DOE/MC/16372-5

SIMULTANEOUS HIGH-TEMPERATURE REMOVAL OF ALKALI AND
PARTICULATES IN A PRESSURIZED GASIFICATION SYSTEM

Fifth Quarterly Project Report Covering the Period
April 1982 through June 1982

P. R. Mulik, Project Manager
M. A. Alvin
D. M. Bachovchin

July 1982

Westinghouse Electric Corporation
Research and Development Center
1310 Beulah Road
Pittsburgh, PA 15235

MASTER

Prepared for
U. S. Department of Energy
Under Contract DE-AC21-81MC16372

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PATENT STATUS

This technical report is being transmitted in advance of DOE patent clearance and no further dissemination or publication shall be made of the report without prior approval of the DOE Patent Counsel.

TECHNICAL STATUS

This technical report is being transmitted in advance of DOE review and no further dissemination or publication shall be made of the report without prior approval of the DOE Project/Program Manager.

ABSTRACT

This program is directed at performing experimental and analytical investigations, deriving system designs, and estimating costs to ascertain the feasibility of using aluminosilicate-based getters for controlling alkali in pressurized gasification systems. Its overall objective is to develop a comprehensive plan for evaluating a scaled-up version of the gettering process as a unit operation or as an integral part of a particulate removal device.

This report briefly summarizes efforts previously completed on thermodynamic projections and system performance projections, together with current work on getter selection and qualification completed during the fifth quarter of the project. Work on the thermodynamic projections has been completed and includes an update of the data base, development of alkali phase diagrams, and projections for several gasification processes. Getter selection and qualification efforts involved four tests -- two with activated bauxite and one each with diatomaceous earth and Novacite® on the thermogravimetric analysis (TGA) system. Finally, system performance projections entailed examination of available kinetic data to ascertain the rate-controlling step, along with modeling efforts to determine the size requirements of a commercial-sized unit.

1. INTRODUCTION

An advanced low-Btu gasification system, when integrated with a combined-cycle power plant, results in one of the most promising concepts for using low-Btu gasifiers and, hence, leads the way to using high-sulfur coal. Using this coal to generate a fuel gas requires the removal of contaminants (especially alkali and particulates) that could lead to corrosion, erosion, and deposition problems on turbine materials. A cleanup system, therefore, is obligatory. In the current study Westinghouse is examining the feasibility of a hot-gas cleaning process to minimize the concentration of alkali in a high-temperature fuel gas with possible simultaneous particulate removal through the use of aluminosilicate materials (getters).

Westinghouse initiated work on the alkali-gettering concept in October 1978 as part of DOE contract DE-AC21-78ET11026. The program continued through October 1980. It consisted of seven tasks: (1) Test Plan, (2) Test Facility Assembly, (3) Getter Selection and Fabrication, (4) Getter Material Characterization, (5) Bench-Scale Evaluation of Getter Performance, (6) System Performance Projections, and (7) Program Definition for Concept Scale-up.

Task 1 was completed early in the program and approved by DOE. The task 2 effort was centered on the design and fabrication of two systems for obtaining kinetic data as a function of pertinent parameters such as getter material, temperature, pressure, extent of conversion, concentration of alkali in the bulk gas stream, composition of the alkali-laden gas, and bulk gas velocity. One of these systems was a batch-type bench-scale reactor to be used for preliminary bench-scale studies. This reactor was completed early in the program and was used to screen three candidate getter materials - kaolin, ash from a low-temperature coal char, and ash from a high-temperature gasifier. The

second unit, consisting of a double-balance thermogravimetric analysis (TGA) system designed to continuously monitor the weight loss of the alkali source and the weight gain of a candidate getter, was designed and built during the course of the program. We plan to use this system extensively under our current DOE contract.

Getter fabrication (task 3) efforts involved preparation of sufficient quantities (1/8" dia x 1/8" long cylinders) of the three types of getter pellets for use in the preliminary bench-scale studies (task 5). Getter characterization work (task 4) involved exposure of all three candidate getters for periods up to six hours at temperatures of 850 and 900°C in an inert gas (argon), N₂/10% H₂, and a simulated fuel gas. All three gases contained approximately 80 ppm sodium chloride (NaCl). The system pressure was 11 atm absolute. Work on task 6 included preliminary estimates of the costs associated with alkali gettering in combined-cycle applications.

