
10	STEAM (H ₂ O)		52.1	52.1	188.74		52.1	52.1	146.77	146.77	62.0	2.16	9.59		2.38	183.03
11	COAL (H ₂ O)	100.00		1.46			1.46									
12	STEAM (H ₂ O)		52.1	52.1	188.74		52.1	52.1	146.77	146.77	62.0	2.16	9.59		2.38	183.03
13	COAL (H ₂ O)	100.00		1.46			1.46									
14	STEAM (H ₂ O)		52.1	52.1	188.74		52.1	52.1	146.77	146.77	62.0	2.16	9.59		2.38	183.03
15	COAL (H ₂ O)	100.00		1.46			1.46									
16	STEAM (H ₂ O)		52.1	52.1	188.74		52.1	52.1	146.77	146.77	62.0	2.16	9.59		2.38	183.03
17	COAL (H ₂ O)	100.00		1.46			1.46									
18	STEAM (H ₂ O)		52.1	52.1	188.74		52.1	52.1	146.77	146.77	62.0	2.16	9.59		2.38	183.03
19	COAL (H ₂ O)	100.00		1.46			1.46									
20	STEAM (H ₂ O)		52.1	52.1	188.74		52.1	52.1	146.77	146.77	62.0	2.16	9.59		2.38	183.03

BASIS: 0.8 TONS DRY COAL/HR

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STREAM NO.	IDENT.	COAL TO GASIFIER	STEAM TO GASIFIER	GASIFIER OFF GAS	ASH FROM GASIFIER	OXYGEN TO GASIFIER	GAS TO SCRUBBER	SCRUBBER GAS OUTLET	PARTICULATE FREE FUEL GAS	CLEANED FUEL GAS TO PREHEAT	RECYCLE GAS & FLY ASH TO GASIFIER	CHAP SLUDGE TO DISPOSAL	ACID GAS TO CLAU	FUEL GAS TO TURBO-EXPANDER
CH ₄				4.41			9.41	9.41	7.57	7.25	1.04		0.32	7.01
H ₂				61.08			61.08	61.08	49.08	48.84	11.97		0.24	47.70
CO				80.77			80.77	80.77	64.93	64.21	15.84		0.72	62.05
CO ₂				16.16			25.74	25.74	21.30	20.72	5.74		12.57	8.62
N ₂				1.96			1.96	1.96	1.58	0.12	0.30		1.58	0.52
H ₂ O				6.22		0.10	0.22	0.22	0.10	0.17	0.04		0.01	0.16
O ₂						38.42								
H ₂ O (L)		32.10	30.12				30.12	24.12	0.92		0.23		0.216	43.42
N ₂			1.62				1.62							
COAL (L/HR)		817.83												
ASH (L/HR)			579.62	105.71			21.6				500.94	21.40	15.71	169.32
TOTAL WPM (L/HR)		32.10	279.71	32.61			21.6	204.27	145.71	124.35	32.45			
H ₂ O (L)	256.34													
TOTAL (L/HR)	1076.22	430.00	2448.24	105.71	1134.04	2448.24	4218.07	3058.04	2408.5	723.615	102.0	637.85	311	1200
PRESSURE (PSIA)		480	380			530			550	530				
TEMPERATURE (°F)		550							100	95

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PROCESS FLOW DIAGRAM
WESTINGHOUSE OXYGEN
BLOWN GASIFIER W/SELEXOL

STREAM NO.	IDENT.	1	2	3	4	5	6	7												
LB. PER HOUR	COAL TO GASIFER	STEAM TO GASIFER	GASIFER OFF GAS	ASH FROM GASIFER	OXYGEN TO GASIFER	CLEARED FUEL GAS TO FUEL CELL	RECYCLE GAS													
CH ₄			9.21			7.51	1.84													
H ₂			61.08			49.08	11.97													
CO			80.77			64.92	15.85													
CO ₂			26.74			21.50	5.24													
N ₂			1.70			0.98	0.72													
CO			0.22		0.18	0.18	0.04													
H ₂																				
O ₂					32.43															
H ₂ O		55.18	38.15			49.81	0.23													
N ₂			1.63																	
COAL (LB/HR)	1617.83																			
ASH (LB/HR)			599.68				500.46													
TOTAL VAPOR (HR)		22.10	219.91		32.61	193.07	32.45													
H ₂ O (L)	256.35																			
TOTAL (LB/HR)	1674.22	428.8	4498.24	162.71	193.04	3005.46	745.64													
PRESSURE (PSIA)		450				350														
TEMPERATURE (°F)		650	1900		830	1600														

ASH: 1.63 FROM 1617.83 COAL/HR

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PROCESS FLOW DIAGRAM
WESTINGHOUSE-OXYGEN
BLOWN GASIFIER -/DOLOMITE

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STREAM No.	IDENT.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
LB. MOLES/HR	COAL TO COAL BIN	STEAM TO GASIFIER	GASIFIER OFF-GAS	ASH FROM GASIFIER	AIR TO GASIFIER	GAS TO SCRUBBER	SCRUBBER GAS OUTLET	PARTICULATE FREE FUEL GAS	CLEANED FUEL GAS TO PREHEAT	RECYCLE GAS & FLY ASH TO GASIFIER	CHAR SLUDGE TO DISPOSAL	ACID GAS TO CLAUD	CONDENSATE TO STORAGE	FUEL GAS TO TURBO-CHARGER			
CH ₄			6.96			6.96	6.96	6.66	6.31	0.50		0.15		6.10			
H ₂			47.10			47.20	47.20	43.83	43.68	3.37		0.15		42.48			
CO			89.66			89.66	89.66	83.28	82.62	6.30		0.66		80.35			
CO ₂			17.97			17.97	17.97	16.64	9.34	1.27		7.35		9.08			
H ₂ O			1.64			1.64	1.64	1.52	0	0.12		1.52		0.3 ppm			
CO ₂			183.53			183.53	183.53	170.87	169.60	13.06		0.87		168.93			
N ₂																	
O ₂																	
H ₂ O (L)			17.01			17.01	48.46	2.07		0.16		2.29		48.87			
COAL (LB/HR)	8000	28.74															
CARBON (LB/HR)			643.98	371.63		28				641.50	3.89			347.69			
ASH (LB/HR)			362.97	214.88	323.97	398.41	324.33	311.55	24.05								
TOTAL WASTE (HR)		28.74															
H ₂ O (L)	75.18																
TOTAL (L/HR)	2078.15	58.76	9676.66	371.63	6190.74	4676.66	4876.63	3114.35	7661.44	1260.70	89.40	461.08	88.4	8754.72			
PRESSURE (PSIA)	415	310	310	300	300	300	270	265	530	375	50	29	26.5	376			
TEMPERATURE (°F)	500		1850	800	900	400	280	120	95		100	100	120	1200

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PROCESS FLOW DIAGRAM
WESTINGHOUSE - AIR
BLOWN GASIFIER - WISELROL

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[illegible]

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PROCESS FLOW DIAGRAM
WESTINGHOUSE - AIR
BLOWN GASIFIER w/METC

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References

[illegible]

BASIS: 1 Ton Dry Coal/Wk

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PROCESS FLOW DIAGRAM
WESTINGHOUSE - AIR
BLOWN GASIFIER w/DOLOMITE

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STREAM NO.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
IDENT.	AIR TO GASIFIER	COAL TO GASIFIER	GASIFIER OFF GAS	COOLED GAS TO SCRUBBER	SCRUBBER GAS EFFLUENT	CO ₂ ABSORBER EFFLUENT	CLARIFIED FUEL GAS	CYCLONE DISCHARGE	FLASH STEAM TO STRIPPER	STEAM TO STRIPPER	STEAM TO CALCINER	PERMANENT FUEL GAS NO TURBO EXPANDER (MMBtu/hr)	N ₂ CO ₂ TO STORAGE	WET GASE TO BIN	N ₂ STRIPPER LAMBER EFFLUENT
CO			94.7	94.7	94.7	94.7	94.7					30.7			
H ₂			41.6	41.6	41.6	41.6	41.6					41.2			
CO ₂			10.3	10.3	10.3	7.2	7.2					7.2			
CH ₄			5.0	5.0	5.0	5.0	5.0					5.7			
H ₂ O (g)	4.9		6.8	6.8	2.8	5.9	5.9		31.1	27.7	37.0	64.7			
H ₂	882.6		106.4	106.4	106.4	106.4	106.4					104.5			
H ₂ S			100 ppm	100 ppm	100 ppm	100 ppm						0.5 ppm			
O ₂	24.8														
CO ₂			10 ppm	10 ppm	10 ppm	10 ppm	5 ppm					402.1			
MOLES/HR	827.7		350.6	350.6	350.6	346.6	346.6		31.7	27.7	37.0	4590.5			
LB/HR	4827.8		8748.8	8748.8	8748.8	8616.6	8616.6		540.3	499.0	660.5	9590.5			
N ₂ CO ₂		7.1						7.7	540.3	499.0	660.5		6.3	0.10	7.9
N ₂ HCO ₂ (g)														0.04	0.62
N ₂ S															
N ₂ H ₂ S														0.03	0.60
N ₂ SO ₂	0.008							0.21					0.01	0.063	0.80
N ₂ SO ₃															
N ₂ OH															
H ₂ O (l)								198.3						13.7	155.9
COAL (LB/HR)		1000 (5% H ₂ O)													
ASH (LB/HR)								16.4						28.3	
N														1.4	
COMPOUND 1								0.05						0.033	
COMPOUND 2								0.31						0.31	
COMPOUND 3								0.29						0.29	
3-O ₂													0.00033	0.00	0.02
SURF TOTAL (LB/HR)			8754.8					4766.5					667.6	223.0	2764.6
TEMP (°F)	250	60	781	270	188	188	1200	300	170	250	450	1200			
PRESSURE (PSIA)	215	245	245	245	245	245	245	245	245	245	245	245			
MM/SEC	MM 28.63		MM 25.01	MM 25.01	MM 25.03	MM 24.86	MM 24.86	SG 1.176	MM 18.016	MM 18.016	MM 18.016	MM 23.05			SG 1.260

STREAM NO.	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
IDENT.	CLARIFIER UNDERFLOW	WASH WATER FROM FILTER	RECYCLE LIQUOR TO STORAGE	CARDIATOR UNDERFLOW	CO ₂ ABSORBER RECY SOLUTION	FLASH DRUM UNDERFLOW	PRECARBONATOR CLARIFIER	EARLY LIQUOR STORAGE	LIQUOR MAKE UP	LIQUOR FROM QUENCH	LIQUOR TO WETTER ROLLERS	CLARIFIER OVERFLOW	CO ₂ TO GAS COOLER	STRIPPER OFF GAS TO CLAVS	VENT GAS TO SCOT
CO															
H ₂															
CO ₂													6.26		
CH ₄													0.31	0.42	0.71
H ₂ O (g)															7.76
H ₂ O (l)															0.10
H ₂															2.06
H ₂ S															
O ₂															
CO ₂															
MOLES/HR															
LB/HR															
N ₂ CO ₂	1.3	0.19	0.33	0.17	4.88	7.7	6.1	7.7	0.39	21.10	13.99	4.77			
N ₂ HCO ₂	0.67	0.00	2.63	3.91	4.37		3.05		3.83			2.39			
N ₂ HCO ₂ (g)				18.38	2.48										
N ₂ S															
N ₂ H ₂ S	0.87	0.06	0.33	0.45	0.60	2.45	2.60	2.45	0.53	6.71	4.26	2.03			
N ₂ SO ₂	0.08	0.01	0.20	0.20	0.20	0.21	0.21	0.21	0.20	0.50	0.31	0.16			
N ₂ SO ₃															
N ₂ OH															
H ₂ O (l)	33.6	22.5	194.23	135.36	158.77	164.80	162.82	164.2	194.23	534.73	837.67	127.26			
COAL (LB/HR)															
ASH (LB/HR)	75.3					75.28	75.28	75.28		75.28					
N	1.4					1.41	1.41	1.41		1.41					
COMPOUND 1	0.05					0.05	0.05	0.05		0.05					
COMPOUND 2	0.31					0.31	0.31	0.31		0.31					
COMPOUND 3	0.29					0.29	0.29	0.29		0.29					
3-O ₂	0.87	0.00061		0.08	0.08	0.29	0.29	0.29		0.29					
SURF TOTAL (LB/HR)	1138.6	536.5	3746.18	2600.22	3079.47	4205.07	4205.07	4205.07	3746.13	12592.78	7677.25	2136.76		79.83	240.10
TEMP (°F)	134	134	134	134	134	170	170	170	149	300	300	160		95	
PRESSURE (PSIA)	22	22	22	22	22	22	22	22	22	22	22	22		15	15
MM/SEC	SG 1.427	SG 1.060	SG 1.050	SG 1.046	SG 1.046	SG 1.206	SG 1.206	SG 1.206	SG 1.046	SG 1.175	SG 1.154	SG 1.260	MM 42.7413	MM 31.8716	MM 28.6715

BASIS: 1 TON (5% MOISTURE) COAL/HR

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R 3 ~

 PROCESS FLOW DIAGRAM
 MCKEEL AIR BLOWN
 GASIFIER

to be about 1013 kPa (10 atm) and temperature about 650°C (1200°F). The maximum sulfur level into the fuel cell is assumed to be 0.5 ppmv. Metals present in the coal, such as Be, Bi, Cd, Hg, Mo, Pb, Sb, Ti, V, Zn, Zr, Ca, Fe, and Mg are assumed to condense below 538°C (1000°F) or are absorbed by fly ash and then removed by the scrubber system. Also removed in the scrubber system are Cl, F, Na, K, and some S, with removal of NH₃. Trace elements that form volatile or water insoluble compounds are As, B, Ge, Sc, and Te, which can be present in the product gas. Currently, the assumed impurities entering the gas cleanup system are COS and H₂S, with trace impurities of organic sulfur and possibly NH₃ with micron-sized particulates.

4.4.1 Criteria for Selection

The gas cleanup system must remove COS along with H₂S and leave CO₂ in the purified gas stream. Selective removal of H₂S and COS is important. A ZnO polisher, however, follows the gas cleanup system to ensure proper sulfur limits, and COS hydrolysis may be located upstream, since most gas cleanup systems are more selective to H₂S than COS. The outlet total sulfur concentration is limited to 0.5 ppmv (but can be flexible).

Trace compounds have not been extensively identified for raw gas, since few advanced commercial gasifier studies have been performed for this purpose. Limits on NH₃ are not set for the MCFC but are assumed to be sufficiently removed by the cold gas cleanup system to ensure proper fuel cell operation. Also, environmental constraints limit NO₂ emissions. NH₃ conversion to NO₂ is generally assumed to be 50% during combustion, which would limit NH₃ to about 0.1% in the feed gas entering a combustion turbine, but no such limitation applies to catalytic combustion after the MCFC.

Acid gases from the wet gas cleanup system should be able to be economically treated for sulfur recovery. A Claus plant has been selected as the sulfur recovery system, followed by a SCOT tail gas

cleanup process. Concentrations of H_2S in the acid gas stream are usually required to be above 20 percent, but a lower limit of at least 15% is acceptable for the least costly Claus plant design. Lower concentrations of 5 to 15% require special arrangements for Claus plant sulfur recovery, which are more expensive.

The gasifier must be able to use a wide variety of coals and must also be load following (follow swings in power). Changes in acid gas partial pressure, therefore, must be expected because of these swings in operation. Depending on the sulfur content of the coal used, the concentrations of H_2S may vary from 0.5 to 1.5%. Such substantial composition variation may not be tolerable for some cold gas cleanup systems.

General operating criteria involving those points discussed in Section 2 are listed here. Some of these points are used for the initial selection of the gas cleanup systems and include, the following:

- The system must be economical to operate and be appropriate for use on coal gas.
- The system should not produce compounds in waste streams that are environmentally unacceptable.
- The gas cleanup system must have good sulfur removal efficiency and must also have low utilities consumption.
- Solvents used by the gas cleanup system should not be degraded by constituents in the gas stream and the solvent must not be detrimental to operations downstream if entrained or vaporized in the purified gas stream.
- The process must at least have proved at the pilot plant stage that it removes sulfur compounds.

In summary, the criteria for selection of a reference wet coal gas cleanup system are:

- Gas Cleanup Specifications
 - Sulfur must be limited to 0.5 ppm or less.
 - The system must be able to at least remove HCN, NH_3 , and Cl.
 - Acid gas must be at least 15% H_2S to the Claus plant.
 - Desulfurization must be selective toward sulfur compounds.
- System Load Follow Requirements
 - The system must be able to handle swings flow and pressure.

- The system must be able to handle changing feed gas concentrations (0.5 to 1.5% H₂S).
- Operational Characteristics
 - The system should not produce dangerous compounds.
 - The system should have good sulfur removal efficiency with low utility consumption.
 - The system solvent must not be degraded by constituents in the feed gas.
 - The system must have demonstrated at least an experimental operation.

4.4.2 Rectisol II Selection

The reference wet cleanup system, based on "process information and data ... extracted from sources available in the public domain" as requested by contract, and based also on the criteria established in this section, is Rectisol II. Its selection is predicated largely on work published by General Electric Company and United Technologies, Inc., as part of their MCFC development programs, followed by the work done by C. F. Braun for the Electric Power Research Institute and published as EPRI Report EM-1333 in January 1980.⁷⁶ On the basis of its capital and operating costs, as provided in Tables 5-1 and 5-2 of the EPRI report, Rectisol II is clearly as good as or better than the other commercially available wet cleanup systems studied, both air blown and oxygen blown. This judgment is made because of its simplicity (Rectisol II does not require the as yet undemonstrated COS hydrolysis step required by other processes) and its operating and maintenance cost (Rectisol II was less expensive in 31 of the 32 cases studied). In addition, Davy McKee in its material and energy balance work presented in Section 4.3 of this report, present better efficiencies for Rectisol II in all wet cleanup configurations studied. We conclude that, based on information in the public domain, Rectisol II should be the reference wet cleanup system.

4.5 RECOMMENDATIONS FOR DETAILED STUDY

Major evaluation criteria were established in Section 4.2 of this report, and a decision matrix was used to derive weighting factors

for the criteria. This section applies those weighted criteria to each of the 17 configurations presented in Section 4.3 and derives rankings for both oxygen- and air-blown gasifier/cleanup sets of configurations. Data in Section 4.3, along with data on investment costs in the reports referenced in Tables 93 and 95, were used to provide relative rankings of the configurations shown in the flow diagrams of Section 4.3. Then the weighting factors were applied to the rankings, and coefficients of merit were derived for each configuration and for each evaluation criterion. Finally, in Tables 94 and 96, the coefficients of merit were summed to obtain a rank for each configuration.

The contractual requirements for this section are that the number of final configurations to be studied in detail "will be a maximum of 12, counting all combinations of gasifiers and cleanup trains." We have chosen for further study the top three ranked processes in Table 96 from a total of five air-blown gasifier configurations. These will be studied in detail, as will six of the top-ranked processes from a total of twelve in Table 94 for the oxygen-blown processes. We recommend that the eighth-ranked process in Table 94 be studied in place of the fourth-ranked process to provide a complete set of four cleanup process variations for a single gasification system.

