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KEY CONTRIBUTIONS IN MHD POWER GENERATION

Quarterly Report for June 1–August 31, 1979

By
J. F. Louis

MASTER

November 1979
Date Prepared

Work Performed Under Contract No. AC01-79ET15518

Massachusetts Institute of Technology
Energy Laboratory
Cambridge, Massachusetts

U. S. DEPARTMENT OF ENERGY

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QUARTERLY REPORT

for the period

1 June 1979 - 31 August 1979

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Date Prepared - November 1979

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ABSTRACT

Activities during the third quarter of the contract period are reported both in summary and in detail. The tasks reported on include: 1) investigation of electrical behavior in the vicinity of electrode and insulating walls; 2) studies of critical performance issues in the development of combustion disk generators; 3) development and testing of electrode modules, including studies of insulator properties; and 4) determination of coal combustion kinetics and ash behavior relevant to two-stage MHD combustors, and investigation of the mixing and flow aerodynamics of a high swirl geometry second stage.

Analysis of data from the first test series under Task 1 revealed a systematic dependence of electrode voltage drops on the cumulative amount of charge passing through a given electrode. Plans for further investigation (in Test Series 2) of the nature and origin of this effect are discussed; this test will focus on transition to arcing phenomena with different surface materials and higher currents. Other experimental work on damage to insulators by magnetically driven arcs indicates a dramatic effect of the magnetic field on arc penetration, with arcs being either extinguished or driven through the insulator depending on field polarity, even for $B < 0.2$ Tesla. Initial isothermal runs have been made in an improved glycerin channel for simulation of slag flow, and various ripple regimes have been identified and mapped. Plasma conductivity calculations which were carried out for a DOE workshop, and which include phosphorus negative ion effects, are reported. The status of the design of Channel II flow components (with 4 Tesla magnet) is also presented.

Under Task 2, experiments on wake nonuniformities in a radial flow disk have been carried out, and comparisons have been made with measure-

ments obtained in an undisturbed reference flow. Results, which are applicable to both linear and disk channel configurations, are consistent with theoretical predictions. The experiment was designed to enhance the wake effect, and the initial tests reduced the open-circuit voltage by 40% relative to the reference flow case, and produced a decrease in measured average effective Hall coefficient from 6.5 to 3.0. Theoretical modeling of the electrodynamics in the disk r-z plane has been carried out for an investigation of the interaction between the side-wall boundary layer and the conductor/insulator segments of a segmented disk wall. The calculations indicate the extent of performance degradation as a function of conductor-to-insulator width ratio, boundary layer thickness, and wall temperature. Other experimental work reported is concerned with the influence of CO and CO₂ radiation on the cesium spectrum.

Room temperature dielectric breakdown measurements were made in Task 3 for magnesium oxide (single crystal) and silicon nitride (hot pressed), and these materials showed the highest breakdown strength of all materials tested to date. Single layered electrodes of composition SZSFLF-6 were tested in the MIT MHD Simulation Facility; only minor damage was observed for electrodes operated at 1-1/2 A/cm² for 22 hours and 39 minutes, while more extensive but not severe damage (including anode melting) was incurred by electrodes operated at 3 A/cm² for 7 hours and 32 minutes. Evidence of resistance increase in electrodes was found in one case, but no microscopic evidence of electrochemical decomposition was found in any test.

The two-color pyrometer system used in Task 4 for measurement of burning particle temperatures has been improved to permit single particle temperatures to be measured as a function of time. Experimental results have been obtained for various particle size ranges (45-53, 75-90, 90-105 mm), furnace temperatures (1500-1800°K), and mixtures of O₂ in Ar, He, and

N_2 (10-100% O_2). A simple diffusion-controlled particle model has been developed for comparison with the experimental data. An initial version of a char/coal combustion model has been completed, with external diffusion, internal pore diffusion, and reaction of the internal surfaces being taken into account. Instantaneous reaction rates are reported as a function of equivalence ratio, particle diameter, gas phase temperature, and pressure, and the trade-offs in reaction rate due to variation of these four parameters are discussed.

Progress is reported on development of the water model test facility for study of the effects of second stage nozzle geometry and input operational variables on the flow aerodynamics and fluid mechanics within the second stage of an MHD combustor. Preliminary tests have been carried out with varying degree of first stage swirl and with zero second stage swirl. In parallel with the above experimental studies, a computer program "SHAPE" has been developed for predicting the flow aerodynamics and flow separation within the second stage of the combustor nozzle sections under isothermal conditions.

OBJECTIVE AND SCOPE OF WORK

The Department of Energy (DOE) is responsible for a national program for the development of commercial open-cycle MHD power generation with the initial objective of establishing the engineering feasibility of MHD power systems utilizing coal or fuel derived from coal.

Research and development in open-cycle coal-fired MHD power generation has been underway at Massachusetts Institute of Technology (MIT) since 1971, the scope of the effort gradually expanding to its present level. The scope and objectives of the present MIT program are as follows:

1. To carry out an experimental investigation of the mechanisms of near-electrode voltage drops, axial breakdown, onset of transverse arcs, arc damage, slag shorting and related phenomena important for the design of MHD electrode and insulating walls, and to develop analytical models in support of these experiments.

2. To investigate, experimentally and analytically, critical performance issues involved in the development of combustion disk generators. Particular emphasis will be given to determination of the effective plasma properties and generator performance as affected by (a) plasma nonuniformities, (b) chemical nonequilibrium, (c) unsteady flow phenomena, (d) boundary layers and slag, and (e) inviscid flow distortion.

3. To perform the engineering design, construction and testing of electrode modules. This work will include: (a) a laboratory-based materials selection investigation, (b) electrode/insulator fabrication, and (c)

performance measurements. In addition, a model of the time-dependent performance based on measured module data will be developed. The major emphasis of the task will be on development of super-hot electrode modules and measurement of dielectric breakdown of insulator materials and coal slag.

4. To research the coal combustion kinetics relevant to the two-stage MHD combustor, focussing on two problem areas: (a) coal oxidation kinetics under fuel-rich conditions, and (b) ash behavior in an MHD combustion environment. This task will also include study of the mixing and flow aerodynamics behavior in a high swirl geometry intended for the second stage of an MHD combustor, using a simple water model test facility.

II. SUMMARY OF PROGRESS TO DATE

TASK 1. ARCING PHENOMENA IN MHD GENERATORS

The major effort during this reporting period has been in preparation for two experiments in the simulation facility. One of them is a second experiment relating to transverse current transfer to the electrodes, and it will investigate several phenomena identified as important by the first experiment. The other planned test is an axial voltage breakdown experiment employing an interelectrode insulator configuration designed to prevent insulator-initiated breakdown. Details of the planning for these experiments are given in the text.

Work has also progressed on the experiments on damage to insulators by magnetically driven interelectrode arcs, as well as on the glycerin-simulated slag flow experiments. Improvements were made to our equilibrium plasma properties computer code, on the occasion of MIT's participation in the DOE conductivity work shop. Finally, design of Channel II and its flow train has continued, and the feasibility of installing a 4 Tesla superconducting magnet is being evaluated.

TASK 2, OPEN CYCLE DISK GENERATOR PROGRAM

The principal results and program status as of this reporting period are summarized as follows:

Nonuniformities Studies in a Radial Flow Disk

The reference flow phase of this study has been completed. With mixtures of Ar/CO₂ effective Hall coefficients up to 7.5 were measured, in agreement with the ideal values. This and other evidence support/indicate that the flow is uniform and in Saha-equilibrium. Aerodynamic profiles/struts were designed, fabricated and used to create well-defined wake nonuniformities. The results of two tests with 25 struts at 3.5 Tesla were analyzed. Relative to the reference flow case, the open-circuit voltage was reduced by 40% and the average measured effective Hall coefficient was reduced from 6.5 to 3.0. These results are consistent with theoretical predictions.

The experiment was designed to produce a strong wake effect (as part of a study of basic phenomena in MHD generators in general); long, cold ($T_w = 300$ K) struts were used. Swirl guide vane wakes for a similar scale experiment would most likely have less severe effects since the blades would be predominately in a region of high favorable pressure gradient and the boundary layer would remain laminar (which leads to a narrower initial wake and hence less rms deviation). The effect of blade temperature will be investigated as well as number of blades and variations of the ideal Hall parameter. Wake growth rate will also be determined experimentally. Quantification and scaling of the effects of this type of nonuniformity will be an asset to the understanding of plasma properties and performance of both linear and disk channel configurations.

Experiments with Inlet Swirl

With swirl, the wakes produced by inlet guide vanes are nonsymmetric. In addition, the trailing edge of the vanes is normally in a region of supersonic flow, thus introducing a recompression shock and expansion wave into the channel. In order to characterize/quantify the swirl vane wake, the existing MIT swirl generator (45° swirl) will be used initially. The generator has been modified to provide a detailed assessment of the wake structure; 80 voltage probes were added in the region behind two vanes, and four additional viewports were added for electron density measurements. Tests with this generator will begin upon completion of the first series of radial flow wake tests.

Disk Generator Modeling

Additional calculations were made using the 2-D uncoupled wake model in order to assess the relative effects of wake growth, $\text{rms}\sigma$ and number of blades/wakes on the open-circuit voltage reduction. The effects are stronger with increasing number of wakes and/or higher $\text{rms}\sigma$. For a constant conductivity deficit (which implies that the free-stream and wake centerline conductivity decay at the same rate) the effect on the voltage is less for wakes with a slow growth rate.

The electrodynamics in the disk r - z plane (i.e., insulator/conductor side wall-boundary layer interaction) was coded and sample results were obtained for a constant height channel. The calculations indicate that:

- (1) The presence of conducting modules causes significant degradation of performance when the width of these modules, l , is greater than the width of the insulating gaps. The smaller the width of the conducting modules, the less degradation of performance relative to the ideal insulating wall case was found (as expected).

- (2) For a given module and gap geometry, the effect of boundary layer thickness for these wall temperatures is relatively small.
- (3) As the conducting module width increases, the effect of wall temperature becomes increasingly important.

Modeling of 1-D flow with chemical nonequilibrium has been completed and implemented on the MIT Energy Laboratory PDP-11/60 computer. A design code has been written and found to be compatible with the performance code when the derived output of one program was used as input to the other. Details of both programs/codes are given in the main text. The design code will be used to design a high performance channel for experiments in the MIT disk facility. Both codes will also be used for further work on establishing effects of chemical nonequilibrium on scaling laws of large-scale disk generators.

Diagnostics

Spectroscopic studies of the influence/effects of radiation from CO and CO₂ molecules on the cesium spectrum were initiated. Spectra for tests with Ar/CO and Ar/CO₂ mixtures were obtained and compared qualitatively. The data, as yet, have not been fully analyzed; however, it appears that the effects on the Cs continuum for the Ar/CO₂ case are minimal. This work will continue into the next reporting period.

TASK 3, ELECTRODE MODULE DEVELOPMENT AND TESTING

Part A.

Room temperature dielectric breakdown measurements were made for magnesium oxide (single crystal) and silicon nitride (hot pressed).

Electrodes of composition SZSFLF-6 were tested for 22 hours and 39 minutes in the MHD Simulation Facility at M.I.T. under a current density of $1\frac{1}{2}$ A/cm².

Electrodes of composition SZSFLF-6 were tested at 3 A/cm^2 in the MHD Simulation Facility at M.I.T. for 7 hours and 32 minutes.

Post-test electrode cross-sections from each of the tests were examined for evidence of electrochemical decomposition and for formation of potassium richness or other second phases.

Part B.

Cooling of the burner modules ..
higher capacity city water pump. Residual pool
of the high energy impactor scrubber accumulated in the ex.
The resulting loss in suction required interruption of the test. This
condition was corrected with the addition of a water spray upstream of the
blower.

In keeping with the Safety Officer's recommendation, remote methods for temperature measurements are being investigated.

The PDP 11/60 computer was used extensively to provide the operator with burner performance and electrode-control feedback.

The electrode tests were of long duration at current densities as high as 3 amps/cm^2 . Other tests were associated with the development of a plasma temperature probe and for correlation of film cooling parameters.

TASK 4, COAL COMBUSTION STUDIES

TASK 4a, KINETIC MODELLING OF 2-STAGE COMBUSTOR

The two-color optical pyrometer system for measurement of burning particle temperatures has been modified to permit single particle temperatures to be measured as a function of time, a major improvement over the previous multiple particle averaging system. Experimental results have been obtained for various particle size ranges (45-53, 75-90, 90-105 μm), furnace temperatures (1500-1800 $^{\circ}\text{K}$), and mixtures of O_2 in Ar, He, and N_2 (10-100% O_2). A simple diffusion-controlled particle model has been developed for comparison with the experimental data.

An initial version of a char/coal combustion model has been completed. The model considers 5 first-order reactions. Concentrations of the gas phase species are calculated from an equilibrium program; 36 species are considered. External diffusion, internal pore diffusion, and reaction of the internal surfaces are taken into account. Instantaneous reaction rates are reported as a function of equivalence ratio (1-4), particle diameter (10-150 μm), gas phase temperature (1500-3000 $^{\circ}\text{K}$), and pressure (1-5 atm.). The trade-offs in reaction rate, due to variation of these 4 parameters, are discussed.

TASK 4b. COMBUSTION AERODYNAMICS AND FLUID MECHANICS OF HIGH-SWIRL SECOND
STAGE

During the last quarter efforts were concentrated on both the theoretical and experimental aspects of this program. The experimental water model test facility has been constructed and allows one to study the effects of second stage nozzle geometry and input operational variables upon flow aerodynamics and fluid mechanics within the second stage of the MHD combustor. Some difficulty was experienced in moving the swirl vanes which are used to vary the degree of swirl in the three annuli independently in the second stage nozzle; it is expected that it can be made operational in early December, 1979. Preliminary tests performed by varying the degree of swirl in first stage and with zero swirl in second stage, using a low intensity slit light source showed some moderate success. These tests revealed that a high intensity slit light beam is necessary for taking still and cine photographs at short exposure times. The fabrication of a slit light beam source incorporating 8 lamps is currently under progress and is expected to be operable in September, 1979.

In parallel with the above experimental studies, a computer program "SHAPE" is being developed for predicting the flow aerodynamics and flow separation within the second stage of the combustor nozzle sections under isothermal conditions. Details of this program are given in the Detailed Description of Technical Progress, Task 4b.

III. DETAILED DESCRIPTION OF TECHNICAL PROGRESS

TASK 1, ARCING PHENOMENA IN MHD GENERATORS

1. Introduction

Successful application of MHD power generation requires efficient and long-lasting channel wall designs. To effect such designs it is necessary to have a good understanding of the mechanisms of current transport in the vicinity of the wall and to develop modes capable of predicting, for example, the conditions for which electrical arcing occurs. In addition, it is important to develop techniques to determine the performance degradation from arcs and the extent of damage to the channel walls. The present task addresses the general problem of current transport to electrodes through a combined experimental and analytical study which includes problems specific to slagging wall operation and non-slagging wall operation. The initial studies, which are of a fundamental nature, are being performed without the complication of a magnetic field. However, the task also includes the designing of a sub-atmospheric channel and the installation of a superconducting magnet. This sub-atmospheric facility, described elsewhere in this section, will allow extension of the experimental work to conditions typical of a full-scale generator operating at high Hall parameter.

The task is divided into several subtasks. Where possible, progress in each subtask is reported separately. During this reporting period major effort has been in preparation for two experiments in the simulation facility. One experiment is a second experiment relating to transverse current transfer processes to the electrodes and will investigate several phenomena identified as important by the first experiment. The other experiment is an axial voltage breakdown experiment employing an interelectrode insulator configuration designed to prevent insulator-initiated breakdown.

Work has also progressed on the arc damage experiment, although late delivery of a DC contactor for the magnet supply prevented experiments at high magnetic fields. Progress has also been made with the slag flow simulation studies, including measurements with the new rig and extension of a linearized stability theory to include the effects of viscosity gradient.

With agreement from DOE, M.I.T. has also participated in the conductivity calculation comparison and we used this as an opportunity to update and improve the data and structure of our equilibrium properties routine.

Work has continued on the definition and design of Channel II, which will serve to extend the investigation of near wall effects to include magnetic interactions. The possible use of a 4 Tesla superconducting magnet is under evaluation, and various portions of the flow train are in their final design phase.

2. Diffuse Discharge and Transition to Arc Experiments

This section summarizes the progress in the experiments and analysis relating to the current transport processes in the vicinity of the electrode walls of the generator. The principal progress has been the definition of a second series of experiments, upgrading of the instrumentation and the reassembly of the channel. The first section briefly describes the channel and facility and the salient results of the first experimental series as background for the experimental run plan. Preparation for the second experiment is then described and the upgrading of the instrumentation discussed.

Previous Experiment and Analysis

The design and construction of a test channel for experiments on the electrical plasma-electrode interface was described in the previous progress report.^[1] The channel is rectangular with flow cross-section of 1.625" x 3.00" and is mounted at the end of the MIT MHD simulation rig combustor. This facility can provide seeded combustion plasma at a rate of 0.6 lb/sec; plasma temperatures up to 3000 K and pressures slightly above 1 atm can be achieved. No magnetic field is applied. The channel itself has two completely ceramic (MgO) walls designed to operate at a surface temperature of approximately 2000 K. Three electrode pairs are mounted in the other walls of the channel. For the experiments reported in Ref. 1 these electrodes were made of 304 stainless steel and designed to operate at temperatures close to 1100 K at a nominal N/O ratio of 0.8. The electrodes are separated by ~ 1/16" alumina insulators. The remaining upstream and downstream sections of the short walls were made of MgO. The central electrode pair was instrumented with a row of voltage probes across each sidewall and partial rows of the probes were provided for the other electrode pairs. Other instrumentation included thermocouples inserted near the electrode surfaces and in the brick and a mirror system for optical access through the exit opening of the channel. The principal results obtained from the experimental runs with this first channel are briefly summarized below and are fully documented in Refs. 1 and 3.

(a) The central sidewall probe readings provided a core plasma conductivity to good agreement with that indicated from the measured plasma temperature at $N/O = 1.0$.

(b) The voltages from the near-wall probes and from the electrodes themselves allowed the determination of voltage-current curves for both anodes and cathodes at $N/O = 1.0$.

(c) Wall overheating made the data at $N/O = 0.7$ unreliable.

(d) Visual observation showed no evidence of anode arcing for current densities up to about 2 A/cm^2 . Cathodes showed arcs even at relatively low currents ($\sim$ approx. 0.5 A/cm^2). Although cathode arcs were visually observed for most conditions, the qualitative behavior of the arcs changed from relatively mobile arcs to less mobile arcs at a moderate current level. The reason for this is not understood.

(e) A two dimensional, turbulent boundary layer computer program was used to calculate values of anode voltage drop as a function of current and these were compared with the measured values. The calculation procedure included only three-body electron recombination and it was found that these rates needed to be increased by a factor of 30 to get good agreement between experiment and theory. Such increases might represent the influence of three body-heavy recombination at the lower temperatures. Cathode voltage drops showed the usual non-zero voltage at low currents; when this value was subtracted the voltage drop is similar in value to the anode drop.

(f) More detailed examination of the experimental data shows that the near anode voltage drop increases gradually as a function of cumulative current through the electrode as shown in Figure 1a. The opposite trend, that is a decrease with cumulative current, is observed on the cathode (Fig. 1b). This is qualitatively similar to the electrolytic polarization effects observed in slag or refractory electrodes (Ref. 1). One possible interpretation is the accumulation of a thin refractory oxide layer on the "clean" electrode surface, showing partially ionic conduction with the corresponding polarization. An immediate question that arises is about the origin and nature of this layer and whether such effects would be observed

on a noble metal electrode for example. If the layer originates from plasma material or from burner material creeping along the wall, there should be little difference to the hysteresis behavior for electrodes of different materials. If the layer is formed in situ from corrosion of the electrode material, significant differences in behavior should result.

Second Experimental Series

Main Experiments

A second experimental series has been planned and implemented based on the results of the first experiment. The principal goals of this experimental series are:

(a) to study the effect of upstream wall temperatures on voltage drop characteristics and the transition to arc threshold current density levels for anodes;

(b) to study the influence of electrode surface material on the voltage drop and on the transition to arc threshold level;

(c) to obtain more detailed information relating to the hysteresis effect; and

(d) to obtain preliminary information relating to the high frequency fluctuations of current and voltage. The new experimental setup and modifications for these experiments are described below.

The channel has the same cross-section and sidewalls as in the previous test, but the electrode walls have been modified as follows:

(a) Only one electrode wall retains the MgO-metal-MgO sequence; the opposite wall starts from the beginning with five water cooled dummy (non-current carrying) stainless electrodes designed for 1100 K followed by the three active electrodes and a downstream MgO section. This will afford an

opportunity to assess the effect of wall temperature discontinuities: the near-wall boundary layer on this wall should be representative of that actually seen by electrodes in a metal-wall generator, while the MgO-metal-MgO wall, more convenient for experimentation, may show distortion effects due to the heated upstream boundary layer. These two cases should help evaluate the calculation procedure used to get the voltage drop.

(b) Only one of the three active electrodes on the "cold wall" side of the channel is bare stainless steel. The others are clad with 15 mil layers of Pt and Cu respectively as shown in Figure 2. This will allow an investigation of the surface effects (as distinct from the thermal one) on arcing and on diffuse discharge voltage drop, and has been prompted in part by the observation of hysteresis effects of opposite sense in stainless anodes and cathodes in our previous experiments.

(c) the central electrode on one side is fitted with an electrically isolated mini-electrode as shown in Figure 2. This mini-electrode is constructed of a 1/8" diameter stainless steel rod insulated from the electrode body by plasma sprayed alumina. The mini-electrode is mounted flush to the surface. Instrumentation is provided for digital recording of the current collected by this mini-electrode and the voltage relative to the body of its parent electrode at frequencies up to 1 MHz. The main purpose of this electrode is to investigate the possible existence of fast moving, short-lived arcs, undetectable by low speed visual or electrical observations. Time resolved voltage and current fluctuation measurements taken with this mini-electrode will be correlated to other fluctuation data (luminosity, see below) to discriminate between acoustic or other large scale fluctuations and those associated with the current collection itself.

(d) The external connection circuits have been modified to allow channelling of the full power supply current to any one of the three electrode pairs, the change being made during the run. This will allow a higher (approx. 30%) current density on the selected electrode at the cost of greater distortion of the current pattern. An additional improvement is the incorporation of an SCR (silicon-controlled rectifier) switch that will simultaneously connect all three electrode pairs to the supply voltage; this should eliminate the transient interelectrode arcs that were observed in the previous experiments and which were attributed to non-simultaneity of the manually switched connections.

(e) To facilitate time correlation of events, a single camera (TV monitor) will be used in the next run for visual records, rather than two as in the past. To retain the capability for obtaining separate "wall" and "plasma" images a beam splitting arrangement similar to that in Ref. 2 has been assembled. A narrow band red filter is used to reject the plasma radiation and accentuate the wall response while a narrow band filter centered on the 4044 Å potassium line is used to accentuate the plasma response.

Secondary Experiments

In addition to the main experiments during this test series, two other matters will be addressed. The first is related to the conditions of the plasma in the channel and includes velocity and temperature measurements at the channel exit. The new measurement devices and upgrading of existing equipment is described below. The second matter relates to questions of the accuracy of the voltage probe measurements and involves a biasing experiment with a probe. The problem and the planned experiment are described below.

Plasma Condition Characterization

(a) Velocity measurements. Two independent velocity measurements will be obtained in an effort to more fully characterize the plasma flow. One of these will be made with a classical Pitot impact probe water cooled to withstand the high total temperature of the flow, and maintained under N_2 purge except during data acquisition. The probe will be mounted across the exit plane of the test section. The other measurement will be made using the luminosity fluctuations of the flame, many of which can be identified as convected acoustic fluctuations. Two lines of sight, spaced about 4" apart in the flow direction, will be provided (Fig. 3), and the resulting photodiode signals correlated for time delay. Figures 4 and 5 show an example of the spectral characteristics of luminosity fluctuations obtained in the simulation facility during a separate experiment. The discrete harmonic nature of the data is to be noted. The fundamental at about 70 Hz is too slow to be a combustor mode and is probably related to a resonance of the whole test shell, including part of the exhaust pipe. The other, seemingly independent, spike at about 8 kHz is likely to be a longitudinal combustor mode propagating in the flowing gas at a speed equal to the flow speed plus the speed of sound. It is of interest to note that almost identical spectra were obtained from measurements of the voltage and the current of a full size electrode in the same test. This indicates that the luminosity fluctuations are a reflection of large scale temperature disturbances that affect directly the instantaneous impedance of each electrode pair. The 8 kHz mode, whose wavelength is approximately 0.15 m, will be used for velocity measurement. A separation of 10 cm between the two lines of sight is thus expected to provide adequate resolution.

(b) Temperature measurement. Substantial improvements have been made to the sodium line-reversal temperature measurement diagnostic. Previously the maximum temperature that could be measured was limited to the apparent filament temperature of the reference tungsten lamp and was about 2500 K. This resulted because an actual reversal was sought; however, an extrapolation technique can be used to extend the method to temperatures beyond the filament temperature. The lamp is set to a fixed current, and the filament temperature is noted (and recalibrated periodically). The lamp is then sighted through the plasma (at the exit flame from the test section) and a chopper wheel interposed between lamp and plasma provides alternative "lamp plus plasma" and "plasma alone" beams to the light detector. A synchronization signal from a photodiode behind the chopper serves as an enabling signal for digital circuitry to send the two pulses of light intensity data to different channels for on-line computation of plasma temperature.

A calibration test is planned for this method: the flame will be stabilized at a temperature low enough for direct reversal and a temperature reading will be made this way. For comparison, the lamp will be dimmed to a lower temperature, and the extrapolation technique applied as described above. After such calibration the extrapolation system will be used throughout.

Voltage Probe Characteristics

Certain systematic deviations from linearity in the measured distribution of voltage across the sidewall in our previous experiments have raised the possibility of measurement errors attributable to voltage differences between the plasma and the probes. Specifically, all probes are connected

to the ground through a large leakage resistance (~ 2 M ohms) which serves as a part of a voltage divider used to match the magnitude of the signal voltages to the levels accepted by the digitizer; on the other hand, the electrode pairs are given equal and opposite voltage from the power supply, which puts the ground level somewhere near the channel centerline. Thus, those probes located near the anode see a locally positive plasma voltage of up to some 120 volts and act as local small cathodes ballasted to the ground. Depending on the detailed geometry, loading and surface properties, the micro-ampere level current drawn by the probe through the ~ 2 M ohm resistance may be sufficient to create a significant cathodic voltage drop, which would falsify the reading of the plasma potential. To test this possibility the complete voltage-current characteristic of one of the probes will be measured during the next run. The data obtained will be used to correct the probe readings or, if necessary, to help redesign the probe measurement system.

The channel has been mostly assembled for testing in the next reporting period.

3. Breakdown Experiments and New Insulator Designs

Experimental and analytical work relating to axial breakdown has established that breakdown can be initiated in the plasma or in the insulator. For many electrode wall designs, the threshold voltage for insulator-initiated breakdown is considerably lower than that for formation of an axial arc in the plasma. Therefore the development of electrode wall designs with higher threshold levels is clearly desirable. One possibility of improved insulator design is a "laminated" insulator shown schematically in Figure 6, which provides good cooling in the region adjacent to the electrode where Joule heating is extreme.

In the present reporting period significant progress has been made in the thermal analysis of this configuration. In addition, a second copper shell test section has been constructed and assembly of the channel and diagnostics initiated.

3a. Heat Transfer Analysis

To evaluate the above approach a heat transfer analysis of the inter-electrode region has been performed. The analysis consists of a solution for the convective heat transfer to the wall for variable wall temperature coupled to a two-dimensional conduction solution for the complex wall construction. A coupled solution is required since the wall temperature distribution affects the heat transfer coefficient. The analysis will be used to choose appropriate dimensions for the components such that insulator breakdown will not occur. The additional heat transfer due to Joule heating is estimated from representative numerical calculations of Ref. 2. The two components of solutions are presented below and some representative results for each are shown.

Plasma Heat Transfer--The convective heat transfer in the absence of Joule heating is modeled as a high speed boundary layer flow over a flat plate with constant freestream conditions and variable wall temperature. The solution for this problem can be represented in terms of the empirical solution for a single step change in wall temperature^[4] for which the local Stanton number, St_x , is represented as

$$St_x = 0.00295 Re_x^{*-0.2} Pr^{*-0.4} [1 - (\zeta/x)^{9/10}]^{-1/9}$$

where ζ is the axial distance as measured from the location of step change, x is the distance from the leading edge and Re_x^* and Pr^* are, respectively,

the Reynolds and Prandtl number evaluated at a reference condition as specified in Ref. 4. For an arbitrary wall temperature distribution, such as indicated in Figure 7, the heat flux is given as

$$q''_0 = \rho U_\infty \left\{ \int_0^x St(x, \zeta) \left(\frac{di_0}{d\zeta} \right) d\zeta + \sum_{i=1}^k St(x, \zeta_i) \Delta i_0, i \right\}$$

where i_0 is the wall enthalpy and the first term accounts for variations of a continuous nature and the second term for discontinuous changes in wall temperature.

Representative calculations of heat flux and convective conductance have been made for a representative surface temperature distribution for the laminated design. For these calculations the plasma conditions were taken as

$$P = 1 \text{ atm}$$

$$T = 2800 \text{ K}$$

$$U = 1000 \text{ m/sec}$$

The assumed temperature distribution and the calculated heat flux and convective coefficient are shown in Figures 7 and 8. The qualitative behavior of the heat transfer to the wall temperature is as expected. High heat transfer rates are experienced on the upstream edge of the upstream electrode and of the upstream cooler piece since the fluid has been in contact with a hot wall immediately upstream. Similarly, the upstream edges of the two small insulators experience lower heat transfer because the oncoming gas has accommodated a lower surface temperature. Conduction in the wall will tend to smooth these spatial distributions in heat flux by allowing axial gradients in surface temperature. The temperature distribution in the central insulator has been assumed to be parabolic resulting in a smooth distribution of heat flux.

The effect of Joule heating and of radiation from the plasma and from the other walls of the channel (which operate at temperatures significantly hotter than this portion of the channel) will be included in the next reporting period.

Wall Heat Conduction--The two-dimensional (i.e. elliptic) heat transfer equations for the complex wall geometry have been solved by considering finite length slabs in the axial direction and infinitesimal elements in the vertical direction as shown in Figure 9. The temperature across the slab is assumed to be constant, but the slabs transfer heat axially to the adjoining slabs. The total thermal resistance between the slabs is the sum of the thermal resistance of the material itself, plus the thermal contact resistance if there is material interface. The model also includes the effect of variable thermal conductivity which is significant especially for the ceramic pieces. The above approach results in a set of n (number of slabs) coupled, second order, ordinary differential equations. The physical boundary conditions are the specified plasma temperature, velocity and pressure and the rear face temperatures which are set by the cooling water temperatures. Since the wall temperature is not known a priori, the plasma side heat transfer rates (or convective coefficients) are not known and the convection and conduction solutions must be effected together. To avoid a lengthy matrix solution, the present technique assumes a surface temperature distribution (and therefore the surface heat transfer rates) and solves the equations as an initial value problem (T_{surface} and $\frac{dT_{\text{surface}}}{dy}$ specified). Iteration of the surface temperature is performed until the solution yields the proper rear face temperature. While the iteration process is somewhat tedious, the numerical methods employed are

standard and some useful results are achieved without major computer program development.