Under the current contract, a basis for evaluating the alkali removal unit operation will be developed, and the results will also be directly applicable to pressurized fluidized-bed combustion (PFBC) systems. To accomplish this objective, the work under the current contract is comprised of four technical tasks: Process Thermodynamic Projection, Getter Selection and Qualification, System Performance Projections, and Program Definition for Concept Scale-up. The overall objective of the proposed program is to develop a comprehensive plan for evaluating a scaled-up version of the gettering process as a unit operation or as an integral part of a particulate removal device. Realization of the primary objective will require that the following interrelated aspects of the problem be taken into consideration: identification of suitable candidate getter by additional bench-scale and TGA studies; utilization of the experimental data to provide a technical, economic, and environmental assessment of the gettering process; specification of appropriate design details for the scale-up studies; and delineation of key tests, operating conditions, and so on, for the conduct of the scale-up studies.

This report briefly summarizes efforts previously completed on thermodynamic projections and system performance projections, together with current work on getter selection and qualification, during the fifth quarter of the project, from April 1, 1982 through June 20, 1982. Work on the thermodynamic projections has been completed and includes an update of the data base, development of alkali phase diagrams, and projections for several gasification processes. Getter selection and qualification efforts involved four tests -- two with activated bauxite and one each with diatomaceous earth and Novacite® on the thermogravimetric analysis (TGA) system. Finally, system performance projections entailed examination of available kinetic data to ascertain the rate-controlling step, along with modeling efforts to determine the size requirements of a commercial-sized unit. In addition, an appendix is included that contains a project summary prepared for presentation at a DOE cross-cut review meeting held in Morgantown during the latter part of June 1982. The purpose of the meeting was to review all projects associated with the Department of Energy's Advanced Research and Technology Development (AR&TD) program in coal gasification.

2. PROJECT SUMMARY

During the fifth quarter of this program, work centered on task 2 (Getter Selection and Qualification). Also included in this report are brief summaries of work previously completed on two other tasks (1 and 3) and the text of a project summary prepared for presentation at a DOE cross-cut review meeting held in Morgantown during the latter part of June. The summary paper is included as an appendix.

Work completed on task 1 (Thermodynamic Projections) includes an update of the data base, development of alkali phase diagrams, and projections for several gasification processes. Task 3 (System Performance Projections) efforts entailed examination of available kinetic data to ascertain the rate-controlling step, along with modeling efforts to determine the size requirements of a commercial-sized unit.

Work on task 2 involved four tests--two with activated bauxite and one each with diatomaceous earth and Novacite® on the TGA system. Runs 26 (diatomaceous earth) and 27 (Novacite®) represented the last two promising getters to be tested on the basis of batch reactor screening tests. The objective of these TGA tests was to find an alternative getter with gettering capacity significantly better than activated bauxite. On the basis of TGA tests and subsequent atomic absorption analyses, the three leading candidate alternative getters include diatomaceous earth, emathlite, and Ebony Novacite®.

Subsequently to run 27, the TGA system was modified to permit the addition of several parts of water vapor to the carrier gas stream. Upon completion of the system modifications, two tests (runs 28 and 29) were made with activated bauxite in the presence of water vapor. The gettering capacity in the presence of water vapor was found to be a factor of two to three times greater than was observed for activated bauxite without moisture in the system.

3. PROJECT STATUS

3.1 TASK 1: THERMODYNAMIC PROJECTIONS

Work on the thermodynamic projections has been completed and includes a data base update, development of alkali phase diagrams, and gasification process projections. Our data base update involved a literature review and subsequent updating of the thermodynamic data base to include aluminosilicate complexes that had been experimentally identified as resulting gettered species. Phase diagrams were then generated to demonstrate the various interactions of the mineral constituents of the feedstock during gasification, the chemical transformations of the released volatile alkali with effluent gas constituents, and the chemical stabilities of potential getter materials.