Approximate cost estimates ($\pm 35\%$) for the nine processes recommended for detailed study have been prepared by Davy McKee and have been studied parametrically with the Westinghouse AHEAD computer program to derive data on overall power plant efficiencies, including fuel expansion turbines, heat recovery steam generation, and supply of steam to the fuel gas to avoid carbon deposition in the fuel gas reheat exchangers and the fuel cells; cathode gas recycle compression, air compression, cathode gas expansion turbines, etc. This work, in Sections 5 and 6, also includes a tenth process for detailed study, using air-blown gasification with hot gas cleanup in a utility application. The suggestion to include this tenth option was made by DOE after review of the matrix evaluation procedure and preliminary results.

Table 93

EVALUATION OF SOLUTIONS FOR EACH REQUIREMENT:
UTILITY CASE (OXYGEN-BLOWN GASIFIER)

Dwg. 4252809

Gasifier/Gas Cleanup	1. Environmental ^a		2. Cost of Electricity ^b		3. Heat Rate ^c		4. Reliability ^d	
	Ranking	Coefficient	Ranking	Coefficient	Ranking	Coefficient	Ranking	Coefficient
Texaco/Rectisol	10	0.152	1	0.015	7	0.106	9	0.136
Texaco/Selexol	4	0.061	0	0	0	0	11	0.167
Texaco/METC	5	0.076	2	0.030	1	0.015	6	0.091
Texaco/Dolomite	1	0.015	6	0.091	2	0.030	2	0.030
Westinghouse/Rectisol	11	0.167	8	0.121	8	0.121	4	0.061
Westinghouse/Selexol	6	0.091	4	0.061	3	0.045	8	0.121
Westinghouse/METC	9	0.136	9	0.136	4	0.061	3	0.045
Westinghouse/Dolomite	2	0.030	11	0.167	6	0.091	1	0.015
BGC/Rectisol	8	0.121	5	0.076	11	0.167	7	0.106
BGC/Selexol	7	0.106	3	0.045	10	0.152	10	0.152
BGC/METC	3	0.045	7	0.106	5	0.076	5	0.076
BGC/Dolomite	0	0	10	0.152	9	0.136	0	0
Weighting Factors		0.182		0.418		0.127		0.273

a) Based on efficiency (Btu in/Btu out) and conditions inherent to the process to cause it to pollute; derived from EPRI AP-1543, EM-1333, AF-416, and AF-642, with additional input from Davy-McKee.

b) Based on capital costs derived from EPRI AP-1543, EM-1333, AF-416, and AF-642, with additional input from Davy-McKee.

c) Based on efficiency (Btu in/Btu out) derived from AP-1543, EM-1333, AF-416, and AF-642, with additional input from Davy-McKee.

d) Based on state of development and complexity.

Table 94
UTILITY CASE (OXYGEN-BLOWN GASIFIER)

Evaluation Criteria	Texaco				Westinghouse				BGC			
	Rectisol	Selexol	METC	Dolomite	Rectisol	Selexol	METC	Dolomite	Rectisol	Selexol	METC	Dolomite
1) x 0.182	0.028	0.011	0.014	0.003	0.030	0.017	0.025	0.005	0.022	0.019	0.08	0
2) x 0.418	0.006	0	0.013	0.038	0.051	0.025	0.057	0.070	0.032	0.019	0.044	0.064
3) x 0.127	0.013	0	0.002	0.004	0.015	0.006	0.008	0.012	0.021	0.019	0.010	0.017
4) x 0.273	0.037	0.046	0.025	0.008	0.017	0.033	0.012	0.004	0.029	0.041	0.021	0
Total	0.084	0.057	0.054	0.053	0.113	0.081	0.102	0.091	0.104	0.098	0.093	0.081
Rank	6	10	11	12	1	8	3	5	2	4	7	9

Table 95

Dwg. 4252B11

EVALUATION OF SOLUTIONS FOR EACH REQUIREMENT:
INDUSTRIAL CASE (AIR-BLOWN GASIFIER)

Gasifier/Gas Cleanup	1. Environmental ^a		2. Cost of Electricity ^b		3. Heat Rate ^c		4. Reliability ^d	
	Ranking	Coefficient	Ranking	Coefficient	Ranking	Coefficient	Ranking	Coefficient
Westinghouse/Rectisol	3	0.3	2	0.2	2	0.2	1	0.1
Westinghouse/Selexol	2	0.2	0	0	0	0	3	0.3
Westinghouse/METC	4	0.4	1	0.1	4	0.4	2	0.2
Westinghouse/Dolomite	0	0	4	0.4	3	0.3	0	0
Rockwell/ZnO	1	0.1	3	0.3	1	0.1	4	0.4
Weighting Factors		0.182		0.418		0.127		0.273

a) Based on efficiency (10^6 Btu in/ 10^6 Btu out) and conditions inherent to the process to cause it to pollute; derived from NASA Technical Memorandum 81687, D.O.E. report on Molten Carbonate Coal Gasification and EPRI EM-1333.

b) Based on capital costs derived from the above sources.

c) Based on efficiency.

d) Based on state of development and complexity.

Table 96
INDUSTRIAL CASE (AIR-BLOWN GASIFIER)

Evaluation Criteria	Westinghouse				Rockwell
	Rectisol	Selexol	METC	Dolomite	ZnO
1) x 0.182	0.55	0.036	0.073	0	0.018
2) x 0.418	0.084	0	0.042	0.167	0.125
3) x 0.127	0.025	0	0.051	0.038	0.013
4) x 0.0273	<u>0.027</u>	<u>0.082</u>	<u>0.055</u>	<u>0</u>	<u>0.109</u>
Total	0.191	0.118	0.221	0.205	0.265
Rank	4	5	2	3	1

Section 5

ENGINEERING ANALYSIS

5.1 INTRODUCTION

The objective of this section is to evaluate and compare coal gasification and gas cleanup processes on a system basis for use in advanced MCFC-based power plants including topping and/or bottoming cycles. Specifically, the goal is to rank systems by efficiency and to select the optimum MCFC operating pressure.

Section 5.2 provides parametric equations and supporting documentation. The equations provide the basis for input/output characteristic and operational characteristic evaluations. The input data, based on coal gasification and gas cleanup system assessments made by Davy McKee, Inc., provide coal gas compositions and system utility requirements as a function of system size and configuration. The output data are power production figures for each power plant element and power consumption figures for each component requiring power.

Section 5.3 then provides a parametric evaluation for each of the ten fuel supply systems to evaluate power plant relative efficiency as a function of MCFC operating pressure. System efficiencies as a function of input heating value content and fuel cell pressure, for utility size and industrial size units, and for both hot and cold gas cleanup have been provided.

5.2 SYSTEM PARAMETERIZATION

Table 97 lists the ten gasification subsystem configurations included in the parametric study of the MCFC system. Four different coal gasification processes are included. The first seven configurations are for utility application and the remaining three for industrial

Table 97

Dwg. 4253856

LIST OF TEN GASIFICATION SUBSYSTEM CONFIGURATIONS

Case	Application	Gasifier	Blast	Cleanup Process	Cell Operating Pressures for Which Performance Calculations Were Made
1	Utility	Westinghouse	Oxygen	Rectisol II	345, 690, 1034, & 2069 kPa (50, 100, 150, & 300 psia)
2	Utility	British Gas Council	Oxygen	Rectisol II	345, 690, 1034, & 2069 kPa (50, 100, 150, & 300 psia)
3	Utility	Westinghouse	Oxygen	Selexol	345, 690, 1034, & 2069 kPa (50, 100, 150, & 300 psia)
4	Utility	Texaco	Oxygen	Rectisol II	345, 690, 1034, & 2069 kPa (50, 100, 150, & 300 psia)
5	Utility	Westinghouse	Oxygen	Iron Oxide (METC)	345, 690, 1034, & 2069 kPa (50, 100, 150, & 300 psia)
6	Utility	Westinghouse	Oxygen	Dolomite	345, 690, 1034, & 2069 kPa (50, 100, 150, & 300 psia)
7	Utility	Westinghouse	Air	Iron Oxide (METC)	345, 690, 1034, & 1724 kPa (50, 100, 150, & 250 psia)
8	Industrial	Rockwell	Air	ZnO	345, 690, 1034, & 1724 kPa (50, 100, 150, & 250 psia)
9	Industrial	Westinghouse	Air	Iron Oxide (METC)	345, 690, 1034, & 1724 kPa (50, 100, 150, & 250 psia)
10	Industrial	Westinghouse	Air	Dolomite	345, 690, 1034, & 1724 kPa (50, 100, 150, & 250 psia)

application. Air blast is used for the industrial cases and for one utility case; oxygen blast is used for all other utility cases.

The first four cases use low-temperature gas cleanup processes, either Rectisol II or Selexol. The last six cases use high-temperature fuel gas cleanup processes. Two different, high-temperature cleanup processes are used with the Westinghouse gasification process, i.e., Fe_2O_3 and dolomite, and a ZnO process is used in combination with the Rockwell molten carbonate gasification process.

One basic design parameter was investigated for each of the ten fuel supply cases: cell operating pressure. In each case performance was analyzed for four nominal values of cell operating pressure - 345, 690, 1034, and 2069 kPaa (50, 100, 150, and 300 psia). Where the fuel gas supply pressure was less than 2069 kPaa (300 psia), a maximum value somewhat less than the fuel supply pressure was used.

Table 98 characterizes the gasifier subsystem for each of the ten cases. Gasifier/fuel cell subsystem interface values are listed for process air, process steam, and auxiliary power requirements for the gasifier subsystem. Also listed are the product fuel gas and the power steam supplied by the gasifier subsystem to the fuel cell subsystem.

Table 99 lists the molten carbonate design parameters specified for all ten cases of this study.

Table 100 describes the coal used as a feedstock for all the gasifier subsystem configurations for the MCFC parametric study except the air-blown Westinghouse gasifier. The coal used for the Westinghouse air-blown gasifier is described in Table 100.

The equations for the parametric study of the MCFC subsystem are given in Appendix A.

5.3 PARAMETRIC STUDIES

This section contains a description of the system configuration developed for use in the parametric study of the molten

Table 98

Dwg. 5601C45

CHARACTERIZATIONS OF TEN GASIFIER SUBSYSTEM CONFIGURATIONS

Description	Case									
	1	2	3	4	5	6	7	8	9	10
Process Air to Gasifier Subsystem										
Pressure, kPaa (psia)	579 (84.0)	579 (84.0)	579 (84.0)	579 (84.0)	579 (84.0)	579 (84.0)	2620 (380)	2241 (325)	2620 (380)	2620 (380)
Flow rate, kg/s (lb/s)	68.90 (151.9)	50.35 (111.0)	70.81 (156.1)	74.89 (165.1)	68.54 (151.1)	67.77 (149.4)	72.62 (160.1)	15.70 (34.6)	15.74 (34.7)	15.60 (34.4)
Process Steam to Gasifier Subsystem										
High Pressure										
Pressure, kPaa (psia)	4240 (615)	4240 (615)	4240 (615)	-	-	-	-	4240 (615)	-	-
Temperature, °C (°F)	427 (800)	427 (800)	427 (800)	-	-	-	-	427 (800)	-	-
Flow rate, kg/s (lb/s)	11.52 (25.4)	1.72 (3.8)	4.04 (8.9)	0.0	0.0	0.0	0.0	1.72 (3.8)	0.0	0.0
Low Pressure										
Pressure, kPaa (psia)	448 (65)	448 (65)	448 (65)	448 (65)	-	-	-	-	-	-
Temperature, °C (°F)	SAT	SAT	SAT	SAT	-	-	-	-	-	-
Flow rate, kg/s (lb/s)	4.31 (9.5)	2.36 (5.2)	14.02 (30.9)	3.27 (7.2)	0.0	0.0	0.0	0.0	0.0	0.0
Power Steam from Gasifier Subsystem										
Pressure, kPaa (psia)	-	-	-	4240 (615)	4240 (615)	4240 (615)	4240 (615)	-	4240 (615)	4240 (615)
Temperature, °C (°F)	-	-	-	427 (800)	427 (800)	427 (800)	427 (800)	-	427 (800)	427 (800)
Flow rate, kg/s (lb/s)	0.0	0.0	0.0	4.81 (10.6)	0.28 (0.61)	0.24 (0.53)	7.17 (15.8)	0.0	1.63 (3.6)	1.59 (3.5)
Product Fuel Gas from Gasifier Subsystem										
Pressure, kPaa (psia)	3558 (516)	3558 (516)	3558 (516)	3558 (516)	2413 (350)	2413 (350)	2000 (290)	1862 (270)	2000 (290)	2000 (290)
Temperature, °C (°F)	649 (1200)	649 (1200)	649 (1200)	649 (1200)	649 (1200)	649 (1200)	649 (1200)	649 (1200)	649 (1200)	649 (1200)
Flow rate, kg/s (lb/s)	47.13 (103.9)	42.05 (92.7)	42.14 (92.9)	41.23 (90.9)	50.03 (110.3)	50.44 (111.2)	102.83 (226.7)	21.95 (48.4)	22.32 (49.2)	22.45 (49.5)
Composition (mole fraction)										
CH ₄	0.0390	0.0597	0.0416	0.0008	0.0393	0.0393	0.0175	0.0142	0.0175	0.0175
H ₂	0.2641	0.2299	0.2801	0.2831	0.2542	0.2542	0.1190	0.1025	0.1190	0.1190
CO	0.3486	0.4376	0.3682	0.4157	0.3362	0.3362	0.2262	0.2455	0.2262	0.2262
CO ₂	0.0893	0.0113	0.0512	0.0668	0.1114	0.1114	0.0454	0.0178	0.0454	0.0454
N ₂	0.0010	0.0034	0.0010	0.0077	0.0009	0.0009	0.4629	0.4590	0.4629	0.4629
H ₂ O	0.2580	0.2581	0.2580	0.2260	0.2580	0.2580	0.1290	0.1610	0.1290	0.1290
Heating Value kJ/kg (Btu/lb)										
Higher	10,709 (4604)	12,909 (5550)	11,995 (5157)	10,258 (4410)	10,086 (4336)	10,086 (4336)	4710 (2025)	4675 (2010)	4710 (2025)	4710 (2025)
Lower	9932 (4270)	12,095 (5200)	11,123 (4782)	9606 (4130)	9353 (4021)	9353 (4021)	4429 (1904)	4433 (1906)	4429 (1904)	4429 (1904)

Table 99
SPECIFIED DESIGN PARAMETERS FOR THE
MOLTEN CARBONATE FUEL CELL

Operating Pressure (base case)	1034 kPaa (150 psia)
Operating Temperature	704°C (1300°F)
Cooling Loop Temperature Differential	93°C (200°F)
H ₂ and CO Anode Conversion Fractions	0.85
Overall O ₂ Utilization Factor	0.50

Table 100
ILLINOIS NO. 6 COAL ANALYSES

Type	As Received ⁷³	As Fired	DAF
PROXIMATE ANALYSIS, wt %			
Moisture	4.2	0.0	0.0
Ash	9.6	10.0	0.0
Fixed carbon	52.0	54.3	60.3
Volatile matter	<u>34.2</u>	<u>35.7</u>	<u>39.7</u>
	100.0	100.0	100.0
ULTIMATE ANALYSIS, wt %			
Carbon	66.60	69.52	77.26
Hydrogen	5.58	5.33	5.92
Oxygen	13.32	10.02	11.14
Nitrogen	1.20	1.25	1.39
Sulfur	3.70	3.86	4.29
Ash	<u>9.60</u>	<u>10.02</u>	<u>-</u>
	100.00	100.00	100.00
HEATING VALUE			
High heating value (HHV), kJ/kg (Btu/lb)	28,459 (12,235)	29,705 (12,771)	33,006 (14,190)
Low heating value (LHV), kJ/kg (Btu/lb)	27,235 (11,709)	28,545 (12,272)	31,717 (13,636)

carbonate fuel cell, a description of the computational techniques used in the engineering analysis of this system, and a summary of the results from the study.

Figure 44 is the generalized flow diagram of the MCFC subsystem developed for the parametric study of the MCFC/coal gasification system. The interface boundary shown on the diagram separates the MCFC and gasifier subsystems. Ambient air passes through an air filter before entering two axial flow compressors in parallel. Compressor No. 1 is for process air supplied to the gasifier subsystem. For oxygen-blown gasifiers this air goes to the air separation plant; for air-blown gasifiers it goes directly to the gasifier. For air-blown gasifiers this compressor is equipped with an intercooler.

The product fuel gas received from the gasifier subsystem has been sulfur polished, humidified to prevent carbon laydown, and reheated to 649°C (1200°F). Since gasification system economics dictates that the product fuel gas supply pressure be well above the fuel cell operating pressure, an expander is used to reduce the pressure to the fuel cell operating pressure. The expander exit temperature varies with cell operating pressure, since the temperature drop across the expander is a function of the pressure ratio. The fuel gas then enters the fuel cell anode, where 85% of the H_2 and CO contained are reacted with O_2 transported through the electrolyte to form H_2O and CO_2 . An equivalent quantity of CO_2 is also transported through the electrolyte. Water-gas shift equilibrium is assumed in calculating the gas composition out of the anode.

The dc power produced by the fuel cell is converted to ac in an inverter.

A booster compressor is used on the anode exhaust gas to balance the pressures in the anode and cathode. Since the maximum inlet temperature for commercially available compressors (centrifugal) is about 400°C (750°F), the exhaust gas from the anode is cooled to 400°C (750°F) by heat exchanger HX1. The booster compressor provides the

Table 101
OHIO NO. 9 COAL ANALYSES

Type	<u>As Received</u> ⁷⁶	<u>As Fired</u>	<u>DAF</u>
PROXIMATE ANALYSIS, wt %			
Moisture	3.6	0.0	0.0
Ash	15.7	16.3	0.0
Fixed carbon	44.9	46.6	55.7
Volatile matter	<u>35.8</u>	<u>37.1</u>	<u>44.3</u>
	100.0	100.0	100.0
ULTIMATE ANALYSIS, wt %			
Carbon	64.83	67.25	80.35
Hydrogen	4.74	4.50	5.38
Oxygen	11.00	8.09	9.66
Nitrogen	1.30	1.35	1.61
Sulfur	2.42	2.51	3.00
Ash	<u>15.71</u>	<u>16.30</u>	<u>-</u>
	100.00	100.00	100.00
HEATING VALUE			
High heating value (HHV), kJ/kg (Btu/lb)	26,958 (11,590)	27,965 (12,023)	33,411 (14,364)
Low heating value (LHV), kJ/kg (Btu/lb)	25,926 (11,146)	26,986 (11,602)	32,238 (13,860)

Figure 44 -- Generalized Molten Carbonate Fuel Cell Subsystem -- Flow Diagram

pressure rise required to overcome the pressure losses in heat exchanger HX1 and the catalytic burner.

Axial-flow air compressor No. 2 supplies combustion air to the catalytic burner at a pressure equal to the discharge pressure from the booster compressor. The combustible constituents in the anode exhaust gas (H_2 , CO, and CH_4) are completely reacted with this combustion air in the catalytic burner. The quantity of combustion air is selected to give 50 % overall oxygen utilization, i.e., an overall air equivalence ratio of 2.0.