The detailed results using the combined plasma and wall solutions and the final design will be presented in the next progress report.

3b. Breakdown Experiment

Preparation for the experiment to test the breakdown threshold voltage of laminated wall concept has begun. A second copper shell (similar to the one used for the transverse discharge experiments) has been constructed to allow the axial breakdown experiment to be assembled while the transverse experiment is being installed in the Simulation Facility and the testing performed. The major diagnostics employed in this experiment are:

- a) basic thermal and electrical behavior of the interelectrode wall components;
- b) visual observation looking down on the interelectrode region; and
- c) light intensity measurements in the plasma immediately above the downstream edge of the upstream electrode.

A special window port will be provided as shown schematically in Figure 6 and dual-filter photography will be used to display the wall and plasma response to the axial discharge. In addition, as shown in Figure 6, access and the appropriate mounting structure will be provided for the plasma radiation probe array described in the previous progress report (see also Sec. 7 of this Task Report). This will allow the measurement of relative temperature for eight lines of sight in the region of expected high Joule heating.

4. Arc Damage in Inter-Electrode Insulators

Inter-electrode arcs have the potential to cause considerable damage to the generator wall. In some experiments (such as on the U25-B) such arcs were observed to be driven into the anode wall (presumably under the influence of the $\vec{J} \times \vec{B}$ force) and extinguished only upon reaching a well cooled containment shell and only after causing significant damage to the generator. In other experiments, inter-electrode arcing occurs without widespread damage even after relatively long term operation. Early considerations at Avco established some rules of thumb about the arc power level required to produce damage to their type of electrode wall. The purpose of the experiments and analysis in this subtask is to study the extent of damage to the walls from inter-electrode arcs and to develop designs and techniques to minimize the effects of such arcing.

For this purpose a small facility shown schematically in Figure 10 has been assembled and preliminary experiments performed. The magnet is a conventional iron core magnet capable of reaching fields of ~ 2 Tesla at a current of 50 amps and with approximately a 1-1/2 inch air gap. At present the gap is relatively large and late delivery of a D.C. contactor has limited the current through the magnet to < 15 amps and thus to a magnetic field of 0.16 Tesla.

Although in the long term a torch will be used to simulate the temperature distribution of an actual generator, the preliminary experiments have been performed without a torch and cooling of the insulator was varied by inserting varying thicknesses of stainless steel between it and the cooled end copper blocks. The arc was initiated and positioned by notching the inter-electrode insulator and placing a small amount of steel wool bridging the electrodes; when the power supply is turned on the steel wool is

vaporized and an arc established in the air. The effect of the magnetic field (even at the low strengths possible) was clear. Without magnetic field the arc caused heating of the inter-electrode insulator but no significant damage to it. With the magnetic field oriented to drive the arc away from the wall the arc was blown off and extinguished. With the magnetic field oriented in the opposite way the arc was driven into the wall, causing significant damage for some conditions. Figure 11 shows a photograph of the damage to the insulator resulting when the arc is driven into the wall; the damage is similar to that observed on examination of the disassembled Channel 1 used in the US/USSR U25-B experiments. The preliminary experiments investigated the effect of cooling and arc current on recession rate and arc damage width and these results are shown in Figures 12 and 13. The cooling was altered by changing the size of the stainless steel cap separating the water cooled copper piece from the inter-electrode. The few data points available indicated a damage width increasing with current and with stainless steel width as expected. No strong trend of recession rate with these parameters can be established with the available data. With the magnetic field available ($\sim .16$ Tesla) times of ~ 10 seconds were required for the arc to pass through $\sim 1/2$ inch of insulator.

More extensive experiments with the above configuration and more realistic cooling configurations are necessary and will be performed in the next reporting period. Preliminary order of magnitude analysis of the factors controlling the recession rate will be considered in the next reporting period.

5. Modeling of Slag Flow with Ripples

Progress has been made both in the experimental apparatus and the theoretical analysis of slag flow in MHD generators. The three channel sections and the feeder section have been assembled with the necessary air velocity measurements. One section has been provided with a cooling tube through which a controlled temperature alcohol flow will be maintained; this will allow simulation of the viscosity gradient present in the actual slag flow situation. Parallel experiments with "waves" made of clay have been initiated to determine the flow distribution around the ripple surfaces. A previous linear stability model for the viscous films has been extended to include viscosity gradients normal to the wall; solution of the resulting equations has not been effected and results from this work are deferred until the next progress report.

5a. Simulation Experiments

Several experiments were performed in the new experimental rig for the purpose of understanding the instability of viscous isothermal films flowing under the shear of a turbulent boundary layer. A typical section of the channel is shown in Figure 14. As described in the previous progress report,^[1] the average shear stress on the surface of the film was controlled by changing the free-stream velocity of air and the mass flowrate of glycerin was adjusted by changing the elevation of the feeding reservoir as well as the feeding tube diameter. Note that throughout the experiments, the feeding of glycerin was protected by a 1/8" thick aluminum plate to prevent any upstream perturbations from developing in the film. The qualitative similarities of Figures 15a and 15b to actual slag flow photograph of Figures 16a and 16b is apparent.

The history of ripple formation followed a general trend as these two parameters were modified. The following is a qualitative presentation of that trend (see Figs. 17 through 19)

- a) For very low air velocities (up to 8 m/sec), a smooth glycerin film was obtained for all values of m . As m was increased, the thickness of the layer increased also, as would be expected from theoretical models.
- b) For higher air speeds (~ 14 m/sec), sinusoidal waves similar to gravity waves were observed at moderate values of m (~ .03 mL/sec). These waves were uniform, flowing in the direction of air motion with minor perturbations. As m was reduced for the same air speed, three dimensional perturbations grew and the waves started to lose some of their sinusoidal character. This happened when part of the wave lagged behind the rest of the wave. Further reduction in m caused the formation of dry areas with a main streamer flowing in the middle of the channel. The streamer maintained the disturbed sinusoidal wave behavior.
- c) At high speeds (~ 30 m/s), the sinusoidal wave behavior was replaced by that of single ripples characterized by a limited spectrum of velocities. These ripples acquired much higher velocities (up to 30 cm/sec) and thinner crests (~ .4 mm) as compared to the sinusoidal waves (ripple speed ~ 4 cm/sec and ripple size ~ 1-2 mm). Some random three-dimensional perturbations were displayed and these developed into individual streamers when m was reduced (~ .03 mL/sec). The final stages reached by the ripples are those of single drops of glycerin flowing in individual rows while transferring their momentum upon collision with each other.

Participation in the DOE Workshop on
Analytical Simulation of MHD Chemical Equilibrium and
Transport Properties, 13-14 September, 1979

Introduction

Invitations to take part in an MHD Analytical Workshop were extended to 30 companies, universities and government agencies. The objectives included assessment of the capabilities within the MHD community for analytical prediction of plasma and transport properties under conditions of chemical equilibrium. Specifications for the "test problem" were drawn up by Dynatrend, and 17 participants to the Workshop submitted partial or complete solution sets, with many of the participants providing multiple solution sets to demonstrate the effect of various assumptions which could be made in meeting the specifications. Compilation of the results and assessment of the conclusions of the Workshop is being carried out by Dynatrend; the following sections deal solely with MIT's participation in this Workshop, but comparisons with some of the results submitted by Aerodyne Research, Inc. and by Westinghouse Electric Corporation are included.

M.I.T. has in the past made extensive use of the NASA Lewis Research Center codes for calculation of MHD plasma properties. However, much of the current experimental work at MIT is coupled into a DEC PDP 11/60 computer, and a great deal of "number-crunching" is also carried out on this machine in a time-sharing mode. Therefore a "stripped-down" version of the NASA code, based on programming effort carried out at Stanford, has been implemented on the PDP 11/60 as "EQUIPRP". This version occupies less than 32K 16 bit words, and is currently dimensioned for up to 8 elements and up to 31 gas phase species. A computer code data sheet is appended.

Unfortunately it has been necessary to discard some of the convenient features of the NASA Lewis Research Center code in order to fit the new program into the 32K available on the minicomputer. For instance, arbitrary addition or deletion of species is no longer a simple procedure; each selection of elements is tied in with a predetermined array of species, and the necessary solution matrix for such a case is stored as an input file. Addition of any new species requires alteration of this input file and the procedures are not automated. Species can be effectively deleted, however, merely by modifying the enthalpy curve fit parameters and thereby forcing the equilibrium concentration of a particular species to be infinitesimal. The most serious drawback is the present inability of the program to handle condensed phases. However, this has not limited the utility of the minicomputer version since relatively little of the current theoretical and experimental work at MIT has involved plasmas in which the slag constituents play a significant role.

The test problem specified the coal composition, the oxidizer stoichiometry, and the seeding details. It also specified the percentage slag rejection, without specifying whether any slag components should be allowed to enter the gas phase prior to slag rejection. Adequate attention to the latter question was beyond the manpower limits available at the time of MIT's participation in preparation for the workshop. Therefore the contract monitor approved a more restricted participation by MIT, wherein the minicomputer version would be used, and only gas phase constituents of the plasma would be considered. It was expected that this exercise would help to delineate the limitations of the usefulness of gas phase calculations when slag constituents are present. It was also hoped that the relatively simple gas phase model could help shed light on the causes of discrepancies between various solution sets for the test problem using the full NASA LeRC code.

Calculations for Workshop Test Problem

Three sets of runs were carried out to test the ability of the EQUIPRP program to predict the plasma properties for the Workshop cases prepared by Dynatrend. The first case, with elements C,H,O,N,K,S,Ar and Al, yielded unsatisfactory results since it was not possible to account for the condensed phase Al-species, and therefore impossible to restrict the mole-fractions of the Al-containing gaseous species. The presence of even 0.05% by weight of Al in the gas phase ensures that AlO_2^- is the dominant negative ion. Therefore these runs were not included in the Workshop package.

The second (designated Case A) uses the elements C,H,O,N,K,S,Ar and P, with thermodynamic data for PO_2 and the negative ions PO_2^- and PO_3^- being obtained from Aerodyne Research Inc. The relative elemental concentrations used are identical with those in the ARI Workshop package, so that species concentrations can be compared directly. The "missing" species, (Si, Fe, Al, Mg, Ca, Na, and Ti) contribute 0.8% of the total mass fraction. Their omission from the MIT runs has two major effects:

- a) whenever the ARI calculations show significant gas phase species containing Fe or Al, the presence of AlO_2^- and FeO_2^- is liable to reduce both the electron concentration and electrical conductivity,
- b) the oxygen tied up in the various compounds of the above elements is not negligible, and this causes a shift in the stoichiometry of the MIT results relative to those of ARI. For this reason a third set of runs has been made, with the relative concentration of the input O-element changed by 2.7%. This set (designated Case B) permits even more direct comparison with ARI results.

Values of electrical conductivity, mobility and collision frequency for the 9 pressure-temperature combinations of the test problem are given in Table 1 for Case A and Case B.

Species Considered in EQUIPRP

CO, CO₂, H₂O, H₂, H, OH, O₂, O, S, SO, SO₂, NO, NO₂, N₂, K, KO, KOH, P, PO, PO₂, Ar, K⁺, PO₂⁻, PO₃⁻, O⁻, OH⁻, NO₂⁻ and e⁻. Thermodynamic properties for PO₂, PO₂⁻ and PO₃⁻ were supplied by ARI. All other thermodynamic properties are from the JANAF data tape supplied by NASA LeRC (latest version received 2/6/79).

Cross-Sections Used in Conductivity Calculations

Cross-sections for Ar, N₂, NO, O₂, O, H₂, OH, H, CO, CO₂, SO₂, H₂O and K, KOH are taken from Ref. 5, and cross-sections for NO₂ and KO are set equal to those for NO and KOH respectively.

Note: Collision Frequency (Sec⁻¹) = $1.76 \times 10^{11} / (\text{Electron Mobility})$.

Sensitivity Analysis

Since the major uncertainties in the plasma properties for the test problem hinge on the magnitudes of the concentrations of PO₂⁻, PO₃⁻, AlO₂⁻ and FeO₂⁻, and since the latter two species are not considered in the MIT calculations there was little point in repeating the calculations with different electron affinities. The effect which is specifically attributable to PO₂⁻ and PO₃⁻ is shown in Table 2, obtained by reducing the input P level to 10% of nominal, and then to zero.

Comparisons with ARI and Westinghouse

The results of varying phosphorus content in Case B are of particular interest when they are compared with other workshop submissions which included Fe and Al species, but which contained different assumptions for the electron affinities of PO_2^- and PO_3^- . Such comparisons are shown in Table 3, using one each of the cases submitted by ARI and by Westinghouse.

At the highest temperature the MIT zero-phosphorus case shows higher σ and Ne (by 18% and 19%, respectively) than the Westinghouse case, which contains negligible contribution from PO_2^- . When P is included to match the ARI input, the MIT results again are somewhat high (15-18% above ARI), since the ARI results show AlO_2^- competing with PO_2^- as the dominant negative ion.

At the lowest temperature considered the discrepancies are much smaller; the MIT zero-P case is only 5-7% higher than Westinghouse, indicating that condensation of Al-species is inhibiting the role of AlO_2^- . The "nominal-P" case shows excellent agreement with ARI, since both calculations yield PO_2^- as the dominant negative ion, to an extent which severely depletes the electron concentration.

Conclusions

If phosphorus is present in the coal slag, and if the thermodynamic data on PO_2^- and PO_3^- proposed by Aerodyne are substantiated, then the minicomputer version which includes phosphorus is unlikely to differ by more than 10-15% at temperatures below 2700 K from results obtained with more sophisticated codes. When phosphorus is not present (or if PO_2^- and PO_3^- concentrations are negligible) then slightly larger discrepancies arise from omission of condensed species, but again these discrepancies are unlikely to exceed 20% unless T exceeds 2700 K.

The above brief discussion underlines one of the main conclusions of the Workshop, that there is a pressing need to design and carry out a definitive experiment to eliminate the present uncertainty in the effects of phosphorus on plasma properties.

Acknowledgement

The cooperation of C.E. Kolb and J. Wormhoudt is gratefully acknowledged.

MHD System/Component Computer Code Data Sheet

Date: August 28, 1979

1. Information Source - J.D. Teare, MIT 31-261 Cambridge, Mass. 02139
(617) 253-7067
2. Code/Name - EQUIPRP
3. Source Language - FORTRAN
4. Code Reference - Based on Stanford code, recent modifications not yet documented.
5. Core Storage Requirements - 32K 16-bit words.
6. Computer Configuration - DEC PDP 11/60
7. Code Analysis Description - Modified versions of Standford code, based on NASA LeRC CEC Conductivity calculation uses Frost's rule. Capable of running with electron temperature not equal to gas (heavy particle) temperature.
8. Input Data Description/Requirements - Choice of elements present restricted to certain pre-coded sets, such as C,H,O,N,K or C,H,O,N,K,S,Ar,P used in present problem. Input requires relative molar concentrations of elements. Thermodynamic and cross-section data used are from JANAF, ARI and SPENCER/PHELPS (Ref. 1)
9. Analysis Assumptions/Limitations - No condensed species present. Hence solution set is offered for comparison with output of other workshop contributors. For this reason, input was specifically matched to ARI cases.
10. Output Data Description - Thermodynamic variables, frozen thermal conductivity, specific heat, Prandtl number, sound speed, plus electrical conductivity mobility and molecular weight. Mole fractions, partial pressures and number densities of all species are also given.

Table 1 Summary of MIT Solution Sets for Workshop Test Problem

Case A					Case B (Reduced Oxygen Input)		
Patm	T °K	σ mho/m	μ T ⁻¹	ν sec ⁻¹	σ mho/m	μ T ⁻¹	ν sec ⁻¹
3.5	2700	8.23	.206	8.54x10 ¹¹	8.36	.206	8.54x10 ¹¹
	2600	4.62	.199	8.84x10 ¹¹	4.73	.199	8.84x10 ¹¹
	2500	2.32	.190	9.26x10 ¹¹	2.41	.190	9.26x10 ¹¹
2.0	2600	7.49	.348	5.06x10 ¹¹	7.61	.347	5.07x10 ¹¹
	2500	3.99	.333	5.29x10 ¹¹	4.10	.333	5.29x10 ¹¹
	2400	1.88	.318	5.53x10 ¹¹	1.96	.319	5.52x10 ¹¹
1.0	2400	3.67	.638	2.76x10 ¹¹	3.78	.638	2.76x10 ¹¹
	2300	1.62	.607	2.90x10 ¹¹	1.70	.608	2.89x10 ¹¹
	2200	0.619	.579	3.04x10 ¹¹	0.647	.580	3.03x10 ¹¹

Table 2
Effect of Reduced Levels of Phosphorus

p = 3.5 atm, T = 2600 K (Case B)

	Nominal Phosphorus	Phosphorus=0.1xNominal	Zero Phosphorus
N _e , x 10 ⁻²⁰ m ⁻³	1.49	1.05	1.90
Conductivity mho/m	4.73	5.95	6.13

Table 3

Comparison of Results from ARI, Westinghouse and MIT

Electron Concentration $\times 10^{-20}$, m^{-3}

p(atm)	T(K)	Aerodyne	Westinghouse	MIT calculations with phosphorus		
				Nominal P	0.1xNominal	Zero P
3.5	2700	2.197	2.44	2.528	2.865	2.911
3.5	2600	1.308	1.65	1.486	1.849	1.904
3.5	2500	0.725	1.08	0.791	1.142	1.209
2.0	2600	1.221	1.39	1.367	1.572	1.600
2.0	2500	0.695	0.912	0.767	0.984	1.019
2.0	2400	0.363	0.575	0.384	0.586	0.628
1.0	2400	0.344	0.461	0.369	0.482	0.500
1.0	2300	0.168	0.280	0.175	0.276	0.298
1.0	2200	0.071	0.162	0.072	0.146	0.171

Electrical Conductivity, mho/m

p(atm)	T(K)	Aerodyne	Westinghouse	MIT calculations with phosphorus		
				Nominal P	0.1xNominal	Zero P
3.5	2700	7.10	8.21	8.36	9.56	9.72
3.5	2600	4.10	5.29	4.73	5.95	6.13
3.5	2500	2.19	3.30	2.41	3.53	3.74
2.0	2600	6.62	7.91	7.61	8.83	9.00
2.0	2500	3.65	4.92	4.10	5.32	5.52
2.0	2400	1.83	2.95	1.96	3.04	3.26
1.0	2400	3.44	4.77	3.78	4.99	5.20
1.0	2300	1.62	2.75	1.70	2.73	2.96
1.0	2200	0.65	1.51	0.66	1.38	1.62

7. Development of Small Fiber Optics Instrument

The 2 x 4 fiber-optics/photodiode array described in the previous progress report has been initially tested in the MHD facility during this reporting period. The test was piggybacked onto another test in the facility. Useable signal levels of ~0.3V were obtained from the detector system with adequate separation of the eight channels. Minor mechanical problems with the firing of the optical fibers are being resolved, and it is expected that the array will be available for use in the forthcoming arcing investigation.

8. Design of Channel II

During the reporting period progress has been made on the over-all subatmospheric facility system definition and on the design, procurement, and installation of key components. A final decision on the layout of the flow train awaits the outcome of an investigation of the feasibility of using a surplus/GFE superconducting MHD magnet which has recently become available. The status of major components is reviewed individually below.

Combustor

The design has remained substantially identical to that reported in the last progress report, viz a 0.35 kg/s natural gas/preheated O₂ enriched air plug-flow unit having a design point residence time of 30 ms. It now appears feasible and desirable to integrate the electrical preheater unit with the combustor itself, and the detailed design is proceeding on this basis. This configuration minimizes the heat loss and simplifies the problem of electrical isolation from the MHD-induced voltages.

Exhaust System

An 8" steam ejector has been specified and ordered, and the necessary modifications to the existing MHD facility scrubber and exhaust train are in process. The condenser/heat exchanger and de-watering cyclone required upstream of the ejector are being designed in detail for local fabrication. The design goal remains the achievement of a 0.2-atm backpressure at the MHD channel exit at the design mass flow rate.

Control System

A design of needed improvements to the existing facility control system has been completed. A decision as to whether or not to proceed with implementation of these improvements awaits the resolution of budgetary issues in FY'80.

Magnet

Since budgetary constraints have precluded the transport and installation of the GFE 1.5 MW DC power supply which it was intended to transfer to this contract from a Westinghouse facility, it has been necessary to look for alternative approaches to procuring the magnet system for this facility. Two alternatives are being looked at:

- (a) Use the existing 1 MW DC power supply and control system, and design and procure a racetrack, copper-coil magnet with or without iron.
- (b) Use an available surplus GFE superconducting saddle-coil MHD magnet, designing and procuring the necessary dewar, power supply and cooling subsystems.

The relative merits of these options in terms of cost, time, experimental flexibility and capability, and instrumentation accessibility will be evaluated over the next few months. Since the SC magnet has assured capability to 3.9T, and the possibility to achieve its design field of 5T given sufficient training, its use is clearly desirable if it is financially possible.

Test Channel

Detailed design of the MHD channel proper must await a decision on the magnet to be used. Preliminary calculations do indicate that a high subsonic channel of up to 0.9m. length and designed for 0.25 kg/sec can be accomodated in the GFE superconducting magnet warm bore. Thus, no integration difficulties are foreseen if this is the route decided upon.

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Figure 1a. Voltage-current characteristics of the anode in condition number 100 of our previous run (Ref. 1). The lines connect the points in the order in which the data were taken.

Figure 1b. Voltage-current characteristics of the cathode in condition number 100 of our previous run (Ref. 1). The lines connect the points in the order in which the data were taken.

Figure 2. Electrode Configuration for the Second Experimental Series.

$$u + c \approx 1500 \text{ m/sec}$$

$$f \approx 9000 \text{ Hz}$$

$$\lambda \approx 15 \text{ cm}$$

Figure 3. Luminosity Fluctuations and Flow Speed Measurement (schematic).

Figure 4. Power spectrum (arbitrary units) of plasma luminosity.

Figure 5. Detail of the low frequency end of Figure 4.

Figure 6. Schematic of Proposed Inter-electrode Insulator Gap Configuration to Alleviate the Heating at the Regions of High Heat Flux.

Figure 7. Convection Coefficient vs. Length. Also shown is the assumed wall temperature distribution.

Figure 8. Heat Flux vs. Length.

Figure 9. Schematic of numerical solution technique for heat conduction in the coupled wall to be used in the breakdown experiments.

Figure 10. Schematic of Experimental Rig to Simulate Damage Caused by Inter-electrode Arcs (Torch is used to simulate temperature in wall components.)

Figure 11. Photographs of insulators taken after runs in the arc damage rig. The damage path is clearly observed.

Figure 12. Effect of Arc Current and Cooling on Damage Width.

Figure 13. Effect of Arc Current and Cooling on Récession Rate.

Figure 14. Longitudinal Section for One Channel with Velocity Measurement Tubes and Cooling Coil.

Figure 15a.

Figure 15b.

Figures 15a and 15b. Photographs of ripple structure observed in glycerin simulated slag flow rig.

$M \sim 0.6$
Inconel-Zirconia

Figure 16a. Slag flow photographs taken at AVCO Everett Research Laboratory. D.B. Stickler and R. DeSaro, "Replenishment Processes and Flow Train Interactions," presented at the 15th Symposium on Engineering Aspects of MHD, Philadelphia, Pennsylvania, May 1976.

Figure 16b. Slag flow photograph taken in the Soviet U-02 facility. Bright spots are arcs and dark spots are craters. D.K. Burenkov et. al, "Study of the Influence of a Slag Film in the Characteristics of Electrodes in the MHD Generator Channel," presented at the 4th US-USSR Colloquium on Magnetohydrodynamic Electric Power Generation, Washington, D.C., October, 1978.

Figure 17. General Behavior of Slag Flow.

Figure 18. Moderate Speed Range [in decreases from 1 to 4].

Figure 19. High Speed Range [in decreases from 1 to 4].

TASK 2, OPEN CYCLE DISK GENERATOR PROGRAM

The potential benefits of the disk generator with swirl (as an alternative to a linear generator) were discussed, and the earlier/previous results were reviewed in detail in Reference 1. Critical performance issues were defined, and the MIT disk program goals were outlined.¹ In particular, the effective plasma properties and generator performance (with and without swirl) as affected by (a) plasma nonuniformities, (b) electric stress limitations, (c) chemical nonequilibrium (in small-scale supersonic generators), (d) unsteady flow phenomena, (e) boundary layers (and inlet boundary layer separation) and slag, and (f) inviscid flow distortion are to be investigated. Theoretical modeling and the development of diagnostics are designed to support the experimental work; a detailed data base is to be developed which can be applied to the design and performance predictions of large-scale disk generators.

Work Accomplished

During this quarter, our major experimental effort has been directed primarily on wake nonuniformity effects in a radial flow generator; theoretical work has emphasized the electrodynamics in the disk r - z plane (i.e., insulator/conductor side wall-boundary layer interaction) and the development of a 1-D design code which includes chemical kinetics effects. Progress in other areas is reported (below) as well.

(a) Nonuniformities Studies in a Radial Flow Disk

Experiments are being conducted in a radial flow generator in order to quantify thermal and velocity wake nonuniformity effects on generator performance. The main goal is to establish experimental reduction formulae

for this type of nonuniformity, and assess the validity of the numerical 2-D wake models,^{1,2} and consequently assess the impact on linear and disk properties and performance.

The experiment is carried out in two phases. First, the reference or undisturbed flow is determined/characterized. This flow should be as free as possible from background nonuniformities, and yield Hall coefficients sufficiently high to simulate those obtained with equilibrium open-cycle combustion products (i.e., $3 \leq \beta \leq 7$). The factors which determine the choice of test gas include stability of the plasma with respect to ionizational nonuniformities (which can occur even in molecular gases), test time (which is a facility limitation) and degree of simulation of combustion gases. These factors were examined in Reference 1. It was concluded that for the experiments with moderate to high interaction (i.e. Saha equilibrium; negligible electron kinetics), Ar/CO₂ mixtures would be used initially. Later tests may include hydrogen addition. Nitrogen was ruled out as a buffer gas on the basis of shock tube boundary layer and bifurcation effects and relatively short test times.

The second phase of the experiment consists of creating well-defined wake nonuniformities, and assessing the results relative to the uniform reference case. Aerodynamic profiles (equally spaced) which emanate from the central stagnation region (see Figures 9 and 10) are used to create the wakes. The trailing edge is located at the sonic point in the generator. The configuration is discussed further below.

Experiments and Analysis of Reference Flow Tests

The "new channel" reported/described in Reference 1 was fabricated and tested this quarter for various Mach numbers and stagnation conditions; the

inlet Mach number was varied by varying the inlet area ratio (channel height/spacing). Figure 1 is a comparison of the new and old channels. For the new channel, the abrupt change in wall angle at $r = 8.8$ cm was eliminated to provide a more uniform flow (without a weak oblique shock) in the disk r - z plane. The inlet turning radius was increased to 1.85 cm, and the channel convergence (3.5° constant wall angle) is started at the sonic radius, $r^* = 7.7$ cm. An assembly drawing of the generator is shown in Figure 2, which illustrates the relative locations of the voltage probes, instrumentation ports (used for pressure and electron density measurements), and interferometer window.

Several tests were conducted for stagnation conditions in the range $2800 \leq T_0 \leq 2950$, $3.5 < p_0 < 6.5$ atm at $B = 3.5$ Tesla, for inlet Mach numbers between $1.25 < M < 1.40$; an initial (at room temperature) mixture of 80% Ar, 20% CO_2 was used. The final operating conditions for the reference flow (which will be used for the wake tests as well) were determined/selected from these data on the basis of the highest achievable measured effective Hall parameter, flow uniformity and constancy of fluid properties. Table I summarizes these conditions.

TABLE I--Summary of Reference Flow Test Conditions

Mixture of Gases (room temp.)	Ar 80%/CO ₂ 20%
Species Concentration at Stagnation Conditions (mole fraction)	Ar .80/CO ₂ .126/CO .071/O ₂ .035
Stagnation Temperature (K)	T ₀ = 2850
Stagnation Pressure (atm)	3.5 < p ₀ < 4.2
Minimum Area A* (cm ²)	78
Cesium Seed Fraction	.20% < SF < .30%
Mass Flow (kg/sec)	2.3
<u>Test Section</u>	
Mach Number <M>	1.40
Test Time (msec)	.7 - .8
<σ> (mho/m) @ B = 3.5 Tesla	25
<β> @ B = 3.5 Tesla	6.5

The reference flow results (for these conditions) are shown in Figures 3 - 8. The calculated profiles were obtained using the two-temperature 1-D model described in Reference 1. Molecular oxygen was included in the model this quarter, extending the number of heavy gas species to four. Although the model accounts for finite rate electron kinetics, the carrier gas composition is assumed to be frozen. The validity of this assumption, however, was verified with the chemical kinetics program/code; species concentrations did not change significantly (from their stagnation values) during the expansion.

The calculated electron density profile is shown in Figure 3; Saha equilibrium predominates throughout the generator since the level of Ne is high ($>10^{20} \text{ m}^{-3}$). Data for Ne have not as yet been fully analyzed (see section (d)). The conductivity and pressure, including the measured values, are indicated in Figures 4 and 5, respectively. The measured

effective and ideal Hall parameters are compared in Figures 6 and 7 for two magnetic field strengths. The agreement between the effective and ideal values suggests that the plasma is stable and uniform. The histograms in Figure 8 further support this conclusion; fluctuations in pressure, voltage and PM tube signals are minimal during the test time. The upper and lower solid curves (bounds) in Figure 6 for the calculated ideal Hall parameter reflect both the uncertainty (error bars) and run-to-run variations in the pressure measurements of Figure 5. That is, $\beta_{ideal} = \beta_{calc} (p_{calc}/p_{exp})$ where the subscript "calc" is the value obtained from the full 1-D model calculation. The energy averaged cross-section data of Spencer and Phelps³ were used. A particularly noteworthy result of these tests is that effective Hall coefficients as high as 7.5 were measured. This is the highest value ever obtained in a disk generator of this small scale.

Wake Experiments

Having established the reference flow conditions for the wake study, the next phase of the experiment was initiated: design and fabrication of the aerodynamic profiles/struts and first tests with wake nonuniformities. In a disk, wakes are created when inlet guide vanes are used to produce swirl (for example); in both linear and disk channels large-scale nonuniformities can also be produced as a result of incomplete mixing of seed and gas causing "streamers" or striations in the flow. Quantification of the effects of this type of nonuniformity will be an asset to the understanding of plasma properties and performance in both linear and disk channel configurations.