The thermodynamic model was used to rank the Lurgi, Shell Koppers, Texaco, Winkler, and Westinghouse gasification systems on the basis of released alkali concentrations at process conditions. In the order of increasing released alkali concentrations for the gasification of Illinois No. 6 coal, the following series applies: Lurgi (0.028-0.035 ppm Na, 0.013-0.016 ppm K), Texaco (18.70-12.3 ppm Na, 4.5-6.4 ppm K), Westinghouse (19-23 ppm Na, 4.3-12 ppm K), Shell Koppers (37.2-45.6 ppm Na, 983 ppm K). Gasification of eastern Kentucky coal in the Winkler process (15.5-132.2 ppm Na, 7.7-101 ppm K) or Wyoming subbituminous coal in the Westinghouse fluidized bed (34-51 ppm Na, 20-32 ppm K) is not projected to emit the potassium concentrations of the Shell Koppers process, but borders on, if not exceeds, those for sodium.

Our most recent process projections have been incorporated into our Third Quarterly Technical Progress Report¹ for the period

October 1981 through December 1981. A complete summary of this task has been incorporated into the Annual Technical Progress Report for the period April 1981 through March 1982. This report should be available in early August.

3.2 TASK 2: GETTER SELECTION AND QUALIFICATION

3.2.1 TGA Testing

Four runs were made in this quarter on the TGA system. These are summarized in Table 1. All were made at 1 atm total pressure. The first two runs used diatomaceous earth and Novacite® and represented the last two promising getters to be tested on the basis of batch reactor screening results. As mentioned in our Annual Technical Progress Report,² the objective of these TGA tests was to find a material with gettering capacity significantly better than activated bauxite.

Both the weight gain and the gas-phase salt concentration for these two materials are given as a function of time in Figures 1 and 2. Both materials demonstrated substantial increases in capacity over that of activated bauxite. On the other hand, both materials adsorbed salt at much lower rates than those previously obtained with activated bauxite. On a weight percentage basis, the diatomaceous earth at a 4.7 wt % gain showed a particularly high capacity. Along with emathlite and Ebony Novacite®, it is the most promising candidate tested to date in our bench-scale and TGA systems. These results have been further confirmed by atomic absorption analyses, as will be described in Section 3.2.2.

Subsequently to run 27, the TGA system was modified to permit the addition of several parts of water vapor to the carrier gas stream. Upon completion of system modifications, two tests (runs 28 and 29) were made to investigate system performance with activated bauxite in the presence of water vapor. Both the weight gain and gas-phase salt concentration for these two runs are shown as a function of time in Figure 3.

Table 1
TGA DATA SUMMARY

<u>Run</u>	<u>Dates</u>	<u>Material</u>	<u>Concentration, ppmv</u>	<u>Temperature, °C</u>	<u>Length, hr</u>	<u>Wt Gain, mg</u>	<u>Original Wt, mg</u>
26	4/6 - 4/21/82	Diatomaceous earth	9.7 - 4.2	850	300	6.5	139.1
27	4/26 - 5/10/82	Novacite®	11.2 - 5.0	850	283	4.9	196.5
28*	6/8 -- 6/21/82	Activated bauxite	22.0 - 6.6	850	257	16.1	204.5
29*	6/28 - 7/5/82	Activated bauxite	24.0 - 8.1	850	113	12.5	204.5

* Water vapor present in carried gas at 4.0 mol %.

Figure 1 -- TGA results for diatomaceous earth

Figure 2 -- TGA results for Novacite

Figure 3 -- TGA results for activated bauxite in the presence of water vapor

In each of these tests (summarized in Table 1), a 204.5 mg activated bauxite pellet was held at 850°C and exposed to salt concentrations on the order of 10 ppmv. During run 28, the pellet gained 5 wt % in the first 110 hours of operation. In this same period, the salt concentration decreased from an initial value of 20 ppmv to 7.5 ppmv. An additional 2.8 wt % gain was obtained in the next 147 hours of operation, in which time the concentration decreased to 6.6 ppmv. At the conclusion of the test, the reactor was opened, and salt was found to have accumulated inside the shroud. As on other similar occasions, we concluded that the run had been allowed to proceed for too long a period of time.