The combustion products from the catalytic burner are blended with recycle gas from the fuel cell cathode cooling loop to provide cathode inlet gas at a temperature $93^{\circ}C$ ($200^{\circ}F$) lower than the fuel cell operating temperature [$704^{\circ}C$ ($1300^{\circ}F$)]. The cathode gas provides the oxygen and the carbon dioxide required for the generation of electricity in the fuel cell electrolyte.

The cathode exhaust gas is split into two streams. A quantity of combustion products equal to the sum of the product fuel gas from the gasifier subsystem and the combustion air from air compressor No. 2 is blown down to provide a system mass balance. The balance of the cathode exhaust gas is recycled through the cathode gas cooling loop to provide an energy balance for the system.

Since the cathode is operating at pressures of 345 kPaa (50 psia) or greater, the blowdown gas is expanded through gas expander No. 2 for power generation. In the diagram, gas expander No. 2 is shown driving the two axial flow air compressors and a generator. In reality, air compressor No. 2 and gas expander No. 2 together are a gas turbine unit driving the generator and air compressor No. 1 in tandem.

The exhaust from the gas turbine expander is cooled to an appropriate temperature [$143^{\circ}C$ ($290^{\circ}F$)] in heat exchanger HX4 and exhausted to the atmosphere through a stack.

The quantity of recycle gas and its temperature are selected to provide the required amount of fuel cell cooling and to meet the specified cathode inlet temperature of 593°C (1100°F). In addition, the recycle gas compressor inlet temperature is limited to 400°C (750°F), and the maximum economic effectiveness of the recuperator for reheating the recycle gas after compression is about 85%. Two heat exchangers (HX2 and HX3) are required in the cathode gas cooling loop to satisfy these requirements and constraints. The duty for the recycle gas compressor is similar to that of the anode gas booster compressor, and a centrifugal compressor is used here also. The compressor pressure rise is equal to the cumulative pressure losses in the cooling loop.

The heat recovered from the four heat recovery heat exchangers in the MCFC subsystem has composite characteristics that are well suited to a subposed steam Rankine cycle. The quantity of heat available, however, is not commensurate with a reheat cycle, so throttle conditions of 12,411 kPag/538°C (1800 psig/1000°F) are used.

An analysis of the gas-side temperature profiles showed that heat exchanger HX4 should be used as the low-level economizer with heat exchanger HX3 and heat exchangers HX1 and HX2 in parallel in series with heat exchanger HX4.

Heat exchanger HX4 incorporates a low-pressure evaporator with an integrated deaerating feedwater heater to provide minimum metal temperatures equal to or higher than 71°C (160°F). This heat exchanger has two possible operating modes using either a nonsteaming or a steaming economizer.

Heat exchanger HX3 has three possible operating modes using:

- A nonsteaming economizer
- A steaming economizer
- A partial once-through evaporator.

The functions of heat exchangers HX1 and HX2 are parallel, and they have two possible operating modes. These are:

- A nonsteaming economizer, followed by a drum-type evaporator and superheater
- A drum-type evaporator followed by a superheater.

The steam turbine has three elements, i.e., high pressure, intermediate pressure, and low pressure. The high-pressure element has a single extraction point to provide 4137 kPag/427°C (600 psig/800°F) process steam to the gasifier subsystem. Alternatively, power steam at 4137 kPag (600 psig) is injected into the steam turbine at the crossover between the high and intermediate pressure turbine elements. Provision is made for extracting low-pressure [345 kPag (50 psig)/sat] process steam for the gasifier subsystem at the crossover between the intermediate-pressure and low-pressure turbine elements.

The steam condenser is assumed to operate at a pressure of 6.75 kPaa (2 in. Hg abs) for all parametric cases.

The drum-type evaporators used in heat exchangers HX1 and HX2 require blowdown for control of dissolved solids in the evaporator loop. For 12,411 kPag (1800 psig) evaporators, the quantity of blowdown should be about 1%.

For those cases where the amount of power steam injected into the steam turbine from the gasifier subsystem exceeds the sum of low-pressure steam extracted from the steam turbine for the gasifier subsystem plus the boiler blowdown, there will be an excess of condensate out of the condensate pump. Provision is made for removing this excess condensate from the condensate return line.

Since the boiler blowdown is saturated liquid at 12,411 kPag (1800 psig), it must be cooled to near ambient temperatures before it is depressurized. This is done most advantageously by using it to heat boiler makeup water in a recuperator, as shown in Figure 44.

5.3.1 Engineering Analysis

The Westinghouse Research and Development Center has a generalized computer program for analyzing engineering systems,

designated by the acronym AHEAD (Advanced Heat Engine Analysis & Design). The AHEAD program has a data structure designed to be accommodated by a generic computer program, GOOP (Generalized Orthonormal Optimization Program), that serves as a driver for the solution of energy and mass balances. AHEAD contains, besides the GOOP package, a library of functional routines that can be called for specific system configurations.

The AHEAD program was used in the parametric study of the MCFC system. Figure 45 is a modification of the generalized flow sheet of the MCFC subsystem shown in Figure 44 that was used as a basis for the mathematical model of the computer program. Figures 46 through 49 give supplemental details for the four heat recovery units in the system. All these figures have station identifications for both gas and steam streams for use in the computer program.

Table 102 lists the component performance data assumed for the MCFC parametric study. These data, in combination with the gasifier subsystem characterizations given in Table 98, the MCFC design parameters given in Table 99, and the coal feedstock technical data given in Tables 100 and 101, constitute the inputs to the AHEAD program required for the calculation of the system performance for each of the ten cases considered.

5.3.2 Results of Parametric Study

Table 103 is the computer printout of the 345 kPaa (150 psia) run for the Case I system configuration. The balance of the computer printouts for the performance runs made for the MCFC parametric study have been submitted to DOE as part of the Task C Topical report for this contract and are available from DOE/METC for inspection.⁷⁷ The results of the various runs for each of the ten cases are summarized in Tables 104a through 104j, and the results for the reference cell operating pressure 1034 kPaa (150 psia) for all ten cases are summarized in Table 105.

Figure 45 -- Flow Diagram for Mathematical Model of Molten Carbonate Fuel Cell Subsystem

Figure 46 -- Heat Exchanger HX1
Flow Diagram

Figure 47 -- Heat Exchanger HX2
Flow Diagram

Figure 48 -- Heat Exchanger HX3
Flow Diagram

Figure 49 -- Heat Exchanger HX4
Flow Diagram

Table 102
ASSUMED COMPONENT PERFORMANCE FOR MOLTEN
CARBONATE FUEL CELL PARAMETRIC STUDY

Ambient Conditions		
Temperature		16°C (60°F)
Pressure	99.3 kPaa (14.4 psia)	
Relative humidity		0%
Turbomachinery		
Expander polytropic efficiency		90%
Axial compressor polytropic efficiency		90%
Centrifugal compressor isentropic efficiency		80%
Pump efficiency		70%
Gas turbine mechanical efficiency	98% of net	
Compressor mechanical efficiency	99%	
Expander mechanical efficiency	98%	
Steam Cycle		
Turbine throttle conditions		
Pressure	12,514 kPaa (1815 psia)	
Temperature	538°C (1000°F)	
Turbine efficiency	See Appendix B	
Condenser pressure	6.75 kPaa (2.0 in. Hg abs)	
Turbine mechanical efficiency	99%	
Evaporator blowdown rate		1%
Low-pressure turbine leaving loss	11.63 kJ/kg(5 Btu/lb)	
Molten Carbonate Fuel Cell		
Pressure differential across electrolyte	0 kPaa (0 psia)	
Heat loss to atmosphere	1-1/2% of cooling load	
Current density	290.9 mA/cm ²	
Performance as function of cell operating pressure	See Appendix A	
Catalytic Burner		
Combustion efficiency	100%	
Heat loss to atmosphere	0%	
Overall air equivalence ratio	2.0	

Table 102 (cont'd)

Heat Exchangers

Heat loss to atmosphere	1-1/2%
Evaporator pinch point temperature differential	22°C (40°F)
Recuperator effectiveness	85%
Stack-gas temperature	143°C (290°F)

Electrical Equipment

Generator efficiency	98.5%
Motor efficiency	95%
Converter efficiency	97%

Pressure Drops

Gas side

Inlet air filter	0.75%
Catalytic burner	5.5%
Superheater elements	1.5%
Evaporator elements	1.25%
Economizer elements	1.25%

Recuperator

Cold side	3.0%
Hot side	3.0%
Exhaust	Balanced by stack effect

Steam side

Feedwater heater	69 kPa (10 psi)
Economizer	138 kPa (20 psi)
Evaporator	Drum type with natural circulation
Superheater	241 kPa (35 psi)
Extraction	
> 690 kPaa (100 psia)	3%
< 690 kPaa (100 psia)	5%

Case 1 - 150 psia

2ASG, A AHEAD=6CFW.

END FLT. ERRORS: NONE. TIME: 0.470 SEC. IMAGE COUNT: 71

2471 AMFAD-CCFH-MCFCI

Table 103 (Cont'd)

MOLDEN CARBONATE FUEL CELL - CASE 1 - TESTS

* * * * * FIRST TEST OF MCFC SYSTEM NO 1 * * * * *

NPAR	12	NPARA	37	AFUEL	2	NDPP	11	NEFF	20	NH2O	0
NGAS	10	NSTEA	45	NSW	0	NMIX	7	NPWR	15	NSHAF	0
NSUPP	13										

* * INPUT PARAMETERS * *

1	2	3	4	5
ATMOS PRESS	ATMOS TEMP	GASFR AIR FL	GASFR AIR P	GASFR DEMAND
14.400	520.00	151.90	24.000	-10780.
6	7	8	9	10
POWER STM PR	POWER STM FL	EXC AIR RAT	H2O IN TEMP	CELL PRESS
615.00	.00000	2.0000	60.000	150.00
11	12	13	14	15
CELL TEMP	CONVA	CONVC	CLPR DENS	LP EXT STM P
1760.0	.85000	.50000	290.93	65.000
16	17	18	19	20
LP EXT STM F	HP EXT STM P	HP EXT STM F	HRSG IN W P	FUEL PRESS
9.5830	915.00	25.400	29.820	516.00
21	22	23	24	25
FUEL TEMP	FUEL FLW	HRSG BD RAT	TOT BD RAT	COND PRSS
1660.0	103.93	.10000-001	.20000	.98235
26	27	28	29	30
STEAM PRESS	STEAM TEMP	BLOWER IN T	STACK TEMP	HRSG OFFSET
1815.0	1000.0	1210.0	750.00	15.000
31	32			
RECIRC QUAL	LEAVING LOSS			
.20000	5.0000			
37	38	39	40	41
FUEL TEMP	COND SR HEAT	CP/CV AIR	CP/CV GAS IN	CP/CV ANODE
42	43	44	45	46
CP/CV EXH	CP/CV LOCF	COMPR4 PRAT	BURN EXC AIR	COND EXT FR
47	48	49	50	51
LP EXT FRAC	CATH O2 REQ	MCFC HEAT	GASFR AIR FR	COOL H2O FRC
52	53	54	55	56
COOL GAS FRC	IP STM FRAC	HRSG1 W FRC	COMPR3 PRAT	EVPRTR1 PRS
57	58	59	60	
EVPRTR2 PRS	EXPDR CAFR	COMPR2 PRAT	COMPR1 PRAT	
GASDAT	.00000	.10000-002	.00000	.26410
	.34860	.25800	.00000	.39000-001
CMOL	1.0000			
HMOL	4.0000			
GASDAT	.00000	.10000-002	.00000	.26410
	.34860	.25800	.00000	.39000-001
CMOL	1.0000			
HMOL	4.0000			

* * INPUT FUEL CHARACTERISTICS * *

FUEL NUMBER	1	2
SUPPLY TC:	FUEL GAS IN	ANODE EXIT
FUEL TYPE	GASEOUS	GASEOUS
MASS FLOW	.00000	.00000
CARBON (C)	.47690	.47690
HYDROGEN (H)	.34210	.34210
NITROGEN (N)	.10000-002	.10000-002
OXYGEN (O)	.26360	.26360
SULFUR (S)	.00000	.00000
WATER (H2O)	.25800	.25800
ASH CONTENT	.00000	.00000
SPEC HT (CP)	.35000	.35000
HIGH HT VAL	4604.3	4604.3
LHV/HHV	.92750	.92750
MOL. WEIGHT	19.529	19.529
AIR/FUEL(ST)	2.7163	2.7163

* INPUT PRESSURE LOSS RATIOS *

1	2	3	4	5
AIR FILTER	TCT HRSG	SPRTR GAS	SPRTR STM	EVPRTR GAS

Table 103 (Cont'd)

MOLDEN CARBONATE FUEL CELL - CASE 1 - TESTS

.75000-002	.45000-001	.15000-001	35.000	.12500-001
ECON GAS	ECON STM	OF WH STM	RECLP COLD	RECLP HOT
.12500-001	20.000	10.000	.30000-001	.30000-001
CAT BURNER				
.55000-001				

• INPUT EFFICIENCIES AND EFFECTIVENESSES •

1 COMPR POLY	2 COMPR GEN	3 COMPR MECH	4 COMPR POLY	5 COMPR GEN
.90000	.98500	.98000	.80000	1.0526
6 COMPR MECH	7 EXPDR POLY	8 EXPDR GEN	9 EXPDR MECH	10 BURNER EFF
1.0101	.90000	.98500	.98000	1.0000
11 SPRHTR ETAG	12 EVPTR ETAG	13 ECON ETAG	14 STURB ETA	15 PUMP ETAG
.98500	.98500	.98500	.97500	.70000
16 RECLP EFFECT	17 RECLP ETAG	18 MCFC CNVTR E	19 MCFC ETAG	20 PUMP MOTORS
.85000	.98500	.97000	.98500	.95000

* • MIXTURE COMPOSITION IDENTIFIERS • •

1 INLET AIR	2 BURNER OUT	3 CATHODE IN	4 RECIRC LOOP
5 FUEL GAS IN	6 ANODE OUT	7 CATHODE OUT	

NAMES OF POWER DEVICES ARE:

1 COMPR GASFR	2 COMPR MAIN	3 COMPR MCFC	4 GAS EXPDR
5 EXHST EXPDR	6 FUEL CELL	7 HP1 STURB	8 IP STURB
9 LB STLRB	10 CONDST PUMP	11 HRSG1 PUMP	12 HRSG2 PUMP
13 RECIRC FAN	14 GASFR DEMD	15 HP2 STURB	

NAMES OF HEAT TRANSFER DEVICES ARE:

1 CONDENSER	2 FUEL CELL	3 SPRHTR 2	4 HP EVPRTR 2
5 LP EVPRTR 2	6 ECON 2	7 SPRHTR 1	8 HP EVPRTR 1
9 HP EVPRTR 1	10 ECON 1	11 RECUPERATOR	12 LOOP ECON
13 STACK ECON			

GOOPZ

M 5 MPRIM 2

NTU	X	BOUN1	BOUN2	XWAY	DC	XSTEP
0	1227.0	500.00	1800.0	1.0000	1227.0	.10000+000
0	148.60	50.000	1000.0	1.0000	148.60	.10000+000
0	50.000	15.000	300.00	1.0000	50.000	.10000+000
0	.50000	.10000+000	.90000	1.0000	.50000	.10000+000
0	100.00	15.000	450.00	1.0000	100.00	.10000+000

TARGET	WAIT
1.0000	1.0000
1560.0	1.0000
1210.0	1.0000
1210.0	1.0000
750.00	1.0000

GOOPZ

Table 103 (Cont'd)

MOLDEN CARBONATE FUEL CELL - CASE 1 - TESTS

OPTIMIZATION PROGRESS SUMMARY

CONTROL CONSTANTS

ISTRT 131.67 ILCOP 1 JSTRT 5
 DOLD 131.67 DNEW .45997-002 CHANG 99.996507

MIX VECTOR 5 1 2
 3 4

TABLE OF X(J) AND ASSOCIATED DEFECTS

J	X(J)	WAIT	VIOLATION	FCN-CONTRIB
1	1332.2405	1.0000000	.00000000	.00000000
2	163.33072	1.0000000	.00000000	.00000000
3	31.453703	1.0000000	.00000000	.00000000
4	654.17533	1.0000000	.00000000	.00000000
5	129.59495	1.0000000	.00000000	.00000000

TABLE OF DEFECT FUNCTIONS

I	PROPERTY	WAIT	DEFECT	FCN-CONTRIB
1	.99999871	1.0000000	-.12964010-005	-.12964010-002
2	1560.0003	1.0000000	-.27465820-003	-.27465820-003
3	1209.9987	1.0000000	-.12512207-002	-.12512207-002
4	1210.0015	1.0000000	-.15258789-002	-.15258789-002
5	749.23222	1.0000000	-.67779541-001	-.67779541-001
6	.00000000	1.0000000	.00000000	.00000000

Table 103 (Cont'd)

MOLDEN CARBONATE FUEL CELL - CASE 1 - TESTS

* * * * * FIRST TEST OF MCFC SYSTEM NO 1 * * * * *

* * ARRAY AND VECTOR LIMITS * *

NPAR	32	NPARA	37	NFUEL	2	NOPP	11	NEFF	20	NH2O	0
NGAS	30	NSTEAD	45	NSW	0	NMIX	7	NPWR	15	NSHAF	0
NSURF	13										

* * INPUT PARAMETERS * *

1 ATMOS PRESS	2 ATMOS TEMP	3 GASFR AIR FL	4 GASFR AIR P	5 GASFR DEMAND
14.400	520.00	151.90	84.000	-107.00
6 POWER STM PR	7 POWER STM FL	8 EXC AIR RAT	9 H2O IN TEMP	10 CELL PRESS
615.00	.00000	2.0000	60.000	150.00
11 CELL TEMP	12 CONVA	13 CONVC	14 CLRR DENS	15 LP EXT STM P
1760.0	.85000	.50000	290.93	65.000
16 LP EXT STM F	17 HF EXT STM P	18 HP EXT STM F	19 HRSG IN W P	20 FUEL PRESS
9.5830	915.00	25.400	29.820	516.00
21 FUEL TEMP	22 FUEL FLOW	23 HRSG BD RAT	24 TOT BD RAT	25 COND PRSS
1660.0	103.93	.10000-001	.20000	.98235
26 STEAM PRESS	27 STEAM TEMP	28 BLOWER IN T	29 STACK TEMP	30 HRSG OFFSET
1815.0	1000.0	1210.0	750.00	15.000
31 RECIRC QUAL	32 LEAVING LCSS			
.20000	5.0000			

* * INTERNAL PARAMETERS * *

37 FUEL TEMP	38 COND SR HEAT	39 CP/CV AIR	40 CP/CV GAS IN	41 CP/CV ANODE
1237.3	.11756+006	1.4007	1.2676	1.2309
42 CP/CV EXH	43 CP/CV LOOP	44 COMPR4 PRAT	45 BURN EXC AIR	46 COND EXT ER
1.2977	1.3281	1.1337	5.1688	.00000
47 LP EXT FRAC	48 CATH O2 REQ	49 MCFC HEAT	50 GASFR AIR FR	51 COOL H2O FRC
.69477-001	2.7733	.14619+006	.21201	.00000
52 COOL GAS FRC	53 IP STM FRAC	54 HRSG1 W FRC	55 COMPR3 PRAT	56 EVPTR1 PRS
.00000	.15551	.65618	1.1017	19.820
57 EVPTR2 PRS	58 EXPDR CAFR	59 COMPR2 PRAT	60 COMPR1 PRAT	
1850.0	.00000	11.100	5.8774	