The basis for the strut design is discussed in detail in Reference 1; summarized briefly, the initial design was predicated on obtaining strong

conductivity wakes/deficits with a corresponding strong reduction in open circuit voltage (i.e. approximately 50%). Two programs were used to estimate this reduction: the available 2-D uncoupled wake code^{1,2} (although only strictly applicable for weak interaction) and the strut boundary layer program⁴ which includes finite-rate electron kinetics in the boundary layer. In order to obtain a strong wake effect, long struts emanating from the center of the stagnation region are required (by virtue of the fact that the wakes are narrow and the electrons are partially frozen in the boundary layer). Fifty flat-plate struts in the form of a "spider" were fabricated. Figure 9 is a cross-section drawing in the r-z plane which illustrates the location of a strut relative to the shock tube stagnation region, nozzle and generator. The blades are 0.30 mm thick (stainless steel) and are supported primarily in the downstream wall and center support sting. Photographs of strut assembly are shown in Figure 10. The trailing edge is located at the generator sonic point, $r^* = 7.7$ cm.

Two experiments were conducted with 25 blades at $B = 3.5$ Tesla (for the reference flow conditions given in Table I). The voltage profiles for these tests are shown in Figure 11; for comparison, the reference flow data are shown as well. Note that with 25 blades a voltage reduction of approximately 40% is obtained. This result is consistent with earlier predictions,¹ although further calculations for the actual experimental conditions (e.g. seed fraction) are necessary. Results for the effective Hall parameter reduction are shown in Figure 12. While in the reference flow case the average is 6.5, with 25 blades the Hall coefficient reduces to about 3.0.

These initial experimental results are encouraging insofar as they represent the first quantitative attempt to characterize nonuniformities of

this nature. It should be mentioned/recalled that the experiment was designed to produce a strong wake effect (as part of a study of basic phenomena in MHD generators in general); long, cold ($T_w = 300$ K) struts were used. Swirl guide vane wakes (characterized further below) for a similar scale experiment would most likely have less severe effects since the blades would be predominately in a region of high favorable pressure gradient and the boundary layer would remain laminar (which leads to a narrower initial wake and hence less rms deviation). The effect of blade heating/ temperature will be investigated as well as the effects of number of blades and variation of the ideal Hall parameter. Application of the results to commercial linear and disk channel performance will be assessed.

(b) Experiments with Inlet Swirl

The swirl flow disk experimental work consists of two parts: (i) determining the effect of swirl-plus-wakes on channel performance; and (ii) demonstrating high performance and efficiency with combustion gas mixtures. With respect to the latter part, a new swirl generator will be designed (for lower Mach number) using the recently developed 1-D chemical kinetics design code (as described in section (d), below). The work this quarter addresses the first phase in a study to characterize/quantify the swirl vane wake. With swirl, the wakes produced by guide vanes are nonsymmetric, since the flow on the suction side of the blade is overexpanded relative to the flow on the pressure side. In addition, the trailing edge of the vane is normally in a region of supersonic flow, thus introducing a recompression shock and expansion wave into the channel.

The first tests will be made in the existing MIT swirl generator^{5,6} (45° inlet swirl). Modifications were recently made to the generator in

order to provide a detailed assessment of the wake structure. Approximately eighty voltage probes were added (see Figure 13) in the region behind the trailing edge of two of the vanes. Both azimuthal and radial profiles can be measured. Additional viewports were provided (labelled x in the figure) to allow electron density measurements to be made in the vane passage and wake regions. The ports can also be used to locate small, closely spaced (~30 mils) voltage probes for further enhancement of wake resolution. Tests with this generator will begin upon completion of the first series of (radial flow) wake tests.

(c) Disk Generator Modeling

Theoretical modeling of the flow and interaction phenomena in disk channels is designed both to be supportive of the small-scale experimental program and to provide a basis for large-scale generator design and performance predictions. The work accomplished this quarter is summarized as follows.

Two Dimensional Modeling of Open-Cycle Disk Generators

The 2-D modeling effort for both small and large-scale disk generator design and performance predictions focussed on:

(i) Effects of wake nonuniformities on the open-circuit voltage and short-circuit current reductions

Additional calculations were made using the uncoupled 2-D wake model of Dvore, Martinez, and Shamma² with prescribed¹ velocity, Hall parameter and conductivity that account for variable wake growth and conductivity decay parameters. Although the code^{1,2} allows for σ , β , and u to vary with

angle θ (azimuthal direction), only conductivity wakes were considered in these initial calculations.

The results are summarized in Table II. The values of rms σ_1 (at the inlet) and rms σ_2 (at the exit) are normalized by $\langle\sigma\rangle$ in the table. $V'_{o.c.}$ and $I'_{s.c.}$ are the open-circuit voltage and short-circuit current of the undisturbed/uniform 1-D flow. The conductivity in the center of the wake and in the free-stream/undisturbed flow at the inlet and at the exit of the channel are denoted as SGWK, SGIN, and SGEXIT, respectively. The results indicate the effects of the number of blades, N , growth of wake width, and rms σ on the disk performance. Clearly the effects are stronger with increasing number of wakes and/or higher rms σ . For a constant conductivity ratio (which implies that the free-stream and wake centerline conductivity decay/decrease at the same rate) the effect on the open-circuit voltage is less for wakes with a slow growth rate. Relative to the open-circuit voltage, the wake effect on the short-circuit current is generally small.

The conductivity wake development in an axisymmetric flow with electron kinetics is not well understood/modeled in general. The simple model used here (and described in Reference 1) should (and will) be supported by detailed wake voltage measurements in the near future. Comparisons of the experiment (section (a)) and the 2-D wake model are currently underway and will be given in the next report.

(ii) Effects of boundary layer and conducting modules on the side walls of disk generators

Previously,¹ we described a model to study the boundary layer effects and the axial field limitation for breakdown on the side walls of disk generators. In the model, the disk walls are assumed to be made of

concentric metallic ring frames (modules) separated by ceramic insulators (Figure 14). The frames are electrically floating and draw no net current. The model consists of solving the coupled 2-D electrodynamics and the 2-D fluid dynamics in the meridional (r, z) plane.

We completed developing an iterative numerical code for the electro-dynamic part of the problem. Given the condition that no net normal current to the module exists (since it is electrically floating), special care was needed to determine the potential on the module as a part of the solution. The code has the feature of variable grid to adjust the refinement of the grid in places of sharp gradients, and it is designed to accept variable conductivity, Hall parameter, and velocity profiles in the radial and magnetic field directions (i.e. in the r and z directions).

We report here a sample calculation for the case of channels with constant height. The calculation domain consisted of one period (see Figure 14), and it is assumed that we have strong convection which implies constant flow properties in the flow/radial direction. Relatively strong conductivity, Hall parameter and velocity gradients, according to the 1/7th Law, in the magnetic field direction are prescribed. The results are presented in Table III and the conditions for these calculations are presented in Table IV.

These calculations indicate that:

- (1) The presence of conducting modules causes significant degradation of performance when the width of these modules, l , is greater than the width of the insulating gaps, g . The smaller the width of the conducting modules, the less degradation of performance relative to the ideal insulating wall case was found (as expected).

- (2) For a given module and gap geometry, the effect of boundary layer thickness for these wall temperatures is relatively small.
- (3) As the conducting module width increases, the effect of wall temperature becomes increasingly important.

TABLE II

Dependence of open circuit voltage and short circuit current reduction on number of blades, N , wake width, and rms σ for $B = 2.0T$; 80% Ar - 20% Co₂, $T_0 = 2500K$, $P_0 = 6.0$ atm, $\chi = .16\%$ Cs. Wake width at inlet = 1.272 mm. ($2.54 \leq \beta \leq 4.67$)

	N	EXIT WAKE WIDTH	INLET rms σ	EXIT rms σ	$\frac{V_{o.c.}}{V'_{o.c.}}$	$\frac{I_{s.c.}}{I'_{s.c.}}$
SGWK/SGIN = .2	50	3.716	.18	.22	.29	.90
	25	3.716	.13	.16	.42	.90
	15	3.716	.10	.12	.59	.95
	50	2.544	.18	.18	.34	.86
	25	2.544	.13	.13	.50	.93
	15	2.544	.10	.10	.68	.97
	50	1.272	.18	.13	.45	.91
	25	1.272	.13	.09	.65	.96
	15	1.272				
SGWK/SGIN = .1	50	3.716	.20	.22	.24	.79
	25	3.716	.14	.16	.36	.89
	15	3.716	.11	.12	.53	.94
	50	2.544	.20	.19	.28	.84
	25	2.544	.14	.13	.44	.92
	15	2.544				
	50	1.272	.20	.13	.38	.89
	25					
	15					
SGWK/SGIN = .1	50	3.716	.20	.20	.28	.82
	25	3.716	.14	.14	.42	.90
	15	3.716	.11	.10	.58	.95
	50	2.544	.20	.16	.34	.86
	25	2.544	.14	.11	.50	.93
	15	2.544				
	50	1.272	.20	.11	.45	.91
	25	1.272	.14	.08	.65	.96
	15	1.272	.11	.06	.73	.98

Table III

Open-circuit voltage for disk generators with boundary layers and conducting modules on the side walls. Conditions for the calculations are presented in Table IV.

Case 1. Boundary layer thickness = 5 cm		
l = width of conducting module g = width of insulating gap	T_W	$V_{o.c.}$
$l = 0, g = 5 \text{ cm}$	2500 2000	717 700
$l = 1 \text{ cm}, g = 4 \text{ cm}$	2500 2000	712 698
$l = 4 \text{ cm}, g = 1 \text{ cm}$	2500 2000	584 624
Case 2. Boundary layer thickness = 10 cm		
$l = 0, g = 5 \text{ cm}$	2500 2000	716 680
$l = 1 \text{ cm}, g = 4 \text{ cm}$	2500 2000	711 679
$l = 4 \text{ cm}, g = 1 \text{ cm}$	2500 2000	586 618

Table IV

Conditions and data for calculations presented in Table III.

core radial velocity	1300 m/s
core azimuthal velocity	0.0
core temperature	2500 K
static pressure	2 atm
magnetic field	5 Tesla
core conductivity	10.2 mho/m
core Hall parameter	2.2
channel height	.40 m
Inlet radius (beginning of the period)	1.20 m
Exit radius (end of the period)	1.25 m

One-Dimensional Flow with Chemical Nonequilibrium

During the last quarter, a design code for the disk generator incorporating nonequilibrium kinetics has been written and implemented on the MIT Energy Laboratory PDP-11/60 computer. The files for the performance code have also been transferred from the MIT Laboratory for Nuclear Science facility to the PDP-11/60 computer. Because it can be used interactively, the PDP-11/60 is excellent for debugging purposes and for incorporation of code modifications.

Both the performance and design codes have two versions. The performance code requires a description of the channel lofting; it may be run with the prescription of either channel height or the gradient of height as a function of the disk radius. In a similar manner, the design code may accept either the values of temperature or the gradients of temperature as a function of radius. Mutual compatibility of those codes has been established with several test runs by using the derived output of one code as input to the other. Under restrained time increment (10^{-7} sec per step) it has been established that the results from both codes agree to at least the third significant digit as regards both the electrical and gas dynamics variables.

The codes provide a one-dimensional description of the disk generator behavior, following the formulation of Louis⁷:

Radial Momentum:

$$\rho u_r \frac{du_r}{dr} + \frac{dp}{dr} = \frac{\rho u_\theta^2}{r} + j_\theta B - \frac{\rho u_r u_\theta f}{\eta} \quad (1)$$

Tangential Momentum:

$$\rho u_r \frac{du_\theta}{dr} = - \frac{\rho u_r u_\theta}{r} - j_r B - \frac{\rho u_\theta f}{\eta} \quad (2)$$

Conservation of Energy:

$$\rho u_r \left\{ \frac{dh}{dr} + u_r \frac{du_r}{dr} + u_\theta \frac{du_\theta}{dr} \right\} = j_r E + \frac{2}{\eta} \dot{Q} \quad (3)$$

where η is the channel height and the terms involving f and Q introduce the effects of wall friction and wall heat loss on the mean flow properties.

The electrical variables are given by the following relationships:

$$j_r = I_{\text{load}}/2\pi r\eta, \quad j_\theta = \beta j_r - \sigma u_r B$$

and $E = -(1 - k) (\beta + S) u_r B$, where

$k = j_r/j_{\text{rsc}}$ and the short circuit radial current density is given

by

$$j_{\text{rsc}} = \sigma (S + \beta) u_r B / (1 + \beta^2).$$

In the above expressions $S = u_\theta/u_r$ is the swirl ratio, B is the magnetic field intensity, and σ , β are the effective values of electrical conductivity and Hall parameter, respectively.

In the "design mode" Equations (1), (2) and (3) do not specify the derivatives of p , h , u_r and u_θ until a design constraint is applied in some manner, for example, by specifying dT/dr as a function of r . When the specification is completed in such a way, then the channel lofting is determined from mass continuity;

$$\text{i.e.} \quad \eta = m/2\pi r \rho u_r. \quad (4)$$

In the "performance mode" Eqn. (4) provides the necessary constraint when rewritten in the form

$$\frac{1}{\eta} \frac{d\eta}{dr} + \frac{1}{r} + \frac{1}{\rho} \frac{d\rho}{dr} + \frac{1}{u_r} \frac{du_r}{dr} = 0,$$

and the equation of state is used to express $\frac{d\rho}{dr}$ in terms of $\frac{dp}{dr}$ and $\frac{dT}{dr}$ or of $\frac{dp}{dr}$ and $\frac{dh}{dr}$.

The above methodology has been used extensively for equilibrium plasma disk calculations, usually with ρ , σ and $\mu = \beta/B$ all evaluated as functions of the state variables p and h .

Under chemical nonequilibrium conditions the major differences arise from the need to express

$$h = \sum_i X_i h_i \quad \text{and} \quad p = \rho R T z,$$

where $z = \sum_i X_i$, and X_i , h_i are the dimensionless concentration and specific enthalpy, respectively, of the i th species in the plasma. The chemical rate equations yield expressions for $\frac{dX_i}{dt}$, so that the overall enthalpy derivative can be expressed as

$$\frac{dh}{dt} = \sum_i h_i \frac{dX_i}{dt} + \frac{dT}{dt} \sum_i X_i \frac{dh_i}{dT} = \sum_i h_i \frac{dX_i}{dt} + C_p \frac{dT}{dt}.$$

Transforming the overall equations to make t the independent variable, with $\frac{d}{dt} = u_r \frac{d}{dr}$, we obtain the master equation*

$$\begin{aligned} \frac{1}{n} \frac{dn}{dt} + \frac{u_r}{r} - \frac{1}{z} \sum_i \frac{dX_i}{dt} - \frac{dT}{dt} \left(\frac{1}{T} + \frac{C_p}{u_r^2} - \frac{\rho C_p}{p} \right) + \frac{j_\theta B u_r}{p} \\ + \left[\frac{1}{\rho u_r^2} - \frac{1}{p} \right] [j_r (E + u_\theta B) - \rho \sum_i h_i \frac{dX_i}{dt}] + \frac{j_\theta B}{p} + \frac{v_\theta^2}{r v_r} = 0 \end{aligned}$$

This equation yields $\frac{dT}{dt}$ in the performance mode (when $\frac{dn}{dr} = \frac{1}{u_r} \frac{dn}{dt}$ is specified) or yields $\frac{dn}{dt}$ when the radial variation of temperature is specified for the design mode.

As previously reported,⁸ the chemical nonequilibrium codes use an implicit integration scheme to deal with the "stiff" equations which describe the time dependence of the species concentrations. The methodology for handling the chemistry is completely generalized, and the choice of species to be included and of reactions and reaction rate constants can

* Friction and wall heat loss terms have been omitted for clarity.

all be specified at run-time. Only one minor constraint is imposed; since the calculation of the plasma properties and electrodynamics requires knowledge of the electron concentration, the convention is adopted that the first member of the species array will always be electrons.

The electrical and gas dynamic variables are integrated in a straightforward, explicit manner using a fourth-order Runge-Kutta integration procedure, operating concurrently with the above implicit method.

An approximation has been introduced into the method of deriving electrical conductivity (σ) and mobility ($\mu = \beta/B$) in the plasma under conditions of chemical nonequilibrium. It is assumed that the gas composition will be sufficiently close to equilibrium to eliminate the need for recalculation of mobility; i.e., mobility is treated as a function of T and p only, derived in tabular form for the equilibrium plasma using EQUIPRP (see discussion under Task 1). Electrical conductivity, on the other hand, is derived from the tabulated EQUIPRP values in terms of the local electron density in the chemical nonequilibrium situation, i.e., $\sigma/\sigma_{EQ} = Ne/(Ne)_{EQ}$.

The validity of these approximations will be assessed as future work progresses; and, if necessary, the method will be replaced by the more conventional use of integrated cross-sections which are summed over the species present in the plasma.

Current work with the design-mode code is addressed to the design of a channel for high interaction experiments in the MIT disk facility. Both codes will also be used for further work on establishing effects of chemical nonequilibrium on scaling laws for large-scale disk generators.

(d) Diagnostics

During this reporting period, several spectroscopic measurements were made in order to assess the contribution/effects of molecular gases on the radiative recombination continuum for the cesium spectrum.

An optical multichannel analyzer, PARC-OMAI, was used to collect the data. As shown in Figure 15, the radiation from the plasma was transferred to the OMA via the fiber optic and relay lens. The data collected was captured in several of the hundred scans of the vidicon tube; the gate mode was not used/available for these tests. The spectral region covered was from 3100 Å to 7900 Å (although only a portion is shown in the figures discussed below) with a spectral resolution of approximately 5 Å. Two spectra are presented. Both were taken without a magnetic field as the OMA is sensitive to the high fields created in the MHD disk generator. The first spectrum presented was taken for Ar/CO₂ (test conditions of Table I) and Cs and is shown in Figure 16. The second was obtained for similar test conditions but for Ar/CO and Cs and is given in Figure 17. A cesium lamp spectrum is also given as a reference in Figure 18. Examination of these spectra indicates that there is an overall higher continuum level for the Ar/CO test as compared to the Ar/CO₂ test.

Qualitatively, it appears that, in the case of Ar/CO₂, the effect of "other" radiation interfering with the Cs continuum is minimal. However, this can only be verified with more detailed measurements; in the next reporting period an analysis of this and additional data will be presented and a comparison will be made with model calculations.

Work Forecast

In the coming months our efforts will be directed primarily towards:

Nonuniformity Studies

Wake experiments in a radial flow generator will continue. Emphasis will be placed on determining the reduction of open-circuit voltage as a function of the number of wakes for Hall coefficients up to 7.5; the effect of blade heating/temperature will be investigated as well. In addition, measurements of the local voltage distribution in the wakes and free stream will be made, as well as the pressure and electron density radial profiles. The results will be analyzed with the 2-D wake models.

Studies in a Swirl Generator

An assessment of the effects of wakes in a 45° swirl generator will begin. The generator and instrumentation for a quantitative experimental study which parallels/complements the radial flow nonuniformities study is ready for testing.

Disk Generator Modeling

The chemical kinetics 1-D design code will be used to (1) design a small-scale experimental channel for performance studies with molecular gases, and (2) establish scaling laws for chemical kinetics in the disk for application to commercial-scale MHD power plants.

With respect to the 2-D modeling effort:

- (a) Application of the electrodynamics code in the (r,z)-meridional plane, to channels with variable height and variable flow properties in the radial direction will be made. The model will

be extended to include the coupling with the fluid dynamics, and an assessment of the Hall field limitation will begin.

- (b) Modification of the present electrodynamics code in the (r, θ) -plane in order to handle narrower wakes and smaller number of blades will be made. This task requires developing an adjustable grid structure that is very fine inside the wakes and more coarse far away from the wakes.
- (c) The small perturbation analysis of wake nonuniformities with high interaction will continue.

Diagnostics

Application of the high-bandwidth A/D equipment to the characterization of plasma nonuniformities will continue. Signal processing codes will be tested as needed. Sensitivity amplification of the laser interferometer system will be examined in accordance with the technique described in Reference 1. In addition, spectroscopic studies will continue; of particular concern is the effect of radiation from CO and CO₂ molecules on the cesium spectrum (in the continuum region where Ne measurements are being made with PM tubes). The spectra obtained this quarter will be analyzed.

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(a) Previous channel (Reference [1])

(b) Reference Flow "New" channel.

Figure 1. Comparison of Reference Flow channel and the old channel configurations.

Figure 2. Drawing of the radial flow generator.

Figure 3. Calculated electron density in the disk for the uniform case. Electrons are in Saha equilibrium. Gas mixture at room temperature: Ar80%/CO₂20%; $T = 2850$ K, $p_0 = 3.5$ atm, SF = .2 5%, $\dot{m} = 2.3$ kg/sec, $A^* = 78$ cm², $B = 3.5$ Tesla.

Figure 4. Calculated conductivity in the disk for the uniform case. Gas mixture at room temperature: Ar80%/CO₂20%
 $T_o = 2850$ K, $p_o = 3.5$ atm, SF = .25%, $\dot{m} = 2.3$ kg/sec, $B = 3.5$ Tesla.

Figure 5. Calculated and measured static pressure in the disk. Gas mixture at room temperature: Ar80%/CO₂20%, $T_o = 2850$ K,
 $3.5 < p_o < 4.2$ atm, $.20\% < SF < .30\%$, $\dot{m} = 2.3$ kg/sec, $A^* = 78$ cm².
_{exp}

Figure 6. Measured effective Hall parameter in the disk. The upper and lower curves, with the error bars, represent the ideal Hall parameter by using the measured pressure. Gas mixture at room temperature: Ar80%/CO₂20%, $T_0 = 2850 \text{ K}$, $3.5 < p_0 < 4.2 \text{ atm}$, $.20\% < SF < .30\%$, $\dot{m} = 2.3 \text{ kg/sec}$, $A^* = 78 \text{ cm}^2$.

Figure 7. Comparison of the average measured effective Hall parameter with the ideal. Gas mixture at room temperature: Ar80%/CO₂20%, $T_o = 2850$ K, $3.5 < p_o < 4.2$ atm, $.20\% < SF < .30\%$, $\dot{m} = 2.3$ kg/sec, $A^* = 78$ cm²

(a) Pressure at $r = 11.1$ cm

(b) Voltage signal at $r = 8.0$ cm

(c) PM Tube signal at $r = 10.5$ cm

Figure 8. Typical static pressure, voltage, and PM-tube histories in the disk for the reference flow tests; τ = test time

Figure 9. Drawing in the r - z plane which illustrates blade/strut location relative to shock-tube, nozzle and generator.

Figure 10. Photographs of the blade/strut assembly; upstream plexiglas nozzle, 25 blades, downstream nozzle and generator wall.

Figure 11. Experimental voltage profile in the disk. (2 run average)
 ● V'_{oc} curve represents the uniform reference case
 ▲ V_{oc} curve represents the created nonuniform plasma by using 25 blades
 (.3 mm thickness) . Gas mixture at room temperature: Ar80%/CO₂20%,
 $T_0=2850$ K, $3.5 < p_0 < 4.2$ atm, $.20\% < SF < .30\%$, $\dot{m}=2.3$ kg/sec, $A^*=78$ cm² .

Figure 12. Comparison of the measured effective Hall parameter in the disk. The upper profiles represent the uniform reference case (fig. 9), the lower profile gives the effective Hall parameter for the created nonuniform plasma by using 25 blades (.3 mm thickness) Gas mixture at room temperature: Ar80%/CO₂20%, $T_0=2850$ K, $3.5 < p_0 < 4.2$ atm, $.20\% < SF < .30\%$, $\dot{m} = 2.3$ kg/sec, $A^* = 78$ cm².

Figure 13. Layout of the Swirl Generator - View from the Inside of the Generator on the Downstream Wall

Figure 14. Schematic of a disk generator with conducting ring modules on the side wall.

Figure 15. Test Setup

C= 0	X= 3203.028	14	328	
TIMING 1		SCAN MODE	1	
X0 0	CHNLS 500	DATA/TRK	500	COMP MODE 0
Y0 200	DELTY 150	TRACKS	1	US/CHNL 120
	DELAY 10DE-6	WIDTH 10DE-6	SINGLE? 1	MS/TRK 60.000
FULL SCALE 500000	CHNL 429			HEAD 1
PREP SCANS 15	SCANS 100 :			TIME 0:321
014: MHD DISK				

Figure 16. Cesium spectrum for Ar/CO₂ test (conditions of Table I).

C= 0	X= 3203.028	23	96	
TIMING 1		SCAN MODE	1	COMP MODE 0
X0 0	CHNLS 500	DATA/TRK	500	US/CHNL 120
Y0 200	DELTY 150	TRACKS	1	MS/TRK 60.000
DELAY 100E-6		WIDTH 100E-6	SINGLE? 1	
FULL SCALE 800000				
PREP SCANS 15		SCANS 100		TIME 131:405
023: MHD DISK				

Figure 17. Cesium spectrum for Ar/CO test ($T_0 = 2900$ K).

Figure 18. Cs Lamp Spectrum

TASK 3. ELECTRODE MODULE DEVELOPMENT AND TESTING

Part A. Insulator Materials

Magnesium oxide - Single crystal magnesium oxide was obtained from Norton Research Corp., Niagara Falls, Ontario, Canada. Specimens were obtained as flat plates approximately 1 cm square by 1.5 mm thick. This material was prepared by melting high-purity magnesium oxide in an electric arc furnace and then slow-cooling the melt.

Dielectric breakdown specimens were prepared by diamond grinding to about .35 mm thickness. For this thickness, it was not possible to induce breakdown at room temperature with the test apparatus; thus, indicating a dielectric breakdown strength in excess of 950 kilovolts/cm.

Silicon nitride - Hot pressed silicon nitride (Noralide NC-132) was obtained from Norton Co., Worcester, MA. The material was obtained as a flat plate 15 cm square by 7 mm thick. Specimens were prepared by diamond sawing and grinding to produce pieces approximately 1 cm square by .75 mm thick. This material was prepared by hot pressing silicon nitride with a small amount of magnesium oxide added as an aid to densification.

Dielectric breakdown specimens were prepared by diamond grinding to about .25 mm thickness. Room temperature dielectric breakdown strength varied from about 300 kv/cm to about 850 kv/cm, although the variation within individual specimens was much less. More specimens will be tested to ascertain the cause of this variation.

Materials and Specimen Preparation*

Aluminum oxide - plasma sprayed specimens of aluminum oxide were prepared at the MHD Electrode Module Fabrication Facility from

* Dielectric breakdown data for these materials was presented in the previous report.

aluminum oxide powder (PP33) obtained from Bay State Abrasives, West-boro, MA. The powder was 99.5% pure and was prepared specifically for plasma spraying. The material was plasma sprayed at the "standard" conditions of 700 amperes current and 40% feed rate. The material was sprayed onto stainless steel "buttons," 1.27 cm diameter by 1.27 mm thickness, to a thickness of about .65 mm; then the material was separated from the substrate and the resulting disks were tested.

Magnesium aluminate - plasma sprayed specimens of magnesium aluminate were prepared at the MHD Electrode Module Fabrication Facility from magnesium aluminate powder (XP1134) obtained from Metco, Westbury, L.I., N.Y., This powder was prepared specifically for plasma spraying. The material was plasma sprayed at "standard" conditions onto stainless steel "buttons," 1.27 cm diameter by 1.27 mm thickness, to a thickness of about .63 mm. The material was separated from the "buttons" and the resulting disks were tested for dielectric breakdown.

Sintered magnesium aluminate was obtained from Trans-Tech, Gaithersburg, MD. Specimens were obtained as flat plates 2.5 cm by 11.25 cm by 1.27 mm thick. Specimens for dielectric breakdown measurements were prepared by diamond sawing and grinding to produce pieces approximately 1.25 cm square by about .5 to 1.27 mm thick.

Magnesium oxide - Sintered magnesium oxide was obtained from Trans-Tech, Gaithersburg, MD. Specimens were obtained as flat plates 2.5 cm by 11.25 cm by 1.4 mm thick. Specimens for dielectric breakdown measurements were prepared by diamond sawing and grinding to produce pieces approximately 1.25 cm square by about .3 to .75 mm thick.

Strontium zirconate - Plasma sprayed specimens of strontium zirconate were prepared at the MHD Electrode Module Fabrication Facility from strontium zirconate powder (118) obtained from Transelco, Penn Yan, NY.

As received, the average particle size of the powder was too small for efficient plasma spraying. This material was spray dried at the MHD Fabrication Facility to produce a larger average particle size which would be suitable for plasma spraying. The spray dried material was plasma sprayed at "standard" conditions onto stainless steel "buttons," 1.27 cm diameter by 1.27 mm thickness, to a thickness of about .63 mm. The material was separated from the "buttons" and the resulting disks were tested for dielectric breakdown.

Sintered strontium zirconate specimens were prepared at the MHD Electrode Module Fabrication Facility from the same material as used for the plasma sprayed specimens. The powder was pressed into disks 1.27 cm diameter by various thicknesses of the order of .5 mm, and then sintered at 1600-1650°C for two hours. This procedure yielded specimens ranging in thickness from .3 to .6 mm. These specimens were subsequently tested for dielectric breakdown.

ELECTRODE TESTING

During the current quarter two additional tests were made in the MHD Simulation Facility. The results of these tests, as well as analysis of test performed in the previous quarter, are reported here. We have continued to test electrodes of the super hot-wall type and of compositions in the $\text{SrZrO}_3 \cdot \text{LaFeO}_{3-\delta} \cdot \text{SrFeO}_3$ ternary system. They were tested with surface temperature greater than 1800°C and for durations of up to 23 hours at $1\frac{1}{2}\text{ A/cm}^2$. The purpose of the tests were to evaluate the effects of testing durations five to ten times longer than previous tests and to evaluate effects of high current densities on electro-chemical corrosion and general durability of the electrodes.

Test 274:

Results of test 274 were reported last quarter but as the test was performed near the end of the quarter no analysis was included in that report. As a review, the electrodes were single-layered and of composition SZSFLF-3($75\%\text{SrZrO}_3 \cdot 25\%\text{La}_{.75}\text{Sr}_{.25}\text{FeO}_3$) and were plasma sprayed into a 0.80cm wide grooved stainless-steel base. The duration of the test was 17 hours and 35 minutes with $1/2\text{ A/cm}^2$ for 15 hours and 15 minutes.

Photo micrographs of the post-test cross sections of a typical cathode and anode are shown in Figures III-1a and III-1b respectively. Electrodes, in general, did not undergo severe deterioration during the test. The surface of the cathode is shown to be irregular as was evident from the irregularity in the surface temperature profile during the test and internal cracking is observed.

Intrusion of small pieces of the electrode into the plasma appeared to have caused some small amount of melting and transfer of material to the

surface of neighboring electrodes. Clear evidence of this was visually observed during the test and extra material appears in some cross sections.

The anode surfaces were not so irregular as the cathode but the entire anode of Figure III-1b was expanded out beyond its original thickness into the plasma. Subsurface cracking accounts for most of this expansion. The formation of potassium rich phases does not appear to have occurred since microprobe analysis indicates very little ($<1\%$) K in the solid matrix, although larger amounts were found in the pores of both the cathode and anode. The composition of neither the cathode nor anode had changed appreciable at any location within the electrode during the test. The small pores had, however, consolidated into large pores of sizes between 10 and 50 μm .