On the basis of the above observation, we decided to repeat the previous test conditions but to discontinue TGA operations prior to the initiation of salt accumulation within the shroud. Consequently, run 29 was made in which the activated bauxite pellet gained 6.0 wt % in 113 hours of operation. During this period the salt concentration decreased from an initial value of 24 ppmv to 8.1 ppmv. The observed weight gain was consistent with that observed in run 28, since the salt concentration was somewhat higher. No salt was found in the shroud at the conclusion of the run. The capacity observed in the presence of water vapor was found to be a factor of two to three times greater than was observed for activated bauxite without moisture present in the system.

The next planned test is with emathlite in the presence of water vapor.

3.2.2 Atomic Absorption Analyses

During the quarter, atomic absorption analyses were completed on all alternative getters tested to date on the TGA system without water vapor. Data are summarized in Table 2. As shown in the table, the weight percent of sodium based on atomic absorption analyses tends either to exceed or to be equivalent to the weight percent gain measured

Table 2

COMPARISON OF TGA DATA WITH ATOMIC ABSORPTION RESULTS

<u>Run</u>	<u>Material</u>	<u>Concentration, ppmv</u>	<u>Temperature, °C</u>	<u>Length, hr</u>	<u>Wt Gain, mg</u>	<u>% Wt Gain</u>	<u>Wt % Na by Atomic Absorb.</u>
20	Vansil®	13.4	900	26	0.3	0.144	0.30
21	Vansil®	12	800	24	0.3	0.160	0.34
22	Ebony Novacite®*	13.9 - 5.7	850	165	2.3	0.833	3.56
23	Ebony Novacite®**	12.1 - 3.1	850	267	14.5	4.71	5.61
24	Zeolite	12.0 - 9.6	850	50	0.8	0.465	2.92
25	Emathlite	11.0 - 3.7	850	284	10.8	5.48	5.45
26	Diatomaceous earth	9.7 - 4.2	850	300	6.5	4.67	4.59
27	Novacite®	11.2 - 5.0	850	283	4.9	2.49	2.15

*Effect masked by carbon oxidation

**Prebaked to remove volatiles

by the TGA system. Additional atomic absorption results for both the unreacted and reacted materials are summarized in Table 3. Background sodium and potassium data for the unreacted alternative getters were previously summarized in our Third Quarterly Technical Progress Report.¹ As Table 3 indicates, and as has been found in previous work, background potassium is displaced as part of the sodium chloride gettering process. In addition, it appears from these results that insoluble sodium is the preferred reaction product, with the possible exception of Vansil. This parallels our previous results obtained for Keystone boiler ash and PDU char and gasifier ash. The PDU materials were obtained from the Westinghouse gasifier process development unit. On the other hand, these data contrast with the results obtained to date for activated bauxite. For this material, soluble sodium represents a substantial fraction of the reaction product. As in our Third Quarterly Technical Progress Report, we shall attempt to correlate the atomic absorption results with the observed weight through an assumed reaction stoichiometry. Part of this effort will most likely include selected chloride analyses of reacted and unreacted pellets.

3.3 TASK 3: SYSTEM PERFORMANCE PROJECTIONS

In our First Quarterly Technical Progress Report,³ the available gettering kinetic data for activated bauxite and Westinghouse PDU char and gasifier ash were analyzed to evaluate the feasibility of proposed gettering system concepts. In this preliminary study we gathered a data base, theorized a general kinetic expression, and used the data to generate rate expressions. The rate expressions in turn were used to size full-scale systems for alkali removal using entrained-bed, packed-bed, and fluidized-bed contactors.