Table 103 (Cont'd)

MOLDEN CARBONATE FUEL CELL - CASE 1 - TESTS

* * * * GAS FLOW STATIONS * * * *

	1	2	3	4	5
GAS STATION					
PRESSURE	14.400	14.292	14.292	14.292	84.000
TEMPERATURE	520.00	520.00	520.00	520.00	908.04
ENTHALPY	28.725	28.725	28.725	28.725	122.74
MASS FLOW	716.49	716.49	151.90	564.59	151.90
COMP POINTER	1.0000	1.0000	1.0000	1.0000	1.0000
GAS STATION	6	7	8	9	10
PRESSURE	158.73	150.00	150.00	144.08	158.73
TEMPERATURE	1103.8	1688.5	1760.0	1210.0	1237.3
ENTHALPY	171.43	345.06	411.57	227.51	236.16
MASS FLOW	564.59	834.96	270.37	270.37	270.37
COMP POINTER	1.0000	2.0000	6.0000	6.0000	6.0000
GAS STATION	11	12	13	14	15
PRESSURE	150.00	150.00	149.86	149.86	150.00
TEMPERATURE	1284.8	1000.0	1560.0	1760.0	1760.0
ENTHALPY	354.74	0.0000	311.61	373.41	373.41
MASS FLOW	103.93	168.44	2167.2	2000.8	1332.2
COMP POINTER	5.0000	7.0000	5.0000	4.0000	4.0000
GAS STATION	16	17	18	19	20
PRESSURE	144.08	139.76	138.01	154.50	149.86
TEMPERATURE	1519.6	1294.6	1210.0	1257.5	1480.4
ENTHALPY	302.11	237.34	213.55	226.86	290.64
MASS FLOW	1332.2	1332.2	1332.2	1332.2	1332.2
COMP POINTER	4.0000	4.0000	4.0000	4.0000	4.0000
GAS STATION	21	22	23	24	25
PRESSURE	150.00	14.767	14.400	516.00	149.75
TEMPERATURE	1760.0	1064.7	749.93	1660.0	1557.8
ENTHALPY	373.41	173.37	85.282	560.87	341.75
MASS FLOW	668.52	668.52	668.52	103.93	270.37
COMP POINTER	4.0000	4.0000	4.0000	5.0000	6.0000
GAS STATION	26	27	28	29	30
PRESSURE	147.75	14.582	145.90	145.90	.00000
TEMPERATURE	1669.2	865.68	1526.1	1225.2	.00000
ENTHALPY	346.37	119.75	303.99	232.33	.00000
MASS FLOW	1332.2	668.52	1332.2	270.37	.00000
COMP POINTER	4.0000	4.0000	4.0000	6.0000	.00000

Table 103 (Cont'd)

MOLDED CARBONATE FUEL CELL - CASE 1 - TESTS

* * * * STEAM FLOW STATIONS * * * *

STEAM STA NO	1	2	3	4	5
PRESSURE	1615.0	915.00	915.00	915.00	615.00
TEMPERATURE	1001.4	822.45	822.45	822.45	730.02
ENTHALPY	1481.0	1407.0	1407.0	1407.0	1368.3
MASS FLOW	163.33	163.33	25.400	137.93	137.93
ENTROPY	1.5747	1.5903	1.5903	1.5903	1.5998
SPEC.WOL.	.43919	.77552	.77552	.77552	1.0795
QUALITY	1.0000	1.0000	1.0000	1.0000	1.0000
SUPERHEAT	.00000	.00000	.00000	.00000	.00000
SUBCOOLING	.00000	.00000	.00000	.00000	.00000
STEAM STA NO	6	7	8	9	10
PRESSURE	615.00	615.00	66.250	66.250	66.250
TEMPERATURE	730.02	730.02	324.95	324.95	324.95
ENTHALPY	1368.3	1368.3	1193.0	1193.0	1193.0
MASS FLOW	.00000	137.93	137.93	9.5830	128.33
ENTROPY	.00000	1.5992	1.6504	1.6504	1.6504
SPEC.WOL.	.00000	1.0795	6.5941	6.5941	6.5941
QUALITY	.00000	1.0000	1.0000	1.0000	1.0000
SUPERHEAT	.00000	.00000	.00000	.00000	.00000
SUBCOOLING	.00000	.00000	.00000	.00000	.00000
STEAM STA NO	11	12	13	14	15
PRESSURE	.98235	.98235	29.620	29.620	29.620
TEMPERATURE	101.14	101.14	101.20	101.20	101.20
ENTHALPY	965.09	69.139	69.262	69.262	69.262
MASS FLOW	128.33	128.33	128.33	.00000	128.33
ENTROPY	1.7646	.13158	.13164	.13164	.13164
SPEC.WOL.	299.81	.16134-001	.00000	.00000	.00000
QUALITY	.88377	.00000	.00000	.00000	.00000
SUPERHEAT	.00000	.00000	.00000	.00000	.00000
SUBCOOLING	.00000	.00000	148.79	148.79	148.79
STEAM STA NO	16	17	18	19	20
PRESSURE	29.620	29.620	1890.0	1870.0	1870.0
TEMPERATURE	92.298	106.10	438.23	594.68	594.68
ENTHALPY	60.390	74.163	418.22	607.46	607.46
MASS FLOW	163.66	164.98	164.98	164.98	164.98
ENTROPY	.11570	.14034	.60925	.60295	.60295
SPEC.WOL.	.16104-001	.16119-001	.00000	.00000	.00000
QUALITY	.00000	.00000	.00000	.00000	.00000
SUPERHEAT	.00000	.00000	.00000	.00000	.00000
SUBCOOLING	.00000	143.89	189.59	31.654	31.654
STEAM STA NO	21	22	23	24	25
PRESSURE	1850.0	1815.0	.00000	1815.0	1870.0
TEMPERATURE	624.83	1000.0	.00000	1000.0	594.68
ENTHALPY	654.44	1480.1	.00000	1480.1	607.46
MASS FLOW	1.0826	107.17	1.3498	56.157	56.157
ENTROPY	.00000	1.5741	.00000	1.5741	.60295
SPEC.WOL.	.00000	.43861	.00000	.43861	.00000
QUALITY	.00000	.00000	.00000	.00000	.00000
SUPERHEAT	.00000	377.83	.00000	377.83	.00000
SUBCOOLING	.00000	.00000	.00000	.00000	31.654
STEAM STA NO	26	27	28	29	30
PRESSURE	1850.0	1850.0	1850.0	1850.0	1850.0
TEMPERATURE	624.83	609.93	624.83	624.83	624.83
ENTHALPY	654.44	630.11	654.44	753.36	1149.0
MASS FLOW	.56724	56.724	294.60	294.60	56.157
ENTROPY	.00000	.62436	.00000	.00000	1.3030
SPEC.WOL.	.00000	.00000	.00000	.00000	.21051
QUALITY	.00000	.00000	.00000	.00000	1.0000
SUPERHEAT	.00000	.00000	.00000	.00000	.00000
SUBCOOLING	.00000	15.000	.00000	.00000	.00000
STEAM STA NO	31	32	33	34	35
PRESSURE	1850.0	1850.0	1850.0	1850.0	1910.0
TEMPERATURE	609.93	624.83	624.83	624.83	231.78
ENTHALPY	630.11	654.44	753.36	1149.0	204.20
MASS FLOW	108.26	562.23	562.23	107.17	164.98
ENTROPY	.82436	.00000	.00000	1.3030	.33280
SPEC.WOL.	.00000	.00000	.00000	.21051	.00000

Table 103 (Cont'd)

MOLDEN CARBONATE FUEL CELL - CASE 1 - TESTS

QUALITY	.00000	.00000	.00000	1.00000	.00000
SUPERHEAT	.00000	.00000	.00000	.00000	.00000
SUBCOOLING	15.000	.00000	.00000	.00000	397.52
STEAM STA NO	36	37	38	39	40
PRESSURE	19.820	19.820	19.820	19.820	19.820
TEMPERATURE	227.48	227.48	227.48	227.48	227.48
ENTHALPY	195.78	195.78	1156.1	195.78	387.86
MASS FLOW	164.98	165.87	20.893	104.46	104.46
ENTROPY	.33510	.33510	1.7328	.00000	.00000
SPEC. VOL.	.16830-CC1	.00000	20.257	.00000	.00000
QUALITY	.00000	.00000	1.00000	.00000	.00000
SUPERHEAT	.00000	.00000	.00000	.00000	.00000
SUBCOOLING	.00000	.00000	.00000	.00000	.00000
STEAM STA NO	41	42	43	44	45
PRESSURE	1650.0	.00000	29.820	.00000	.00000
TEMPERATURE	624.83	.00000	60.000	.00000	.00000
ENTHALPY	654.44	.00000	28.143	.00000	.00000
MASS FLOW	1.3198	.32976	35.313	.00000	.00000
ENTROPY	.00000	.00000	.55490-CC1	.00000	.00000
SPEC. VOL.	.00000	.00000	.00000	.00000	.00000
QUALITY	.00000	.00000	.00000	.00000	.00000
SUPERHEAT	.00000	.00000	.00000	.00000	.00000
SUBCOOLING	.00000	.00000	.00000	.00000	.00000

* * * * GAS COMPOSITIONS * * * *

GAS COMP NO	1	2	3	4	5
COMPOSITIONS	INLET AIR	BURNER OUT	CATHODE IN	RECIRC LOOP	FUEL GAS IN
EXC. DRY AIR	1.00000	.00000	.00000	.00000	.00000-001
(CO2)	.00000	.19286	.13989	.10555	.89300-001
WATER VAPOR	.00000	.12328	.13702	.14513	.25800
(SO2)	.00000	.00000	.00000	.00000	.00000-002
NITROGEN	.00000	.53712	.60172	.63995	.10000-002
ARGON	.00000	.91364-002	.94996-002	.97145-002	.00000
HYDROGEN H2	.00000	.00000	.00000	.00000	.26410
(CO)	.00000	.00000	.00000	.00000	.34860
(CH4)	.00000	.00000	.00000	.00000	.39000-001
(C2H6)	.00000	.00000	.00000	.00000	.00000
OXYGEN(O2)	.00000	.13760	.11186	.96634-001	.00000
(H2S)	.00000	.00000	.00000	.00000	.00000
MOL. WEIGHT	28.969	30.447	29.379	28.746	19.525
GAS CONSTANT	53.320	50.755	52.600	53.757	79.130
GAS COMP NO	6	7			
COMPOSITIONS	ANODE OUT	CATHODE OUT			
EXC. DRY AIR	.00000	.00000			
(CO2)	.59492	.66667			
WATER VAPOR	.31633	.00000			
(SO2)	.00000	.00000			
NITROGEN	.05755-003	.00000			
ARGON	.00000	.00000			
HYDROGEN H2	.26957-001	.00000			
(CO)	.33475-CC1	.00000			
(CH4)	.25645-CC1	.00000			
(C2H6)	.00000	.00000			
OXYGEN(O2)	.00000	.33333			
(H2S)	.00000	.00000			
MOL. WEIGHT	33.391	40.010			
GAS CONSTANT	46.260	38.623			

* * * * FUEL CHARACTERISTICS * * * *

FUEL NUMBER	1	2
FUEL TYPE	FUEL GAS IN	ANODE EXIT
MASS FLOW	103.93	270.37
CARBON (C)	.47690	.65604
HYDROGEN (H)	.34210	.78246-001
NITROGEN (N)	.10000-002	.65755-003
OXYGEN (O)	.26360	.61365
SULFUR (S)	.00000	.00000
WATER (H2O)	.25800	.31635
ASH CONTENT	.00000	.00000
SPEC HT (CP)	.35000	.28193
HIGH HT VAL	4404.3	515.51
LHV/HHV	.92750	.91483

Table 103 (Cont'd)

MOLDEN CARBONATE FUEL CELL - CASE 1 - TESTS

MOL. WEIGHT 19.529 33.391
 AIR/FUEL(ST) 2.7163 .33688

* HEAT EXCHANGERS -- NOS. AND EFFECTIVENESSES *

1 COMPR FCLY .90000	2 COMPR GEN .98500	3 COMPR MECH .98000	4 COMPR3 POLY .80000	5 COMPR3 GEN 1.0526
6 COMPR3 MECH 1.0101	7 EXPDR POLY .90000	8 EXPDR GEN .98500	9 EXPDR MECH .98000	10 BURNER EFF 1.0000
11 SPRHTR ETAQ .98500	12 EVPRTT ETAQ .98500	13 ECON ETAQ .98500	14 STURB ETA .97500	15 PUMP ETA1 .70000
16 RECUP EFFECT .85000	17 RECUP ETAQ .98500	18 MCFC CNVTR E .97000	19 MCFC ETAQ .98500	20 PUMP MOTORS .95000

* * PRESSURE LOSSES -- NOS. AND LOSSES * *

1 AIR FILTER .75000-CC2	2 TCT HRSG .45000-CC1	3 SPRHTR GAS .15000-UC1	4 SPRHTR STM 35.000	5 EVPRTT GAS .12500-001
6 ECON GAS .12500-CC1	7 ECON STM 20.000	8 OFWH STM 10.000	9 RECUP COLD .30000-CC1	10 RECUP HOT .30000-CC1
11 CAT BURNER .55000-CC1				

* * * UNIT POWERS -- NOS AND POWERS * * *

1 COMPR GASFR -14529.	2 COMPR MAIN -81985.	3 COMPR MCFC -2661.9	4 GAS EXPDR 17566.	5 EXHST EXPDR .13606+006
6 FUEL CELL .17341+006	7 HF1 STURB 11579.	8 IP STURB 24132.	9 LB STURB 26764.	10 CONDST PUMP -15.811
11 HRSG1 PLMP -1389.6	12 HRSG2 PLMP .00000	13 RECIRC FAN -19950.	14 GASFR DEMD -10780.	15 HP2 STURB 4781.9

NET POWER = .26297+006

* * * HEAT EXCHANGER UA -- NOS. AND UA * * *

1 CONDENSER .00000	2 FUEL CELL .89774+006	3 SPRHTR 2 .30408+006	4 HP EVPRTT 2 .38746+006	5 LP EVPRTT 2 .00000
6 ECON 2 19451.	7 SPRHTR 1 .17886+006	8 HP EVPRTT 1 .36647+006	9 HP EVPRTT 1 .66428+006	10 ECON 1 30223.
11 RECUPERATOR .81340+007	12 LOOP ECON .41606+006	13 STACK ECON .75836+006		

* * * SEARCH RESULTS * * *

1	X(I)	BOUN1(I)	BOUN2(I)
1	1332.2	500.00	1800.0
2	163.33	50.000	1000.0
3	31.654	15.000	300.00
4	65618	10000+000	90000
5	189.59	15.000	450.00
J	FTARG(J)	TARGET(J)	FCN(J)
1	1.0000	1.0000	-.12964-002
2	1560.0	1560.0	-.27466-003
3	1210.0	1210.0	-.12512-002
4	1210.0	1210.0	-.15259-002
5	749.93	750.00	-.67780-001

* * * * CASE COMPLETED * * RUN ENDED * * * *

ORJEFIN: RJESPF.RJEFIN . . .

Table 104a
MOLTEN CARBONATE FUEL CELL PARAMETRIC STUDY
PERFORMANCE SUMMARY

Case 1	Run				
	1	2	3	4	5
Cell Pressure - kPaa (psia)	345 (50)	690 (100)	993 (144)	1034 (150)	2069 (300)
Exhaust Expander Power - kW	80090	117010	134220	136060	164700
Combustion Air Compressor Power - kW	36887	63524	80014	81985	119350
Net Gas Turbine Power - kW	43203	53486	54206	54075	45350
Fuel Gas Expander Power - kW	29750	22423	18075	17566	8239
Steam Turbine Power - kW					
HPI element	12215	11591	11571	11579	12101
HP2 element	5093	4788	4778	4782	5038
IP element	25703	24162	24112	24132	25421
LP element	28637	26801	26741	26764	28301
Total (net)	71648	67342	67202	67257	70861
Fuel Cell Power (net) - kW	157940	168040	172880	173410	181790
System Gross Power - kW	302541	311291	312363	312308	306240
Auxiliary Power Requirements - kW					
Process air compressor	14529	14529	14529	14529	14529
Fuel gas booster compressor	2662	2662	2662	2662	2662
Recycle gas compressor	20687	20049	19951	19950	20228
Condensate pump	17	16	16	16	17
Boiler feedwater pump	1466	1391	1389	1390	1452
Gasifier subsystem auxiliaries	10780	10780	10780	10780	10780
Total auxiliary power	50141	49427	49327	49327	49668
Net System Power Output - kWe	252400	261860	263040	262970	256570
Coal Feed Rate kg/s (lb/hr)	21. 34 (169400)	21. 34 (169400)	21. 34 (169400)	21. 34 (169400)	21. 34 (169400)
Coal HHV kJ/kg (Btu/lb)	29. 703 (12, 770)	29. 703 (12, 770)	29. 703 (12, 770)	29. 703 (12, 770)	29. 703 (12, 770)
Heat Rate kJ/kWh (Btu/kWh)	9043 (8571)	8716 (8261)	8677 (8224)	8679 (8226)	8895 (8431)

Table 104b

MOLTEN CARBONATE FUEL CELL PARAMETRIC STUDY
PERFORMANCE SUMMARY

Case 2	Run			
	1	2	3	4
Cell Pressure kPaa (psia)	345 (50)	690 (100)	1034 (150)	2069 (300)
Exhaust Expander Power - kW	84294	123090	143090	173150
Combustion Air Compressor Power - kW	40038	68951	88988	129540
Net Gas Turbine Power - kW	44256	54139	54102	43610
Fuel Gas Expander Power - kW	27250	20567	16120	7562
Steam Turbine Power - kW				
HPI element	13573	12955	12927	13490
HP2 element	6505	6203	6189	6464
IP element	32825	31301	31231	32620
LP element	38036	36219	36136	37791
Total (net)	90939	86678	86483	90365
Fuel Cell Power (net) - kW	161470	171600	176980	185390
System Gross Power - kW	323915	332984	333685	326927
Auxiliary Power Requirements - kW				
Process air compressor	10617	10617	10617	10617
Fuel gas booster compressor	2523	2523	2523	2523
Recycle gas compressor	21587	20777	20568	20647
Condensate pump	25	21	21	22
Boiler feedwater pump	1629	1555	1552	1619
Gasifier subsystem auxiliaries	8931	8931	8931	8931
Total auxiliary power	45312	44424	44212	44359
Net System Power Output - kWe	278600	288560	289470	282560
Coal Feed Rate kg/s (lb/hr)	22.43 (178,000)	→		
Coal HHV kJ/kg (Btu/lb)	29,703 (12,770)	→		
Heat Rate kJ/kWh (Btu/kWh)	8608 (8159)	8311 (7877)	8285 (7853)	8488 (8045)