Tests 276, 277, 278

Results of this series of tests were also reported in the previous semi-annual report, and analysis of results are presented here. The electrodes were three layered plasma-sprayed electrodes on the grooved stainless steel base (described in the discussion of Test 274). The layers were a 1mm thick LASF-5 ($\text{La}_{0.9}\text{Sr}_{0.1}\text{FeO}_3$) inner layer, a 0.75mm middle layer of 1 part LASF-5 to 2 parts SZSFLF-3, and a 0.75mm SZSFLF-3 outer layer. A current density of 1 A/cm^2 was applied for 11 hours and 53 minutes of the total test duration of 13 hours and 15 minutes. The average surface temperature was near 1800°C .

The layered structure allowed us to apply a higher current than the single layer SZSFLF-3 electrodes of 274, but the consequence of layer structure was less mechanical strength. The outer layers on most of the electrodes was delaminated and lost during the test. Pieces of the outer layers of electrodes on the anode side were lost even before the application of current. These electrodes had been fabricated separately from electrodes used for cathodes and so the delamination was probably fabrication related. Most of the remainder of the electrodes' outer-layers were lost during the first hour of applied current, and may have been in some way current related

failures. Damage was also incurred during two accidental shutdowns during a latter portion of the test.

Figures III-2a and III-2b are photographs of the center section of a cathode and anode placed midway up the stack. Neither of these two electrodes lost their entire outer layers during the test. The large horizontal crack midway through the cathode is between the LASF-5 layer and the mixed middle layer. It appeared that electrodes failed at this interface. The mixed layer maintained discrete phases of LASF-5 and SZSFLF-3 near the colder edge but homogenized into a single phase at the hotter edge. The interface of this layer with the outer SZSFLF-3 was not discernible.

The electrodes which had lost most of their outer layers functioned surprisingly well during the remainder of the test. Nevertheless since damage was mostly layer related, single layered-electrodes or improved layering will be necessary. The next two tests used a single layered electrode of increased electrical conductivity. Electrodes plasma-sprayed with a continuous compositional variation are in the planning stage.

Tests 282, 283, 284

Electrodes tested were of the composition SZSFLF-6 ($50\%ZrSrO_3 \cdot 50\%La_{.75}Sr_{.25}FeO_3$). A discussion of properties of SZSFLF-6 was contained in the previous quarterly but briefly its melting temperature is $2300^\circ C$ and conductivity is constant over a wide range of temperatures. The affect of P_{O_2} on conductivity has not been measured. Electrodes were single layered and plasma-sprayed on the stainless steel bases of the same design as the previous two tests. The total duration of the test was 25 hours and 48 minutes. Of that time 22 hours and 39 minutes were at a current density of $1\frac{1}{2} A/cm^2$. The test was performed over a three day period with the facility shut down over night. A heat gun was directed at the electrodes during the shutdown to minimize damage due to water reaction with the potassium.

The general appearance of the electrodes was very good during the entire test. Some small amounts of surface damage progressively worsened during the

three day test. Near the very beginning of the test some roughening at the most-upstream and downstream electrodes was observed and so they were subsequently maintained at 1 A/cm^2 rather than $1 \frac{1}{2} \text{ a/cm}^2$ but nevertheless exhibited the most damage during the test. A slightly roughened appearance of the surface of the cathodes developed in the first few hours of the test but electrodes did not further deteriorate during the entire first day. The most marked change in appearance of the electrode surfaces was at the beginning of the second and third day. Some small portions of the most upstream electrode detached during each of these two start-ups and the general appearance of other electrodes was less uniform at the beginning of each day, than at the end of the previous day. The cause may have been thermal shock or creep related damage but likely was related to hydration of potassium in the pores.

Anodes exhibited no observable deterioration during the entire first day. The surface was very smooth and uniform in appearance for this period. Some deterioration was noted, as with the cathode, at the beginning of the second and third day. The basis for the difference in deterioration between cathode and anode may be electrochemical in nature or possibly related to surface electron emissivity at the cathode. The former affect will be discussed below and the extent of the latter is unknown at this time. An increase in surface temperature should completely eliminate the problem if it is electron emission related.

Post-test cross sections of a typical cathode and anode are shown in Figure III-3a and III-3b. The main feature of deterioration are the cracks both parallel and perpendicular to the surface. These appear to be no worse in the cathode than the anode though the surface of the anode is flatter. Microprobe examination of the cathode and anode revealed another strong difference between the two. The composition of the cathode was uniformly the same throughout

the electrode but this was not true of the anode. A large amount of potassium rich second phase was present throughout the region between the largest horizontal crack and the stainless steel base. In order to check whether this was generally the case a second anode was examined and the same thing was observed. This type of phenomenon was not previously observed in other tests and is not expected for the anode. One observation which may explain the result is that there is an abnormally large gap at the stainless steel ceramic interface in these particular electrodes. If potassium were to fill the gap then the electrical potential would drive the potassium into the subsurface porous region of the electrodes. Once there it could react rapidly with the electrode.

The results of this test is very encouraging. Providing our judgement that most damage was incurred during the shutdown periods is correct, durability at constant operation would be very good. Operation for many times this length of time would be expected.

Test 285

Single layered electrodes of composition SZSFLF-6 performed so well that a identical test was performed except that a current density of 3 A/cm^2 was applied. The total duration of the test was 8 hours and 56 minutes. The total time over which 3 A/cm^2 was applied was 7 hours and 32 minutes. The current was step-wise increased in increments of $1/2 \text{ A/cm}^2$ in the usual manner. In this test the most upstream electrode did not carry a current and the second upstream and the most downstream electrode carried only 1 A/cm^2 . Also there were seven rather than the usual six electrodes in the stack. These precautions were taken because it was usually observed that the upstream electrodes exhibited the most deterioration and often lost material which deposited on downstream electrodes.

Electrodes behaved generally well during the test but deterioration proceeded more rapidly than Tests 282, 283, and 284. Cathodes again

developed a non-uniform, roughed surface and exhibited some streaking from protrusion melting early in the test while the anodes remained smooth. At 2 hours and 45 minutes into the test, however, a large piece of the third most upstream anode suddenly melted and spread over the anode stack. The power was temporarily shut down but was started soon after and the voltage returned to its normal level. The test proceeded normally until 15 minutes before shut down when the same event occurred again but with a more up-stream anode. The power was shut off and the test discontinued after this second event.

Arcing was not exhibited at the cathode or anode surface even at 3 A/cm^2 . There was some interelectrode arcing between the second and third upstream most electrode when the second electrode was at 1 A/cm^2 , but disappeared in a short time.

The extent of electrode deterioration may be seen in the post-test cross section of Figure III-4a and III-4b. A comparison Fig III-3a and III-4a shows that deterioration of cathodes at 3 A/cm^2 is more extensive than the deterioration for cathodes at $1 \frac{1}{2} \text{ a/cm}^2$. Extensive melting at the anode surface is observed in Figure III-4b and in cross sections of other anodes. No clue was found as to the cause of this sudden melting. For instance, microprobe analysis revealed no compositional changes, ie. no high potassium subsurface second phase formed as in the previous test. Future tests at high current densities will determine whether this anode failure is a general phenomenon or whether it was caused merely by a chance detachment of a large electrode piece.

The results of this test is also encouraging since we have shown that local high current densities which may be encountered in a MHD channel can be handled for at least a short period of time. Furthermore, improvement in the properties of these electrodes may allow long term constant operation at 3 A/cm^2 .

Electrochemical and Mechanical Deterioration of Electrodes

To monitor electrochemical changes or mechanical deterioration during the test it is useful to examine the current-voltage characteristics. The previous progress report contained several figures describing run conditions and the current-voltage characteristics for Run 274 which are repeated in Figures III-5 through III-9. Fig. III-5, III-6 and III-7 provide a record of the test conditions for the first 16 hours of Run 274. The missing links in the traces were caused by computer hardware problems subsequently repaired by the manufacturer. The air flow trace (crosses) shows the periodic cycling of the supply air compressor, and the small dips occurring approximately every 25 minutes in the fuel flow trace (circles) reveal the momentary pressurization of the fuel supply twin tank. The large drop in the oxygen flow and the corresponding increase in the air flow at approximately 20:00:00 hours indicates the on-line refilling of the liquid oxygen supply tank. The instantaneous weight of the seed supply tank (exes) depicts the seed usage during the test. The seed weight has been scaled by a factor of 0.001 to allow plotting in the same graph with the other burner inputs. Note the refilling periods.

The voltage and current of electrode pair No. 4 are depicted in Fig. III-8 and III-9. The voltage rose in the first few hours of the test, and then the rate of the rise diminished. Since voltage is measured across both electrodes and plasma, changes in the voltage may either reflect a change in the plasma resistance or in the electrode resistances. Figs. III-5 through III-7 indicate that run conditions, are rather constant and by comparing these figures with Figs. III-8 and III-9 it can be seen that changes in the run conditions, as for instance at 12:37 hours, change the voltage very little. Thus resistance changes are likely in the electrodes.

In the other three tests no change in the voltage occurred during the test. Since these electrodes being tested, however, were a lower electrical

resistance design, changes in electrode resistance may not have shown up.

Figure III-10 is the V vs I curve for the four tests. The points on the curves were taken in the early portion of the test when the current density was increased step-wise. Table III-1 contains estimated electrodes resistances, total resistances from Fig. III-10 and calculated core resistivities. The electrode resistances were calculated from resistivities measured on dense samples at 0.2 atm P_{O_2} and from electrode thickness and conducting areas. The estimates may be off in magnitude due to porosity, uncertainty in electrode conducting area, electro-chemical effects, etc. but the relative values should be about correct. The calculated core resistivity was taken from a computer program developed at NASA's Lewis Research Center and modified at M.I.T. to provide values of electrical conductivity and transport properties. Core resistivities should be in about the same ratio to each other as total plasma resistances since boundary layer resistances are affected by run conditions in a similar manner to the core.

Test Number	Table III-1		Calculated Plasma Core Resistivity
	Calculated Electrode Resistance	Measured Total Resistance	
274	$\sim .83 \mu \Omega$	10.6-18 μ	0.043 μm
277	~ 0.25	5.26	0.045
282	~ 0.05	6.67	.053
285	~ 0.05	5.62	.048

Table III-1 shows that total resistances in tests 277, 282 and 285 are in about the same ratios as the core resistivities, but Test 274 stands out as an anomaly. It is concluded that only in test 274 are the electrode resistances sufficiently large to contribute significantly to the total resistance. Thus by subtracting out the plasma resistance ($\sim 5 \mu$) the electrode resistance is calculated to be 5.6 μ to 13 μ . Thus electrode resistances are considerably underestimated.

Also from these results the boundary layer voltage, $\Delta V = \Delta V_{\text{anode}} + \Delta V_{\text{cathode}}$ may be calculated. The calculations are not included here but

considering Joule heating of the plasma it is estimated ΔV increases linearly from 0 to 36 volts as the current is increased to $> 1 \text{ A/cm}^2$, then remains constant at approximately 36 volts.

The increase in resistance of the electrodes during Test 274 may have resulted either from physical damage of electrodes or from an electrical or electrochemical effect. Unfortunately there is no definite evidence supporting either of these mechanisms but indications are that it is a combination of the two.

Heat flux results measured during the tests were examined to determine whether physical damage to the electrodes including cracks, etc. reduced the heat flux in the same way it increased the resistance. The data indicated that heat flux did not vary during the tests except for Test 274 where the heat flux increased by approximately the amount expected for Joule heating. Unfortunately there was sufficient scatter in the data that mechanical damage was difficult to detect.

Cross sections of both cathodes and anodes in Test 274 were examined by microprobe analysis for evidence of electrochemical decomposition. No products of decomposition such as free iron were found in the cathode. There was some question as to whether small precipitates of iron might reoxidize in the few minutes between the time the current was shut-off and the time the electrodes were cooled at the end of the test. Nowhere, however, was Fe contents as high as FeO. Furthermore at the anode no detectable oxide layer formed at the stainless steel interface.

An estimate was made of the expected decomposition thickness. The rate at which the decomposed layer grows is given by the equation: ⁽¹⁾

$$(1) \quad J_{Ox} = \frac{i_{ion}}{F} = \frac{RT \sigma_{ion}}{4F^2 L} \ln \frac{P_{O_2}(0)}{P_{O_2}(L)} + \frac{i_{el} \sigma_{ion}}{\sigma_{el} F}$$

Where J_{Ox} is in equivalents of $O^{-2}/\text{cm}^2 \text{ sec}$ and represents either oxidation of the iron base or decomposition of electrodes.

T is the absolute temperature (assumed Constant)

F is Faraday's Constant

L is the electrode thickness

i_{el} is the electronic current

σ is the conductivity (assumed to be constant)

t_{ion} is the ionic transference number

R is the gas constant

The two terms on the right of Eq. (1) are of opposite sign and approach each other in magnitude as equilibrium is approached. Considering only the second term, the Faraday's law term, and estimating that $t_{ion} = 10^{-3}$ the calculated thickness of the decomposed layer after 20 hours would be 0.3 mm.

Since microprobe and microscopic analysis of the post-test cross section did not reveal any metallic iron, nor any change in the phase composition, it is possible that cracks and open porosity allowed the plasma PO_2 to be established throughout the cross section. There are several possible ways that the mechanical damage may be related to electrochemical degradation. For example, during the test 285 portions of the anodes detached and melted. Oxygen partial pressure internally in the anode, resulting from local high oxygen transport could be sufficiently high to exceed the mechanical strength of the material and failure would result. In the cathode small cracks may form where electrochemically there was a low PO_2 . This would account for the progressive damage at the cathode. Also this combination of factors may have contributed both to a resistivity rise in Test 274 and mechanical damage.

A final observation is that electrodes of SZSFLF-6 degraded less rapidly than those of SZSFLF-3, which has a lower conductivity. The implication is that the degradation rate is dependent on the electrode materials' conductivity, since these materials should be similar in their other properties. It is possible to speculate as to the origin of the degradation by considering that the electrochemical degradation would be related to the iR product, whereas ohmic heating degradation would depend on i^2R . Three different tests may be compared by using Table III-1. They are listed in the order of severity of electrode degradation.

TABLE III-1.

	<u>iR</u>	<u>I²R</u>
Test 285	(3)(0.05) = 0.15	(9)(0.05) = 0.45
Test 274	(0.5)(0.83) = 0.42	(0.25)(0.83) = 0.21
Tests 282, 283, 284	(1.5)(0.05) = 0.075	(2.25)(0.05) = 0.112

The order of decreasing i^2R values would indicate degradation is related to ohmic heating rather than to the electrochemistry. A more sophisticated analysis, which would account for the affect of resistivity on P_{O_2} and the affect of non-uniformities in electrodes must be applied to expect a realistic method of matching current densities to materials properties.

Reference

1. J. Misusaki, W. R. Cannon, and H. K. Bowen, "Electrochemical Degradation of Ceramic Electrodes," submitted to the J. Am. Ceram. Soc.

Figure III-1(a) Cathode from Test 274, Fourth from upstream

Figure III-1(b) Anode from Test 274, Third upstream in stack.

Figure III-2(a) Cathode from Tests 276, 277, and 278, fourth upstream in stack.

Figure III-2(b) Anode from Tests 276, 277, and 278, fourth upstream in stack.

Figure III-3(a) Cathode from Tests 282, 283, and 284, third upstream in stack.

Figure III-3(b) Anode from Tests 282, 283, and 284, third upstream in stack.

Figure III-4(a) Cathode from Test 285, fourth from upstream.

Figure III-4(b) Anode from Test 285, fifth from upstream.

Figure III-5 Test Conditions-Run No. 274

Figure III-6. Run Conditions-Test 274, continued

Figure III-7. Run Conditions-Test 274, continued

Figure III-8. Voltage and Current for number 4 up-stream pair-Run 274

Figure III-9. Voltage and Current for number 4 up-stream electrode pair-Run 274, continued.

Figure III-10. Voltage-Current density relationship in the initial portion of the tests indicated in the figure. The previous three figures show an increasing voltage with time at $1/2 \text{ A/cm}^2$ for Test 274. This is indicated by the arrow.

Part B.

The MHD Test Facility Complex

The MHD Small Scale Simulation Facility, designed exclusively for electrode development testing and used extensively for other MHD-related tests as well, was also used in the reporting period for a series of tests for the U.S. Air Force on Film Cooling applicable to gas turbine components.

Facility Development

Infrastructure

The recently installed city water pump of higher capacity than what was in service before has considerably improved the cooling of the burner modules. The higher draw of this pump limits the water supply to other test facilities in the laboratory, a condition that will be corrected by MIT with the installation of an additional six-inch diameter feeder from the city's water main.

Facility Components

Residual potassium carbonate not completely removed by the high energy impactor scrubber accumulated in the blower and drained out between tests. On long endurance tests this accumulation caused the blower to progressively lose efficiency until it was finally necessary to shut down the experiment. This condition was corrected with the installation of a water spray just upstream of the blower impeller and continuous drain at the bottom of the impeller housing.

The resistance thermometry wiring inside the test chamber was further protected from convective and radiative heating for a longer life cycle.

A versatile wiring diagram which will permit utilization of the forthcoming ten DC rectifiers in a variety of configurations for different ranges of currents and voltages was designed.

Instrumentation

Electrode and Plasma Temperatures

The recommendation from the Safety Officer to use remote methods to measure the electrode and plasma temperatures is receiving priority attention. In this vein, a commercially available Fiber Optic Thermal Monitoring device was tested under typical burner operating conditions. A bifurcated fiber bundle is being considered for application on the electrode temperature measurements, for which the radiation intensity at two different wave lengths would be needed by one of the methods under evaluation.

Data Acquisition

Test data from burner input and electrode electrical parameters was acquired and stored using the PDP 11/60 computer in the Energy Laboratory Data Acquisition Center. The computer was used extensively during the tests to provide the operator with burner performance and electrode-control feedback; periodic printed output provided the operator with on-line reporting of burner performance, and a CRT display supplied information on electrode electrical performance and individual voltage-current characteristics. Real-time graphic output supplied information on such time-varying phenomena as electrode-plasma resistance, and a more detailed graphical view of experimental conditions was produced for post-test analysis.

Facility Operations

Testing during the reporting period was of three different categories: for Electrode Development; for the Development of a Plasma Temperature Probe; and for Correlation of Film Cooling Parameters. A list of all tests performed appears in Table F-1 indicating representative test parameters.

Electrode Development Testing

Electrode development tests for extended test times were continued during the reporting period with excellent results. Test runs numbers 282/4 and 285 for 25.5 hours and 11 hours respectively are reported in detail in Part A of this Task. Test 282/4 was performed with an applied current density of 1.5 amps/cm^2 and test 285 was performed at 3 amps/cm^2 . This is the highest current density applied to any of our electrodes.

Plasma Temperature

A number of tests were performed in the selection of components for a plasma temperature probe under development which will be used in conjunction with the December 1979 tests of the U-25 MHD channel in Moscow.

Film Cooling

A series of tests were performed for the U.S. Air Force on the application of film cooling under high temperature gas, to validate performance parameters derived from short duration testing in a pebble bed heated blow-down test apparatus.

Diffused and Arcing Current Transfer

The modular test section constructed and tested during the previous reporting period has been refurbished, modified and installed again in the Facility for another series of tests. Detailed plans for the projected test series are reported under Task 1 in this report.

TABLE F-1

ELECTRODE DEVELOPMENT AND ELECTRO-FLUID MECHANICS TESTS
IN MHD SIMULATION FACILITY.

Run Sequence No.	Electrode Stack Nos.	Date	Total Durtn. (h)	Seed Durtn. (h)	Current Durtn. (h)	$\dot{m}$ Total (kg/s)	N_2/O_2	ϕ_{O_2}	Seed (%K)	Slag (kg/s)	Current Density (A/cm ²) max	T_o (K)	P_o (atm)	Mach No.	Q_{hot} (W/cm ²)	Q_{cold} (W/cm ²)	σ (mho/m)	Remarks
279		6/28	.35			.170	.864	.890				2634	1.103	.652				Temp. Probe
280		7/2	.35			.177	0	1.076				2999	1.063	.627				Temp. Probe
281	255-256	7/3	.08			.149	1.125	.527				1961	1.001	.505				Thermal Integrity
282-3-4	255A-256C	7/10- 12-16	25.5	23.69	23.49	.248	.356	1.022	.977		1.5	2896	1.134	.694	100.3	187.2	22.52	Endurance
285	259A-260C	7/19	10.93	8.42	8.37	.258	.399	.960	1.117		3	2864	1.155	.717	112.3	217.9	23.76	Endurance, High J
286		7/25	.73	.33		.229	.500	1.034	.49			2818	1.119	.678			14.69	Temp. Probe
287		7/26	.57			.199	1.020	.979				2632	1.080	.632				USAF Film Cooling
288		7/26	1.03			.247	1.779	.629				1988	1.178	.735				USAF Film Cooling
289		7/26	.02			.247	1.779	.629				1988	1.178	.735				USAF Film Cooling
290		8/3	1.03			.273	1.878	.536				1572	1.102	.622				USAF Film Cooling
291		8/15	2.13			.263	1.813	.511				1218	1.071	.324				USAF Film Cooling
292		8/17	1.45			.287	1.023	.501				1750	1.137	.435				USAF Film Cooling

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TASK 4, COAL COMBUSTION STUDIES

TASK 4a, KINETIC MODELLING OF 2-STAGE COMBUSTOR

Introduction

There are two parts to this section of the report. The first part presents experimental and modeling results for single particle temperature-time histories during combustion. The second part presents modeling results from a simulation study of fuel-rich, high temperature char combustion.

DETERMINATION OF TEMPERATURE AND BURNING TIMES FOR SINGLE COAL PARTICLES

Particle Temperature

An important input to the development and validation of a model of coal particle combustion is the knowledge of particle temperatures during burnout. To this end, the method of two-color optical pyrometry has been used to determine the temperatures of single pulverized coal particles burning in a range of argon/oxygen and helium/oxygen mixtures. This measurement technique utilizes the known variation of radiant energy emission as a function of wavelength and temperature as its basis of operation.

A Simple Particle Burning Model

A simple diffusion-controlled particle combustion model has been developed for comparison with experiment. The basic assumptions in this model are:

- i) Volatiles are instantaneously released and burned. The residual char is modeled as a shrinking, burning carbon sphere with a density of the char residue.
- ii) Pseudo steady-state heat and mass transfer are rapidly attained.
- iii) The combustion rate is mass transfer limited.
- iv) The primary reaction $2C + O_2 \rightarrow 2CO$ occurs on the surface of the particle.

- v) The oxidation of CO to CO₂ occurs far enough away from the particle surface that it has little or no influence on particle temperature.
- vi) The two modes of heat transfer are conduction and radiation; convection is negligible.
- vii) The emissivity of the particle is unity.
- viii) The effects of oxygen dissociation in the boundary layer are negligible.
- ix) Ash does not influence the combustion rate.

A steady-state energy balance about a burning particle gives:

$$-K \frac{dT}{dr} = \frac{R \cdot (-\Delta H_{rxn})_T - Q}{4\pi r^2}$$

where k is the gas thermal conductivity, $(-\Delta H_{rxn})$ is the heat of reaction at temperature T , R is the reaction rate in gram-moles O₂/sec., and Q is the radiative heat loss term.

$$Q = 4\pi r_p^2 \sigma (T_p^4 - T_w^4)$$

For a diffusion-controlled model, R equals the rate at which O₂ arrives at the particle surface. From assumption (ii) we know that

$$-4\pi r^2 N_{O_2} = \text{constant} = R$$

where N_{O_2} is the radial flux of oxygen.

Since the primary reaction is the formation of carbon monoxide, the flux of CO will be twice that of O₂ in the opposite direction:

$$-2 N_{O_2} = N_{CO}$$

Fick's Law states that

$$N_{O_2} = -c D \frac{dX_{O_2}}{dr} + X_{O_2} (N_{O_2} + N_{CO})$$

Combining the last three equations:

$$\frac{dX_{O_2}}{1 + X_{O_2}} = \frac{R}{4\pi c D} \frac{dr}{r^2}$$

This equation is now solved in conjunction with the energy balance to yield a particle temperature and reaction rate. Values for the thermal conductivity, k , and diffusivity, d , are taken to be those of the ambient oxygen/diluent mixture at the appropriate temperature.

Experimental Apparatus and Procedure

Single particles are entrained into a carrier gas stream using a combined vibrating feeder/dilution chamber system. The carrier gas and suspended particle are then injected axially into the laminar flow furnace shown schematically in Figure 1. The temperature of the furnace can be varied between 1000°K and 1800°K. The main combustion gas to the furnace comprises oxygen (10 to 100%) in either argon, helium, or nitrogen

The axial feeder tube doubles as the optical access light emitted from the incandescent burning particle is collected at the top of this tube and conveyed out of the system by a fibre optic. The fibre optic is bifurcated and conducted to the photomultiplier detectors (EMI-Gencom Model 9824 B) whose spectral response regions are defined by interference filters at 450 ± 2 nm and 550 ± 2 nm, respectively. The narrow solid angle defined by the feeder tube precludes radiation from the hot furnace walls reaching the detectors and the normal background signal is negligibly low.

Figure 1. Laminar Flow Furnace

The signals from the photomultipliers are recorded simultaneously on a dual beam oscilloscope and the display photographed for subsequent analysis. A typical oscillograph is shown in Figure 2. As the particle is ignited and heats up, the emitted intensities rise. All the while, however, the particle is moving away from the injector so that the intensities soon peak and begin decreasing. The signal disappears when the particle is consumed so that we also obtain an accurate measure of the total burnout time of the individual particles.

An important part of the measurements is the calibration of the overall optical system. The temperature is calculated as a function of the ratio of the intensities at the analysis wavelengths. Therefore, only a relative sensitivity calibration is required; this is obtained by viewing a tungsten strip lamp of known temperature (and emissivity) without changing the optical system.

Results

Table I summarizes the experimental conditions investigated. So far we have concentrated on the effects of oxygen concentration and inert diluent (Ar or He). However, we also have preliminary data to show the effects of furnace gas temperature and particle size as well as the differences arising in changing from coal to char feedstock. Average burnout times and particle temperature histories obtained in the various runs are summarized in Table II. Detailed results are presented graphically in the Appendix for Single Particle Burnout Histories (see page 147).

Figure 2. Traces from a particle burning in an oxygen-rich environment.

TABLE I.

Summary of Experiments

<u>Run</u>	<u>% O₂</u>	<u>Inert</u>	<u>Temperature (K)</u>	<u>Particle</u>	<u>Particle Diameter (μm)</u>
B1	100%	--	1753 K	Coal	90-105μm
B2	50	He	1753	Coal	90-105
B3	35	He	1753	Coal	90-105
B4	20	He	1753	Coal	90-105
E1	100	--	1791	Coal	75-90
E2	75	He	1791	Coal	75-90
E3	50	He	1791	Coal	75-90
E4	40	He	1791	Coal	75-90
E5	30	He	1791	Coal	75-90
F1	75	Ar	1791	Coal	75-90
F2	50	Ar	1791	Coal	75-90
F3	40	Ar	1791	Coal	75-90
F4	30	Ar	1791	Coal	75-90
F5	20	Ar	1791	Coal	75-90
F6	10	Ar	1791	Coal	75-90
G1	100	--	1536	Coal	75-90
G2	50	Ar	1536	Coal	75-90
G3	30	Ar	1536	Coal	75-90
J1	100	--	1536	Char	75-90
J2	100	--	1536	Coal	75-90
K1	100	--	1536	Coal	90-105
K2	100	--	1536	Coal	45-53

TABLE I. Averages of Temperatures for Five Dimensionless Time Intervals

Run	Average Burnout Time	Dimensionless Time Interval				
		0-0.20	0.20-0.40	0.40-0.60	0.60-0.80	0.80-1.00
B1	--	3313 $\pm$ 346	3450 $\pm$ 250	3245 $\pm$ 276	3090 $\pm$ 272	--
B2	--	2580 $\pm$ 234	2720 $\pm$ 215	2703 $\pm$ 137	2742 $\pm$ 168	2654 $\pm$ 146
B3	--	2285 $\pm$ 191	2411 $\pm$ 220	2427 $\pm$ 124	2469 $\pm$ 175	2466 $\pm$ 163
B4	--	2038 $\pm$ 144	2138 $\pm$ 154	2143 $\pm$ 133	2195 $\pm$ 263	--
E1	9.6 $\pm$ 3.3	3170 $\pm$ 158	3316 $\pm$ 140	3155 $\pm$ 139	3177 $\pm$ 250	--
E2	13.0 $\pm$ 3.3	2745 $\pm$ 213	3023 $\pm$ 228	2905 $\pm$ 244	2845 $\pm$ 245	2728 $\pm$ 500
E3	13.5 $\pm$ 3.5	2470 $\pm$ 176	2667 $\pm$ 141	2846 $\pm$ 197	2795 $\pm$ 288	2932 $\pm$ 316
E4	15.9 $\pm$ 4.2	2491 $\pm$ 279	2541 $\pm$ 162	2566 $\pm$ 191	2611 $\pm$ 159	2742 $\pm$ 367
E5	24.6 $\pm$ 7.4	2271 $\pm$ 165	2390 $\pm$ 210	2345 $\pm$ 208	2350 $\pm$ 245	2516 $\pm$ 224
F1	15.8 $\pm$ 3.9	2940 $\pm$ 366	3363 $\pm$ 174	3225 $\pm$ 135	3113 $\pm$ 111	--
F2	19.5 $\pm$ 5.4	2718 $\pm$ 272	3000 $\pm$ 175	2966 $\pm$ 152	2925 $\pm$ 180	2912 $\pm$ 99
F3	24.5 $\pm$ 5.8	2704 $\pm$ 190	2932 $\pm$ 103	2947 $\pm$ 127	2880 $\pm$ 120	2844 $\pm$ 217
F4	34.9 $\pm$ 8.2	2632 $\pm$ 193	2741 $\pm$ 136	2828 $\pm$ 149	2786 $\pm$ 189	2709 $\pm$ 251
F5	50.0 $\pm$ 12.0	2285 $\pm$ 144	2422 $\pm$ 139	2479 $\pm$ 119	2497 $\pm$ 127	--
F6	136 $\pm$ 34	2146 $\pm$ 126	2182 $\pm$ 106	2255 $\pm$ 150	2344 $\pm$ 108	--
G1	12.5 $\pm$ 3.4	3183 $\pm$ 256	3365 $\pm$ 298	3207 $\pm$ 217	3175 $\pm$ 204	--
G2	20.4 $\pm$ 5.3	2862 $\pm$ 227	3070 $\pm$ 204	2945 $\pm$ 180	2763 $\pm$ 216	--
G3	33.7 $\pm$ 7.9	2624 $\pm$ 160	2688 $\pm$ 174	2709 $\pm$ 167	2759 $\pm$ 179	2700 $\pm$ 300
J1	10.4 $\pm$ 4.4	3907 $\pm$ 354	3941 $\pm$ 360	3675 $\pm$ 345	3606 $\pm$ 384	3540 $\pm$ 414*
J2	8.3 $\pm$ 3.2	3417 $\pm$ 531	3812 $\pm$ 419	3485 $\pm$ 481	3255 $\pm$ 334	--
K1	10.7 $\pm$ 5.6	3548 $\pm$ 427	4014 $\pm$ 318	3782 $\pm$ 365	3542 $\pm$ 320	--
K2	5.3 $\pm$ 1.7	3421 $\pm$ 309	3580 $\pm$ 216	3477 $\pm$ 263	3238 $\pm$ 278	2909 $\pm$ 105

* Originally 3835 $\pm$ 680 before point T = 4719 K was removed.

i) Burnout Times

Average burnout times for about 100 particles at each condition as a function of oxygen partial pressure are shown in Figure 3 for argon and helium inert gases. As expected, the burnout time decreases from high values at low oxygen concentrations to a minimum in pure oxygen. The furnace temperature has no appreciable effect on the results. However, changing from argon to helium reduces the burning lifetime 10 - 20%.