More recently this study has been updated for activated bauxite on the basis of current data from the following four sources:

- Westinghouse TGA System
- Westinghouse Bench-Scale System

Table 3

DETAILED ATOMIC ABSORPTION RESULTS FOR ALTERNATIVE GETTERS

Run	Material	<u>Background Total Alkali</u>		<u>Reacted Getter Analysis</u>			
		<u>Wt % Na</u>	<u>Wt % K</u>	<u>Water Soluble</u> <u>Wt % Na</u>	<u>Insoluble</u> <u>Wt % Na</u>	<u>Water Soluble</u> <u>Wt % K</u>	<u>Insoluble</u> <u>Wt % K</u>
20	Vansil®	0.24	0.028	NA*	0.30	NA*	<0.05
21	Vansil®	0.24	0.028	NA*	0.34	NA*	<0.05
22	Ebony Novacite®	0.057	2.2	0.047	3.51	<0.01	<0.02
23	Ebony Novacite®	0.057	2.2	0.028	5.58	<0.01	<0.02
24	Zeolite	1.7	0.40	0.010	2.91	<0.01	0.18
25	Emathlite	0.09	0.83	0.058	5.39	<0.01	<0.02
26	Diatomaceous earth	0.45	0.62	0.095	4.49	<0.01	<0.02
27	Novacite®	<0.01	0.044	0.22	1.93	<0.01	<0.02

*NA - not analyzed and therefore included in the insoluble fraction.

- o General Electric TGA Data (made available at the February 1982 Contractor Review Meeting)
- o Argonne National Laboratory Bench-Scale Data.

Using these data, we have evaluated the relative importance of film diffusion, pore diffusion, and adsorption kinetics. In turn, these analyses have been used for two purposes. These were to determine the preferred contacting device and the size requirements for a full-scale unit. Particular emphasis was placed on a comparison between a granular packed-bed unit and an entrained-flow system.

We found that the intrinsic rates were low, so it would not have been feasible to increase the overall rate by using fine particles. As a result of the low intrinsic rates, long solid residence times must be provided, so packed beds, containing relatively large sorbent particles, are still the best option. This information is summarized in our Annual Technical Progress Report.²

Currently, we are preparing to update these studies on the basis of the results generated with water vapor in the system. Of particular interest will be those obtained with the leading candidate getter materials -- diatomaceous earth, emathlite, and Ebony Novacite®.

3.4 TASK 4: PROGRAM DEFINITION FOR CONCEPT SCALE-UP

Work has begun on this task, in the sense that it is a logical extension of our efforts in Task 3. As such, preliminary emphasis is on the nature of the contactor to be employed, not only in a full-scale system, but also in a pilot- or bench-scale unit and an associated test program, which would be required to ensure an orderly transition from our TGA system to the commercial unit.

4. REFERENCES

1. Mulik, P. R., M. A. Alvin, and D. M. Bachovchin, Simultaneous High-Temperature Removal of Alkali and Particulates in a Pressurized Gasification System, Third Quarterly Technical Progress Report, October 1981 - December 1981, Westinghouse Research and Development Center, Pittsburgh, PA, Contract No. DE-AC21-81MC16372, DOE Report DOE/MC/16372-3.
2. Mulik, P. R., M. A. Alvin, and D. M. Bachovchin, Simultaneous High-Temperature Removal of Alkali and Particulates in a Pressurized Gasification System, Annual Technical Progress Report, April 1981 - March 1982, Westinghouse Research and Development Center, Pittsburgh, PA, Contract No. DE-AC21- 81MC16372, DOE Report DOE/MC/16372-4.
3. Mulik, P. R., M. A. Alvin, D. M. Bachovchin, and T. E. Lippert, Simultaneous High-Temperature Removal of Alkali and Particulates in a Pressurized Gasification System, First Quarterly Technical Progress Report, April 1981 - June 1981, Westinghouse Research and Development Center, Pittsburgh, PA, Contract No. DE-AC21-81MC16372, DOE Report DOE/MC/16372-1.

APPENDIX

STATUS OF DOE CONTRACT DE-AC21-81MC16372

DEVELOPMENT OF A PROCESS FOR THE SIMULTANEOUS
HIGH TEMPERATURE REMOVAL OF ALKALI AND PARTICULATES
IN PRESSURIZED GASIFICATION SYSTEMS

Contractor

Westinghouse Electric Corp.
Research and Development Center
1310 Beulah Road
Pittsburgh, PA 15235

Prepared For

DOE Contractors Review Meeting
AR & TD Gasification Projects
June 22-24, 1982
Morgantown, WV

Contract Number: DE-AC21-81MC16372

Contract Title: Development of a Process for the Simultaneous High-Temperature Removal of Alkali and Particulates in Pressurized Gasification Systems

Objective: Perform experimental and analytical investigations, system design and cost estimates to ascertain the feasibility of utilizing aluminosilicate based getters for controlling alkali in pressurized gasification systems.