Table 104c

MOLTEN CARBONATE FUEL CELL PARAMETRIC STUDY
PERFORMANCE SUMMARY

Case 3	Run			
	1	2	3	4
Cell Pressure - kPaa (psia)	345 (50)	690 (100)	1034 (150)	2069 (300)
Exhaust Expander Power - kW	79127	115560	134350	162600
Combustion Air Compressor Power - kW	36940	63615	82103	119520
Net Gas Turbine Power - kW	42187	51945	52247	43080
Fuel Gas Expander Power - kW	27989	21123	16559	7772
Steam Turbine Power - kW				
HPI element	12620	11970	11955	12489
HP2 element	5863	5546	5538	5799
IP element	29589	27985	27949	29266
LP element	28816	26903	26860	28430
Total (net)	76888	72404	72302	75984
Fuel Cell Power (net) - kW	159690	169790	175160	183530
System Gross Power - kW	306754	315262	316268	310366
Auxiliary Power Requirements - kW				
Process air compressor	14931	14931	14931	14931
Fuel gas booster compressor	2566	2566	2566	2566
Recycle gas compressor	21046	20298	20117	20263
Condensate pump	17	16	16	17
Boiler feedwater pump	1514	1437	1435	1499
Gasifier subsystem auxiliaries	12880	12880	12880	12880
Total auxiliary power	52954	52128	51945	52156
Net System Power Output - kWe	253800	263140	264320	258211
Coal Feed Rate kg/s (lb/hr)	21. 91 (173900)	→		
Coal HHV kJ/kg (Btu/lb)	29, 703 (12, 770)	→		
Heat Rate kJ/kWh (Btu/kWh)	9232 (8750)	8904 (8439)	8865 (8402)	9074 (8600)

Table 104d

MOLTEN CARBONATE FUEL CELL PARAMETRIC STUDY
PERFORMANCE SUMMARY

Case 4	Run			
	1	2	3	4
Cell Pressure - kPaa (psia)	345 (50)	690 (100)	1034 (150)	2069 (300)
Exhaust Expander Power - kW	64507	94270	109630	132740
Combustion Air Compressor Power - kW	29563	50912	65707	95651
Net Gas Turbine Power - kW	34944	43358	43923	37089
Fuel Gas Expander Power - kW	25797	19533	15345	7225
Steam Turbine Power - kW				
HPI element	9314	8743	8670	9027
HP2 element	4555	4276	4240	4415
IP element	24835	23427	23246	24127
LP element	28106	26428	26212	27262
Total (net)	66810	62874	62368	64831
Fuel Cell Power (net) - kW	160250	170370	175730	184120
System Gross Power - kW	287801	296135	297366	293265
Auxiliary Power Requirements - kW				
Process air compressor	15792	15792	15792	15792
Fuel gas booster compressor	2450	2450	2450	2450
Recycle gas compressor	22928	22558	22294	22271
Condensate pump	17	16	16	16
Boiler feedwater pump	1118	1049	1041	1083
Gasifier subsystem auxiliaries	8710	8710	8710	8710
Total auxiliary power	51015	50575	50303	50322
Net System Power Output - kWe	236790	245560	247070	242950
Coal Feed Rate kg/s (lb/hr)	18.67 (148200)	→		
Heating Value of As-Fired Load (dry) kJ/kg (Btu/lb)	29,703 (12,770)	→		
Heat Rate kJ/kWh (Btu/kWh)	8432 (7992)	8131 (7707)	8082 (7660)	8219 (7790)

Table 104e

MOLTEN CARBONATE FUEL CELL PARAMETRIC STUDY
PERFORMANCE SUMMARY

Case 5	Run			
	1	2	3	4
Cell Pressure - kPaa (psia)	345 (50)	690 (100)	1034 (150)	2069 (300)
Exhaust Expander Power - kW	80775	118030	137260	166180
Combustion Air Compressor Power - kW	36926	63592	82072	119470
Net Gas Turbine Power - kW	43849	54438	55188	46710
Fuel Gas Expander Power - kW	26611	18331	12885	2510
Steam Turbine Power - kW				
HPI element	12526	11951	11969	12542
HP2 element	6126	5845	5853	6134
IP element	31020	29601	29645	31060
LP element	36973	35282	35334	37021
Total (net)	86645	82679	82801	86757
Fuel Cell Power (net) - kW	155660	165680	171000	179310
System Gross Power - kW	312765	321128	321874	315287
Auxiliary Power Requirements - kW				
Process air compressor	14453	14453	14453	14453
Fuel gas booster compressor	2705	2705	2705	2705
Recycle gas compressor	21163	20783	20841	21395
Condensate pump	22	21	21	22
Boiler feedwater pump	1503	1434	1437	1505
Gasifier subsystem auxiliaries	7370	7370	7370	7370
Total auxiliary power	47216	46766	41827	47450
Net System Power Output - kWe	265550	274360	275050	267830
Coal Feed Rate kg/s (lb/hr)	21.23 (168500)	→		
As-Fired (dry) HHV kJ/kg (Btu/lb)	29,703 (12,770)	→		
Heat Rate kgJ/kWh (Btu/kWh)	8549 (8103)	8275 (7843)	8254 (7823)	8476 (8034)

Table 104f

MOLTEN CARBONATE FUEL CELL PARAMETRIC STUDY
PERFORMANCE SUMMARY

Case 6	Run			
	1	2	3	4
Cell Pressure - kPaa (psia)	345 (50)	690 (100)	1034 (150)	2069 (300)
Exhaust Expander Power - kW	81434	118990	138380	167530
Combustion Air Compressor Power - kW	37227	64111	82742	120450
Net Gas Turbine Power - kW	44207	54879	55638	47080
Fuel Gas Expander Power - kW	26828	18480	12990	2530
Steam Turbine Power - kW				
HPI element	12628	12049	12066	12645
HP2 element	6176	5892	5901	6184
IP element	31259	29828	29871	31299
LP element	37257	35552	35603	37305
Total (net)	87320	83321	83441	87433
Fuel Cell Power (net) - kW	156930	167030	172400	180780
System Gross Power - kW	315285	323710	324469	317823
Auxiliary Power Requirements - kW				
Process air compressor	14290	14290	14290	14290
Fuel gas booster compressor	2728	2728	2728	2728
Recycle gas compressor	21336	20953	21012	21570
Condensate pump	22	21	21	22
Boiler feedwater pump	1516	1446	1448	1518
Gasifier subsystem auxiliaries	7290	7290	7290	7290
Total auxiliary power	47182	46728	46789	47418
Net System Power Output - kWe	268110	276990	277680	270410
Coal Feed Rate kg/s (lb/hr)	21.00 (166700)	—————→		
As-Fired (dry) HHV Value kJ/kg (Btu/lb)	29,703 (12,700)	—————→		
Heat Rate kJ/kWh (Btu/kWh)	8377 (7940)	8108 (7685)	8088 (7666)	8305 (7872)

Table 104g

MOLTEN CARBONATE FUEL CELL PARAMETRIC STUDY
PERFORMANCE SUMMARY

Case 7	Run			
	1	2	3	4
Cell Pressure - kPaa (psia)	345 (50)	690 (100)	1034 (150)	1724 (250)
Exhaust Expander Power - kW	90784	132510	154010	178300
Combustion Air Compressor Power - kW	35140	60516	78103	103600
Net Gas Turbine Power - kW	55644	71994	75907	74700
Fuel Gas Expander Power - kW	41319	26930	17392	4130
Steam Turbine Power - kW				
HPI element	11438	10940	11023	11540
HP2 element	5594	5350	5391	5644
IP element	30994	29766	29970	31246
LP element	36942	35478	35722	37242
Total (net)	84968	81534	82106	85672
Fuel Cell Power (net) - kW	162480	172520	177850	184070
System Gross Power - kW	344411	352978	353255	348572
Auxiliary Power Requirements - kW				
Process air compressor	29099	29099	29099	29099
Fuel gas booster compressor	4030	4030	4030	4030
Recycle gas compressor	15424	16571	17658	19462
Condensate pump	22	21	21	22
Boiler feedwater pump	1373	1313	1323	1385
Gasifier subsystem auxiliaries	389	389	389	389
Total auxiliary power	50337	51423	52520	54387
Net System Power Output - kWe	294075	301555	300735	294195
Coal Feed Rate kg/s (lb/hr)	23.47 (186300)
As-Fired (dry) of Coal HHV kJ/kg (Btu/lb)	27,965 (12,023)
Heat Rate kJ/kWh (Btu/kWh)	8036 (7616)	7837 (7428)	7858 (7448)	8033 (7613)

Table 104h

MOLTEN CARBONATE FUEL CELL PARAMETRIC STUDY
PERFORMANCE SUMMARY

Case 8	Run			
	1	2	3	4
Cell Pressure - kPaa (psia)	345 (50)	690 (100)	1034 (150)	1724 (250)
Exhaust Expander Power - kW	19255	28105	32664	37816
Combustion Air Compressor Power - kW	7401	12746	16450	21820
Net Gas Turbine Power - kW	11854	15359	16214	15996
Fuel Gas Expander Power - kW	8612	5463	3373	466
Steam Turbine Power - kW				
HPI element	2436	2332	2350	2458
HP2 element	1060	1009	1018	1071
IP element	5351	5093	5139	5404
LP element	6378	6070	6125	6441
Total (net)	15225	14504	14632	15374
Fuel Cell Power (net) - kW	35375	37561	38722	40077
System Gross Power - kW	71066	72887	72941	71913
Auxiliary Power Requirements - kW				
Process air compressor	5890	5890	5890	5890
Fuel gas booster compressor	872	872	872	872
Recycle gas compressor	3684	3938	4178	4575
Condensate pump	4	4	4	4
Boiler feedwater pump	292	280	282	295
Gasifier subsystem auxiliaries	950	950	950	950
Total auxiliary power	11692	11934	12176	12586
Net System Power Output - kWe	59375	60953	60766	59327
Coal Feed Rate kg/s (lb/hr)	4.35 (34500)	—————→		
As-Fired (dry) HHV kJ/kg (Btu/lb)	29,703 (12,770)	—————→		
Heat Rate kJ/kWh (Btu/kWh)	7795 (7419)	7594 (7228)	7617 (7250)	7802 (7426)

Table 1041

MOLTEN CARBONATE FUEL CELL PARAMETRIC STUDY
PERFORMANCE SUMMARY

Case 9	Run			
	1	2	3	4
Cell Pressure - kPaa (psia)	345 (50)	690 (100)	1034 (150)	1724 (250)
Exhaust Expander Power - kW	19691	28742	33405	38673
Combustion Air Compressor Power - kW	7622	13126	16940	22470
Net Gas Turbine Power - kW	12069	15616	16465	16203
Fuel Gas Expander Power - kW	8962	5841	3772	896
Steam Turbine Power - kW				
HPI element	2481	2373	2391	2503
HP2 element	1213	1161	1170	1224
IP element	6749	6483	6528	6804
LP element	8044	7727	7781	8110
Total (net)	18487	17744	17870	18641
Fuel Cell Power (net) - kW	35242	37419	38575	39925
System Gross Power - kW	74760	76620	76682	75665
Auxiliary Power Requirements - kW				
Process air compressor	6310	6310	6310	6310
Fuel gas booster compressor	874	874	874	874
Recycle gas compressor	3345	3594	3830	4221
Condensate pump	5	5	5	5
Boiler feedwater pump	298	285	287	300
Gasifier subsystem auxiliaries	84	84	84	84
Total auxiliary power	10916	11152	11390	11794
Net System Power Output - kWe	63844	65467	65292	63870
Coal Feed Rate kg/s (lb/hr)	5.09 (40400)	→		
As-Fired (dry) HHV of Coal kJ/kg (Btu/lb)	27,965 (12,023)	→		
Heat Rate kJ/kWh (Btu/kWh)	8026 (7608)	7827 (7419)	7849 (7439)	8024 (7605)

Table 104j

MOLTEN CARBONATE FUEL CELL PARAMETRIC STUDY
PERFORMANCE SUMMARY

Case 10	Run			
	1	2	3	4
Cell Pressure - kPaa (psia)	345 (50)	690 (100)	1034 (150)	1724 (250)
Exhaust Expander Power - kW	19823	28935	33629	38933
Combustion Air Compressor Power - kW	7673	13214	17054	22621
Net Gas Turbine Power - kW	12150	15721	16575	16312
Fuel Gas Expander Power - kW	9022	5880	3798	902
Steam Turbine Power - kW				
HPI element	2498	2389	2407	2520
HP2 element	1221	1168	1177	1232
IP element	6781	6513	6550	6837
LP element	8083	7763	7816	8149
Total (net)	18583	17833	17950	18738
Fuel Cell Power (net) - kW	35478	37670	38834	40193
System Gross Power - kW	75233	77104	77157	76145
Auxiliary Power Requirements - kW				
Process air compressor	6260	6260	6260	6260
Fuel gas booster compressor	880	880	880	880
Recycle gas compressor	3368	3618	3855	4250
Condensate pump	5	5	5	5
Boiler feedwater pump	300	287	289	302
Gasifier subsystem auxiliaries	82	82	82	82
Total auxiliary power	10895	11132	11371	11779
Net System Power Output - kW	64339	65973	65796	64366
Coal Feed Rate kg/s (lb/hr)	5.05 (40100)	→		
As-Fired (dry) HHV of Coal kJ/kg (Btu/lb)	27,965 (12,023)	→		
Heat Rate kJ/kWh (Btu/kWh)	7906 (7494)	7711 (7308)	7731 (7328)	7904 (7491)

Table 105

MOLTEN CARBONATE FUEL CELL PARAMETRIC STUDY - PERFORMANCE SUMMARY

Dwg. 4253857

Case	1	2	3	4	5	6	7	8	9	10
Cell Pressure kPaa (psia)	1034 (150)	1034 (150)	1034 (150)	1034 (150)	1034 (150)	1034 (150)	1034 (150)	1034 (150)	1034 (150)	1034 (150)
Exhaust Expander Power - kW	136060	143090	134350	109630	137260	138380	154010	32664	33405	33629
Combustion Air Compressor Power - kW	81985	88988	82103	65707	82072	82742	78103	16450	16940	17054
Net Gas Turbine Power - kW	54075	54102	52247	43923	55188	55638	75907	16214	16465	16575
Fuel Gas Expander Power - kW	17566	16120	16559	15345	12885	12990	17392	3373	3772	3798
Steam Turbine Power - kW										
HPI element	11579	12927	11955	8670	11969	12066	11023	2350	2391	2407
HP2 element	4782	6189	5538	4240	5853	5901	5391	1018	1170	1177
IP element	24132	31231	27949	23246	29645	29871	29970	5139	6528	6550
LP element	26764	36136	26860	26212	35334	35603	35722	6125	7781	7816
Total (net)	67257	86483	72302	62368	82801	83441	82106	14632	17870	17950
Fuel Cell Power (net) - kW	173410	176980	175160	175730	171000	172400	177850	38722	38575	38834
System Gross Power - kW	312308	333685	316268	297366	321874	324469	353255	72941	76682	77157
Auxiliary Power Requirements - kW										
Process air compressor	14529	10617	14931	15792	14453	14290	29099	5890	6310	6260
Fuel gas booster compressor	2662	2523	2566	2450	2705	2728	4030	872	874	880
Recycle gas compressor	19950	20568	20117	22294	20841	21012	17658	4178	3830	3855
Condensate pump	16	21	16	16	21	21	21	4	5	5
Boiler feedwater pump	1390	1552	1435	1041	1437	1448	1323	282	287	289
Gasifier subsystem auxiliaries	10780	8931	12880	8710	7370	7290	389	950	84	82
Total auxiliary power	49327	44212	51945	50303	46827	46789	52520	12176	11390	11371
Net System Power Output - kWe	262970	289470	264320	247070	275050	277680	300735	60766	65292	65796
Coal Feed Rate kg/s (lb/hr)	21.34 (169400)	22.43 (178000)	21.91 (173900)	18.67 (148200)	21.23 (168500)	21.00 (166700)	23.47 (186300)	4.35 (34500)	5.09 (40400)	5.05 (40100)
Coal HHV kJ/kg (Btu/lb)	29703 (12770)	29703 (12770)	29703 (12770)	29703 (12770)	29703 (12770)	29703 (12770)	27965 (12023)	29703 (12770)	27965 (12023)	27965 (12023)
Heat Rate kJ/kWh (Btu/kWh)	8679 (8226)	8285 (7853)	8865 (8402)	8082 (7660)	8254 (7823)	8088 (7666)	7858 (7448)	7617 (7250)	7849 (7439)	7731 (7328)

Figures 50 and 51 show the effect of the gasification process or system performance for oxygen-blown gasifiers with Rectisol II fuel gas cleanup. Figure 50 compares the three gasification processes on the basis of net system power, and Figure 51 compares them on the basis of system heat rate.

Figures 52 and 53 show the effect of the fuel gas cleanup process on system performance for the Westinghouse oxygen-blown gasifier. Figure 52 compares the four cleanup processes on the basis of net system power, and Figure 53 compares them on the basis of system heat rate.

Figures 54 and 55 show the effect of gasifier blast on system performance. Figure 54 compares oxygen and air blowing on the basis of net system power, and Figure 55 compares them on the basis of system heat rate.

Figures 56 and 57 compare the performance of three optional systems for industrial applications. Figure 56 compares the three systems on the basis of net system output, Figure 57 on the basis of system heat rate.

These results will be incorporated into a comparison of cost of electricity, reliability, and operability in Section 6, Summary Analyses.

Figure 50 -- Effect of Gasification Process
on Net System Power

Figure 51 -- Effect of Gasification Process
on System Heat Rate

Figure 52 -- Effect of Fuel Gas Cleanup Process on Net System Power

Figure 53 -- Effect of Fuel Gas Cleanup Process on System Heat Rate

Figure 54 -- Effect of Gasifier Blast on Net System Power

Figure 55 -- Effect of Gasifier Blast on System Heat Rate

Figure 56 -- Comparison of Power Output Systems for Industrial Application

Figure 57 -- Comparison of Heat Rate Systems for Industrial Application

Section 6

SUMMARY ANALYSES

6.1 INTRODUCTION

The previous five sections of this report have developed the bases for the selection of optimal coal gas supply systems for a MCFC power plant configuration. Section 6.2 contains flow diagrams for the ten coal gas supply systems (chosen for detailed study in Section 4 and reviewed for efficiency in Section 5), using a schematic diagram as shown in Figure 58 for the MCFC power system developed to utilize the coal gas. The configurations shown are ranked on the basis of system efficiency, investment, cost of electricity, operability, and environmental effects. Section 6.3 provides insights into part-load performance of the lowest-cost cold cleanup and hot cleanup utility size systems. Section 7 will then provide conclusions about optimum configuration selection and recommendations for future development of hot gas cleaning concepts for MCFC power plants using coal.

This report does not attempt to optimize the coal gas supply and MCFC power systems. Relative rankings of commercial and developmental systems were carefully assessed. The absolute accuracy of the cost and efficiency information is less critical to relative rankings. Investment cost estimates, $\pm 35\%$, were made to assess order-of-magnitude total installed costs. Efficiency estimates assumed present state-of-the-art expansion turbines, compressors, and the like. The GE and UTC concepts for MCFC power plants are understood to contain advanced system components for spent fuel pressure boost, hot gas recycle compression, and so on, which could provide higher efficiency and lower investment than is shown in this report. The results in this report are applicable

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Figure 58 -- Generalized Molten Carbonate Fuel Cell Subsystem -- Flow Diagram

only to relative rankings of coal gasification and gas cleanup processes for use in MCFC power plants.