In Figure 4, the burnout times in argon are compared with those predicted on the basis of the single diffusion-controlled combustion mechanism described above. At high oxygen concentrations there appears to be reasonable agreement between predictions and measurement. However, the model underpredicts the burnout times by increasing amounts at lower oxygen concentrations, until for the 10% oxygen mixture the discrepancy exceeds a factor of two.

ii) Temperature

The variation of temperature during burnout in a number of argon/oxygen mixtures is shown in Figure 5. A dimensionless time scale (fraction of total burning time) is used to account for differences in burning times between runs, and for individual particles within a run. For comparison, the model predictions are also shown and it is apparent that, particularly at higher O_2 concentrations, the model is not capable of predicting even qualitatively the temperature trends during burnout.

When average mean particle temperatures are compared with those predicted, it is seen for Ar/ O_2 mixtures in Figure 6 that the model does qualitatively predict the observed trends. The agreement appears best at low partial pressures of O_2 but this may not be realistic since model and experiment must converge at the furnace temperature at zero oxygen concentration (no combustion).

Figure 3.
Comparison of Burnout Times

Figure 4.
Burnout Times vs. O_2 Partial Pressure
in an O_2 -Ar System

Figure 5.
A Comparison of Experimentally
Determined Temperature Profiles
with Model Predictions

Figure 6.
Average Temperatures vs. O_2 Partial
Pressure in an Ar- O_2 System

For helium as the diluent, temperatures are observed to be somewhat lower than the argon. Precisely the opposite is predicted by the model (Figure 7). Furthermore, the model predicts higher temperatures in 50% Ar/50% He mixtures than in 100% oxygen and this also is not observed experimentally. Clearly, the simple model is not able to handle realistically the complexities of the transport properties of a mixture containing He.

iii) Particle Size

Preliminary tests of the influence of particle size on burning temperature are summarized in Table II (E and K series). Larger particles burn hotter, and, of course, longer than smaller particles under the same conditions. The model prediction of a " d^2 " burning law is not borne out by experiment. Comparison of burnout times in runs K_1 , E_1 and K_2 leads to a ratio of 2:1.8:1 as opposed to the predicted ratio of 4:2.8:1 respectively.

If the lignite coal feed is replaced by a char made from the same coal, observed temperatures and burning behavior change remarkably. The char burns slower than the parent coal, but, as shown in Figure 8, considerably hotter at the same time.

Discussion

Coal particles burn hotter and faster in a more oxygen-rich environment. This is consistent with improved transfer of oxygen to the particle when the ambient concentration is increased and is semi-quantitatively predicted by the simple model.

When helium is substituted for argon as the inert diluent, the particles burn faster and cooler at all oxygen partial pressures. This seemingly paradoxical result can be ascribed qualitatively to the influence of He in improving heat transfer being greater than the increases in mass transfer rates in this gas. The linear mixing laws used in estimating

Figure 7.
Average Temperatures vs. O_2 Partial
Pressure in a He- O_2 System

Figure 8.
Char vs. Coal in 100% O₂
(J Series)

average transport coefficients in our preliminary model are obviously inadequate to describe these phenomena and the model predictions poorly resemble the experimental results.

These observations point the way to the development of a physically more realistic model of carbon particle combustion. Such a model, which is currently being developed, will include:

- multicomponent transport effects (diffusivities and thermal conductivities)
- a full treatment of reactions in the boundary layer to include CO oxidation and its concomitant heat release.
- the formation of dissociation products, such as O-atoms, which may be significant at the high temperatures being observed.

This more advanced model can be expected to reproduce more accurately some of the trends encountered experimentally.

The reasons for the failure of the " d^2 " burning law predicted by the model are probably two-fold -- firstly, the problems associated with the model, as described above, and secondly, the existence of a particle size distribution in the coal feedstock. Therefore, we will compliment our development of a new model with measurements of burning times, and temperatures, using coal particles having a well-characterized size distribution.

Conclusions and Directions of Future Work

The measurements of particle temperature and burning lifetime provide a means of validating a combustion model. The current model is inadequate to predict coal particle burning histories. Its major weakness seems to be its neglect of multicomponent diffusion and thermal conductivity coefficients. Therefore, we are currently engaged in developing a new model to take account of these effects. Furthermore, the new model will

allow for finite heterogeneous reaction rates and homogeneous reactions in the boundary layer.

Further experimental work is required to characterize accurately the effects of particle size, coal char versus coal feedstock, and coal types. The apparatus will also be redesigned to allow reliable measurements to be made at the lower oxygen partial pressures also relevant to practical systems.

APPENDIX FOR SINGLE PARTICLE BURNOUT HISTORIES

(See Table I for run conditions.)

SIMULATION OF FUEL-RICH HIGH TEMPERATURE COAL (AND CHAR) COMBUSTION

Model Description

A computer model was developed to simulate the combustion of coal or char for a range of particle sizes, temperatures and pressures. Five reactions were considered:

These reactions were taken as first order processes based on the surface partial pressure of the reactant. Spherical particle geometry and a fixed set of pore characteristics were used, and external diffusion, internal pore diffusion, and reaction on the internal surfaces were taken into account.

At the high temperatures of interest in MHD combustion systems, the homogeneous gas phase reactions are much faster than the rate of the char gasification reactions considered here. It is assumed that the gas phase is at equilibrium as a first order approximation to the real behavior. The equilibrium assumption is not completely valid, as evidenced for example by non-equilibrium amounts of OH and other species in combustion gases^[11,12], but serves as a basis for calculation.

Equilibrium calculations were presented in a previous report.^[19] The mixture existing in the gas phase at any point in time during the

combustion process is characterized by an effective fuel/air equivalence ratio. This is the basis for using the equilibrium calculations, and allow the steady state model given earlier to be applied to any instantaneous gas composition surrounding the particle, which changes with the extent of burnout in an actual combustor. The gas compositions studied here are fuel-rich, and correspond to those existing in the later stages of char burnout in combustors operating at fuel-rich stoichiometry (for the coal/air feed). These conditions are encountered in the first stage of 2-stage combustor systems for magnetohydrodynamic power generation. The same 2-stage concept is also being considered for the possible reduction of pollutant emissions in the fuel-rich first stage in conventional combustors operating at lower temperatures than MHD combustors.

Kinetics

The symbol notation used in the following development is explained on page 195. The reaction rate based on the film resistance in the gas phase is (Appendix A):

$$-\frac{1}{S_{EX}} \frac{dN_A}{dt} = \frac{K_A}{RT_{BL}} (p_{Ag} - p_{AS}) \quad (1)$$

The reaction rate can also be expressed in terms of reaction on the internal particle surface and on the outer particle surface as:^[1]

$$-\frac{1}{V_p} \frac{dN_A}{dt} = k_A \xi_A f_{IN} C_{As} + k_A f_{EX} C_{AS} \quad (2)$$

Using the relation $p_{AS} = RT_p C_{AS}$ and eliminating the surface concentration between the two rate expressions gives:

$$-\frac{1}{S_{EX}} \frac{dN_A}{dt} = \frac{C_{Ag}}{\left(\frac{T_{BL}}{T_g}\right) \frac{1}{K_A} + \left(\frac{T_p}{T_g}\right) \frac{S_{EX}/V_p}{k_A (\xi_A f_{IN} + f_{EX})}} \quad (3)$$

The rate calculated on this basis assumes that the particle is isothermal, as justified by Field et.al.[3]

The effectiveness factor for a spherical particle is^[4]

$$\xi_A = \frac{3}{\phi_A} \left[\frac{1}{\tanh \phi_A} - \frac{1}{\phi_A} \right] \quad (4)$$

where the Thiele modulus is given by

$$\phi_A = \left(\frac{r_p^2 k_A}{D_{A,EFF}} \right)^{1/2} \quad (5)$$

The effective diffusivity is given by^[5]

$$\frac{1}{D_{A,EFF}} = \frac{\tau}{\theta} \left[\frac{1}{D_{A,KN}} + \frac{1}{D_{A,M}} \right] \quad (6)$$

The Knudsen diffusivity is given by

$$D_{A,KN} = 9700 \bar{r}_{pore} (T_p/M_A)^{1/2} \text{ cm}^2/\text{sec} \quad (7)$$

with T_p in $^{\circ}\text{K}$. The molecular diffusivity in the pores is calculated by the following mixture equation, assuming concentrations equal to the gas phase concentrations for each species:

$$D_{A,M} = \frac{(1 - Y_A)}{\sum_{j \neq A} \frac{Y_j}{D_{Aj}}} \quad (8)$$

$$\text{where } D_{Aj} = \frac{0.001858 (T_p)^{3/2}}{P \sigma_{Aj}^2 \Omega_D} \left[\frac{M_A + M_j}{M_A M_j} \right]^{1/2} \quad (9)$$

The parameters in the above equations are calculated at the particle temperature, except as indicated.

The particle is assumed to be isothermal, and its temperature is determined from the known gas temperature and the following energy balance:

$$\sum [R_i (-\Delta H_{rx,i})] = h(T_p - T_g) + (1 - \epsilon_g)\sigma (T_p^4 - T_w^4) + \epsilon_g\sigma (T_p^4 - T_g^4) \quad (10)$$

ALL

REACTANTS

The concept of controlling resistances is discussed in Appendix H, where criteria are given to determine the rate-controlling step for each reaction.

Parameter Assignment

The calculation of the heat transfer coefficient is discussed in Appendix B. The calculation of the heat of reaction for the five reactions is described in Appendix D.

The intrinsic kinetics used for this study are presented in Appendix E. The physical properties of the pore structure of a typical char are given in Appendix F.

The energy transfer in an MHD combustor is modeled according to the energy balance given in Equation (10). The emissivity of the gas phase, ϵ_g , was taken as 0.3,^[18] and the wall temperature was specified as follows:

$$T_w = T_g \quad (T_g \leq 2000^\circ\text{K}) \quad (11)$$

$$T_w = 2000^\circ\text{K} \quad (2000^\circ\text{K} \leq T_g \leq 3000^\circ\text{K}) \quad (12)$$

The latter condition was based on the need in MHD combustors to avoid vaporizing the mineral species present in the slag which forms in the combustor.

The major variables at our disposal include the gas temperature, the total pressure, the particle size, and the fuel/air equivalence ratio. The ranges of these variables covered in this study are:

$$\begin{aligned}
 1500^{\circ}\text{K} &\leq T_g \leq 3000^{\circ}\text{K} \\
 1 \text{ atm} &\leq P_{\text{TOT}} \leq 5 \text{ atm} \\
 10 \text{ } \mu\text{m} &\leq dp \leq 150 \text{ } \mu\text{m} \\
 1.0 &\leq \phi \leq 4.0
 \end{aligned}$$

The gaseous species considered in the equilibrium calculations are shown below:

CO ₂	Ar	CO	C ₂ H ₂	HCN	NH	S
H ₂ O	C	COS	C ₂ H ₄	H ₂	NH ₃	SO
O ₂	CH	CS	C ₂ H ₆	H ₂ O ₂	NO	SO ₂
O	CH ₄	CS ₂	C ₂ N ₂	H ₂ S	N ₂	S ₂
OH	CN	C ₂	H	N	N ₂ O	

Assumptions

- Spherical particle.
- Gas Phase at equilibrium.
- Gas is fuel-rich mixture of coal and air, specified by an effective fuel/air equivalence ratio.
- External diffusion properties calculated at average of gas and particle temperatures.
- Intrinsic reactions are first order kinetics processes.
- Pore structure properties assumed to be those of a raw char sample.

- Pore structure does not change and is well characterized by a single average pore size and surface per unit weight for cylindrical pores.
- Particle is isothermal throughout.
- Steady state conditions exist.
- Transport properties are calculated by mixture relations using concentrations of each species in bulk gas, both for properties inside pores and in external diffusion film.
- Assumed parameters for energy balance included $\epsilon_g = 0.3$ and specification of the wall temperature.
- Convective heat transfer coefficient described by Nusselt number of 2; mass transfer coefficient for each species described by Sherwood number of 2.

Calculation Procedure

The gas temperature, total pressure, particle size, and bulk gas phase mole fractions of the 36 gas species are input parameters to a computer program. The program then sets the values of constants to be used later in the calculations. An initial estimate of the particle temperature is taken as equal to the gas temperature.

Next, the internal physical properties and rate coefficient are computed, allowing the internal effectiveness factor to be calculated. The external mass transfer coefficient is then obtained, allowing a rate to be calculated for a particular species. When this has been done for all five reacting species, the program then calculates heats of reaction and a heat transfer coefficient, and the results are used in the energy balance. The particle temperature is taken as the unknown in the energy balance, and the initial or prior estimate of T_p is used to find the root of the fourth order polynomial in T_p , by Newton's method. The solution of the equation for T_p allows a comparison to be made between the initial or prior value of T_p and the new value. These will differ because the rates in the energy

balance, as well as the heat transfer coefficient, which are taken as constant when solving for the new value of T_p , are actually functions of the particle temperature.

When the new value of T_p agrees with the estimate from the previous iteration, the results are printed. These consist of the values of T_p , the total rate of reaction, the fraction of total rate due to each reactant, the controlling resistances for each reactant, and then a listing of the transport and reaction parameters for each reactant species. The results of a sample run are shown on the next three pages.

Presentation and Discussion of Results

In the graphical results presented below, the results for $\phi > 2.4$ are excluded because of the appearance of solid carbon as an equilibrium product and the consequent lowering of the oxidant concentrations. Also, results for $\phi < 1.1$ are excluded because of the large shifts in the equilibrium values of the oxidant concentrations near stoichiometric mixture conditions, and the resultant masking of some of the important trends indicated below.

The total reaction rate due to all five species is shown in Figure 9 for $P = 1$ atm, for single spherical particles of 10, 50 and 150 μm at equivalence ratios of 1.1 and 2.4. The total rate is seen to increase with gas temperature. The rate is higher for the larger particle sizes. The total rate is also higher for a given particle size at a lower effective fuel/air equivalence ratio in the gas phase. This latter effect is shown more clearly in Figures 10 and 11, which show the information from Figure 9 in an expanded scale for particle sizes of 10 μm (Figure 10) and 150 μm (Figure 11), and which show the entire range of equivalence ratios.

SAMPLE RESULTS

SUMMARY OF INPUT DATA

GAS TEMPERATURE	3000.0 K
TOTAL PRESSURE	1.0 ATM
MEAN PORE RADIUS	1.8E-06 CM
DENSITY	1.96 G/CC
INTERNAL AREA DENSITY	1.650E 06 CM*CM/G
TORTUOSITY	1.4142
POROSITY	0.7450
EQUIVALENCE RATIO	2.4000

GAS PHASE MOLE FRACTIONS

I	SPECIES	MOLE FRACTION
1	CO2	1.8900518E-03
2	H2O	4.8021317E-03
3	O2	3.5710979E-06
4	O	2.1270583E-04
5	OH	7.3962028E-04
6	AR	5.8051592E-03
7	C	3.6851010E-09
8	CH	6.2281708E-10
9	CH4	5.5721528E-11
10	CN	1.9120524E-07
11	CO	3.2760898E-01
12	COS	8.0702213E-06
13	CS	2.6810735E-06
14	CS2	7.9942192E-09
15	C2	1.1520315E-13
16	C2H2	3.8771063E-11
17	C2H4	6.7291845E-16
18	C2H6	4.4061208E-21
19	C2N2	1.8220499E-12
20	C3H8	0.0000000E 00
21	CH3OH	0.0000000E 00
22	H	5.3341463E-02
23	HCN	3.2360887E-06
24	H2	1.1550310E-01
25	H2O2	1.6990466E-10
26	H2S	6.6431822E-05
27	N	9.6492648E-06
28	NH	7.1331956E-07
29	NH3	1.8990520E-07
30	NO	1.6120442E-04
31	N2	4.8811338E-01
32	N2O	6.4501769E-09
33	S	1.4700403E-03
34	SO	2.1890600E-04
35	SO2	6.6461822E-06
36	S2	3.1780871E-05

RESULTS FOR GIVEN PARTICLE SIZE

PARTICLE DIAMETER	1.50E-02	CM
GAS TEMPERATURE	3000.0	K
CHAR TEMPERATURE	2654.8	K
B.L. TEMPERATURE	2827.4	K
WALL TEMPERATURE	2000.0	K
THERMAL CONDUCTIVITY AT TB	4.187E-04	CAL/(CM*SEC*K)
HEAT TRANS COEFF	5.583E-02	CAL/(CM*CM*SEC*K)

TOTAL RATES OF REACTION

2.093E-05	MOLES C/(CM*CM*SEC)
1.480E-08	MOLES C/SEC

FRACTION OF TOTAL RATE

I= 1	1.28E-01
I= 2	5.27E-01
I= 3	1.79E-03
I= 4	7.97E-02
I= 5	2.62E-01

RATE RELATIVE TO O2

I= 1	7.17E 01
I= 2	2.93E 02
I= 3	1.00E 00
I= 4	4.44E 01
I= 5	1.46E 02

CONTROLLING RESISTANCES

I= 1	NO DOMINANT RESISTANCE
I= 2	NO DOMINANT RESISTANCE
I= 3	NO DOMINANT RESISTANCE
I= 4	EXT MASS TRANSFER CONTROL
I= 5	EXT MASS TRANSFER CONTROL

CO2 REACTION PARAMETERS

HT OF RX AT PARTICLE TEMP	36053.8	CAL/MOLE C
RX RATE COEFFICIENT	2.9747241E 06	SEC**-1
KNUDSEN DIFFUSIVITY	1.3606004E-01	CM*CM/SEC
MOLECULAR DIFFUSIVITY	7.2713813E 00	CM*CM/SEC
EFF PORE DIFFUSIVITY	7.0359822E-02	CM*CM/SEC
THIELE MODULUS	4.8766E 01	
INTERNAL EFFECTIVENESS	6.0256E-02	
BOUND LAYER DIFFUSIVITY	8.0722381E 00	CM*CM/SEC
MASS TRANS COEFFICIENT	1.0762984E 03	CM/SEC
EXTERNAL RESISTANCE	8.7565E-04	SEC/CM
INTERNAL RESISTANCE	1.9710E-03	SEC/CM
EXT/INT RESISTANCE	4.4426E-01	
RX RATE PER EXT AREA	2.6973529E-06	MOLES C/(CM*CM*SEC)
RX RATE	1.9066464E-09	MOLES C/SEC

H2O REACTION PARAMETERS

HT OF RX AT PARTICLE TEMP	30866.6	CAL/MOLE C
RX RATE COEFFICIENT	4.9589927E 06	SEC**-1
KNUDSEN DIFFUSIVITY	2.1263213E-01	CM*CM/SEC
MOLECULAR DIFFUSIVITY	1.1635099E 01	CM*CM/SEC
EFF PORE DIFFUSIVITY	1.1000418E-01	CM*CM/SEC

THIELE MODULUS	5.0356E 01	
INTERNAL EFFECTIVENESS	5.8392E-02	
BOUND LAYER DIFFUSIVITY	1.2921361E 01	CM*CM/SEC
MASS TRANS COEFFICIENT	1.7228481E 03	CM/SEC
EXTERNAL RESISTANCE	5.4704E-04	SEC/CM
INTERNAL RESISTANCE	1.2199E-03	SEC/CM
EXT/INT RESISTANCE	4.4839E-01	
RX RATE PER EXT AREA	1.1040520E-05	MOLES C/(CM*CM*SEC)
RX RATE	7.8040843E-09	MOLES C/SEC

O2 REACTION PARAMETERS

HT OF RX AT PARTICLE TEMP	-29545.3	CAL/MOLE C
RX RATE COEFFICIENT	1.2751909E 09	SEC**-1
KNUDSEN DIFFUSIVITY	1.5956266E-01	CM*CM/SEC
MOLECULAR DIFFUSIVITY	9.2470702E 00	CM*CM/SEC
EFF PORE DIFFUSIVITY	8.2631701E-02	CM*CM/SEC
THIELE MODULUS	9.3169E 02	
INTERNAL EFFECTIVENESS	3.2164E-03	
BOUND LAYER DIFFUSIVITY	1.0263934E 01	CM*CM/SEC
MASS TRANS COEFFICIENT	1.3685245E 03	CM/SEC
EXTERNAL RESISTANCE	6.8867E-04	SEC/CM
INTERNAL RESISTANCE	8.3115E-05	SEC/CM
EXT/INT RESISTANCE	8.2857E 00	
RX RATE PER EXT AREA	3.7595190E-08	MOLES C/(CM*CM*SEC)
RX RATE	2.6574474E-11	MOLES C/SEC

O REACTION PARAMETERS

HT OF RX AT PARTICLE TEMP	-90805.8	CAL/MOLE C
RX RATE COEFFICIENT	5.4125251E 10	SEC**-1
KNUDSEN DIFFUSIVITY	2.2565569E-01	CM*CM/SEC
MOLECULAR DIFFUSIVITY	1.2525653E 01	CM*CM/SEC
EFF PORE DIFFUSIVITY	1.1677163E-01	CM*CM/SEC
THIELE MODULUS	5.1061E 03	
INTERNAL EFFECTIVENESS	5.8741E-04	
BOUND LAYER DIFFUSIVITY	1.3903039E 01	CM*CM/SEC
MASS TRANS COEFFICIENT	1.8537386E 03	CM/SEC
EXTERNAL RESISTANCE	5.0841E-04	SEC/CM
INTERNAL RESISTANCE	9.1980E-06	SEC/CM
EXT/INT RESISTANCE	5.5274E 01	
RX RATE PER EXT AREA	1.6694535E-06	MOLES C/(CM*CM*SEC)
RX RATE	1.1800671E-09	MOLES C/SEC

OH REACTION PARAMETERS

HT OF RX AT PARTICLE TEMP	-38257.8	CAL/MOLE C
RX RATE COEFFICIENT	8.7412280E 09	SEC**-1
KNUDSEN DIFFUSIVITY	2.1885381E-01	CM*CM/SEC
MOLECULAR DIFFUSIVITY	1.2223674E 01	CM*CM/SEC
EFF PORE DIFFUSIVITY	1.1326421E-01	CM*CM/SEC
THIELE MODULUS	2.0835E 03	
INTERNAL EFFECTIVENESS	1.4391E-03	
BOUND LAYER DIFFUSIVITY	1.3566849E 01	CM*CM/SEC
MASS TRANS COEFFICIENT	1.8089133E 03	CM/SEC
EXTERNAL RESISTANCE	5.2101E-04	SEC/CM
INTERNAL RESISTANCE	2.5914E-05	SEC/CM
EXT/INT RESISTANCE	2.0105E 01	
RX RATE PER EXT AREA	5.4938786E-06	MOLES C/(CM*CM*SEC)
RX RATE	3.8833939E-09	MOLES C/SEC

Figure 9. (P = 1 atm)

Figure 10. ($P = 1 \text{ atm}$; $d_p = 10 \mu\text{m}$)

Figure 11. ($P = 1 \text{ atm}$, $d_p = 150 \mu\text{m}$)

Figure 12. (P = 5 atm).

Figure 13. ($P = 5$ atm; $d_p = 10\mu\text{m}$)

Figure 14. ($P = 5$ atm; $d_p = 150\mu\text{m}$)

The effect of increasing the total pressure to 5 atm on the total rate of reaction is seen by comparing the curves in Figures 9, 10 and 11 with those presented for the same particle sizes and equivalence ratios in Figures 12, 13 and 14. The rates are higher for 5 atm for the same particle size and equivalence ratio, with the exception of rates for the smallest particle size, smallest equivalence ratio, and highest temperature combinations.

Now that the total rates of reaction have been presented, it is desirable to show what part of the total rate under any set of conditions is due to each of the five reactions. Figures 15, 16 and 17 show cumulative fractions of the total rate for each species, at 1 atm and $\phi = 1.1$, for particle sizes of 10, 50 and 150 μm respectively. Figures 18, 19 and 20 show the curves for these three sizes at a fuel equivalence ratio $\phi = 2.4$. These six figures correspond to the six curves presented in Figure 9.

Examination of any of these figures shows that CO_2 and H_2O account for the entire rate at the lower temperatures (less than 2000 $^\circ\text{K}$), but as the temperature is raised to 3000 $^\circ\text{K}$ the fraction of the total rate due to these species decreases as the reactions with O_2 , O and OH become important.

Comparing Figures 15, 16 and 17, it is seen that increasing the particle size results in decreasing the contributions of O_2 , O and OH to the total rate at the higher temperatures. This trend is even more pronounced for the higher fuel equivalence ratio, $\phi = 2.4$, in Figures 18, 19 and 20. With $\phi = 2.4$, the contribution of O_2 is negligible for the range of particle sizes given here. Comparing Figure 15 with Figure 18, 16 with 19, or 17 with 20 shows that CO_2 and H_2O account for more of the total rate at higher temperatures when $\phi = 2.4$ compared to $\phi = 1.1$. The amount due to H_2O is much larger than that due to CO_2 at $\phi = 2.4$.

Figure 15. ($P = 1 \text{ atm}$; $d_p = 10\mu\text{m}$; $\phi = 1.1$)

Figure 16. ($P = 1$ atm; $d_p = 50\mu\text{m}$; $\phi = 1.1$)

Figure 17. ($P = 1 \text{ atm}$; $d_p = 150 \mu\text{m}$; $\phi = 1.1$)

Figure 18. ($P = 1 \text{ atm}$; $d_p = 10 \mu\text{m}$; $\phi = 2.4$)

Figure 19. ($P = 1 \text{ atm}$; $d_p = 50 \mu\text{m}$; $\phi = 2.4$)

Figure 20. ($P = 1 \text{ atm}$; $150\mu\text{m}$; $\phi = 2.4$)

Figure 21. ($P = 1 \text{ atm}$; $d_p = 10 \mu\text{m}$; $\phi = 1.1$)

Figure 22. ($P = 5 \text{ atm}$; $d_p = 150 \mu\text{m}$; $\phi = 1.1$)

Figure 23. ($P = 5$ atm; $d_p = 10\mu\text{m}$; $\phi = 2.4$)

Figure 24. ($P = 5$ atm; $d_p = 150\mu\text{m}$; $\phi = 2.4$)

Figures 21 to 24 present the cumulative fractions for 5 atm, and are seen to show the same trends as the previous six graphs. (Note that the graphs for 50 μ m particles are omitted for 5 atm case.) With the higher pressure, the dissociation of molecular compounds is decreased, and thus the contributions of O and OH are diminished as compared to the 1 atm case. Under very fuel-rich conditions, both O₂ and O are negligible, and OH is important at high temperatures and for smaller particles. The domination of CO₂ and H₂O is again seen for wide ranges of temperatures and particle size, as well as effective fuel/air equivalence ratio.

It is important to note that the gas temperature and particle temperature will differ, due to both the enthalpy changes of the five reactions and the assumptions of wall temperature in the energy balance, the latter of which affects the radiation terms. Tables 3 and 4 shows the temperatures of both reactive and inert coal particles calculated by the steady state model in the presence of equilibrium gases under wide ranges of T_g and ϕ , at pressures of 1 and 5 atm respectively.

The inert particle temperature is equal to the gas temperature for $T \leq 2000^\circ\text{K}$, corresponding to the condition $T_w = T_g$ in Equation (11). For $T_g > 2000$, the inert particle temperatures are seen to be less than T_g , corresponding to the condition $T_w = 2000^\circ\text{K}$ in Equation (12). The deviation from T_g is greatest for $d_p = 150\mu\text{m}$ at $\phi = 1.1$, and is about 500°K for the 5 atm case.

The deviation of the particle temperature from the temperature which an inert particle would reach is shown in Figure 25. Deviations below a value of zero indicate the importance of the endothermic CO₂ and H₂O reactions. At higher temperatures, the dissociation to O₂, O, and OH results in positive deviations. These deviations are seen to be more pronounced for gases whose composition is closer to stoichiometric.

Table 3 Calculated Temperatures of Reacting and Inert Particles

A. Temperature of Reacting Particles (P = 1 atm)

$T_{\text{gas}} (^{\circ}\text{K})$	1500	1750	2000	2250	2500	2750	3000
$d_p = 10\mu\text{m}$ $\phi = 1.1$	1499	1744	1983	2153	2486	3029	3538
$\phi = 1.7$	1500	1749	1998	2221	2436	2695	3040
$\phi = 2.4$	1500	1750	2000	2237	2463	2691	2943
$d_p = 150\mu\text{m}$ $\phi = 1.1$	1473	1687	1909	2002	2159	2403	2707
$\phi = 1.7$	1492	1728	1963	2089	2213	2378	2623
$\phi = 2.4$	1500	1749	1998	2158	2295	2449	2655

B. Temperature of Inert Particles (P = 1 atm)

$T_{\text{gas}} (^{\circ}\text{K})$	1500	1750	2000	2250	2500	2750	3000
$d_p = 10\mu\text{m}$ $\phi = 1.1$	1500	1750	2000	2153	2339	2579	2858
$\phi = 1.7$	1500	1750	2000	2226	2437	2657	2909
$\phi = 2.4$	1500	1750	2000	2237	2463	2690	2939
$d_p = 150\mu\text{m}$ $\phi = 1.1$	1500	1750	2000	2092	2207	2354	2544
$\phi = 1.7$	1500	1750	2000	2132	2258	2406	2601
$\phi = 2.4$	1500	1750	2000	2160	2298	2452	2655

Table 4 Calculated Temperatures (P = 5 atm)

A. Temperature of Reacting Particles

$T_{\text{gas}} (^{\circ}\text{K})$	1500	1750	2000	2250	2500	2750	3000
$d_p = 10\mu\text{m}$ $\phi = 1.1$	1498	1724	1924	2047	2255	2661	3227
$\phi = 1.7$	1500	1747	1989	2203	2399	2599	2874
$\phi = 2.4$	1500	1750	2000	2238	2467	2685	2913
$d_p = 150\mu\text{m}$ $\phi = 1.1$	1439	1579	1761	1839	1962	2171	2465
$\phi = 1.7$	1469	1676	1894	2017	2137	2273	2466
$\phi = 2.4$	1498	1746	1994	2159	2305	2439	2602

B. Temperature of Inert Particles

$T_{\text{gas}} (^{\circ}\text{K})$	1500	1750	2000	2250	2500	2750	3000
$d_p = 10\mu\text{m}$ $\phi = 1.1$	1500	1750	2000	2149	2313	2520	2771
$\phi = 1.7$	1500	1750	2000	2228	2443	2647	2869
$\phi = 2.4$	1500	1750	2000	2239	2470	2688	2915
$d_p = 150\mu\text{m}$ $\phi = 1.1$	1500	1750	2000	2092	2202	2336	2496
$\phi = 1.7$	1500	1750	2000	2136	2265	2347	2554
$\phi = 2.4$	1500	1750	2000	2167	2313	2447	2609

FIGURE 25. Deviation of Char Temperature from Inert Partical Temperature.