Contractor: Westinghouse Electric Corporation
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1310 Beulah Road
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Program Manager: Dr. P. R. Mulik
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METC Project Manager: Hsiao-Ya L. Lai

Contract Period of Performance: April 9, 1981 - April 9, 1983

Project Background:

Under DOE Contract DE-AC21-78ET11026, the Westinghouse Electric Corporation examined the feasibility of a hot gas cleaning process to minimize the concentration of alkali in a high-temperature fuel gas with simultaneous particulate removal through the use of aluminosilicate materials (getters). The program consisted of seven tasks: (1) test plan, (2) test facility assembly, (3) getter selection and fabrication, (4) getter material characterization, (5) bench-scale evaluation of getter performance, (6) system performance projections, and (7) program definition for concept scale-up.

The contract extended through October 1980 with extensive work being completed on six of the seven tasks. Specifically, work completed included the DOE-approved test plan (Task 1); design and construction of a high temperature-high pressure (HTHP) bench-scale reactor and a unique dual balance HTHP thermogravimetric analysis (TGA) system for detailed investigation of gettering kinetics (Task 2); selection of three getters (kaolin, char ash, and gasifier ash) and development of pellet fabrication techniques for the bench-scale reactor studies (Task 3); getter material characterization associated with the bench-scale reactor studies (Task 4); the scheduled bench-scale reactor studies (Task 5); and preliminary system performance projections based on the bench-scale kinetic studies (Task 6).

The experimental and analytical investigations, preliminary systems design, and cost estimates completed under this program demonstrated the feasibility of utilizing aluminosilicate based getters for controlling alkali in pressurized gasification systems. On this basis, this work was extended to the current contract which will enable us to resolve several questions, raised during the completed program, regarding alkali getter selection and application.

Description of Work:

The overall objective of the current program is to develop a comprehensive plan for evaluating a scaled-up version of the gettering process as a unit operation or as an integral part of a particulate removal device. Realization of this primary objective requires that the following inter-related aspects of the problem be taken into consideration: identification of a candidate getter by additional bench-scale studies as well as by comprehensive TGA studies and attrition studies; utilization of the data generated by the experimental studies to provide a technical, economic, and environmental assessment of the gettering process; specification of appropriate design details as to the specific reactor and equipment configurations for the scale-up studies; and delineation of key tests, operating conditions, etc., for conduct of the scale-up studies.

To realize the foregoing objectives, the Westinghouse program is composed of four technical tasks. The tasks are: (1) process thermodynamic projections, (2) getter selection and qualification, (3) system performance projections, and (4) program definition for concept scale-up. Tasks 1, 3, and 4 are basically analytical investigations which depend upon the experimental kinetic and particle attrition studies to be conducted in conjunction with Task 2. Task 1 input includes phases and compounds identified by x-ray diffraction analysis of reacted getter pellets; the quantity of volatile alkali in the coal-derived fuel gas is then predicted thermodynamically. Task 3 is directed to analysis of the experimental data in three areas: kinetic modeling studies using the bench-scale and TGA system data, process modeling, and an engineering assessment of the alkali gettering system. In Task 4, input from the other tasks will be used to meet the overall objective of the program.

Present Status/Accomplishments/Future Plans:

During the first year of this program, work has centered on Tasks 1 through 3. Work has also been initiated on Task 4.

The work on Task 1 has been completed and includes a data base update, development of alkali phase diagrams, and gasification process projections. Our data base update involved a literature review and subsequent updating of the thermodynamic data base to include aluminosilicate complexes which had been experimentally identified as resulting gettered species. Phase diagrams were then generated to demonstrate the various interactions of the mineral constituents of the feedstock during gasification, the chemical transformations of the released volatile alkali with effluent gas constituents, and the chemical stabilities of potential getter materials.