6.2 PROCESS CONFIGURATION RANKINGS

6.2.1 Configurations

Flow diagrams for the ten coal gas supply configurations for the MCFC power systems are presented here. Seven configurations for the utility size power plants have been studied. These are:

<u>Flow Diagram No.</u>	<u>System</u>
B1 and B2	BGC-Lurgi Slagging Oxygen-Blown Gasifier - Rectisol II
T1 and T2	Texaco Oxygen-Blown Gasifier - Rectisol II
W1 and W2a	Westinghouse Oxygen-Blown Gasifier - Rectisol II
W3 and W4a	Westinghouse Oxygen-Blown Gasifier - Selexol
W5 and W6a	Westinghouse Oxygen-Blown Gasifier - METC Iron Oxide
W7 and W8a	Westinghouse Oxygen-Blown Gasifier - Dolomite
W17 and W18	Westinghouse Air-Blown Gasifier - METC Iron Oxide

Three configurations have been studied for the industrial size power plants. These are:

<u>Flow Diagram No.</u>	<u>System</u>
R1, R2 and R3	Rockwell Air-Blown Gasifier - ZnO
W13 and W14	Westinghouse Air-Blown Gasifier - METC Iron Oxide
W15 and W16	Westinghouse Air-Blown Gasifier - Dolomite

25 26 27

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PROCESS FLOW DIAGRAM
WESTINGHOUSE OXYGEN
BLOWN GASIFIER w/ METC

26a

[illegible]

Basis: 0.8 Ton Dry Coal/hr

SNT 2 OF 2

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PROCESS FLOW DIAGRAM
WESTINGHOUSE OXYGEN
BLOWN GASIFIER - IDOLMITE

14 92

429

432

434

[illegible]

DATE: 16 MAR 1961

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Davy McKee

ENGINEERS AND CONSTRUCTORS

PROCESS FLOW DIAGRAM
WESTINGHOUSE-AIR
FLOWN GASIFIER - IMETC

W 14

[illegible]

SNT 2 OF 2

Davy McKee
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PROCESS FLOW DIAGRAM
WESTINGHOUSE - AIR
BLOWN GASIFIER - /DOLOMITE

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The process of selecting configurations for detailed study was reported in Section 4 of this effort. In summary, we can point out that both the BGC-Lurgi slagging gasifier and the Texaco gasifier were greater in detail by EPRI,⁷³ and their inclusion forms a basis by which to compare results from this report and from the several other EPRI reports on coal gasification/electric power generation systems.^{76,78,79} Because of the tar and oil content of the BGC/Lurgi product gas, however, and of the proprietary nature of Texaco data on raw coal gas temperature and solids content, neither of those systems could be used to compare hot (dry) desulfurization and cold (wet) desulfurization. The fluidized-bed gasification systems developed by IGT⁸⁰ and Westinghouse⁸¹ under DOE sponsorship are appropriate for such a comparison. The IGT and Westinghouse systems are similar, but only Westinghouse has extensive operating data in the public domain for gasification system operation at pressures appropriate for MCFC fuel gas supply. Thus, the Westinghouse system was chosen for this study, but results for the Westinghouse system may be assumed also to represent IGT system results. The Rockwell molten salt gasifier⁸² was finally selected to compare with Westinghouse gasification for air-blown system study (the Rockwell system has not operated in the oxygen-blown mode). Data on air-blown BCC/Lurgi gasification are unavailable, as are data on air-blown Texaco gasification that would permit a valid hot (dry) coal gas cleanup system design and cost comparison with wet cleanup as conventionally applied to Texaco gasification. Westinghouse air-blown gasification was used for both utility and industrial applications. The preliminary process screening had indicated that costs of industrial size systems would be more favorable if air-blown gasification were used.

6.2.2 Efficiency

Section 5 of this report evaluated MCFC power plants parametrically as a function of coal gas supply system configuration and of fuel cell pressure. The data from that section are summarized in Table

106. Data were obtained for a power plant configuration such as is shown in Figure 58. This system configuration was intended to provide realistic, relative power production efficiencies but not optimal, absolute efficiencies. The data used to derive power output from the fuel cells were obtained from experimental work performed in mid-1980 by Energy Research Corporation. The technology has advanced significantly since that time, and more optimistic data are now available for fuel cell power output. These data, however, have not been correlated for output as a function of cell operating pressure and so could not be used in this study. Higher power output from the MCFC units, however, and lower power output from the bottoming cycle components would provide significantly higher overall efficiencies. The use of methane reforming also would boost MCFC output and system efficiency. Energy Research Corporation has under development internal cell reforming catalyst configurations that could be effective in converting methane into MCFC power. These configurations for catalyst utilization have not yet been developed to provide adequate data in the public domain for inclusion of internal methane reforming results in this report.

For the three industrial size systems, many applications would benefit from lower power costs and higher system efficiency by the use of steam production in a cogeneration system configuration. The cogeneration mode of operation provides an opportunity for future evaluations of industrial coal gasification hot cleanup MCFC applications.

The data in Table 106 are numbers that represent net power output divided by total coal HHV input. As discussed in Section 5, the numbers are not intended to indicate absolute system efficiencies. We can see from the tabulation that:

- 1034 kPaa (150 psia) is a more efficient operating pressure than 345 kPaa (50 psia) or 1724 kPaa (250 psia) for all systems studied. Actually, for the air-blown systems the maximum efficiency MCFC system pressure is slightly lower than 1034 kPaa (150 psia), and for the oxygen-blown systems it is at or slightly above 1034 kPaa (150 psia). Within the accuracy of this study, and for cathode-cooled MCFC units, the 1034 kPaa (150 psia) pressure is clearly nearly optimum for power output.

Table 106
SYSTEM EFFICIENCY

System Designation	Net Power Output ÷ Coal HHV Input		
	345 kPaa (50 psia)	1034 kPaa (150 psia)	1724 kPaa (250 psia)
A. Utility Size			
BGC/O ₂ /Rectisol II	156.5	162.6	160.6
Texaco/O ₂ /Rectisol II	159.8	166.7	164.6
(W)/O ₂ /Rectisol II	149.0	155.2	153.0
(W)/O ₂ /Selexol	145.9	152.0	150.2
(W)/O ₂ /METC	157.6	163.2	160.8
(W)/O ₂ /dolomite	160.8	166.6	164.2
(W)/air/METC	167.6	171.5	167.6
B. Industrial Size			
Rockwell/Air	172.8	176.1	171.8
(W)/air/METC	167.7	171.7	167.8
(W)/air/dolomite	170.3	174.3	170.4

- Hot gas cleanup (state-of-the-art dolomite and METC iron oxide) and dolomite) provides higher system efficiencies than wet scrubbing (Rectisol II and Selexol) for the Westinghouse gasification system. A similar increase in hot cleanup efficiency over wet scrubbing efficiency would probably be applicable to the Texaco gasification system. Data to prove that, however, were unavailable for this study.
- Texaco coal gas provides higher MCFC system efficiencies than does Westinghouse coal gas, because of zero steam consumption and low methane content in the Texaco gas.
- The BGC/Lurgi system has low oxygen and steam consumption, providing a higher efficiency for MCFC service in the cold cleanup mode than the Westinghouse gasification system, in spite of the higher methane content of the BGC gas.

- The Rockwell gasification system, with bulk gas desulfurization and dehalogenation within the gasifier and with a sulfur recovery system that uses no high-level energy, only low-pressure steam, for carbonate melt regeneration, has the highest overall efficiency of all systems studied.
- Westinghouse air-blown gasification with hot gas cleanup is about 5% more efficient than Westinghouse O₂-blown gasification with hot gas cleanup. The O₂-blown systems use more net power for oxygen production and compression than the net power required for air compression to the air-blown gasification systems at 2241 to 2620 kPaa (325 to 380 psia). The use of the term "net power" is significant, since much of the power required to compress air for the air-blown systems is recovered in gas expansion turbines, but almost none of the power required for air compression for air separation is so recovered.

6.2.3 Investment

Davy McKee Corporation, as a subcontractor to Westinghouse, has prepared investment estimates for the ten coal gas fuel supply systems for this study. The results of their work are presented in Tables 107 and 108. The estimates, with $\pm 35\%$ accuracy, were factored by Davy McKee using proprietary scaling factors. Sources in the public domain, including EPRI,^{73,79} NASA,⁸³ ERDA,⁸⁴ and DOE⁸⁵ reports, were used for all base costs. The $\pm 35\%$ estimated costs are adequate for comparing systems on an economic basis when the investment difference between systems is beyond the range of the stated accuracy and are first quarter 1982 costs, without escalation. System capacity was used as the parameter for individual processing unit cost factor application. Costs derived for coal gasification, heat recovery, and bulk gas desulfurization were lumped together by Davy McKee. Some of the individual processing unit investment costs, in Davy McKee's judgment, were not accurate to within $\pm 35\%$. Adding together combinations of unit costs, however, cancelled out such inaccuracies and provided $\pm 35\%$ accurate totals, as reported in Tables 107 and 108. Westinghouse, using cost data from References 76, 78, and 79, has estimated investments by factoring the cost of all items in Table 109 other than gasification, waste heat recovery, and desulfurization. The costs are all total installed, including all equipment, materials, installation and construction labor, engineering, indirect construction, and tax costs. Specifically, they

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2/19/82

Table 107

SUMMARY OF GASIFICATION, HEAT RECOVERY, AND DESULFURIZATION INVESTMENT COSTS,
(\$1000)
250 MW Utility Cases

	$\frac{1}{0_2}$	$\frac{2}{0_2}$	$\frac{3}{0_2}$	$\frac{4}{0_2}$	$\frac{5}{0_2}$	$\frac{6}{0_2}$	$\frac{7}{\text{AIR}}$
COST CATEGORY	B.G.C. W/ RECTISOL II	TEXACO W/ RECTISOL II	WESTINGHOUSE W/RECTISOL II	WESTINGHOUSE W/SELEXOL	WESTINGHOUSE W/METC	WESTINGHOUSE W/DOLomite	WESTINGHOUSE W/METC
DIRECT COSTS:							
Equipment (All)	30,600	27,800	31,100	34,100	18,700	17,300	20,600
Material (D/P)	15,600	14,200	15,900	18,100	10,300	9,700	11,200
Material (S/C)	1,900	1,700	1,900	2,100	1,100	1,000	1,300
Labor (S/C)	9,100	8,200	9,200	10,300	5,300	4,900	5,900
Labor (D/H)	6,200	5,600	6,400	6,700	4,700	4,500	5,000
FIELD INDIRECTS (1)	7,700	7,000	7,900	8,400	5,800	5,500	6,100
PRO-SERVICE (2)	13,100	11,900	13,400	14,700	8,500	7,900	9,200
TAXES	2,400	2,200	2,400	2,700	1,500	1,400	1,100
INSURANCE	900	800	900	1,000	600	500	600
TOTALS	87,500	79,400	89,100	98,100	56,500	52,700	61,000

1) INCLUDES CONSTRUCTION FEE

2) INCLUDES PRO-SERVICE FEE

(D/P) is Davy McKee purchased.

(D/H) is Davy McKee hired.

(S/C) is subcontracted.

Table 108

SUMMARY OF GASIFICATION, HEAT RECOVERY, AND DESULFURIZATION INVESTMENT COSTS,
(\$1000)

50 MW Industrial Cases

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COST CATEGORY	8	9	10
	AIR ROCKWELL	AIR WESTINGHOUSE W/METC	AIR WESTINGHOUSE W/DOLOMITE
Direct Costs:			
Equipment (All)	11,000	8,000	8,200
Material (D/P)	5,700	4,400	4,500
Material (S/C)	7,900	500	500
Labor (S/C)	Incl. Above	2,200	2,300
Labor (D/H)	1,900	2,000	2,000
Field Indirects (1)	2,500	2,500	2,500
Pro-Services (2)	5,300	3,600	3,700
Taxes	600	600	700
Insurance	300	200	300
TOTALS	35,200	24,000	24,700

(1) Includes Construction Fee

(2) Includes Pro-Service Fee

(D/P) is Davy McKee purchased.

(D/H) is Davy McKee hired.

(S/C) is subcontracted.

Table 109

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INVESTMENT SUMMARY

Area	BGC/O ₂ / Rectisol II	Tex./O ₂ / Rectisol II	Ⓢ/O ₂ / Rectisol II	Ⓢ/O ₂ / Selexol	Ⓢ/O ₂ / Metc	Ⓢ/O ₂ / Dolomite	Ⓢ/Air/ Metc	Rockwell/ Air	Ⓢ/Air/ Metc	Ⓢ/Air/ Dolomite
Coal Receiving and Preparation	12.0	15.0	18.3	18.3	18.1	18.1	20.0	9.0	9.2	9.2
Coal Gasification, Heat Recovery and Bulk Gas Desulfurization	87.5	79.4	89.1	98.1	56.5	52.7	61.0	35.2	24.0	24.7
Sulfur Polishing	1.9	1.9	1.9	1.9	4.4	4.4	6.2	3.0	3.0	3.0
Molten Carbonate Fuel Cells & DC/AC Inverters	48.7	48.4	47.8	48.2	47.1	47.5	49.0	10.7	10.6	10.7
Other Power Equipment	163.0	131.4	147.1	149.1	157.8	158.8	152.1	37.9	41.5	41.8
Air Compression or Air Separation and Oxygen Compression	38.5	48.5	46.0	47.0	45.8	45.0	14.8	4.6	4.8	4.7
Hot Cleanup Ancillary Equipment	—	—	—	—	1.9	4.9	2.7	—	1.0	2.3
BFW & Condensate Treatment	1.2	0.3	1.6	1.6	1.6	1.6	1.6	0.1	0.7	0.7
General Facilities	26.5	24.4	26.4	27.3	25.0	25.0	23.1	7.5	7.1	7.3
Total Cost	379.3	349.3	378.2	391.5	358.0	358.0	330.5	108.0	101.9	104.4

^a Above in Millions of First Quarter 1982 Dollars.

have the same basis and scope as costs in the "total cost, \$1,000" captioned column of Table 4-7, page 4-51 of Reference 73. An allowance has been made for hot gas dechlorination. An investment equal to that used for ZnO polishing has been chosen arbitrarily to represent the cost of a system utilizing materials such as barium carbonate (BaCO_3) for dechlorination. All other hot gas cleanup is based either on the cost data in Reference 79 or on the cost data for dolomite desulfurization in Reference 84.

The tabulation shows that

- The hot gas cleanup (METC and Dolomite) configurations require less investment than does wet scrubbing (Rectisol II and Selexol) for the Westinghouse gasification system. A similar incremental decrease in hot cleanup investment from wet scrubbing investment would probably be applicable to the Texaco gasification system, but data were unavailable to prove that for this study.
- Higher investment in sulfur and ash removal and salt recycle systems for the Rockwell air-blown gasification produced higher investment costs relative to the Westinghouse gasification system with hot cleanup.
- Air-blown gasification requires lower investment than oxygen-blown gasification in the total system costs because of the high costs of separating air to produce oxygen.
- The opportunity to provide lower cost power through development of less expensive power production equipment should be obvious from the large portion of the total investment that is estimated for power production equipment.

6.2.4 Cost of Electricity

The cost of electricity (COE) for the ten systems whose efficiency and investment costs were tabulated earlier in this report is presented in Table 110. The basis for COE is EPRI's "Technical Assessment Guide"⁸⁶ and the calculation method used in Reference 73. Reiterating briefly the major assumptions derived from those two EPRI reports, we find:

Table 110

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FIRST YEAR COST OF ELECTRICITY

	Utility Systems							Industrial Systems		
	BGC/O ₂ / RII	Texaco/O ₂ / RII	⊗/O ₂ / RII	⊗/O ₂ / Selex.	⊗/O ₂ / METC	⊗/O ₂ / Dolomite	⊗/Air/ METC	Rockwell/ Air	⊗/Air/ METC	⊗/Air/ Dolomite
Fixed Operating Cost, \$ 10 ⁶ /Yr										
Operating/Maintenance Labor	7.26	6.86	7.22	7.38	6.90	6.85	6.68	4.33	3.80	3.81
Maintenance Materials	5.84	5.25	5.80	6.04	5.31	5.23	4.97	1.76	1.61	1.62
Admin./Support Labor	2.18	2.06	2.17	2.21	2.07	2.06	2.00	1.30	1.14	1.14
Variable Operating Costs, \$ 10 ⁶ /Yr										
Coal	15.47	12.88	14.72	15.11	14.65	14.49	15.24	3.00	3.31	3.28
Catalysts & Chem.	0.09	0.08	0.08	0.08	2.24	3.17	4.42	0.88	1.01	1.43
Ash & Dolomite Disposal	0.31	0.25	0.33	0.34	0.33	1.54	0.59	0.06	0.11	0.39
Raw Water	0.28	0.24	0.28	0.29	0.27	0.26	0.29	0.05	0.06	0.06
Fixed Capital Charges, \$ 10 ⁶ /Yr •	87.16	80.82	86.79	89.65	82.45	82.52	76.97	24.32	23.03	23.57
Total Operating Cost, \$ 10 ⁶ /Yr	118.59	108.44	117.39	121.10	114.17	116.12	111.34	35.70	34.07	35.30
Cost of Electricity, mills/kWh	66.8	71.6	72.8	74.7	67.7	68.2	60.4	95.8	85.1	87.5

• Includes Replacement of MCF Units Every 6 Years.

- Coal cost, \$1.05/GJ (\$1.11/10⁶ Btu) (dry)
- Zinc oxide cost, \$35/dm³ (\$125/ft³)
- Ash and sulfated dolomite disposal cost, \$4.99/Mg (\$5.50/ton)
- Dolomite cost, \$9.07/Mg (\$10/ton)
- 70% capacity factor
- 30 year plant life
- No credit for by-products
- Raw water cost \$0.19/l (\$0.50/1,000 gal)
- COE on a first year, nonescalated basis
- Operating labor, \$18/hr, average
- Cost of capital as defined on p. 2-18 of Reference 73
- Fuel cells replaced every 6 years, etc.
- Zinc sulfide production returned to zinc oxide vendor.

We have not added contingency to the investment costs from Table 109, but we have increased them by 16.5% to allow for funds required during construction, inventory, preproduction, etc.

The tabulation shows that:

- The hot gas cleanup (METC and Dolomite) systems provide lower COE than does wet scrubbing (Rectisol II and Selexol) for the Westinghouse oxygen-blown gasification system. A similar incremental decrease in hot-cleanup-derived COE relative to wet scrubbing COE would probably be applicable to the Texaco gasification system, but data to prove that were unavailable for this study.
- The complex Rockwell system has high investment costs per unit of power output and is, therefore, not competitive in COE with the Westinghouse systems with hot gas cleanup.
- Low-methane coal gas (Texaco) provides higher efficiency in a MCFC application, and this, along with a slightly lower investment per unit of power output than the Westinghouse system, as derived for Texaco from optimistic EPRI cost data, provides a slight advantage in COE when wet scrubbing (Rectisol II) is used.
- The lowest COE from a coal gasification wet scrubbing combination is for the BGC/Lurgi slagging system. The air-blown Westinghouse gasification with hot gas cleanup, however, provides significantly lower COE. The BGC/Lurgi system provides a

coal gas that in our judgment is unsuitable for hot cleanup. Hot cleanup, however, with an air-blown gasification system, utility size, clearly has an economic advantage over the BGC/Lurgi system with cold (wet) cleanup.