The reaction rate may be controlled by either the internal or external resistance, as discussed in Appendix G. Figures 26 and 27 show, for d_p of 10 and 150 μm respectively, the ratio of external to internal resistance as a function of gas temperature. The slight changes due to fuel equivalence ratio are more likely due to differences in particle temperature. The O, OH and O_2 curves show higher ratios than CO_2 and H_2O since the internal resistance is much smaller (due to high reaction rates) and since the external resistances for all species are roughly equal.

The increase in the external/internal resistance with increase in gas temperature is due primarily to the decrease in internal resistance, due to the intrinsic Arrhenius kinetics. Also, the external resistance to diffusion is not very temperature sensitive. By comparing Figures 26 and 27 it is seen that the ratio of resistances is much larger for 150 μm than for 10 μm particles, for all species. This result is achieved at a balance between two opposing factors. First, the external resistance is larger for the larger particles, in proportion to d_p . Secondly, the internal resistance is also larger, due to the increased difficulty in overcoming the effects of internal pore diffusion for the larger particles.

This latter effect is manifested as a decrease in internal effectiveness as diameter is increased, which increases the internal resistance according to Equation (G.2). This is seen by comparing Figures 28 and 29, which show effectiveness factors for each species at $d_p = 10 \mu\text{m}$ and $d_p = 150 \mu\text{m}$, respectively. The effectiveness factors are not greatly affected by equivalence ratio. Note that the CO_2 and H_2O utilize the internal surface more efficiently than O_2 , O and OH.

Figure 26. (P = 1 atm; $d_p = 10\mu\text{m}$)

Figure 27. ($P = 1 \text{ atm}$; $d_p = 150 \mu\text{m}$)

Figure 28. ($P = 1 \text{ atm}$; $d_p = 10 \mu\text{m}$)

Figure 29. ($P = 1 \text{ atm}$; $d_p = 150 \mu\text{m}$)

A model to simulate coal combustion in the presence of a gas phase (which is effectively fuel-rich) has been presented. The rates due to reaction of char with CO_2 , H_2O , O_2 , O and OH are calculated based on first order kinetics, taking into account the effects of external film diffusion and internal pore diffusion.

This model was applied to char oxidation in MHD combustors where an effectively fuel-rich gas phase would exist. The results give the instantaneous reaction rate due to each species for the given particle size, gas temperature, and pressure. The trade-offs in reaction rate due to changes in d_p , T_g , ϕ and P were shown and discussed. At temperatures below 2500°K , H_2O and CO_2 are the dominant oxidizing species. Above this temperature, significant contributions from O_2 , O and OH are found. The contribution of O_2 is most important at high T_g for equivalence ratios near stoichiometric, while OH is more important for effective ϕ values which are fuel-rich ($\phi = 1.0$ and greater). Finally, the particle temperatures reached for reacting and inert particles were presented. These are determined by the parameters chosen for the energy balance and the enthalpy change of the dominant reactions.

Notation

Symbols and Units

A_g	specific internal area (cm^2/g)
c	total concentration (moles/cm^3)
C	species concentration (moles/cm^3)
d	diameter (cm)
D	diffusion coefficient (cm^2/sec)
f	fraction of total area
h	heat transfer coefficient ($\text{cal}/\text{cm}^2 \text{sec } ^\circ\text{K}$)
ΔH	enthalpy change (cal/mole)
k	intrinsic reaction rate coefficient (sec^{-1})
k^1	surface reaction rate coefficient ($\text{moles}/\text{cm}^2 \text{sec atm}$)
K	external mass transfer coefficient (cm/sec)
m	mass (g)
M	molecular weight (g/mole)
N	moles (moles)
$\tilde{N}$	molar flux ($\text{moles}/\text{cm}^2 \text{sec}$)
n_{AV}	Avogadro's number (6.023×10^{23} molecules/mole)
p	partial pressure (atm)
P	total pressure (atm)
r	radial position (cm)
r_p	particle radius (cm)
r_{pore}	average or mean pore radius (cm)
R	gas constant ($1.9872 \text{ cal}/\text{mole } ^\circ\text{K}$)
R	reaction rate per external surface ($\text{moles C}/\text{cm}^2 \text{sec}$)
S	area (cm^2)
t	time (sec)

T	temperature ($^{\circ}\text{K}$)
v_g	specific pore volume (cm^3/g)
V_p	particle volume (cm^3)
x	dummy variable name
y	mole fraction
ϵ_g	gas emissivity
ϵ/k	Lennard-Jones parameter ($^{\circ}\text{K}$)
ξ	ratio of rate of reaction with pore diffusion to rate if pore diffusion was absent, based on surface concentration
λ	thermal conductivity ($\text{cal}/\text{cm sec } ^{\circ}\text{K}$)
μ	viscosity ($\text{g}/\text{cm sec}$)
ϕ	Thiele modulus, Eqn. (5) or fuel/air equivalence ratio
ρ	density (g/cm^3)
σ	Stefan-Boltzmann constant ($1.355 \times 10^{-12} \text{ cal}/\text{sec cm}^2 \text{ } ^{\circ}\text{K}^4$)
σ_i	Lennard-Jones parameter ($\text{\AA}$)
σ_{ij}	Binary Lennard-Jones parameter ($\text{\AA}$)
τ	tortuosity of porous particle ($\sqrt{2}$)
θ	porosity of porous particle
Ω	collision integral
Φ	parameter defined by Eqn. (B.3)

Subscripts

A	species A
B	bulk
BL	boundary layer or diffusion film
C	Carbon
CO ₂	Carbon Dioxide
D	diffusional mass transport
EFF	effective
EX	external
g	gas
H ₂ O	Steam
i	species i
IN	internal
j	species j
K	thermal or energy transport
KN	Kundsen
M	molecular
MIX	mixture
O	Oxygen Atoms
O ₂	Oxygen Molecules
OH	Hydroxyl Radicals
p	particle
rx	reaction
s	surface of particle
SK	skeletal
TOT	total
μ	viscous momentum transport

Appendix A Reaction Rate Due to External Diffusion

The molar flux of species A in the r direction is^[2]

$$\tilde{N}_{Ar} = -c D_{A,MIX} \frac{dY_A}{dr} + Y_A (\tilde{N}_{ir}) \quad (A.1)$$

Neglecting total molar bulk flow, and using the mean boundary layer properties at temperature $T_{BL} = (T_p + T_g)/2$, (A.2)

$$\tilde{N}_{Ar} = - \frac{D_{A,MIX}}{RT_{BL}} \frac{dp_A}{dr} \quad (A.3)$$

Since no reaction of A occurs in the gas phase, a mass balance on A for $r \geq r_p$ gives^[3]

$$4 \pi r^2 M_A \tilde{N}_{Ar} = 4 \pi r_p^2 M_A \tilde{N}_{Ar_p} = \text{constant} \quad (A.4)$$

Thus,

$$r_p^2 \tilde{N}_{Ar_p} = r^2 \tilde{N}_{Ar} = - r^2 \frac{D_{A,MIX}}{RT_{BL}} \frac{dp_A}{dr} \quad (A.5)$$

Integrating between the limits $p_A = p_{AS}$ at $r = r_p$ and $p_A = p_{Ag}$ at $r = \infty$,

$$- r_p \frac{RT_{BL}}{D_{A,MIX}} \tilde{N}_{Ar_p} = p_{Ag} - p_{AS} \quad (A.6)$$

The reaction rate per unit external surface is then

$$- \frac{1}{S_{EX}} \frac{dN_A}{dt} = - \tilde{N}_{Ar_p} = \frac{2 D_{A,MIX}}{d_p RT_{BL}} (p_{Ag} - p_{AS}) \quad (A.7)$$

Defining an external mass transfer coefficient for species A as

$$K_A = \frac{2 D_{A,MIX}}{d_p} \quad (A.8)$$

where $D_{A,MIX}$ is evaluated at T_{BL} , it follows that

$$-\frac{1}{S_{EX}} \frac{dN_A}{dt} = \frac{K_A}{RT_{BL}} (p_{Ag} - p_{AS}) \quad (A.9)$$

The evaluation of $D_{A,MIX}$ is done by using equations (8) and (9) at the mean boundary layer temperature. Lennard-Jones parameters are described more fully in Appendix C.

Appendix B Heat Transfer Coefficient and Gas Phase Thermal Conductivity

The heat transfer from the particle surface to the surrounding gas due to convection is assumed to be described using a Nusselt number equal to two. That is,

$$h = 2 \frac{\lambda_g}{d_p} \quad (B.1)$$

The gas phase thermal conductivity is given by^[2]

$$\lambda_g = \sum_i \left[\frac{Y_i \lambda_i}{\sum_j Y_j \phi_{ij}} \right] \quad (B.2)$$

where the summations are over all gaseous species present in the system, and where

$$\phi_{ij} = \frac{1}{\sqrt{8}} \left[1 + \left(\frac{\mu_i}{\mu_j} \right)^{1/2} \left(\frac{M_i}{M_j} \right)^{1/4} \right] \left[1 + \frac{M_i}{M_j} \right]^{-1/2} \quad (B.3)$$

The pure species properties are calculated from:

$$\lambda_i = 1.9891 \times 10^{-4} \frac{\sqrt{T/M_i}}{\sigma_i^2 \Omega_K} \frac{\text{cal}}{\text{cm sec } ^\circ\text{K}} \quad (B.4)$$

$$\mu_i = 2.6693 \times 10^{-5} \frac{\sqrt{T M_i}}{\sigma_i^2 \Omega_\mu} \frac{\text{g}}{\text{cm sec}} \quad (B.5)$$

where T is in $^\circ\text{K}$, M in g/mole, σ in $\text{\AA}$, and Ω is dimensionless. The temperature is taken as the mean boundary layer temperature, eqn. (A.2), and the composition is assumed to be the same as that of the bulk gas phase outside the transport film.

Appendix C Lennard-Jones Parameters for Property Estimates

The equations for diffusivity, thermal conductivity, and viscosity are based on kinetic theory using the Lennard-Jones potential function. The Lennard-Jones parameters for all of the species considered as gas phase constituents are listed in Table (C.1). To obtain binary parameters from the values listed in the table, the following two relations are used:^[6]

$$\sigma_{ij} = (\sigma_i + \sigma_j)/2 \quad (C.1)$$

$$\frac{\epsilon_{ij}}{K} = \left[\left(\frac{\epsilon_i}{K} \right) \left(\frac{\epsilon_j}{K} \right) \right]^{1/2} \quad (C.2)$$

Finally, the collision integrals Ω_o , Ω_K and Ω_μ are assumed to be equal to the values of $\Omega^{(1,1)*}$ given in reference [6]; these are listed as a function of the dimensionless temperature (KT/ϵ) in Table (C2).

The data given in Table (C2) were fitted over two regions with a parabola on a log-log scale. Thus, the collision integral can be calculated via the following equation

$$\Omega^{(1,1)*} = 10 \left\{ A + B \left[\log_{10} \left(\frac{KT}{\epsilon} \right) \right] + C \left[\log_{10} \left(\frac{KT}{\epsilon} \right) \right]^2 \right\} \quad (C.3)$$

Table (C1) Lennard-Jones Parameters from Ref. (7)

Species	σ_i (Å)	$\epsilon_i/k(^{\circ}\text{K})$	Species	σ_i (Å)	$\epsilon_i/k(^{\circ}\text{K})$
Ar	3.542	93.3	HCN	3.630	569.1
C	3.385	30.6	H ₂	2.827	59.7
CH	3.370	68.6	H ₂ O	2.641	809.1
CH ₄	3.758	148.6	H ₂ O ₂	4.196	289.3
CN	3.856	75.0	H ₂ S	3.623	301.1
CO	3.690	91.7	N	3.298	71.4
COS	4.130	336.0	NH	3.312	65.3
CO ₂	3.941	195.2	NH ₃	2.900	558.3
CS	4.216	199.4	NO	3.492	116.7
CS ₂	4.483	467.0	N ₂	3.798	71.4
C ₂	3.913	78.8	N ₂ O	3.828	232.4
C ₂ H ₂	4.033	231.8	O	3.050	106.7
C ₂ H ₄	4.163	224.7	OH	3.147	79.8
C ₂ H ₆	4.443	215.7	O ₂	3.467	106.7
C ₂ N ₂	4.361	348.6	S	3.839	847.0
C ₃ H ₈	5.118	237.1	SO	3.993	301.0
CH ₃ OH	3.626	481.8	SO ₂	4.112	335.4
H	2.708	37.0	S ₂	4.519	847.0

Table (C2) Values of $\Omega^{(1,1)*}$ from Ref. (6)

kT/ϵ_{ij}	$\Omega^{(1,1)*}$	kT/ϵ_{ij}	$\Omega^{(1,1)*}$	kT/ϵ_{ij}	$\Omega^{(1,1)*}$
1.70	1.140	3.1	0.9406	4.8	0.8492
1.75	1.128	3.2	0.9328	4.9	0.8456
1.80	1.116	3.3	0.9256	5	0.8422
1.85	1.105	3.4	0.9186	6	0.8124
1.90	1.094	3.5	0.9120	7	0.7896
1.95	1.084	3.6	0.9058	8	0.7712
2.0	1.075	3.7	0.8998	9	0.7556
2.1	1.057	3.8	0.8942	10	0.7424
2.2	1.041	3.9	0.8888	20	0.6640
2.3	1.026	4.0	0.8836	30	0.6232
2.4	1.012	4.1	0.8788	40	0.5960
2.5	0.9996	4.2	0.8740	50	0.5756
2.6	0.9878	4.3	0.8694	60	0.5596
2.7	0.9770	4.4	0.8652	70	0.5464
2.8	0.9672	4.5	0.8610	80	0.5352
2.9	0.9576	4.6	0.8568	90	0.5256
3.0	0.9490	4.7	0.8530	100	0.5130

The values of the constants A,B, and C are given in Table (C3) for the two ranges of dimensionless temperature covered. The value of $\Omega^{(1,1)*}$ so calculated is good to within 1.2% of the values listed in Table (C2).

Table (C3) Values of Constants to Calculate $\Omega^{(1,1)*}$

Constant Name	Value ($1.7 \leq \frac{kT}{\epsilon} \leq 7$)	Value ($7 \leq \frac{kT}{\epsilon} \leq 100$)
A	0.1355	0.04563
B	-0.3920	-0.1839
C	0.1296	0.009320

Appendix D Heats of Reaction

The heats of reaction for the following five reactions are needed for the program:

The pure component enthalpy of these species is available in the form of a polynomial function of temperature, [8]

$$\frac{H_i^0}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T} \quad (\text{D.6})$$

The values of the constants for each species appear in Table (D1), valid for $1000^\circ\text{K} \leq T \leq 5000^\circ\text{K}$.

These temperature expansions are used to derive polynomial expansions for the enthalpy of reaction in the form

$$\frac{\Delta H_{\text{RX},i}^0}{R} = AT + BT^2 + CT^3 + DT^4 + ET^5 + F \quad (\text{D.7})$$

The results of these calculations are shown in Figure (D1).

Table (D1) Enthalpy Expansion Coefficients from Ref. (8)

Species	C(s)	CO	CO ₂
a ₁	0.13506 E 1	0.29841 E 1	0.44608 E 1
a ₂	0.19182 E- 2	0.14891 E- 2	0.30982 E- 2
a ₃	-0.84040 E- 6	-0.57900 E- 6	-0.12393 E- 5
a ₄	0.16449 E- 9	0.10365 E- 9	0.22741 E- 9
a ₅	-0.11673 E-13	-0.69354 E-14	-0.15526 E-13
a ₆	-0.65714 E 3	-0.14245 E 5	-0.48961 E 5

Species	O ₂	O	OH
a ₁	0.36220 E 1	0.25353 E 1	0.29131 E 1
a ₂	0.73618 E- 3	-0.14372 E- 4	0.95418 E- 3
a ₃	-0.19652 E- 6	-0.11360 E- 7	-0.19084 E- 6
a ₄	0.36202 E-10	0.66005 E-11	0.12731 E-10
a ₅	-0.28946 E-14	-0.61182 E-15	+0.24804 E-15
a ₆	-0.12020 E 4	+0.29230 E 5	+0.39647 E 4

Species	H ₂	H ₂ O
a ₁	0.31002 E 1	0.27168 E 1
a ₂	0.51120 E- 3	0.29451 E- 2
a ₃	0.52644 E- 7	-0.80224 E- 6
a ₄	-0.34910 E-10	0.10227 E- 9
a ₅	0.36945 E-14	-0.48472 E-14
a ₆	-0.87738 E 3	-0.29906 E 5

FIGURE D1

COEFFICIENTS FOR VALUES OF ENTHALPY OF GIVEN RX FOR
TEMPERATURES IN THE RANGE 1000 TO 5000 DEGREES KELVIN

THE FORM OF THE EQUATION IS

DELTA H OF RX/GAS CONSTANT = $AT+BT**2+CT**3+DT**4+ET**5+F$

WHERE T = DEGREES KELVIN AND THE CONSTANTS A THROUGH F ARE GIVEN BELOW

CO₂+C=2 CO

1.4684090E-01	-1.0190588E-03	3.0722243E-07
-4.6152194E-11	2.6659827E-15	2.1128124E 04

H₂O+C=H₂+CO

2.0070022E 00	-1.4315137E-03	3.7209833E-07
-4.9504523E-11	2.6558128E-15	1.5440356E 04

.5 O₂+C=CO

-1.8740134E-01	-3.9858801E-04	1.1988939E-07
-1.9735519E-11	1.2369192E-15	-1.2987098E 04

O+C=CO

-9.1168839E-01	-2.0735640E-04	9.0922396E-08
-1.6860453E-11	1.0698262E-15	-4.2818354E 04

CH₄+C=CO+.5 H₂

2.6054745E-01	-5.6383493E-04	1.5952413E-07
-2.2756770E-11	1.2673085E-15	-1.7991485E 04

Appendix E Estimates of Intrinsic Reaction Coefficients

E.1 CO₂ and H₂O

Gasification rates of 75-100 μ m Montana Rosebud coal char in CO₂ and in H₂O at temperatures up to 1800°C and residence times from 0.25 to 0.5 seconds were measured in a laboratory scale laminar flow reactor at MIT.^[9] The results are correlated for the H₂O reaction by the expression

$$-\frac{1}{S_{TOT}} \frac{dm_c}{dt} = \frac{0.2 \text{ grams C}}{\text{cm}^2 \text{ sec atm}} \exp \left(\frac{-41000 \text{ cal/mole}}{RT_p} \right) p_{H_2O,S} \quad (E.1)$$

To equate this to the intrinsic reaction coefficient of the form of eqn.

(2), the conversion factor for the reaction (D.2) given here is used:

$$\frac{dN_{H_2O}}{dt} = \frac{dm_c}{dt} \frac{1 \text{ mole H}_2\text{O}}{12 \text{ grams C}} \quad (E.2)$$

Also, as given in Appendix F, we use the values of the ratio S_{TOT}/V_p given in ref. (9). Finally, for the data in ref. (9) at 1480°K and 1764°K, $\xi \sim 1$, $f_{IN} \sim 1$, and $f_{EX} \sim 0$. The use of eqns. (2), (E.1) and (E.2) along with this information results in an intrinsic rate coefficient for H₂O of

$$k_{H_2O} = \left(\frac{4.43 \times 10^6}{\text{sec}^\circ\text{K}} \right) T_p \exp \left(\frac{-41,000 \text{ cal/mole}}{RT_p} \right) \quad (E.3)$$

The data in reference (9) for the reaction of CO₂ with the coal char shows a limitation due to pore diffusion at the highest temperature studied. The rate at the lower temperatures was roughly 60% of the rate of the H₂O - C reaction at the same temperatures, and if it is assumed that the intrinsic kinetics were measured under these experimental conditions, the result is a rate coefficient given by

$$k_{CO_2} = \left(\frac{2.66 \times 10^6}{\text{sec}^{\circ}\text{K}} \right) T_p \exp \left(\frac{-41,000 \text{ cal/mole}}{RT_p} \right) \quad (\text{E.4})$$

E.2 Oxygen

Pulverized semi-anthracite particles have been burned in O_2 in a laminar furnace at partial pressures of 0.1 and 0.2 atmospheres.^[10] The results were analyzed in terms of the internal pore structure and its effect on the observed rate, as well as the effect of the diffusion of O_2 to the particle surface. This is an analysis which must be done in order to obtain the intrinsic reactivity, which was reported as:

$$- \frac{1}{S_{TOT}} \frac{dm_c}{dt} = \left(\frac{55 \text{ grams C}}{\text{cm}^2 \text{ sec atm}} \right) \exp \left(\frac{-40,000 \text{ cal/mole}}{RT_p} \right) p_{O_2} S \quad (\text{E.5})$$

Using the values of skeletal density and internal area per unit weight for the particles as reported in reference [10], and using $\xi = 1$ and $f_{IN} + f_{EX} = 1$, the following rate coefficient for the O_2 -C reaction is derived using equations (2), (E.5), (D.3), and (F.3):

$$k_{O_2} = \left(\frac{9.42 \times 10^8}{\text{sec}^{\circ}\text{K}} \right) T_p \exp \left(\frac{-40,000 \text{ cal/mole}}{RT_p} \right) \quad (\text{E.6})$$

E.3 O Atoms and OH Radicals

Direct data on the gasification rate of carbon due to reaction with O atoms or OH radicals was not available; however, some information on efficiency of collisions resulting in reaction was found. The OH collision efficiency for carbon atom removal has been estimated by Fenimore and Jones to be about 0.1 for soot in ethylene air flames at temperatures of 1530 to

1890°K. Millikan^[12] inferred that soot in fuel-rich hydrocarbon flames was oxidized by OH rather than CO₂ or H₂O. Graham et.al.^[13] attribute the higher reaction probabilities for the H₂O-C reaction in their work compared to low pressure studies on pyrolytic carbon to the dissociation of water, yielding reactive OH radicals which they estimate can govern almost completely the rate of reaction at 2600°K. Blackwood and McTaggart^[14] passed the products of an electric discharge in water vapor over carbon at room temperature, and attributed the large reaction rate to OH as well as to O atoms. Rosner and Allendorf^[15] used the fast reaction:

to generate OH in a flow system, employing a microwave discharge. The OH collision efficiency was found to be 4×10^{-3} at 1800°K, which was 100 times lower than the efficiency for O atoms and 10 times less than that for O₂. This latter result is surprising, and conflicts with the data reported earlier by Fenimore and Jones. The OH radicals in Rosner and Allendorf's work are rapidly consumed by gas-phase and surface reactions not involving the C reaction, and it is not clear that the concentration of OH which reacted with the C was precisely known.

The above discussion points out the uncertainty in the experimental measurements of the rate of reaction of carbon with the species O and OH. Since the rate of the O₂-C reaction is known, it was decided for the present study to take the rates of O and OH as some multiple of the O₂ rate, in proportion to their different collision efficiencies.

The rate of reaction can be expressed as follows:

$$-\frac{n_{AV}}{S_{EX}} \frac{dN_i}{dt} = \left(\frac{\text{Flux of } i}{\text{Molecules}} \right) \left(\frac{\text{C atoms reacted}}{\text{collision}} \right) \left(\frac{\text{moles } i}{\text{moles C}} \right) \quad (\text{E.8})$$

where the flux is the collision rate of i molecules with the surface, per unit surface. In the studies mentioned above, reaction occurred only on the surface, so the rate can also be expressed as

$$- \frac{1}{S_{EX}} \frac{dN_i}{dt} = k_i^1 p_i \quad (E.9)$$

Now, the flux of i molecules striking the surface is proportional to partial pressure and molecular weight according to:

$$\text{Flux} \propto \frac{p_i}{M_i^{1/2}} \quad (E.10)$$

Therefore, from equations (E.8) and (E.9), we have

$$k_i^1 \propto \frac{\text{Efficiency}}{M_i^{1/2} \left(\frac{\text{moles C}}{\text{moles i}} \right)} \quad (E.11)$$

for equal temperatures and partial pressures. In this relation, the intent is a comparison of the O and OH reaction rates with that of O_2 .

A collision efficiency, C atoms reacted per collision of reactant molecule, was assumed to be 0.6 for O atoms and 0.04 for O_2 atoms, based on Rosner and Allendorf's experiments.^[15] Their data for OH was ignored, and instead the collision efficiency of 0.1 reported by Fenimore and Jones^[11] was used in this study. Using these values, we calculated that:

$$k_O^1 = 42.4 k_{O_2}^1 \quad (E.12)$$

$$k_{OH}^1 = 6.86 k_{O_2}^1 \quad (E.13)$$

To apply these surface reaction rate coefficients to the case of a porous coal or char particle, we simply note that for any particle, the internal area per unit volume is a constant, and thus for equal partial pressures of reactant

$$k_0 = 42.4 k_{O_2} \quad (E.14)$$

$$k_{OH} = 6.86 k_{O_2} \quad (E.15)$$

Finally, using the expression (E.6), we have

$$k_0 = \left(\frac{4.00 \times 10^{10}}{\text{sec}^\circ\text{K}} \right) T_p \exp \left(\frac{-40,000 \text{ cal/mole}}{RT_p} \right) \quad (E.16)$$

$$k_{OH} = \left(\frac{6.46 \times 10^9}{\text{sec}^\circ\text{K}} \right) T_p \exp \left(\frac{-40,000 \text{ cal/mole}}{RT_p} \right) \quad (E.17)$$

The rate expressions given here were used over a larger temperature range than that under which they were experimentally determined. The extrapolation of these expressions to higher temperatures is done with little confidence in view of the highly non-Arrhenius behavior of gas-carbon reactions at these temperatures, as evidenced in references [3], [15] and [16].

Appendix F Pore Structure of Chars

The pore structure of a coal or char particle is characterized by the specific internal surface area, A_g , the specific internal pore volume, V_g , and the distribution of internal volume over the range of pore diameters. The pore size distribution may be analyzed in terms of a single value of the average pore radius, $\bar{r}_{\text{pore}}$, such as done in this study.

The physical properties of Montana Rosebud char samples used in a study of gasification of char in CO_2 and O_2 at temperatures between 1500 and 1825°K by Mandel^[17] are given in Table (F1). This is the same char which was used to obtain the CO_2 and H_2O gasification parameters in Appendix E. The porosity listed in Table (F1) is calculated from the relation

$$\theta = 1 - (\rho_B / \rho_{SK}) \quad (\text{F.1})$$

The average pore radius is calculable from the given properties using the relation^[5]

$$\bar{r}_{\text{pore}} = \frac{2V_g}{A_g} = \frac{2\theta}{A_g \rho_B} \quad (\text{F.2})$$

Using this equation, $\bar{r}_{\text{pore}} = 181\text{\AA} = 1.81 \times 10^{-6} \text{ cm}$ for the char used in the above mentioned studies. An additional relationship which is useful in the derivation of the intrinsic kinetics in Appendix E is:

$$\frac{S_{\text{TOT}}}{V_p} = \rho_{SK} A_g \quad (\text{F.3})$$

This equation allows the ratio on the left side of eqn. (F.3) to be evaluated from known pore structure properties.

Table (F1) Physical Properties of Montana Rosebud Char (from Ref. (17))

Specific Internal Surface Area, A_g	$1.65 \times 10^6 \text{ cm}^2/\text{g}$
Bulk Particle Density, ρ_B	0.50 g/cm^3
Particle Skeletal Density, ρ_{SK}	1.96 g/cm^3
Porosity, θ	0.745

Appendix G Controlling Resistances

The concept of controlling resistance arises from the general conductance equation,

$$\text{Flux} = \frac{\text{Driving Force}}{\text{Sum of Resistances}} \quad (\text{G.1})$$

Equation (1) is of this form, with a driving force of $p_{Ag} \sim p_{AS}$ and a resistance given by RT_{BL}/K_A . Equation (3) is similar to this form, but the terms in its denominator can be considered as resistance terms. Thus the resistance to external diffusion is given by $T_{BL}/T_g K_A$, while the resistance to the combined effects of pore diffusion and reaction on the particle surface is given by:

$$\frac{T_p S_{EX}/V_p}{T_g k_A (\xi_A f_{IN} + f_{EX})} \quad (\text{G.2})$$

To determine which of these terms is the larger resistance, we simply compare their magnitude. For external mass transfer to be the controlling step, it must have the largest resistance, that is

$$\frac{T_{BL}}{T_g K_A} \gg \frac{T_p S_{EX}/V_p}{T_g k_A (\xi_A f_{IN} + f_{EX})} \quad (\text{G.3})$$

for mass transfer control.

If the right hand term is actually much larger than the external resistance term, then internal diffusion and reaction controls the rate due to its larger resistance.

The resistance for internal diffusion and chemical reaction also includes the possible effects of reaction on the exterior surface of the

particle. This contribution is seen from Equation (2), which is reproduced below:

$$-\frac{1}{V_p} \frac{dN_A}{dt} = k_A \xi_A f_{IN} C_{AS} + k_A f_{EX} C_{AS} \quad (2)$$

The first term on the right side is a result of diffusional effects in the pores through the term ξ_A , and reaction on the internal surface through the term f_{IN} . The second group, $k_A f_{EX} C_{AS}$, reflects the extra reaction due to the external surface. Under different conditions, either of these terms can be controlling, although usually the external surface term is negligible. The criterion for internal diffusion and reaction to be dominant is

$$\xi_A f_{IN} \gg f_{EX} \quad (G.4)$$

or

$$\xi_A S_{IN} \gg S_{EX}. \quad (G.5)$$

These criteria were used in the computer model in the following form:

1. The ratio of external diffusion resistance to total internal resistance was calculated.

If this ratio exceeded 10, external mass transfer control existed according to Eqn. (G.3).

2. If the ratio of external to internal resistances is between 0.1 and 10, there is no dominant resistance.
3. If the ratio external to internal is less than 0.1, the internal resistance term dominates. Additionally, if the term $\xi_A f_{IN}/f_{EX}$ is greater than 10, the internal reaction and pore diffusion is dominant, according to Eqn. (G.4). If the term $\xi_A f_{IN}/f_{EX}$ is less than 0.1, reaction on the external surface dominates. If the term lies between 0.1 and 10, neither term is dominant, and only their combined sum controls (over the external diffusion term).