With respect to process projections, the thermodynamic model was utilized to rank the Lurgi, Shell Koppers, Texaco, Winkler, and Westinghouse gasification systems on the basis of released alkali concentrations at process conditions. In the order of increasing released alkali concentrations for the gasification of Illinois #6 coal, the following series applies: Lurgi (0.028-0.035 ppm Na, 0.013-0.016 ppm K), Texaco (18.70-12.3 ppm Na, 4.5-6.4 ppm K), Westinghouse (19-23 ppm Na, 4.3-12 ppm K) and Shell Koppers (37.2-45.6 ppm Na, 983 ppm K). Gasification of Eastern Kentucky Coal in the Winkler process (15.5-132.2 ppm Na, 7.7-101 ppm K) or Wyoming subbituminous coal in the Westinghouse fluidized-bed (34-51 ppm Na, 20-32 ppm K) is not projected to emit the potassium release concentrations in the Shell Koppers process, but borders, if not exceeds those for sodium.

Work on Task 2 involved a number of additional bench-scale unit and TGA tests. The bench-scale studies involved runs with activated bauxite in an inert carrier gas containing NaCl, KCl, and NaCl/water vapor. In addition, a series of screening tests were conducted to evaluate 20 candidate getter materials. The 11 atm NaCl and KCl exposures with activated bauxite were conducted at 1123 K and 1153 K in an argon environment containing 80 ppmv NaCl or KCl for durations of 1, 3, and 6 hours. For both temperatures studied, it was found that potassium was gettered at a rate approximately ten times that observed for sodium. Likewise, the presence of water vapor (4.6 mol %) at 1123 K and 11 atm enhanced the NaCl gettering by activated bauxite by a factor of about 2.

The limited rate, capacity and other problems, primarily potassium release, associated with the getters tested initially led us to direct part of our bench-scale efforts to evaluating new candidate getters. A number of the 20 candidates tested had higher gettering capacities than activated bauxite. Test conditions for these screening tests were 1123 K, 6 hours exposure, 11 atm pressure and 80 ppmv NaCl.

TGA studies were focused on ancillary tests needed to define a good operating procedure, preliminary tests with a number of getters (activated bauxite, shattered activated bauxite, boiler ash, char ash, and gasifier ash), and 8 runs involving a detailed evaluation of activated bauxite. The activated bauxite series involved 8 runs at 1123 K and 1173 K, atmospheric pressure with salt concentrations (NaCl) of approximately 0.8, 3, and 10 ppmv. Six of the tests were terminated upon saturation of the pellets with respect to NaCl while two tests were continued by terminating the salt flow to enable desorption to occur. It was found that: capacity is higher at 1123 K than at 1173 K at each gas phase concentration; capacity is greater at high gas phase concentrations at each temperature, and that the desorption is not completely reversible at either temperature level studied. In addition, the TGA system has been utilized to conduct 8 screening tests of the most promising alternative getters identified in the bench-scale unit screening tests. The results revealed that three of the candidates--ebony novacite, emathlite, and diatomaceous earth-- represent substantial improvements over activated bauxite in terms of gettering capacity.

The Task 3 effort involved two aspects. First, we examined the activated bauxite data from all available sources using two reversible sorption mechanisms. The mechanisms were the Langmuir isotherm and the BET two-parameter model. For the Langmuir model the necessary constants were obtained from all available Westinghouse data. The model generated by this technique was then used to determine average errors for our data and those of Argonne National Laboratory (ANL) and General Electric (GE). Average errors obtained were ANL ($\pm 18\%$), GE ($\pm 41\%$), and Westinghouse ($\pm 18\%$).

In the case of the BET model, the two parameters required were obtained using both the Westinghouse and GE data. Average errors obtained were ANL ($\pm 10\%$), GE ($\pm 35\%$), and Westinghouse ($\pm 28\%$).