- For industrial use, the air-blown hot gas cleanup systems are more expensive than the five times larger utility systems. The cost of wet scrubbing small-scale industrial systems would also be higher by about the same proportion as they are higher than hot cleanup in the utility system evaluation. Thus, the lowest cost wet system (BGC/Rectisol II) would probably be at least 7 or 8 mills/kWh more expensive than the 88 mills/kWh shown for the low-cost industrial system. Further, the elimination of utility transmission and distribution costs would possibly justify the 88 mill on-site cost relative to the 63 mill central station cost for air-blown/Westinghouse/METC systems.
- About a 2.5 mills/kWh savings in zinc oxide cost could be subtracted from the COE for those systems using the METC iron oxide process if the zinc ferrite process now under development at METC fulfills its promise of much more effective bulk desulfurization. Also, if the RESOXTM process is substituted for the Allied Chemical SO₂ reduction process used in the cost estimates for the METC process, further investment and efficiency benefits could be expected through the use of coal rather than coal-derived gas for the reduction of SO₂.

6.2.5 Operability

The equipment used for power generation after clean, pressurized, hot coal gas has been produced is common to all systems studied. The discussion of operability differences, therefore, must concentrate on that portion of the system used to produce the clean hot coal gas. Five major subsystems - coal gasification, heat recovery from hot coal gas, coal gas desulfurization/sulfur recovery, oxidant supply, and condensate treating - will be reviewed.

The gasification subsystems reviewed in this study are:

- BGC/Lurgi slagging
- Texaco entrained slagging
- Rockwell molten salt
- Westinghouse (or IGT) fluidized bed.

Operability questions relate to system:

- Flexibility
- Reliability
- Availability.

In terms of flexibility, for a variety of coal feedstocks and for turndown and load change, the short residence time, high-temperature Texaco unit clearly is superior. The Rockwell gasifier and the Westinghouse gasifier are at more moderate temperature levels than Texaco and have substantially greater residence times for their carbon inventory. They are configured, however, to provide equal, if not greater, feedstock flexibility but are slower to respond to load change. Lastly, the BGC/Lurgi unit has the lowest product gas temperature and the least feedstock flexibility. Its flexibility for a wide variety of coals is limited by coal ash fusion characteristics and coal free-swelling index. Many coals that have high free-swelling indices are processed at significantly lower capacity. Also, fine coal, below 8 mm in size, can be processed only at very low capacity, if at all. The BGC/Lurgi's ability to respond to load change is of the same order as the fluidized-bed units, but its capability for turndown operation is somewhat greater. Ranking in terms of flexibility must be:

- 1) Texaco
- 2) Rockwell
- 3) Westinghouse
- 4) BGC/Lurgi.

Reliability can be judged on the basis of severity of process operating conditions. Here, the slagging gasifiers suffer from the need to maintain sufficiently high temperature in a portion of their reactor to assure slag flowability but at the same time to protect the reactor pressure shell from the erosive/corrosive action of coal slag and from its high temperature. Thus, at the present state of development, both BGC/Lurgi and Texaco systems have yet to demonstrate long-term

reliability of slag flow and slag containment. As an example, the Ruhrchemie semicommercial entrained-flow reactor, designed for multi-thousand-hour tests at a nominal 150 Mg/d (165 ton/day) capacity, has processed only 45,360 Mg (50,000 tons) of coal in four years, although a full-time design capacity is $4 \times 365 \times 150$ (165) or 219,000 Mg (240,900 tons) for that same period of time.⁸⁷ In the same context, the Rockwell unit has been prevented from achieving many of its test goals by problems associated with containing and maintaining the molten salt bath and preventing salt plugs from forming in the gas and salt flow passages. The fluidized-bed units do not have molten salt or molten slag problems. They do have to control the reactor so that slag or other kinds of molten materials such as FeS do not form and cause clinkers or gas flow deposition plugs. Such a set of constraints, however, can be routinely programed with the hot gas temperature control equipment developed by Westinghouse and IGT. Fluidized beds do require fines recycle equipment to provide fine particulate consumption in the gasifier. This requirement, however, has been handled by reliable, proven equipment designs in PDU-scale systems. Ranking in terms of reliability must be:

- 1) Westinghouse
- 2) Texaco
- 3) BGC/Lurgi
- 4) Rockwell.

Availability has not been demonstrated for any of the systems under consideration. By analogy with similar systems in commercial operation, however, some judgments can be made. The availability of complex, moving-bed Lurgi reactors, with their high tar-content gas, their internal rotating grate and distributor, and their hot ash lock-hopper valves, has not been good. Many years of modifying equipment and of training maintenance personnel were required to obtain acceptable availability for the Sasol I Lurgi units.⁸⁸ Similar problems may now be surfacing for Sasol II Lurgi units. Rockwell needs such a complex salt

cleanup system for ash and sulfur recovery that the likely availability for such a system is low, unless additional redundancy is provided for the already too high capital cost system. The Texaco system has demonstrated good availability when gasifying oil-derived liquids. The oil gasification experience, however, based on operation in a sooty mode that protected refractory and heat exchange materials, may not apply to nonsooty coal gas with its enormously higher slag content. Heat recovery and slag management, both, have yet to demonstrate high availability in commercial size Texaco systems. Fluidized beds, on the other hand, as demonstrated by Winkler in low-pressure commercial gasification operation since the 1920s, have acceptable availability. Fluid coking and fluid cat cracking units, as well as Exxon's Flexicoking gasifiers, have all shown good availability. Sasol's pressurized, fluidized-bed Fischer Tropsch reactors are likewise operating with good availability. Ranking in terms of availability must be:

- 1) Westinghouse
- 2) Texaco
- 3) BGC/Lurgi
- 4) Rockwell.

If the above operability judgments are quantified by assigning four points for (1), three points for (2), and so forth, both Texaco and Westinghouse tie for acceptable operability, with BGC/Lurgi and Rockwell well behind them.

When considering operability of heat recovery from hot coal gas for the purpose of this study, only one judgment is required. For Westinghouse, Texaco, and Rockwell processes (the BGC/Lurgi uses water quench and has no hot coal gas heat recovery) the heat recovery systems are in such an early stage of development that few facts are available on which to base an operability judgment, but substantially less heat recovery equipment is required for those coal gas systems using hot gas cleanup. The only valid judgment that can be made for this study, therefore, is that good operability should be more readily obtainable

for heat recovery that precedes hot gas desulfurization than for the more complex and extensive heat recovery that precedes cold (wet) coal gas desulfurization.

Coal gas desulfurization/sulfur recovery operability judgment is also simple. Systems such as Selexol and Rectisol have been used on coal gases successfully at many installations (Sasol, Westfield, Ruhrchemie, Coleshill, Montebello, etc.). The operability of such systems, base load, is unquestioned. The load change rate may have restrictions, such as no more than 0.5% load change per minute, placed on these basically operable systems. This restriction may, indeed, limit the load change rate for any MCFC power plant but should not be a problem. Systems such as METC, iron oxide, with air regeneration and SO_2 reduction to S, have not been operated, nor has the dolomitic desulfurization with air oxidation of CaS to CaSO_4 . No such combination of processes exists at any location and, therefore, no operability judgment can be made on them, other than that a test program should be instituted to investigate such system operability if the economic incentives of hot gas desulfurization justify it. Removal of all 3 μm particles and larger, along with dehalogenation, may also be required for MCFC fuel gas supply. Little operability information is available for such systems since only a few have been tested, and then for operating test periods of only a day or two. The judgment of hot gas cleanup system operability is left for the future.

Oxidant supply operability clearly favors the air-blown gasification systems. Air separation plants for oxygen production are subject to both scheduled annual shutdown for rime removal and maintenance and to unscheduled shutdown. Some unscheduled shutdowns can be tolerated without a gasification system shutdown if liquid oxygen standby storage/vaporization is provided. The potential for oxygen compressor failure, and long shutdowns for air separation plant failure, inevitably limit availability more for a system with air separation than for a system with only air compression. We judge, therefore, that air-blown systems are somewhat more operable than oxygen-blown systems.

Condensate treating system operability is also susceptible to simple analysis. With hot gas cleanup for Texaco, Westinghouse, and Rockwell systems, there is no condensate, so the operability of condensate treatment in such cases is by definition faultless. The BGC/Lurgi system requires complex treatment of condensates, including NH_3 recovery, phenol extraction, activated carbon adsorptive cleanup, steam stripping, and incineration via stripper off-gas routing through Claus processes. Similarly, for cold cleanup the Texaco, Westinghouse, and Rockwell gases require adsorptive/stripping treatment for condensates. Thus, hot cleanup for those gasification systems that can use it potentially provides the greatest operability.

To summarize the operability review, then, the Texaco and Westinghouse systems, air-blown if possible, with hot gas cleanup, have superior operability potential. The actual operability of the METC/ SO_2 production/ SO_2 reduction and the Dolomite/ CaSO_4 production needs to be demonstrated.

6.2.6 Environmental Effects

The need to dispose of the mineral matter contained in coal is a common denominator for all coal gasification systems. Some form of sulfur production is another such common denominator. A third is the emission of products of combustion from the process using the coal gas. Other than those three necessary products of coal utilization, all other environmental intrusions are avoidable. Waste water, for example, can be recycled 100% for zero discharge, if necessary. The central fact about all environmental intrusions from these MCFC power systems is that the investment cost estimate includes all equipment necessary to control emissions in accordance with today's accepted regulations for new power plants and new chemical plants in areas of Illinois suitable for such plant siting. Fugitive dust, runoff from coal and ash storage, water emissions, vent gases, carbon dioxide, sulfur production tail gas, and so on have all been cleaned up to meet anticipated environmental regulations. The tar/oil from the BGC/Lurgi process is recycled to

extinction in the gasifier, and the water condensed is cleaned to the required level prior to disposal. The sulfided dolomite from dolomitic hot gas desulfurization is oxidized to nonleaching sulfate prior to disposal with coal ash. The Texaco slag slurry and condensate water bled from the Texaco gas cooling system are carefully treated, as shown on drawing EXTF-1-1, in Reference 73. The Westinghouse ash agglomerate is shown to be so resistant to leaching⁸⁹ that runoff from ash agglomerate percolation with rainwater is of drinking water quality. The salt contaminated ash from the Rockwell process is disposed of in sealed pond areas. Ammonia is recovered and sold from those processes in which ammonia is condensed prior to wet scrubbing. In hot gas cleanup processes the uncondensed ammonia is converted mostly to N_2 and H_2O in the postanode catalytic combustor. To repeat for the sake of emphasis, the capital costs include all appropriate environmental protection measures.

That having been said, there do remain a few issues involving environmental effects:

- Dolomitic desulfurization provides a sulfated dolomite solid waste that increases the solid waste quantity substantially, by a factor of more than four,⁸⁴ over that of METC desulfurization.
- Zinc oxide polishing, in the case of METC and dolomitic bulk desulfurization, increases the production of ZnS by a factor of more than a hundred over that required with Rectisol II or Selexol bulk desulfurization. This report is based on purchased ZnO, wherein ZnS is returned for reprocessing to ZnO at a ZnO production unit. Such reprocessing is polluting to some extent, so that indirectly the hot gas desulfurization systems result in pollution at the ZnO manufacturer's site.
- The amount of coal used, and ash and products of combustion emitted, are a function of system efficiency, so the more efficient systems are less environmentally intrusive than the less efficient ones, all other things being equal. Thus, hot gas cleanup promotes a lesser degree of intrusion into the environment.

Aside from these few comments, all systems by design must be environmentally acceptable.

6.3 PART-LOAD PERFORMANCE ANALYSES

Part-load performance calculations were made for the utility size MCFC system for the two lowest cost-of-electricity cases from Table 5 at the reference cell operating processes of 1034 kPaa (150 psia):

<u>Gasifier</u>	<u>Blast</u>	<u>Cleanup Process</u>
BGC	Oxygen	Rectisol II
Westinghouse	Air	Iron Oxide (METC)

Net system power and heat rates were calculated at fuel cell current values of 80 and 60%.

Industrial systems are commonly operated base loaded. Part-load performance, accordingly, is of less interest for industrial size systems. In any case, conclusions for the utility size systems are also valid for the industrial size.

The following assumptions were made for the gasifier and the fuel cell subsystems of the MCFC system:

- Gasifier subsystem
 - Process air
 - Flow rate - proportional to fuel gas supply
 - Pressure - constant
 - Fuel gas supply
 - Pressure - constant
 - Temperature - constant
 - Composition - constant
 - Process steam
 - Flow rate - proportional to fuel gas supply
 - Conditions - constant
 - Power steam
 - Flow rate - proportional to fuel gas supply
 - Conditions - constant

- Auxiliary power requirements - proportional to fuel gas supply
- Fuel Cell Subsystem
 - Fuel cell
 - Operating pressure - constant
 - Operating temperature - constant
 - Anode conversion of H_2 and CO - constant
 - Overall air equivalence ratio - constant
 - Booster compressor inlet temperature - constant
 - Recycle compressor inlet temperature - constant
 - Low-pressure evaporator pressure - constant
 - Condenser pressure - constant.

The assumptions were made to provide a rational basis for gas expander and compressor performance evaluation as a function of throughput. The control systems required to provide the assumed conditions of operation were then designed into the MCFC system concept. Figure 59 is a flow diagram of the MCFC subsystem showing the controls required to operate the system at part load under the assumptions made.

A bypass line with a control valve is required in the cold flow stream through the product gas reheater to maintain the supply temperature at a constant value.

The expanders for the product fuel gas and the combustion products are equipped with variable inlet nozzle vanes that will be capable of maintaining constant pressure profiles over a flow range of about 20%. For further reduction in flow rate, throttle valves are installed in the expander inlet lines.

Heat exchanger HX1 has a bypass line with a control valve on the hot stream to maintain a constant temperature at the inlet of the booster compressor.

Heat exchangers HX1 and HX2 have bypass lines with control valves on the hot gas streams to maintain a constant temperature profile in the fuel cell cooling loop.

Both the booster compressor and the recycle compressor have throttle valves in the outlet lines for flowrate control. We have assumed that centrifugal compressors for 399°C (750°F) gas temperature with variable geometry for flow control are not commercially available.

The axial flow compressors for process air and combustion air are equipped with variable inlet guide vanes capable of reducing the flow rate by about 20%. For further reduction in flow rate, compressor discharge air bleeds are used.

Performance calculations have been made using the system shown in Figure 59. Tables 111 and 112 are summaries of the part-load performance of the MCFC system for BGC/O₂ and W/air cases at the reference fuel cell pressure of 1034 kPaa (150 psia).

For both cases the net system power is nearly proportional to the fuel cell current down to 80% cell current. At lower load fractions, the power output is less than proportional to the fuel cell current.

At 80% cell current the heat rate is about 99% of the full load value for both cases. At 60% cell current the heat rate is about 20% higher than the full load value for both cases.

The decrease in power and increase in the heat rate at loads under about 80% is due to the use of throttle valves in the expander inlet lines and air bleeds in the axial compressor outlet lines. The part load performance of centrifugal compressors is superior to that of axial compressors at capacities below about 80%, but axial compressors are superior to centrifugals in full load efficiency and cost.

Figure 59 -- Flow Diagram for Mathematical Model of Molten Carbonate Fuel Cell Subsystem

Table 111

PART-LOAD POWER SUMMARY FOR BGC/O₂/RECTISOL II

Fuel Cell Operating Pressure - 150 psia			
Fuel Cell Current - %	100	80	60
Exhst Expdr - kW	143,090	111,868	70,901
Comp Main - kW	88,988	73,015	73,015
GT Net - kW	54,102	38,853	(2,114)
Gas Expdr (Net) - kW	16,120	12,574	6,854
HP1 Steam Turbine	12,927		
HP2 Steam Turbine	6,189		
IP Steam Turbine	31,231		
LP Steam Turbine	36,136		
ST Net - kW	86,483	66,592	50,160
Fuel Cell (Net) -kW	176,980	152,494	122,533
System Gross - kW	333,685	270,513	177,433
Auxiliaries			
Compr Gasfr	10,617	8,711	8,711
Compr MCFC	2,523	2,109	1,696
Reclrc Fan	20,568	16,571	12,835
Condst Pump	21	16	12
Hrsg Pump	1,552	1,195	900
Gasfr Demand	8,931	7,145	5,359
Total - kW	44,212	35,747	29,513
System Net - kW	289,470	234,766	147,920
Coal Feed Rate - kg/s	22.43	17.94	13.46
- (lb/hr)	(178,000)	(142,400)	(106,800)
Coal HHV - kJ/kg	29,703	29,703	29,703
(Btu/lb)	(12,770)	(12,770)	(12,770)
Heat Rate - kJ/kWh	8,285	8,173	9,728
(HHV) - (Btu/kWh)	(7,853)	(7,746)	(9,220)

Table 112

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PART-LOAD POWER SUMMARY FOR WESTINGHOUSE/AIR/METC

Fuel Cell Operating Pressure - 150 psia			
Fuel Cell Current - %	100	80	60
Exhst Expdr - kW	154,010	120,405	75,312
Comp Main - kW	78,103	64,084	64,084
GT Net - kW	75,907	56,321	12,228
Gas Expdr (Net) - kW	17,392	13,566	5,275
HP1 Steam Turbine	11,023		
HP2 Steam Turbine	5,391		
IP Steam Turbine	29,970		
LP Steam Turbine	35,722		
ST Net - kW	82,106	61,580	48,032
Fuel Cell (Net) - kW	177,850	153,079	122,905
System Gross - kW	353,255	284,546	188,440
Auxillaries			
Compr Gasfr	36,974	30,285	30,285
Compr MCFC	4,030	3,369	2,709
Recirc Fan	17,658	13,443	10,771
Condst Pump	21	16	13
Hrsg Pump	1,323	1,025	836
Gasfr Demand	389	311	233
Total - kW	60,395	48,449	44,847
System Net - kW	292,860	236,097	143,593
Coal Feed Rate - kg/s	23.47	18.78	14.08
- (lb/hr)	(186,300)	(149,040)	(111,780)
Coal HHV - kJ/kg	29,703	29,703	29,703
- (Btu/lb)	(12,023)	(12,023)	(12,023)
Heat Rate - kJ/kWh	8,069	8,008	9,875
- (Btu/kWh)	(7,648)	(7,590)	(9,359)

Section 7

CONCLUSIONS

The definition of process information in Section 2 identified several efficient, competitive, "second generation" coal gasification systems capable of fueling MCFC power plants. Conventional wet scrubbing coal gas cleanup systems were also identified that could potentially provide gas of adequate cleanliness to MCFC power plants. A review of the effects of coal gas contaminants on MCFC systems in Section 3 indicated that further MCFC experimental work was required to identify and model the many potentially deleterious effects of trace chemical and particulate contaminants on MCFC performance at elevated pressure. Specifically, chemisorption of sulfur species under pressure, corrosion caused by halogens, electrolyte modification caused by heavy metals, and cathode contamination by particulates from fuel and air need further investigation. Section 2 also identified hot gas cleanup systems that had demonstrated capabilities currently inadequate for cleaning coal gas to MCFC specifications, but the potential cost and efficiency and operability advantages of hot gas cleaning systems shown in analyses prepared in Sections 4 through 6 could justify development of hot gas cleaning in an attempt to meet MCFC requirements. If the MCFC system requirements prove too stringent for hot gas cleanup, the development effort would still be justifiable for application to coal gas, combined-cycle power plants.