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TASK 4b. COMBUSTION AERODYNAMICS AND FLUID MECHANICS OF HIGH-SWIRL SECOND STAGE

Introduction

For any MHD system the overall cycle efficiency of the plant depends upon the relative fraction of power extracted in the MHD generator. The overall efficiency can be increased by minimizing the external losses, including those in the diffuser, and selecting the burner pressure which will maximize the net MHD power. MHD channels are designed to operate with an accelerating sub-sonic flow in the channel. The flow is initially supersonic, but the addition of the seed material reduces it to sub-sonic due to the increased electromagnetic interaction. For a normal (divergent) channel, continual expansion and acceleration of gas over the channel length is produced if the combustor (stagnation) pressure is high enough. However, the burner pressure affects the residence time, and an optimum value of 4 atm., at the burner inlet, has been found. At lower combustor pressures, the stagnation pressure in the channel rises abruptly indicating the existence of a normal shock or a strong shock system. If subscript 1 and 2 denote the region upstream and downstream, respectively, of a shock, then

$$\frac{P_{01}}{P_2} = \frac{\frac{P_{01}}{P_1}}{\frac{P_2}{P_1}} = \frac{\left[1 + \frac{\gamma-1}{2} M_1^2\right]^{\frac{\gamma}{\gamma-1}}}{1 + \frac{2\gamma}{\gamma-1} (M_1^2 - 1)}$$

where γ is the ratio of specific heats, P_{01} is the combustor stagnation pressure, and M is the Mach Number. For no pressure recovery behind the shock, $P_2 = 1$ atm., and if $P_{01}/P_2 = 2.9$ atm., then 2.9 atm. pressure is theoretically required to push the shock to the channel exit. However,

experiments show that the pressure actually required is ~ 4.7 atm., and this excess of 1.8 atm. represents a very large loss which must be minimized, by the addition of a diffuser section. It has been found that at a given pressure the shock moves downstream with the addition of a diffuser. However, the pressure range required here is between 4 to 9 atmospheres in order to achieve supersonic flow at the combustor exit (typically it is required to have a Mach Number of about 1.6).

The diffuser section must allow sufficient pressure recovery to establish near supersonic flow through the generator at combustor pressures between 4 - 9 atmospheres. The pressure recovery in the diffuser section is dependent upon the area ratio, length, boundary layer blockage at the entrance and the height to width ratio. For a thin boundary layer the performance increases with an increasing area ratio as long as no separation occurs. The tendency for separation increases with increased blockage (inviscid core area/geometrical area) due to the boundary layer. Experimentally it was found that maximum pressure recovery occurs if the diffuser is operated in the transitory stall regime, but without flow separation. The formation and sweep-through of the separated regions is accompanied by large pressure perturbations which, in the case of subsonic flow, could propagate upstream to serve as a source of instability in the channel flow. A diffuser pressure recovery factor of 0.6 is required. Secondly, the gasses entering the diffuser have a temperature range of 2500 to 3000°F. For a separated flow a hot spot is formed at the point of separation, with consequent damage to the wall material. Then again, for a non-separated flow, a stream of cool fluid may be forced to flow along the diffuser surface, thereby insulating the surface from the hot exhaust gasses and reducing the wall cooling requirement. It is thus essential that the design of the diffuser should prevent flow separation.

Object

The object of the present program is to develop a computer code for predicting the occurrence of flow separation, if any, in the diffuser section of an MHD combustor generator system. The prediction of flow separation can be achieved either by experimental or theoretical methods. Experimental methods require a large layout and any design change requires a new rig. It is because of this that theoretical models are preferable.

The program SHAPE is being developed to predict flow separation with water as the working medium. It computes the two-dimensional, steady-state, swirling flow using the cartesian co-ordinate system. This code employs the vorticity-stream function approach together with a two-equation $(k - \epsilon)$ model of turbulence. This approach was selected as the stream function map will visually indicate the flow separation by a divergence of the streamlines. Secondly, this approach also reduces by one the number of equations to be solved, and in the process eliminates the pressure term. The axial and radial velocity distribution, if required, can also be calculated.

Governing Equations

The governing equations have been developed in Appendix A and are given in their final form below.

a) Vorticity Equation

$$\frac{\partial}{\partial x} \left(\omega \frac{\partial \psi}{\partial y} \right) - \frac{\partial}{\partial y} \left(\omega \frac{\partial \psi}{\partial x} \right) - \frac{1}{\rho} \left\{ \frac{\partial}{\partial x} \left[\frac{\partial}{\partial x} (\mu \omega) \right] + \frac{\partial}{\partial y} \left[\frac{\partial}{\partial y} (\mu \omega) \right] \right\} = 0 \quad (1)$$

b) Stream Function Equation

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = \omega \quad (2)$$

c) Swirl Velocity Equation

$$\frac{\partial}{\partial x} (w \frac{\partial \psi}{\partial y}) - \frac{\partial}{\partial y} (w \frac{\partial \psi}{\partial x}) - \frac{1}{\rho} \left\{ \frac{\partial}{\partial x} (\mu \frac{\partial w}{\partial x}) + \frac{\partial}{\partial y} (\mu \frac{\partial w}{\partial y}) + \frac{\partial p}{\partial r} \right\} = 0 \quad (3)$$

d) Turbulent Energy Equation

$$\rho \left\{ \frac{\partial}{\partial x} (k \frac{\partial \psi}{\partial y}) - \frac{\partial}{\partial y} (k \frac{\partial \psi}{\partial x}) \right\} - \frac{\partial}{\partial x} (\Gamma_k \frac{\partial k}{\partial x}) - \frac{\partial}{\partial y} (\Gamma_k \frac{\partial k}{\partial y}) - S_k = 0 \quad (4)$$

e) Dissipation Function Equation

$$\rho \left\{ \frac{\partial}{\partial x} (\epsilon \frac{\partial \psi}{\partial y}) - \frac{\partial}{\partial y} (\epsilon \frac{\partial \psi}{\partial x}) \right\} - \frac{\partial}{\partial x} (\Gamma_\epsilon \frac{\partial \epsilon}{\partial x}) - \frac{\partial}{\partial y} (\Gamma_\epsilon \frac{\partial \epsilon}{\partial y}) - S_\epsilon = 0 \quad (5)$$

where

$$S_k = P_s - \rho \epsilon \quad S_\epsilon = \frac{\epsilon}{k} (C_1 P_s - C_2 \rho \epsilon) \quad (6)$$

$$P_s = \mu_t \left[2 \left\{ \left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial x} \right)^2 \right\} + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 + \left(\frac{\partial w}{\partial x} \right)^2 + \left(\frac{\partial w}{\partial y} \right)^2 \right] \quad (7)$$

All the above equations can be put into the general form given below. The values of the parameters a, b, c and d for the different variables (vorticity, stream function, swirl velocity, turbulent energy and dissipation function), denoted by ϕ , are given in Table 1.

$$a_\phi \left\{ \frac{\partial}{\partial x} (\phi \frac{\partial \psi}{\partial y}) - \frac{\partial}{\partial y} (\phi \frac{\partial \psi}{\partial x}) \right\} - \frac{\partial}{\partial x} \left\{ b_\phi \frac{\partial}{\partial x} (c_\phi \phi) \right\} - \frac{\partial}{\partial y} \left\{ b_\phi \frac{\partial}{\partial y} (c_\phi \phi) \right\} + d_\phi = 0 \quad (8)$$

Solution Procedure

In the solution procedure attention is confined to a finite array of points distributed throughout the flow field as the nodal points of a grid. The above differential equations are reduced to a set of simultaneous, algebraic finite difference equations which relate the values of the variables at each node to the values prevailing at the neighbouring nodes. These difference equations are then solved by an iterative procedure using the Gauss-Seidel method, wherein the new values of the variable under consideration is used as it becomes available. This produced a rapid rate of

convergence, thereby reducing the computer time. The convergence of the equations is indicated when the maximum value of the residual defined as

$$\text{Residual} = 1 - \frac{\phi_P^{(N-1)}}{\phi_P^{(N)}}$$

falls below the reference value of 0.0001. The final value of the stream function is then printed out.

a) Grid nodes and notation--Fig. 1 shows some of the internal grid nodes. The intersection of the solid lines mark the grid nodes where all the variables (ω , ψ , w , k , ϵ , μ_t and μ_{eff}) are stored. The dotted line outlines the area associated with a grid node, say P, and the control volume for the node is composed of this area together with a depth of unity into the page. As this depth is common to all terms concerned with volumes, it is suppressed in the subsequent discussion and the computer program. The distance between the grid nodes in the axial direction is kept constant, except for a small region in the center, while that in the radial direction is gradually expanded/contracted on the grounds of accuracy and economy. A fine mesh is used near the wall. In the program we consider a vertical section covering one half of the diffuser. A 27 x 36 rectangular mesh is employed during the calculation.

Finite Difference Equation--The finite difference equation is formed by transforming the general differential equation (Eqn. 8) by integrating it over the control volume for the ϕ in question, and then expressing the resulting forms through grid point values. In the transformation it is assumed that ϕ is located at point P for the control volume marked. This development is shown in Appendix B. When the convection and diffusion terms, labelled (i) to (iv) in Eqn. B2, are integrated over the control volume they give rise to the integral of convection and diffusion fluxes

across the control volume surface, via application of Gauss divergence theorem. A proper representation of these terms is essential to the accuracy and convergence of the numerical procedure. This code employs the "upwind-differencing" scheme for the formation of the difference equation. This scheme has a first order accuracy, but its use for the first order terms of the equation causes the stability of the solution procedure to be far greater than could be obtained by using central-differencing scheme, which has a second order accuracy. This is true especially for high Reynolds number flows. However, it has been found that upwind-differencing (as well as all schemes associated with one-sided differencing) gives rise to a false diffusion of ϕ into the equations. The importance of this false diffusion is related to the ratio of Γ_{false} to Γ_{eff} , which is written as

$$\frac{\Gamma_{\text{false}}}{\Gamma_{\text{eff}}} \approx 0.36 R_{\text{loc}} \sigma_{\text{eff}} \left(\frac{\mu_{\text{lam}}}{\mu_{\text{eff}}} \right) \left(\frac{h}{L} \right) \sin(2\alpha)$$

where R_{loc} is the Reynolds number ($\rho VL/\mu$) based on a typical length L .

From the above we see that Γ_{false} is important only for laminar flow, as in the case of turbulent flows $\sigma_{\text{eff}} \approx 1$ and $\mu_{\text{eff}} \gg \mu_{\text{lam}}$. Thus it is not incorporated in the present code, thereby limiting the applicability of the code to turbulent flows.

The general difference equation is given below.

$$\begin{aligned} & A_E(\phi_P - \phi_E) + A_W(\phi_P - \phi_W) + A_N(\phi_P - \phi_N) + A_S(\phi_P - \phi_S) \\ & - B_E(c_{\phi E} \phi_E - c_{\phi P} \phi_P) - B_W(c_{\phi W} \phi_W - c_{\phi P} \phi_P) - B_N(c_{\phi N} \phi_N - c_{\phi P} \phi_P) \\ & - B_S(c_{\phi S} \phi_S - c_{\phi P} \phi_P) - d_{\phi P} V_P = 0 \end{aligned} \quad (9)$$

This algebraic equation is then transformed to the successive-substitution formula, which is solved iteratively for each of the Eqns. (1) to (5). The

successive-substitution formula is written as

$$\phi_P = C_E' \phi_E + C_W' \phi_W + C_N' \phi_N + C_S' \phi_S - d_{\phi P} / \Sigma_{AB}' \quad (10)$$

where

$$C_i' = (A_i' + B_i' c_{\phi i}) / \Sigma_{AB}'$$

$$\Sigma_{AB}' = A_E' + A_W' + A_N' + A_S' + c_{\phi P} (B_E' + B_W' + B_N' + B_S').$$

Boundary Conditions--The boundary conditions for the stream function equation are relatively simple as the stream function must have a constant value along the length of an impermeable wall. This value may be zero or any other fixed value. Similarly, the center-line value is fixed. The inflow and outflow boundaries are specified as

$$\psi(1,J) = \psi(2,J) \quad \text{and} \quad \psi(IMAX-1,J) = \psi(IMAX,J)$$

The vorticity boundary conditions are very important, as vorticity is produced at the no slip boundary, and it is the diffusion and subsequent advection of this wall produced vorticity which actually drives the problem. The relations given below and recommended in Ref. 2 are used in the code. For the straight portion of the diffuser

$$\omega_w = \frac{3(\psi_{w+1} - \psi_w)}{\Delta n^2} - \frac{1}{2} \omega_{w+1}$$

where w denotes the wall boundary, and Δn^2 is the distance normal to the wall.

For the curved portion of the diffuser

$$\omega_{iw,jw} = \frac{2\psi_{iw-1,jw} + \psi_{iw,jw+1} - 2\psi_{iw,jw}}{\Delta n^2}$$

where $\Delta n^2 = \frac{\Delta x^2}{1 + \beta^2}$ and $\beta = \frac{\Delta x}{\Delta y}$

The vorticity value at the center-line is taken as zero, because of the symmetric nature of the problem, and the inflow and outflow boundary is

denoted by

$$\omega(1,J) = \omega(2,J) \quad \text{and} \quad \omega(IMAX-1,J) = \omega(IMAX, J)$$

The swirl velocity in the immediate vicinity of a solid wall is equal to that of the wall itself. Thus, in our case, w has a value of zero along the wall boundary as well as along the center line boundary. The inflow and outflow boundaries are represented by

$$w(1,J) = w(2,J) \quad \text{and} \quad w(IMAX,J) = w(IMAX-1, J)$$

For the turbulence equations the wall values are difficult to generate. Secondly, for ease of computation, the computation is not carried out at or near the wall nodes. In the code the following wall functions are employed for calculating the value of k and ϵ at the near-wall nodes. If p denotes the near wall nodes, then

$$k_p = \frac{(\tau/\rho)_w}{C_\mu^{1/2}} \quad \text{and} \quad \epsilon = \frac{C_\mu^{3/4} k_p^{3/2}}{\kappa y_p}$$

where $\tau_w = \frac{U_\tau}{y} \sim \frac{\mu y^+}{\ln(Ey^+)} \quad \text{and} \quad y^+ = \rho k^{1/2} C_\mu^{1/4} \frac{y}{\mu}.$

The centerline line, inflow and outflow boundaries are all denoted by

$$\phi(1,J) = \phi(2,J) \quad \phi(IMAX, J) = \phi(IMAX-1,J)$$

$$\phi(I,1) = \phi(I,2)$$

Nomenclature used in the text

a, b, c	Coefficients in the modified general elliptic equation
c_1, c_2	Constants in the source term for the dissipation function
C_D	Constant in the source term for the turbulent energy
D	Source term in the general substitution formula
d	Source term in the modified general equation
$\vec{F}$	Body force acting on the fluid
k	Turbulent energy
p	Pressure
P_s	A function in the source terms for k and ϵ
u	Axial velocity
URF	Under-relaxation factor
v	Velocity in the r -direction, or radial velocity
V_P	Volume associated with a grid node P
w	Swirl velocity
ω	Vorticity
ψ	Stream function
ϵ	Dissipation function
μ	Effective viscosity (turbulent + laminar)
μ_t	Turbulent viscosity
ρ	Density
τ	Shear stress
Γ	Effective exchange coefficient = μ/σ
σ	Effective Schmidt number
ϕ	Any general variable

Nomenclature used in Computer Program

AE,AW,AN,AS	Convection coefficients for the successive-substitution formula
BE,BW,BN,BS	Diffusion coefficients for the successive-substitution formula
CAPPA	A constant in the turbulence equations
CMU,CD,C1,C2	Constants in the equations for k and ϵ
DEN	Density of the fluid
ELOG	A constant in the turbulence equations
EPS	Dissipation function
IMAX,JMAX	Maximum values of the grid nodes in x- and y-directions
MUREF	Laminar viscosity
P	Pressure
PS	A function in the source term for k and ϵ
RE	Reynold's number
RSVT,RSSF, RSW,RSEPS, RSTE	The maximum value of the residual, during each iteration, for vorticity, stream function, swirl velocity, dissipation function and turbulent energy respectively
SIGTE,SIGEPS	Effective Schmidt number for k and ϵ respectively
SRFN	Stream function
SWNB	Swirl number
T	Temperature
TE	Turbulent energy
TAU	Shear stress
TVIS	Turbulent viscosity
UVEL	Axial velocity
URFVT,URFSF, URFW,URFEP, URFTE,URFVIS	Under-relaxation factors for vorticity, stream-function, swirl velocity, dissipation function, turbulent energy and effective viscosity, respectively

VORT	.Vorticity
VANE	Angle of the vanes producing the swirl
VISCOS	Effective viscosity
W	Swirl velocity

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Flow Chart for Each Equation

Appendix A

The Governing Equations in Cartesian Co-ordinates (x,y,z)

The Vorticity Equation:

The general Navier Stokes equation is given as

$$\rho \frac{D\vec{V}}{Dt} = \vec{F} - \nabla p + \nabla \cdot \vec{\tau}$$

where ρ = density of the fluid p = pressure

$\vec{V}$ = velocity $\vec{F}$ = body force $\vec{\tau}$ = stress

For a 2-D (x,y) case we have, with $\vec{V} = \hat{i}u + \hat{j}v + \hat{k}w$

$$\rho \left\{ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right\} = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} \quad (A1)$$

$$\rho \left\{ \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right\} = -\frac{\partial p}{\partial y} + \frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} \quad (A2)$$

$$\text{Now } \tau_{xx} = -p + 2\mu \frac{\partial u}{\partial x} \quad \tau_{yy} = -p + 2\mu \frac{\partial v}{\partial y} \quad \tau_{xy} = \tau_{yx} = \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)$$

$$\text{Then } \frac{\partial \tau_{xx}}{\partial x} = -\frac{\partial p}{\partial x} + 2 \left(\frac{\partial u}{\partial x} \cdot \frac{\partial u}{\partial x} + \mu \frac{\partial^2 u}{\partial x^2} \right)$$

$$\frac{\partial \tau_{yy}}{\partial y} = -\frac{\partial p}{\partial y} + 2 \left(\frac{\partial v}{\partial y} \cdot \frac{\partial v}{\partial y} + \mu \frac{\partial^2 v}{\partial y^2} \right)$$

$$\frac{\partial \tau_{xy}}{\partial x} = \frac{\partial \mu}{\partial x} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) + \mu \left(\frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 v}{\partial x^2} \right)$$

$$\frac{\partial \tau_{xy}}{\partial y} = \frac{\partial \mu}{\partial y} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) + \mu \left(\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 v}{\partial x \partial y} \right)$$

$$\text{For a steady-state case } \frac{\partial u}{\partial t} = \frac{\partial v}{\partial t} = 0$$

Here the density is a constant. Then substituting in Eqn. (A1) and (A2)

$$\rho\left\{u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right\} = -\frac{\partial p}{\partial x} - \frac{\partial p}{\partial x} + 2\left(\frac{\partial u}{\partial x} \cdot \frac{\partial u}{\partial x} + \mu\frac{\partial^2 u}{\partial x^2}\right) + \frac{\partial u}{\partial y}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) + \mu\left(\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 v}{\partial x \partial y}\right) \quad (A3)$$

$$\rho\left\{u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y}\right\} = -\frac{\partial p}{\partial y} - \frac{\partial p}{\partial y} + 2\left(\frac{\partial u}{\partial y} \cdot \frac{\partial v}{\partial y} + \mu\frac{\partial^2 v}{\partial y^2}\right) + \frac{\partial u}{\partial x}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) + \mu\left(\frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 v}{\partial x^2}\right) \quad (A4)$$

Eliminate the pressure from the above equations by differentiating (A3) with respect to y and (A4) with respect to x and subtracting.

$$\begin{aligned} \rho\left\{\frac{\partial}{\partial y}\left(u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right) - \frac{\partial}{\partial x}\left(u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y}\right)\right\} &= -2\frac{\partial^2 p}{\partial x \partial y} + 2\frac{\partial}{\partial y}\left(\frac{\partial u}{\partial x} \cdot \frac{\partial u}{\partial x} + \mu\frac{\partial^2 u}{\partial x^2}\right) \\ &+ \frac{\partial}{\partial y}\left\{\frac{\partial u}{\partial y}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) + \mu\left(\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 v}{\partial x \partial y}\right)\right\} + 2\frac{\partial^2 p}{\partial x \partial y} - 2\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial y} \cdot \frac{\partial v}{\partial y} + \mu\frac{\partial^2 v}{\partial y^2}\right) \\ &- \frac{\partial}{\partial x}\left\{\frac{\partial u}{\partial x}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) + \mu\left(\frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 v}{\partial x^2}\right)\right\} \end{aligned}$$

$$\text{Defining vorticity } \omega = \frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} \quad u = \frac{\partial \psi}{\partial y} \quad v = -\frac{\partial \psi}{\partial x}$$

$$\begin{aligned} \text{L.H.S} &= \rho\left[\frac{\partial u}{\partial y} \cdot \frac{\partial u}{\partial x} + u\frac{\partial^2 u}{\partial x \partial y} + \frac{\partial v}{\partial y} \cdot \frac{\partial u}{\partial y} + v\frac{\partial^2 u}{\partial y^2} - \frac{\partial u}{\partial x} \cdot \frac{\partial v}{\partial x} - u\frac{\partial^2 v}{\partial x^2} - \frac{\partial v}{\partial x} \cdot \frac{\partial v}{\partial y} - v\frac{\partial^2 v}{\partial x \partial y}\right] \\ &= \rho\left[\frac{\partial u}{\partial x}\left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}\right) + \frac{\partial v}{\partial y}\left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}\right) + u\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}\right) + v\frac{\partial}{\partial y}\left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}\right)\right] \\ &= \rho\left[\frac{\partial u}{\partial x}(\omega) + \frac{\partial v}{\partial y}(\omega) + u\frac{\partial}{\partial x}(\omega) + v\frac{\partial}{\partial y}(\omega)\right] \\ &= \rho\left[\frac{\partial}{\partial x}(\omega u) + \frac{\partial}{\partial y}(\omega v)\right] \\ &= \rho\left[\frac{\partial}{\partial x}(\omega\frac{\partial \psi}{\partial y}) - \frac{\partial}{\partial y}(\omega\frac{\partial \psi}{\partial x})\right] \end{aligned}$$

$$\begin{aligned} \text{R.H.S} &= -2\frac{\partial^2 p}{\partial x \partial y} + 2\left(\frac{\partial^2 u}{\partial x \partial y} \cdot \frac{\partial u}{\partial x} + \frac{\partial u}{\partial x} \cdot \frac{\partial^2 u}{\partial x \partial y} + \frac{\partial u}{\partial y} \cdot \frac{\partial^2 u}{\partial x^2} + \mu\frac{\partial^2 u}{\partial x^2 \partial y}\right) + \frac{\partial^2 u}{\partial y^2} \cdot \frac{\partial u}{\partial y} \\ &+ \frac{\partial u}{\partial y} \cdot \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial y^2} \cdot \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \cdot \frac{\partial^2 v}{\partial x \partial y} + \frac{\partial u}{\partial y}\left(\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 v}{\partial x \partial y}\right) + \mu\left(\frac{\partial^3 u}{\partial y^3} + \frac{\partial^3 v}{\partial x \partial y^2}\right) \end{aligned}$$

$$\begin{aligned}
 & + 2 \frac{\partial^2 p}{\partial x \partial y} - 2 \left(\frac{\partial^2 u}{\partial x \partial y} \cdot \frac{\partial v}{\partial y} + \frac{\partial u}{\partial y} \cdot \frac{\partial^2 v}{\partial x \partial y} + \frac{\partial u}{\partial x} \cdot \frac{\partial^2 v}{\partial y^2} + \mu \frac{\partial^3 v}{\partial x \partial y^2} \right) - \left\{ \frac{\partial^2 u}{\partial x^2} \cdot \frac{\partial u}{\partial y} \right. \\
 & + \frac{\partial u}{\partial x} \cdot \frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 u}{\partial x^2} \cdot \frac{\partial v}{\partial x} + \frac{\partial u}{\partial x} \cdot \frac{\partial^2 v}{\partial x^2} + \frac{\partial u}{\partial x} \left(\frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 v}{\partial x^2} \right) + \mu \left(\frac{\partial^3 u}{\partial x^2 \partial y} + \frac{\partial^3 v}{\partial x^3} \right) \Big\} \\
 & = -2 \frac{\partial^2 p}{\partial x \partial y} + 2 \frac{\partial^2 u}{\partial x \partial y} \cdot \frac{\partial u}{\partial x} + 2 \frac{\partial u}{\partial x} \cdot \frac{\partial^2 u}{\partial x \partial y} + 2 \frac{\partial u}{\partial y} \cdot \frac{\partial^2 u}{\partial x^2} + 2 \mu \frac{\partial^3 u}{\partial x^2 \partial y} + \frac{\partial^2 u}{\partial y^2} \cdot \frac{\partial u}{\partial y} \\
 & - \frac{\partial^2 u}{\partial x^2} \cdot \frac{\partial u}{\partial y} + 2 \frac{\partial^2 p}{\partial x \partial y} - 2 \frac{\partial^2 u}{\partial x \partial y} \cdot \frac{\partial v}{\partial y} - 2 \frac{\partial u}{\partial x} \cdot \frac{\partial^2 v}{\partial y^2} + \frac{\partial u}{\partial y} \cdot \frac{\partial^2 u}{\partial y^2} + \mu \frac{\partial^3 u}{\partial y^3} \\
 & + \frac{\partial^2 u}{\partial y^2} \cdot \frac{\partial v}{\partial x} - \frac{\partial^2 u}{\partial x^2} \cdot \frac{\partial v}{\partial x} - \frac{\partial u}{\partial x} \cdot \frac{\partial^2 u}{\partial x \partial y} + \frac{\partial u}{\partial y} \cdot \frac{\partial^2 v}{\partial x \partial y} + \mu \frac{\partial^3 v}{\partial x \partial y^2} - \frac{\partial u}{\partial x} \cdot \frac{\partial^2 v}{\partial x^2} \\
 & + \frac{\partial u}{\partial y} \cdot \frac{\partial^2 u}{\partial y^2} - 2 \mu \frac{\partial^3 v}{\partial x \partial y^2} - \frac{\partial u}{\partial x} \cdot \frac{\partial^2 u}{\partial x \partial y} + \frac{\partial u}{\partial y} \cdot \frac{\partial^2 v}{\partial x \partial y} - \mu \frac{\partial^3 u}{\partial x^2 \partial y} - \frac{\partial u}{\partial x} \cdot \frac{\partial^2 v}{\partial x^2} \\
 & - 2 \frac{\partial u}{\partial y} \cdot \frac{\partial^2 v}{\partial x \partial y} - \mu \frac{\partial^3 v}{\partial x^3}
 \end{aligned}$$

$$\begin{aligned}
 1 & \equiv \frac{\partial u}{\partial x} \cdot \frac{\partial^2 u}{\partial x \partial y} + \mu \frac{\partial^3 u}{\partial x^2 \partial y} = \frac{\partial}{\partial x} \left[\mu \frac{\partial^2 u}{\partial x \partial y} \right] \\
 2 & \equiv -\frac{\partial u}{\partial x} \cdot \frac{\partial^2 v}{\partial x^2} - \mu \frac{\partial^3 v}{\partial x^3} = -\frac{\partial}{\partial x} \left[\mu \frac{\partial^2 v}{\partial x^2} \right] \\
 3 & \equiv \frac{\partial u}{\partial x} \cdot \frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 u}{\partial x^2} \cdot \frac{\partial u}{\partial y} - \frac{\partial^2 u}{\partial x^2} \cdot \frac{\partial u}{\partial y} \\
 & = \frac{\partial}{\partial x} \left[\frac{\partial u}{\partial x} \cdot \frac{\partial u}{\partial y} \right] - \frac{\partial^2 u}{\partial x^2} \cdot \frac{\partial u}{\partial y} \\
 4 & \equiv -\frac{\partial u}{\partial x} \cdot \frac{\partial^2 v}{\partial x^2} - \frac{\partial^2 u}{\partial x^2} \cdot \frac{\partial v}{\partial x} = -\frac{\partial}{\partial x} \left[\frac{\partial u}{\partial x} \cdot \frac{\partial v}{\partial x} \right] \\
 5 & \equiv \frac{\partial u}{\partial y} \cdot \frac{\partial^2 u}{\partial y^2} + \mu \frac{\partial^3 u}{\partial y^3} = \frac{\partial}{\partial y} \left[\mu \frac{\partial^2 u}{\partial y^2} \right] \\
 6 & \equiv -\frac{\partial u}{\partial y} \cdot \frac{\partial^2 v}{\partial x \partial y} - \mu \frac{\partial^3 v}{\partial x \partial y^2} = -\frac{\partial}{\partial y} \left[\mu \frac{\partial^2 v}{\partial x \partial y} \right]
 \end{aligned}$$

$\frac{\partial}{\partial x} \left[\mu \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} \right) \right] \equiv \frac{\partial}{\partial x} \left[\mu \frac{\partial \omega}{\partial x} \right]$

$\frac{\partial}{\partial x} \left[\frac{\partial u}{\partial x} \left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} \right) \right] - \frac{\partial^2 u}{\partial x^2} \cdot \frac{\partial u}{\partial y}$

$\equiv \frac{\partial}{\partial u} \left[\frac{\partial u}{\partial x} \cdot \omega \right] - \frac{\partial^2 u}{\partial x^2} \cdot \frac{\partial u}{\partial y}$

$\frac{\partial}{\partial y} \left[\mu \frac{\partial}{\partial y} \left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} \right) \right] \equiv \frac{\partial}{\partial y} \left[\mu \frac{\partial \omega}{\partial y} \right]$

$$\begin{aligned}
 7 &= \frac{\partial \mu}{\partial y} \cdot \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 \mu}{\partial y^2} \cdot \frac{\partial u}{\partial y} = \frac{\partial}{\partial y} \left[\frac{\partial \mu}{\partial y} \cdot \frac{\partial u}{\partial y} \right] \\
 8 &= -\frac{\partial \mu}{\partial y} \cdot \frac{\partial^2 v}{\partial x \partial y} - \frac{\partial^2 \mu}{\partial y^2} \cdot \frac{\partial v}{\partial x} + \frac{\partial^2 \mu}{\partial y^2} \cdot \frac{\partial v}{\partial x} \\
 &= + \frac{\partial}{\partial y} \left[-\frac{\partial \mu}{\partial y} \cdot \frac{\partial v}{\partial x} \right] + \frac{\partial^2 \mu}{\partial y^2} \cdot \frac{\partial v}{\partial x}
 \end{aligned}$$

$$\begin{aligned}
 &\frac{\partial}{\partial y} \left[\frac{\partial \mu}{\partial y} \left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} \right) \right] + \frac{\partial^2 \mu}{\partial y^2} \cdot \frac{\partial v}{\partial x} \\
 &= \frac{\partial}{\partial y} \left[\frac{\partial \mu}{\partial y} (\omega) \right] + \frac{\partial^2 \mu}{\partial y^2} \cdot \frac{\partial v}{\partial x}
 \end{aligned}$$