Secondly, bench-scale gettering data for kaolin and several ash materials previously collected by Westinghouse and ANL data for activated bauxite were used to determine kinetic expressions. Intrinsic rates were low, so it would not be feasible to significantly increase the overall rate by using fine particles. Furthermore, long solid residence times must be provided so packed bed proved to be the most viable option. With such an approach, bed depths of about 10 m for kaolin or bauxite and 1 m for ash, with the beds replaced annually were estimated as determined by bed saturation capacity. More recently, the system performance projections for activated bauxite have been updated using ANL data along with TGA data from recent Westinghouse and GE studies. Particular attention was focused on the rate controlling step (s) and the preferred contacting device--entrained flow or packed bed reactor. Our previous conclusions have remained unchanged.

Future plans are to evaluate the most promising getter (emathlite) identified in the screening tests after the TGA system has been modified for operation with water vapor. Subsequently, the kinetic model for the gettering process will be finalized and a detailed assessment will be made of the commercial feasibility of the gettering process.

Advantages/Disadvantages/Potential:

Hot-gas cleanup systems if developed have the potential to remove contaminants from the fuel gas without any significant cooling. As such, the heat rate improvement advantage for hot-gas cleanup over cold-gas cleanup is estimated to be about 500 to 600 Btu/kWh for combustion turbine inlet temperatures of about 2000 to 2200°F. At the same time, hot gas cleaning circumvents problems associated with heat recovery in cold cleaning systems. For example, constituents of the fuel gas, such as soot, ash, and other particulates, along with any tars which may be present, could produce deposits on heat exchange surfaces. In an operating system, the performance spread could be greater than the 500 to 600 Btu/kWh indicated above.

The limited rate, capacity and other problems, primarily potassium release, associated with a number of getters tested initially have been cause for concern. While systems based on these getters are feasible, the economics associated with their implementation indicate that an improvement in alkali capacity is desirable. The results of our preliminary screening and TGA tests on several new candidate getters are encouraging. They indicate a substantial improvement in capacity which, if verified in additional studies, will establish gettering via aluminosilicates as a viable hot gas cleaning process.

Figure 1 — Project schedule.

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4. ORIGINATING SOURCE (OS) RDC	5. CONTRACT NO. (CN) DE-AC21-81MC16372	
6. FUNDING SOURCE/SPONSOR (FS) Department of Energy	7. NOTES (NT) This work was prepared for Morgantown Energy Technology Center	
8. AUTHOR/S (AU) Mulik, P. R.; Alvin, M. A.; Bachovchin, D. M.		

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9. TITLE (TI) SIMULTANEOUS HIGH-TEMPERATURE REMOVAL OF ALKALI AND PARTICULATES IN A PRESSURIZED GASIFICATION SYSTEM, FIFTH QUARTERLY TECHNICAL PROGRESS REPORT APRIL-JUNE, 1982	
10. DATE (DA) - YYMMDD 820728	11. PAGES, REFS., TABLES, FIGS. (PA) 21 p. 3 refs. 3 tabs. 4 illus.
12. KEYWORDS (KW) ALKALI. PARTICULATE. REMOVAL. SYSTEMS. PERFORMANCE. PROJECTIONS. ALUMINOSILICATES. GETTERING. MECHANISM. BAUXITE. THERMOGRAVIMETRY. COAL. GASIFICATION. SIMULTANEOUS.	

13. **ABSTRACT** (AB) - PURPOSE, SCOPE, APPROACH, RESULTS, CONCLUSIONS, SIGNIFICANCE

This program performs experimental and analytical investigations, system designs, and cost estimates to ascertain the feasibility of using aluminosilicate-based getters for controlling alkali in pressurized gasification systems. This report briefly summarizes efforts previously completed on thermodynamic projections and system performance projections, together with current work on getter selection and qualification. Work on the thermodynamic projections has been completed and includes an update of the data base, development of alkali phase diagrams, and projections for several gasification processes. Getter selection and qualification efforts involved four tests, two with activated bauxite and one each with diatomaceous earth and Novacite on the thermogravimetric analysis (TGA) system. Finally, system performance projections entailed examination of available kinetic data to ascertain the rate-controlling step, along with modeling efforts to ascertain the size requirements of a commercial-sized unit.

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