As was discussed in Sections 5 and 6, only relative, not absolute, conclusions are appropriate for the nonoptimized system efficiency/cost analyses provided in this report. Optimization would provide presumably lower-cost, higher-efficiency systems, although the costs and efficiencies arrived at in this study do not appear to be unacceptable. Hot gas cleanup, particularly with an air-blown

pressurized fluidized-bed (or entrained-bed, by analogy) coal gasification system has clear cost and efficiency advantages. In addition, the Rockwell molten salt system is assessed to be of little interest for MCFC power plants. The cell operating pressure of about 1034 kPaa (150 psia), with coal gasification above that pressure, provides an efficient combination.

Additional advantages would accrue from the use of a more effective bulk desulfurization unit, such as the zinc ferrite system METC is now developing instead of the METC iron oxide system with ZnO polishing evaluated here. Zinc ferrite could cut the cost of ZnO use by about 2.5 mills/kWh and could also provide smaller reactors and perhaps a more concentrated stream of SO₂ for reduction to sulfur, both of which would reduce capital cost. We conclude that such hot gas cleanup development work, along with the development of hot gas filtration and dehalogenation, should be funded by DOE for the long-term benefits to be derived from innovative power system concepts.

Section 8

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APPENDIX A
PARAMETRIC EQUATIONS OF PERFORMANCE OF MOLTEN CARBONATE
FUEL CELL SUBSYSTEM

The basic equations used in the parametric study of the molten carbonate fuel cell system are as follows:

OVERALL SYSTEM MASS BALANCE

$$ABE \times MWA + GAE \times MWGAE = PBD \times MWBD. \quad (A-1)$$

$$ABE = GAE \times (A/G) \text{ overall}. \quad (A-2)$$

$$(A/G) \text{ overall} = (A/G) \text{ st} \times (\phi_{air}) \text{ overall}. \quad (A-3)$$

Substituting gives:

$$GAE \times [(A/G) \text{ st} \times (\phi_{air}) \text{ overall} \times MWA + MWGAE] \\ = PBD \times MWP. \quad (A-4)$$

GAE, (A/G) st, (ϕ_{air}) overall, MWA, MWGAE,
and MWD are known or specified.

Solve for ABE and PBD.

ANODE MASS BALANCE

$$GAE \times MWAE + OEL \times MWO + CDEL \times MWCD = GAO \times MWA0. \quad (A-5)$$

$$OEL = (HAE + CMAE) \times CONVA/2. \quad (A-6)$$

$$HAE = YHAE \times GAE \quad (A-7)$$

$$CMAE = YCMAE \times GAE. \quad (A-8)$$

$$CDEL = 2 \times OEL. \quad (A-9)$$

Substituting gives:

$$\begin{aligned} &GAE \times [MWAE + (YHAE + YCMAE) \times CONVA/2 \times MWO \\ &+ 2 \times (YHAE + YCMAE) \times CONVA/2 \times MWCD] \\ &= GAO \times MWA0. \end{aligned} \quad (A-10)$$

GAE, MWAE, YHAE, YCMAE, CONVA, MWO, and MWCD are known or specified.

Solve for GAO $\times$ MWA0.

$$\begin{aligned} DW &= -DH \\ DCD &= -DCM \\ \therefore GAO &= GAE + CDEL. \end{aligned} \quad (A-11)$$

Combining equations (A-6) through (A-9) and (A-11) gives:

$$GAO = GAE \times [1 + (YHAE + YCMAE) \times CONVA]. \quad (A-12)$$

GAE, YHAE, YCMAE and CONVA are known or specified.

Solve for GAO.

$$MWA0 = (GAO \times MWA0)/GAO. \quad (A-13)$$

ANODE OUTLET COMPOSITION

The water-gas shift reaction

is controlling, and the equilibrium coefficient for this reaction is:

$$K = \frac{(p\text{H}_2\text{O}) (p\text{CO})}{(p\text{CO}_2) (p\text{H}_2)}. \quad (\text{A-14})$$

Appendix D has a computer subroutine that calculates the equilibrium composition for the water-gas shift reaction using the value of equilibrium coefficient that corresponds to the fuel cell operating temperature.

CATALYTIC BURNER MASS AND ENERGY BALANCE

Composition of Combustion Products from Catalytic Burner

Products Composition = ϕ (fuel gas composition, ϕ_{air})

MWBO = ϕ (products composition).

Mass Balance

$$\text{GBE} \times \text{MWGBE} + \text{ABE} \times \text{MWA} = \text{PBO} \times \text{MWBO}. \quad (\text{A-15})$$

$$\text{GBE} = \text{GAO}$$

$$\text{MWGBE} = \text{MWAO}.$$

Substituting gives:

$$\text{GAO} \times \text{MWAO} + \text{ABE} \times \text{MWA} = \text{PBO} \times \text{MWBO}. \quad (\text{A-16})$$

GAO, MWAO, ABE, MWA, and MWBO are known or specified. Solve for PBO.

Energy Balance

$$\begin{aligned} & \text{GBE} \times \text{MWGBE} \times (\text{HGBE} + \text{LHVGBE}) + \text{ABE} \times \text{MWA} \times \text{HABE} \\ & = \text{PBO} \times \text{MWBO} \times \text{HBO}. \end{aligned} \quad (\text{A-17})$$

$$\text{GBE} = \text{GAO}$$

$$\text{MWGBE} = \text{MWAO}$$

$$\text{LHVGBE} = \text{LHVAO}.$$

Substituting gives:

$$\begin{aligned} & \text{GAO} \times \text{MWAO} \times (\text{HGBE} + \text{LHVAO}) + \text{ABE} \times \text{MWA} \times \text{HABE} = \text{PBO} \\ & \times \text{MWBO} \times \text{HBO} \end{aligned} \quad (\text{A-18})$$

GAO, HAO, LHVAO, ABE, HABE, HGBE, PBO, MWAO, MWA, and MWBO are known or specified.

Solve for HBO.

Fuel Cell Energy Balance

$$\begin{aligned} & \text{GAE} \times \text{MWAE} \times (\text{HAE} + \text{LHVAE}) + \text{PBO} \times \text{MWBO} \times \text{HBO} \\ & + \text{PRC} \times \text{MWBD} \times \text{HRC} = \text{GAO} \times \text{MWAO} \times (\text{HAO} + \text{LHVAO}) \\ & + \text{PBD} \times \text{MWBD} \times \text{HBD} + \text{PRC} \times \text{MWBD} \times \text{HBD} + \text{PWRFC}. \end{aligned} \quad (\text{A-19})$$

$$\text{PWRFC} = V \times \text{TOTAL I}/1000$$

$$V = \text{EAVG} - \text{ECR} \times \text{TOTAL I}/(\text{Area} \times 1000). \quad (\text{A-20})$$

$$\text{EAVG} = (\text{EIN} + \text{EOUT})/2. \quad (\text{A-21})$$

$$\begin{aligned} \text{EIN} = & \text{FCT} (\text{EO}, \text{O}, \text{D} + \text{O}, \text{O}, \text{D} + \text{O}, \text{HAE}, \text{WAE}, \text{CDAE}, \\ & \text{CMAE}, \text{GAE}, \text{OCE}, \text{CDCE}, \text{GCE}, \text{T}, \text{PA}, \text{PC}). \end{aligned} \quad (\text{A-22})$$

$$\begin{aligned} \text{EOUT} = & \text{FCT} (\text{EO}, \text{CONVA}, \text{CONVC}, \text{HAE}, \text{WAE}, \text{CDAE}, \\ & \text{CMAE}, \text{GAE}, \text{OCE}, \text{CDCE}, \text{GCE}, \text{T}, \text{PA}, \text{PC}). \end{aligned} \quad (\text{A-23})$$

Appendix D has subroutines for the computation of EIN and EOUT as functions of the indicated parameters. An expression for the effective cell resistance of a state-of-the-art molten carbonate fuel cell is as follows:

$$\begin{aligned} \text{ECR} &= a + b \times \text{PA}^c \\ &= 542.0 + 790.0 \times \text{PA}^{-0.2723} \text{ m}\Omega \text{ cm}^2. \end{aligned} \quad (\text{A-24})$$

$$\text{AREA} = (\text{TOTAL I} \times 1000) / \text{TCD}. \quad (\text{A-25})$$

Combining gives:

$$\begin{aligned} V &= (\text{EIN} + \text{EOUT}) / 2 - (542.0 + 790.0 \times \text{PA}^{-0.2723}) \\ &\quad \times \text{TCD} \times 10^{-6}. \end{aligned} \quad (\text{A-26})$$

$$\text{TOTAL I} = \text{TAMPF} \times \text{CONFA}. \quad (\text{A-27})$$

$$\text{TAMPF} = (\text{HAE} + \text{CMAE}) / 5.182 \times 10^{-6}. \quad (\text{A-28})$$

$$\text{HAE} = \text{YHAE} \times \text{GAE}. \quad (\text{A-29})$$

$$\text{CMAE} = \text{YCMAE} \times \text{GAE}. \quad (\text{A-30})$$

Combining equations (A-27) through (A-30) gives:

$$\text{TOTAL I} = \text{GAE} \times \text{CONVA} \times (\text{YHAE} + \text{YCMAE}) / 5.182 \times 10^{-6} \quad (\text{A-31})$$

Combining equations (A-26) and (A-31) gives:

$$\begin{aligned} \text{PWRFC} &= [(\text{EIN} + \text{EOUT}) / 2 - (542.0 + 790.0 \times \text{PA}^{-0.2723}) \\ &\quad \times \text{TCD} \times 10^{-6}] \times [\text{GAE} \times \text{CONVA} \times (\text{YHAE} + \text{YCMAE})] / 5.182 \\ &\quad \times 10^{-3}. \end{aligned} \quad (\text{A-32})$$

For state-of-the-art molten carbonate fuel cells,

$$\text{CONVA} = 0.85$$

$$\text{TCD} = 290.9 \text{ mA/cm}^2.$$

Substituting gives:

$$\begin{aligned} \text{PWRFC} = & [(EIN + EOUT)/2 - (0.1577 + 0.2298 \times PA^{-0.2723})] \\ & \times 164.0 \times GAE \times (YHAE + YCMAE). \end{aligned} \quad (A-33)$$

Combining equations (A-19) and (A-33) gives:

$$\begin{aligned} & GAE \times MWAE \times (HAE + HVAE) + PBO \times MWBO \times HBO \\ & + PRC \times MWBD \times HRC = GAO \times MWA0 \times (HA0 + LHVA0) \\ & + PBD \times MWBD \times HBD + PRC \times MWBD \times HBD + [(EIN + EOUT)/2 \\ & - (0.1577 + 0.2298 \times PA^{-0.2723})] \times 164.0 \times GAE \\ & \times (YHAE + YCMAE). \end{aligned} \quad (A-34)$$

The values for all of the terms in equation (A-34) are known or specified, except for HRC and PRC.

BLENDING OF RECYCLE GAS WITH BURNER EFFLUENT

$$\begin{aligned} & PRC \times MWBD \times HRC + PBO \times MWBO \times HBO \\ & = PRC \times MWBD \times HRC @ 1100^{\circ}\text{F} + PBO \times MWBO \times HBO @ 1100^{\circ}\text{F} \end{aligned} \quad (A-35)$$

Here, again, the values of all of the terms in equation (A-35) are known, except for PRC and HRC.

The gas temperature at the cathode inlet is specified as 93°C (200°F) less than the fuel cell operating temperature of 704°C (1300°F). An infinite number of combinations of recycle gas flow rate and recycle gas temperature will satisfy this constraint. Only one combination, however, will satisfy both this temperature constraint and the cathode cooling requirement. This combination can be solved by combining equations (A-34) and (A-35).

TURBOMACHINERY PERFORMANCE CALCULATIONS

Air Compressors

TIN-GIVEN

PIN - GIVEN

POUT - GIVEN

$HIN = \phi(TIN)$

$PRIN = \phi(TIN)$

$PRC = POUT/PIN$

$PROUT = PRIN \times PRC$

$HOUT' = \phi(PROUT)$

$DHC' = HOUT' - HIN$

$DHC = DHC' / ETAC$

$HOUT = HIN + DHC$

$TOUT = \phi(HOUT)$

Gas Expanders

TIN GIVEN

PIN - "

POUT - "

$HIN = \phi(TIN, COMP)$

$PRIN = \phi(TIN, COMP)$

$PRE = POUT/PIN$

$PROUT = PRIN \times PRE$

$HOUT' = \phi(PROUT, COMP)$

$DHE' = HIN - HOUT'$

$DHE = DHE' \times ETAE$

$HOUT = HIN - DHE$

$TOUT = \phi(HOUT, COMP)$

STEAM TURBINE PERFORMANCE CALCULATIONS

The steam turbine expansion line tabulated in Appendix B was used in the steam turbine calculations. A low-pressure end having a loss of 12 kJ/kg (5 Btu/lb) was assumed for all runs.

HEAT EXCHANGER EFFECTIVENESS

$$\epsilon = \frac{C_c[(t_c)_{\text{out}} - (t_c)_{\text{in}}]}{C_{\text{min}}[(t_h)_{\text{in}} - (t_c)_{\text{in}}]}$$

or

$$\epsilon = \frac{C_h[(t_h)_{\text{in}} - (t_h)_{\text{out}}]}{C_{\text{min}}[(t_h)_{\text{in}} - (t_c)_{\text{in}}]}$$

$$C_c = W_c \times (C_p)_c$$

$$C_h = W_h \times (C_p)_h.$$

NOMENCLATURE

GAS STREAMS

ABE	molar flow rate of combustion air at burner entrance, kgmol/s
(A/G) overall	overall molar ratio of air to fuel
(A/G) st	stoichiometric molar ratio of air to fuel
AREA	cell area, cm ²
CDEL	molar flow rate of carbon dioxide through electrolyte, kgmol/s
CMAE	molar flow rate of carbon monoxide at anode entrance, kgmol/s
CONVA	fraction of hydrogen and carbon monoxide converted in anode
DCD	carbon dioxide increment, kgmol/s
DH	hydrogen increment, kgmol/s
DW	water increment, kgmol/s
EAXG	average no load voltage, V
ECR	effective cell resistance, mΩ·cm ²
EIN	no load voltage at inlet, V
EOUT	no load voltage at outlet, V
GAE	molar flow rate of fuel gas at anode entrance, kgmol/s
GAO	molar flow rate of fuel gas at anode outlet, kgmol/s
GBE	molar flow rate of fuel gas at burner entrance, kgmol/s
HABE	enthalpy of air at burner inlet, kJ/kg
HAE	molar flow rate of hydrogen at anode entrance, kgmol/s
HBD	enthalpy of combustion products blown down from cathode cooling loop, kJ/kg
HBO	enthalpy of products at burner outlet, kJ/kg
HGBE	enthalpy of fuel gas at burner entrance, kJ/kg
HRC	enthalpy of recycled products, kJ/kg

HRC @ 593°C (1100°F) - enthalpy of recycle products @ 593°C (1100°F), kJ/kg
HBO @ 593°C (1100°F) - enthalpy of burner outlet products @ 593°C (1100°F), and kJ/kg

LHVAE	lower heating value of fuel gas at anode entrance, kJ/kg
LHVAO	lower heating value of fuel gas at anode outlet, kJ/kg
LHVGBE	lower heating value of fuel gas at burner entrance, kJ/kg
MWA	molecular weight of air
MWAE	molecular weight of fuel gas at anode entrance
MWAO	molecular weight of fuel gas at anode outlet
MWBO	molecular weight of products at burner outlet
MWCD	molecular weight of carbon dioxide
MWGBE	molecular weight of fuel gas at burner entrance
MWO	molecular weight of oxygen
OEL	molar flow rate of oxygen through electrolyte, kgmol/s
PA	anode pressure, atm
PBD	molar flow rate of combustion products blown down from cathode recycle loop, kgmol/s
PBO	molar flow rate of products at burner outlet, kgmol/s
PC	cathode pressure, atm
PRC	molar flow rate of recycled products, kgmol/s
PWRFC	gross electrical power generated by fuel cell, kW
TAMPF	total ampere flow, A
TCD	total current density, mA/cm ²
TOTAL I	total fuel cell current, A
V	fuel cell voltage under load, V
YCMAL	mole fraction of carbon monoxide at anode entrance
YHAE	mole fraction of hydrogen at anode entrance
(ϕ_{air})overall	overall air equivalence ratio

TURBOMACHINERY

COMP	gas composition
DHC'	ideal compressor enthalpy rise, kJ/kg
DHC	actual compressor enthalpy rise, kJ/kg

DHE'	ideal expander enthalpy drop, kJ/kg
DHE	actual expander enthalpy drop, kJ/kg
ETAC	compressor isentropic efficiency
ETAE	expander isentropic efficiency
HIN	inlet enthalpy, kJ/kg
HOUT'	ideal enthalpy at outlet, kJ/kg
HOUT	actual enthalpy at outlet, kJ/kg
PIN	inlet pressure, kPa
POUT	outlet pressure, kPa
PRC	compressor pressure ratio
PRE	expander pressure ratio
PRIN	relative pressure at inlet
PROUT	relative pressure at outlet
TIN	inlet temperature, °C
TOUT	outlet temperature, °C

HEAT EXCHANGERS

(Cp)c	specific heat of colder stream, kJ/kg·°C
(Cp)h	specific heat of hotter stream, kJ/kg·°C
(tc) in	inlet temperature of colder stream, °C
(tc) out	outlet temperature of colder stream, °C
(th) in	inlet temperature of hotter stream, °C
(th) out	outlet temperature of hotter stream, °C
Wc	colder stream flow rate, kg/s
Wh	hotter stream flow rate, kg/s
ϵ	heat exchanger effectiveness

APPENDIX B
STEAM TURBINE PERFORMANCE

The steam turbine throttle conditions assumed in this study are as follows:

Pressure - 12,514 kPaa(1815 psia)
Temperature - 538°C (1000°F)

The steam turbine expansion line typical for the above throttle conditions is as follows:

<u>Pressure KPaa (psia)</u>	<u>Temperature, °C (°F)</u>	<u>Enthalpy, kJ/kg (Btu/lb)</u>
12514 (1815)	537.8 (1000)	3442.7 (1480.1)
8274 (1200)	476.7 (890)	3337.8 (1435.0)
4137 (600)	385 (725)	3177.8 (1366.2)
2069 (300)	304.4 (580)	3033.6 (1304.2)
689.5 (100)	193.3 (380)	2829.6 (1216.5)
365.4 (53)	140.4 (287.7) sat.	2656.3 (1142.0)
69.0 (10)	89.6 (193.2)	2514.4 (1081.0)
34.5 (5)	72.3 (162.2)	2440.0 (1049.0)
6.8 (0.982) 2 in. Hg	38.4 (101.1)	2279.5 (980.0)