Then

$$\begin{aligned}
 \text{R.H.S} &= \frac{\partial}{\partial x} \left(\mu \frac{\partial \omega}{\partial x} \right) + \frac{\partial}{\partial x} \left[\frac{\partial \mu}{\partial x} (\omega) \right] + \frac{\partial}{\partial y} \left[\mu \frac{\partial \omega}{\partial y} \right] + \frac{\partial}{\partial y} \left[\frac{\partial \mu}{\partial y} (\omega) \right] + \text{Rem} \\
 &= \frac{\partial}{\partial x} \left[\frac{\partial}{\partial x} (\mu \omega) \right] + \frac{\partial}{\partial y} \left[\frac{\partial}{\partial y} (\mu \omega) \right] + \text{Rem}
 \end{aligned}$$

where

$$\begin{aligned}
 2 \text{ Rem} &= \frac{\partial^2 \mu}{\partial x \partial y} \cdot \frac{\partial u}{\partial x} - \frac{\partial^2 \mu}{\partial x \partial y} \cdot \frac{\partial v}{\partial y} - \frac{\partial \mu}{\partial x} \cdot \frac{\partial^2 v}{\partial y^2} - \frac{\partial \mu}{\partial x} \cdot \frac{\partial^2 u}{\partial x \partial y} + \frac{\partial \mu}{\partial y} \cdot \frac{\partial^2 u}{\partial x^2} \\
 &\quad + \frac{\partial \mu}{\partial y} \cdot \frac{\partial^2 v}{\partial x \partial y} + \frac{\partial^2 \mu}{\partial y^2} \cdot \frac{\partial v}{\partial x} - \frac{\partial^2 \mu}{\partial x^2} \cdot \frac{\partial u}{\partial y} \\
 &= -\frac{\partial \mu}{\partial x} \left[\frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 u}{\partial x \partial y} \right] + \frac{\partial \mu}{\partial y} \left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 v}{\partial x \partial y} \right] + \frac{\partial^2 \mu}{\partial x \partial y} \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right) + \frac{\partial^2 \mu}{\partial y^2} \cdot \frac{\partial v}{\partial x} - \frac{\partial^2 \mu}{\partial x^2} \cdot \frac{\partial u}{\partial y} \\
 &= -\frac{\partial \mu}{\partial x} \left[\frac{\partial}{\partial y} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right] + \frac{\partial \mu}{\partial y} \left[\frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right] + \frac{\partial^2 \mu}{\partial x \partial y} \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right) + \frac{\partial^2 \mu}{\partial y^2} \cdot \frac{\partial v}{\partial x} - \frac{\partial^2 \mu}{\partial x^2} \cdot \frac{\partial u}{\partial y} \\
 &= \frac{\partial^2 \mu}{\partial x \partial y} \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right) + \frac{\partial^2 \mu}{\partial y^2} \cdot \frac{\partial v}{\partial x} - \frac{\partial^2 \mu}{\partial x^2} \cdot \frac{\partial u}{\partial y}
 \end{aligned}$$

where we see that the Rem is negligible.

$$\text{Hence } \rho \left[\frac{\partial}{\partial x} \left(\omega \frac{\partial \psi}{\partial y} \right) - \frac{\partial}{\partial y} \left(\omega \frac{\partial \psi}{\partial x} \right) \right] = \frac{\partial}{\partial x} \left[\frac{\partial}{\partial x} (\mu \omega) \right] + \frac{\partial}{\partial y} \left[\frac{\partial}{\partial y} (\mu \omega) \right]$$

$$\text{or } \frac{\partial}{\partial x} \left(\omega \frac{\partial \psi}{\partial y} \right) - \frac{\partial}{\partial y} \left(\omega \frac{\partial \psi}{\partial x} \right) - \frac{1}{\rho} \left\{ \frac{\partial}{\partial x} \left[\frac{\partial}{\partial x} (\mu \omega) \right] + \frac{\partial}{\partial y} \left[\frac{\partial}{\partial y} (\mu \omega) \right] \right\} = 0 \quad (\text{A5})$$

Turbulence Equations:

The $k - \epsilon$ model of turbulence is employed, and the governing equations are as given by S.B. Pope in his paper, "Calculation of Separated Boundary Layers."

$$\frac{\partial \rho \epsilon}{\partial t} + \frac{\partial \rho u_i \epsilon}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\mu_{eff}}{\sigma_\epsilon} \cdot \frac{\partial \epsilon}{\partial x_i} \right) + \frac{\epsilon}{k} (C_1 P_S - C_2 \rho \epsilon) \quad (A6)$$

$$\frac{\partial \rho k}{\partial t} + \frac{\partial \rho u_i k}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\mu_{eff}}{\sigma_k} \cdot \frac{\partial k}{\partial x_i} \right) + P_S - \rho \epsilon \quad (A7)$$

where $P_S = \frac{\partial u_i}{\partial x_j} \tau_{ij}$

Writing $\frac{\mu_{eff}}{\sigma_i} = \Gamma_i$ $s_\epsilon = \frac{\epsilon}{k} (C_1 P_S - C_2 \rho \epsilon)$ $s_k = P_S - \rho \epsilon$ $\frac{\partial}{\partial t} = 0$

we obtain

$$\frac{\partial}{\partial x} (u \rho \epsilon) + \frac{\partial}{\partial y} (v \rho \epsilon) = \frac{\partial}{\partial x} \left(\Gamma_\epsilon \frac{\partial \epsilon}{\partial x} \right) + \frac{\partial}{\partial y} \left(\Gamma_\epsilon \frac{\partial \epsilon}{\partial y} \right) + s_\epsilon \quad (A8)$$

$$\frac{\partial}{\partial x} (u \rho k) + \frac{\partial}{\partial y} (v \rho k) = \frac{\partial}{\partial x} \left(\Gamma_k \frac{\partial k}{\partial x} \right) + \frac{\partial}{\partial y} \left(\Gamma_k \frac{\partial k}{\partial y} \right) + s_k \quad (A9)$$

Writing u and v in terms of stream function ψ , we obtain

$$\rho \left\{ \frac{\partial}{\partial x} \left(\epsilon \frac{\partial \psi}{\partial y} \right) - \frac{\partial}{\partial y} \left(\epsilon \frac{\partial \psi}{\partial x} \right) \right\} - \frac{\partial}{\partial x} \left(\Gamma_\epsilon \frac{\partial \epsilon}{\partial x} \right) - \frac{\partial}{\partial y} \left(\Gamma_\epsilon \frac{\partial \epsilon}{\partial y} \right) - s_\epsilon = 0 \quad (A10)$$

$$\rho \left\{ \frac{\partial}{\partial x} \left(k \frac{\partial \psi}{\partial y} \right) - \frac{\partial}{\partial y} \left(k \frac{\partial \psi}{\partial x} \right) \right\} - \frac{\partial}{\partial x} \left(\Gamma_k \frac{\partial k}{\partial x} \right) - \frac{\partial}{\partial y} \left(\Gamma_k \frac{\partial k}{\partial y} \right) - s_k = 0 \quad (A11)$$

Next we will evaluate the value of P_S .

$$P_S = \frac{\partial u}{\partial x} \tau_{xx} + \frac{\partial u}{\partial y} \tau_{xy} + \frac{\partial v}{\partial x} \tau_{yx} + \frac{\partial v}{\partial y} \tau_{yy} + \frac{\partial w}{\partial x} \tau_{xz} + \frac{\partial w}{\partial y} \tau_{yz}$$

Now

$$\tau_{xx} = -p + 2\mu \frac{\partial u}{\partial x} \quad \tau_{yy} = -p + 2\mu \frac{\partial v}{\partial y} \quad \tau_{yx} = \tau_{xy} = \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)$$

$$\tau_{xz} = \mu \frac{\partial w}{\partial x} \quad \tau_{yz} = \mu \frac{\partial w}{\partial y}$$

Thus

$$\begin{aligned}
 P_s &= \frac{\partial u}{\partial x}(-p + 2\mu_t \frac{\partial u}{\partial x}) + \frac{\partial u}{\partial y} \{ \mu_t (\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}) \} + \frac{\partial v}{\partial x} \{ \mu_t (\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}) \} + \frac{\partial v}{\partial y}(-p + 2\mu_t \frac{\partial v}{\partial y}) \\
 &\quad + \frac{\partial w}{\partial x}(\mu_t \frac{\partial w}{\partial x}) + \frac{\partial w}{\partial y}(\mu_t \frac{\partial w}{\partial y}) \\
 &= -p(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}) + 2\mu_t \{ (\frac{\partial u}{\partial x})^2 + (\frac{\partial v}{\partial y})^2 \} + \mu_t \{ (\frac{\partial u}{\partial y})^2 + 2\frac{\partial u}{\partial y} \cdot \frac{\partial v}{\partial x} + (\frac{\partial v}{\partial x})^2 \} \\
 &\quad + \mu_t \{ (\frac{\partial w}{\partial x})^2 + (\frac{\partial w}{\partial y})^2 \} \\
 &= \mu_t [2\{ (\frac{\partial u}{\partial x})^2 + (\frac{\partial v}{\partial y})^2 \} + (\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x})^2 + (\frac{\partial w}{\partial x})^2 + (\frac{\partial w}{\partial y})^2] \\
 &= \mu_t [2\{ [\frac{\partial}{\partial x}(\frac{\partial \psi}{\partial y})]^2 + [\frac{\partial}{\partial y}(\frac{\partial \psi}{\partial x})]^2 + \{ \frac{\partial}{\partial y}(\frac{\partial \psi}{\partial y}) - \frac{\partial}{\partial x}(\frac{\partial \psi}{\partial x}) \}^2 + (\frac{\partial w}{\partial x})^2 + (\frac{\partial w}{\partial y})^2 \}] \quad (A12)
 \end{aligned}$$

Swirl Velocity Equation:

From the Navier-Stokes Equation we have

$$\rho \{ u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} \} = \vec{F} - \frac{\partial p}{\partial r} + \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y}$$

when $r^2 = x^2 + y^2$. Now the components of the body force due to the swirl velocity are $-\rho w \frac{\partial u}{\partial x}$ and $-\rho w \frac{\partial v}{\partial y}$ in the x and y directions. Thus,

$$\begin{aligned}
 \rho \{ u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} \} &= -\rho w \frac{\partial u}{\partial x} - \rho w \frac{\partial v}{\partial y} - \frac{\partial p}{\partial r} + \frac{\partial}{\partial x}(\mu \frac{\partial w}{\partial x}) + \frac{\partial}{\partial y}(\mu \frac{\partial w}{\partial y}) \\
 \text{or } u \frac{\partial w}{\partial x} + w \frac{\partial u}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial v}{\partial y} - \frac{1}{\rho} \{ \frac{\partial}{\partial x}(\mu \frac{\partial w}{\partial x}) + \frac{\partial}{\partial y}(\mu \frac{\partial w}{\partial y}) + \frac{\partial p}{\partial r} \} &= 0 \\
 \text{or } \frac{\partial}{\partial x}(uw) + \frac{\partial}{\partial y}(vw) - \frac{1}{\rho} \{ \frac{\partial}{\partial x}(\mu \frac{\partial w}{\partial x}) + \frac{\partial}{\partial y}(\mu \frac{\partial w}{\partial y}) + \frac{\partial p}{\partial r} \} &= 0 \\
 \text{or } \frac{\partial}{\partial x}(w \frac{\partial \psi}{\partial y}) - \frac{\partial}{\partial y}(w \frac{\partial \psi}{\partial x}) - \frac{1}{\rho} \{ \frac{\partial}{\partial x}(\mu \frac{\partial w}{\partial x}) + \frac{\partial}{\partial y}(\mu \frac{\partial w}{\partial y}) + \frac{\partial p}{\partial r} \} &= 0 \quad (A13)
 \end{aligned}$$

Appendix B

Development of Successive-Substitution Formula

This development is similar to that in Ref. 1. The starting point is the general equation

$$a_{\phi} \left\{ \frac{\partial}{\partial x} \left(\phi \frac{\partial \psi}{\partial y} \right) - \frac{\partial}{\partial y} \left(\phi \frac{\partial \psi}{\partial x} \right) \right\} - \frac{\partial}{\partial x} \left\{ b_{\phi} \frac{\partial}{\partial x} (c_{\phi} \phi) \right\} - \frac{\partial}{\partial y} \left\{ b_{\phi} \frac{\partial}{\partial y} (c_{\phi} \phi) \right\} + d_{\phi} = 0 \quad (B1)$$

Integrating this equation over the control volume gives

$$\begin{aligned} & \int_{x,w}^{x,e} \int_{y,s}^{y,n} a_{\phi} \left\{ \frac{\partial}{\partial x} \left(\phi \frac{\partial \psi}{\partial y} \right) - \frac{\partial}{\partial y} \left(\phi \frac{\partial \psi}{\partial x} \right) \right\} dx dy - \int_{x,w}^{x,c} \int_{y,s}^{y,n} \left\{ \frac{\partial}{\partial x} \left[b_{\phi} \frac{\partial}{\partial x} (c_{\phi} \phi) \right] + \frac{\partial}{\partial y} \left[b_{\phi} \frac{\partial}{\partial y} (c_{\phi} \phi) \right] - d_{\phi} \right\} \\ & \hspace{25em} = 0 \\ \text{or } & \int_{y,s}^{y,n} a_{\phi} \left\{ \phi_e \left(\frac{\partial \psi}{\partial y} \right)_e - \phi_w \left(\frac{\partial \psi}{\partial y} \right)_w \right\} dy - \int_{x,w}^{x,e} a_{\phi} \left\{ \phi_n \left(\frac{\partial \psi}{\partial x} \right)_n - \phi_s \left(\frac{\partial \psi}{\partial x} \right)_s \right\} dx \\ & \hspace{10em} - (i) \hspace{10em} (ii) \\ & - \int_{y,s}^{y,n} \left\{ b_{\phi e} \left[\frac{\partial}{\partial x} (c_{\phi} \phi) \right]_e - b_{\phi w} \left[\frac{\partial}{\partial x} (c_{\phi} \phi) \right]_w \right\} dy - \int_{x,w}^{x,e} \left\{ b_{\phi n} \left[\frac{\partial}{\partial y} (c_{\phi} \phi) \right]_n - b_{\phi s} \left[\frac{\partial}{\partial y} (c_{\phi} \phi) \right]_s \right\} dx \\ & \hspace{10em} (iii) \hspace{10em} (iv) \\ & + \int_{x,w}^{x,e} \int_{y,s}^{y,n} d_{\phi} dx dy = 0 \hspace{15em} (B2) \\ & \hspace{10em} (v) \end{aligned}$$

In the above (i) and (ii) are the convection terms, (iii) and (iv) are the diffusion terms and (v) is the source term. Each of these terms will next be dealt with as a group.

Convection terms:--Only one of the four integrals will be evaluated as the treatment of the others will follow similar lines. Denoting the integral by I_c , we have

$$I_c = a_{\phi p} \int_{y,s}^{y,n} \phi_e \left(\frac{\partial \psi}{\partial y} \right)_e dy \quad (B3)$$

$$\text{Writing } \bar{\phi}_e \equiv \frac{\int_{y,s}^{y,n} \phi_e \left(\frac{\partial \psi}{\partial y} \right)_e dy}{\int_{y,s}^{y,n} \left(\frac{\partial \psi}{\partial y} \right)_e dy} = \frac{I_c}{a_{\phi p} (\psi_{ne} - \psi_{se})} \quad (B4)$$

where $\bar{\phi}_e$ is the average value of ϕ_e and will generally exist. In all the derivations the subscripts follow the notation of Fig. (1). Then equation (B3) may be written as

$$I_c = a_{\phi p} \bar{\phi}_e (\psi_{ne} - \psi_{se}) \quad (B5)$$

Next we have to evaluate $\bar{\phi}_e$. The following assumptions are made to simplify the task. First, ϕ is assumed uniform within each area denoted by broken lines in Fig. (1) and has the value prevailing at point P. The second assumption is that $\bar{\phi}_e$ assumes the ϕ -value possessed by the fluid upstream of the e-face of the area. This assumption indicates that the direction (and magnitude) of flow across the e-face is connected to $(\psi_{ne} - \psi_{se})$. The upwind differencing scheme, which is used here, implies that if the flow is from P to E i.e. $(\psi_{ne} - \psi_{se})$ is positive, then $\bar{\phi}_e$ must equal ϕ_p . However, if $(\psi_{ne} - \psi_{se})$ is negative i.e. the flow is from E to P, then $\bar{\phi}_e$ must equal ϕ_E . This is incorporated by writing Eqn. (B5) as

$$I_c = a_{\phi p} \left[\phi_E \left\{ \frac{(\psi_{ne} - \psi_{se}) - |\psi_{ne} - \psi_{se}|}{2} \right\} + \phi_p \left\{ \frac{(\psi_{ne} - \psi_{se}) + |\psi_{ne} - \psi_{se}|}{2} \right\} \right] \quad (B6)$$

Another assumption that is made is that the value of the stream-function at a particular corner is equal to the average of the values of the four neighboring nodes. Thus,

$$\psi_{ne} = \frac{\psi_N + \psi_E + \psi_{NE} + \psi_P}{4} \quad (B7)$$

If we write

$$A_E = a_{\phi p} [(\psi_{se} - \psi_{ne}) + |\psi_{se} - \psi_{ne}|]/2$$

then Eqn. (B6) can be written as

$$I_c \equiv A_E(\phi_p - \phi_E)$$

By performing a similar procedure for the other integrals, the expression for the sum of the integrals of all the convection terms, denoted by I_{con} , is

$$I_{con} = A_E(\phi_p - \phi_E) + A_W(\phi_p - \phi_W) + A_N(\phi_p - \phi_N) + A_S(\phi_p - \phi_S) \quad (B8)$$

where

$$\begin{aligned} A_E &= a_{\phi p} [(\psi_{se} - \psi_{ne}) + |\psi_{se} - \psi_{ne}|]/2 \\ A_W &= a_{\phi p} [(\psi_{nw} - \psi_{sw}) + |\psi_{nw} - \psi_{sw}|]/2 \\ A_N &= a_{\phi p} [(\psi_{ne} - \psi_{nw}) + |\psi_{ne} - \psi_{nw}|]/2 \\ A_S &= a_{\phi p} [(\psi_{sw} - \psi_{se}) + |\psi_{sw} - \psi_{se}|]/2 \end{aligned} \quad (B9)$$

Diffusion terms:--Here again, because of the similarity of the terms, only one integral will be developed, and the others will follow a similar pattern. Denoting the integral by I_d , we have

$$I_d = \int_{y,s}^{y,n} b_{\phi e} \left[\frac{\partial}{\partial x} (c_{\phi} \phi) \right]_e dy \quad (B10)$$

Assuming a linear variation of b_{ϕ} , c_{ϕ} and ϕ , we have

$$b_{\phi e} = \frac{b_{\phi E} + b_{\phi p}}{2} \quad \left[\frac{\partial}{\partial x} (c_{\phi} \phi) \right]_e = \frac{C_{\phi E} \phi_E - C_{\phi p} \phi_p}{x_E - x_p}$$

Eqn. (B10) may now be integrated to give

$$I_d = \frac{b_{\phi E} + b_{\phi p}}{2} \cdot \frac{C_{\phi E} \phi_E - C_{\phi p} \phi_p}{x_E - x_p} \cdot (y_n - y_s)$$

$$= \frac{b_{\phi E} + b_{\phi D}}{4} \cdot (C_{\phi E \phi E} - C_{\phi D \phi D}) \cdot \frac{y_N - y_S}{x_E - x_P} \quad (B11)$$

The expression for the sum of integrals of all the diffusion terms, denoted by I_{diff} , is

$$I_{diff} = B_E(C_{\phi E \phi E} - C_{\phi D \phi D}) + B_W(C_{\phi W \phi W} - C_{\phi D \phi D}) + B_N(C_{\phi N \phi N} - C_{\phi D \phi D}) + B_S(C_{\phi S \phi S} - C_{\phi D \phi D}) \quad (B12)$$

where

$$B_E = \frac{b_{\phi E} + b_{\phi D}}{4} \cdot \frac{y_N - y_S}{x_E - x_P} \quad B_W = \frac{b_{\phi W} + b_{\phi D}}{4} \cdot \frac{y_N - y_S}{x_P - x_W}$$

$$B_N = \frac{b_{\phi N} + b_{\phi D}}{4} \cdot \frac{x_E - x_W}{y_N - y_P} \quad B_S = \frac{b_{\phi S} + b_{\phi D}}{4} \cdot \frac{x_E - x_W}{y_P - y_S} \quad (B13)$$

Source Terms:--The final integral to be evaluated is

$$I_{sor} = \int_{y,s}^{y,n} \int_{x,w}^{x,e} d_{\phi} dx dy \quad (B14)$$

As d_{ϕ} may assume various forms according to the particular variable under study, the integration cannot be immediately performed. However, assuming that d_{ϕ} is uniform over the area of integration and takes on the value at P leads to

$$I_{sor} \approx d_{\phi P} V_P \quad (B15)$$

where

$$V_P = \left(\frac{y_N - y_S}{2} \right) \cdot \left(\frac{x_E - x_W}{2} \right) \quad (B16)$$

Successive-Substitution Formula:--By combining the above, the integration of the general differential equation (B1) results in the following algebraic equation:

$$A_E(\phi_P - \phi_E) + A_W(\phi_P - \phi_W) + A_N(\phi_P - \phi_N) + A_S(\phi_P - \phi_S) - B_E(C_{\phi E \phi E} - C_{\phi D \phi D}) - B_W(C_{\phi W \phi W} - C_{\phi D \phi D}) - B_N(C_{\phi N \phi N} - C_{\phi D \phi D}) - B_S(C_{\phi S \phi S} - C_{\phi D \phi D}) - d_{\phi P} V_P = 0 \quad (B17)$$

Then, by separating ϕ_p and simplifying, we obtain the successive-substitution formula as

$$\phi_p = C_E \phi_E + C_W \phi_W + C_N \phi_N + C_S \phi_S + D \quad (B18)$$

where

$$C_i = (A_i + B_i C_{\phi i}) / \Sigma_{AB} \quad D = -d_{\phi p} V_p / \Sigma_{AB}$$

$$\Sigma_{AB} = A_E + A_W + A_N + A_S + C_{\phi p} (B_E + B_W + B_N + B_S)$$

The above formula can be written in another form, as follows. By writing

$$A_i' = A_i / V_p \quad \text{and} \quad B_i' = B_i / V_p$$

$$\text{we have } C_i' = (A_i' + B_i' C_{\phi i}') / \Sigma_{AB}' \quad D' = -d_{\phi p} / \Sigma_{AB}'$$

$$\Sigma_{AB}' = A_E' + A_W' + A_N' + A_S' + C_{\phi p} (B_E' + B_W' + B_N' + B_S')$$

Thus

$$\phi_p \approx C_E' \phi_E + C_W' \phi_W + C_N' \phi_N + C_S' \phi_S - d_{\phi p} / \Sigma_{AB}' \quad (19)$$

Appendix C

Subroutine Tasks

Subroutine

Task

MAIN	Controls and monitors the entire sequence of calculations: computes and sets up the grid system; initialization, initial values for the variables, initial output; the iteration loop with call to update boundary values; check for residuals and intermediate output; and, after termination of the iteration loop, final output.
SOLVE	It has two chapters, the first dealing with the solution of vorticity and stream function equations, and the second with the swirl velocity equation. The convection coefficients for the successive substitution formula are obtained by a call to CONVEC, while the diffusion coefficients are assembled internally by each section.
MUTRB	Solves the equations for turbulent energy (k) and the dissipation function (ϵ), and thus provides current values of turbulent and effective viscosities. The convection coefficients are obtained by a call to CONVEC while the diffusion coefficients are internally assembled. The wall functions are employed for calculating the near-wall-node values of k and ϵ .

BOUND It has three chapters; the first dealing with the boundary values of vorticity and stream function, the second with the boundary values for k and ϕ , and the third with the boundary values of swirl velocity. The boundary values, with the exception of those for vorticity, are fixed and are not updated after each iteration. The wall vorticity is updated during each iteration by a call to BOUND(1) from MAIN.

CONVEC Calculates the volume and the convection coefficients for the successive-substitution formula.

PRINT Prints out an entire variable field according to a standard format.

Table 1

$$a_{\phi} \left\{ \frac{\partial}{\partial x} \left(\phi \frac{\partial \psi}{\partial y} \right) - \frac{\partial}{\partial y} \left(\phi \frac{\partial \psi}{\partial x} \right) \right\} - \frac{\partial}{\partial x} \left\{ b_{\phi} \frac{\partial}{\partial x} (c_{\phi} \phi) \right\} - \frac{\partial}{\partial y} \left\{ b_{\phi} \frac{\partial}{\partial y} (c_{\phi} \phi) \right\} + d_{\phi} = 0$$

ϕ	a_{ϕ}	b_{ϕ}	c_{ϕ}	d_{ϕ}
ω	ρ	1	μ_{eff}	0
ψ	0	1	1	$-\omega$
w	ρ	μ_{eff}	1	$-\frac{\partial p}{\partial r}$
k	ρ	Γ_k	1	$-S_k \equiv -P_s + \rho \epsilon$
ϵ	ρ	Γ_{ϵ}	1	$-S_{\epsilon} \equiv -c_1 P_s \frac{\epsilon}{k} + c_2 \rho \frac{\epsilon^2}{k}$

where $P_s \equiv \mu_t \left\{ 2 \left[\left\{ \frac{\partial}{\partial x} \left(\frac{\partial \psi}{\partial y} \right) \right\}^2 + \left\{ \frac{\partial}{\partial y} \left(\frac{\partial \psi}{\partial x} \right) \right\}^2 \right] + \left[\frac{\partial^2 \psi}{\partial y^2} - \frac{\partial^2 \psi}{\partial x^2} \right]^2 + \left(\frac{\partial w}{\partial x} \right)^2 + \left(\frac{\partial w}{\partial y} \right)^2 \right\}$

Fig. 1

IV. CONCLUSIONS

TASK 1. ARCING PHENOMENA IN MHD GENERATORS

- (1) Analysis of data from Test Series 1 revealed **systematic** variations of electrode voltage drops with cumulative current. Test Series 2 will investigate the nature and origin of this effect.
- (2) The spectra of fluctuations in plasma luminosity and in electrode voltages and currents were found to be very similar, and to contain harmonics of acoustic modes of the channel shell, as well as faster combustor modes. In Test Series 2, use will be made of these fast modes in an attempt to measure flow speed by a correlation technique.
- (3) Preparations for Test Series 2 (a refinement of Series 1, devoted to transition to arcing phenomena, including tests with different surface materials and higher currents) are complete. The test itself has been delayed by a malfunction of the compressed air supply system, but is expected to take place within the next reporting period.
- (4) Design is complete and construction 80% complete for Test Series 3. This will focus on interelectrode insulator performance, with a new design conceived for elimination of insulator-induced breakdown.
- (5) Tests on damage to insulators by magnetically driven arcs indicate a dramatic effect of the magnetic field on arc penetration. Arcs will be either extinguished or driven through the insulator depending on field polarity, even for $B \leq 0.2$ Tesla.
- (6) An improved channel for glycerin simulation of slag flow has been built, and preliminary (isothermal) tests run. The channel will allow bottom cooling of the layer, to simulate conditions in slag. Different ripple regimes have been identified and mapped.
- (7) Calculation of plasma conductivity with our simplified equilibrium properties code, incorporating negative phosphorus ion effects, showed reasonable agreement with more complex calculations made at ARI and Westinghouse.

- (8) Design of Channel II flow components has continued. Final channel design awaits evaluation of the feasibility of incorporating a surplus 4 Tesla superconducting magnet.

TASK 2. OPEN CYCLE DISK GENERATOR PROGRAM

The principal conclusions for this reporting period are:

- (1) The radial flow wake nonuniformities study is successful, and the results are providing basic quantitative information on the effects of this type of nonuniformity which has application/inference to linear as well as disk generator performance. Test plans for future work have been formulated.
- (2) A detailed experimental study of the swirl vane wake is underway; the generator and instrumentation are ready for testing.
- (3) Two-dimensional electrodynamics modeling (in the r-z plane) has led to initial quantitative results for the effects of segmented side wall-boundary layer interactions; the side wall consists of alternating/periodic (in the radial direction) metallic (electrically floating) rings and insulators. The model is being extended to include the coupling with the fluid dynamics; the code will be particularly useful in Hall field breakdown/limitation modeling.
- (4) Chemical kinetics modeling is complete. Both performance and design codes will be used to establish the effects of chemical nonequilibrium on scaling laws of large-scale disk generators. The design code will be used to design a high performance channel for experiments in the MIT disk facility.
- (5) Spectroscopic studies of the influence of radiation from CO and CO₂ molecules on the cesium spectrum were initiated. The results are important for both the interpretation of PM-tube data and for the determination of electron density and temperature from the spectral features (i.e., line-to-continuum and continuum slop techniques).

TASK 3, ELECTRODE MODULE DEVELOPMENT AND TESTING

Part A.

Magnesium oxide (single crystal) and silicon nitride (hot pressed) have the highest dielectric breakdown strength of the materials tested to date.

Only minor damage of single layered SZSFLF-6 electrodes was incurred by operating at $1\frac{1}{2}$ A/cm² for 22 hours and 39 minutes, and this damage was considered to be periodic shut-down related.

More extensive but not severe damage was incurred by operating single layered SZSFLF-6 electrodes at 3 A/cm² for 7 hours and 32 minutes. Of particular importance was anode melting.

Evidence of resistance increase in electrodes of Test 274 was found, but no microscopic evidence was found in any test for electrochemical decomposition.

Part B.

Cooling effectiveness of the burner modules was improved with the installation of a higher pressure cooling water pump.

Accumulation of residual potassium carbonate in the exhaust system was corrected with the addition of a water spray.

TASK 4, COAL COMBUSTION STUDIES

TASK 4a, KINETIC MODELLING OF TWO-STAGE COMBUSTOR

A two-color optical pyrometer system has been upgraded to allow for single particle temperature measurements as a function of burnout time. A simple diffusion-controlled particle combustion model was developed for comparison with experimental data. However, this current model is inadequate to predict coal particle burning histories. Experimental data will be improved by better characterized coal feedstocks. Improvements to the model will include allowances for multicomponent diffusion and thermal conductivity coefficients, finite heterogeneous reaction rates, and homogeneous reactions in the boundary layer.

The initial version of a char/coal combustion model has been completed. The model was applied to char oxidation in MHD combustors under fuel rich conditions. The trade-offs in reaction rate due to changes in the particle diameter, the gas temperature, the fuel equivalence ratio, and pressure were presented and discussed. At temperatures below 2500°K , H_2O and CO_2 are the dominant oxidizing species. Significant contributions from O_2 , O , and OH are found at temperatures above 2500°K . At high gas temperatures the contribution of O_2 is greatest near the stoichiometric ratio, while OH becomes more important under fuel rich conditions. Results from this preliminary study point out areas where additional research is imperative to optimize combustion under the high temperature, fuel rich conditions of the two stage MHD combustor.

TASK 4b, COMBUSTION AERODYNAMICS AND FLUID MECHANICS OF HIGH-SWIRL SECOND STAGE

The program called "SHAPE" has been developed to provide theoretical calculations of the flow aerodynamics within the second stage nozzle of the MHD Combustor. This program provides the stream function, static pressure, axial and swirl velocity distribution for the effect of input swirl number, Reynolds number and second stage nozzle geometry. The program has been run successfully for high swirl number (> 1.0). The difficulties encountered in operating the swirl vane blades in the three concentric annuli are expected to be overcome soon and it is expected that the water model facility will be fully operational in the middle of December.