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Revised Users Manual, Pulverized Coal Gasification or Combustion - 2-Dimensional (87-PCGC-2)

Final Report, Volume 2

P.J. Smith
L.D. Smoot
B.S. Brewster

December 1987

Work Performed Under Contract No.: DE-AC21-85MC22059

For
U.S. Department of Energy
Office of Fossil Energy
Morgantown Energy Technology Center
Morgantown, West Virginia

By
Combustion Laboratory
Chemical Engineering Department
Brigham Young University
Provo, Utah

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or Combustion – 2-Dimensional (87-PCGC-2)**

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Office of Fossil Energy
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P.O. Box 880
Morgantown, West Virginia 26507-0880

By
Combustion Laboratory
Chemical Engineering Department
Brigham Young University
Provo, Utah 84602

December 1987

DISCLAIMER

The initial development of this computer code and user's manual was originally sponsored by the United States Government, the Electric Power Research Institute, and Brigham Young University. Recent enhancements (e.g. radiation submodel, energy equation) have been sponsored by BYU and several U.S. industries, the State of Utah and the U.S. Government who are members of the Brigham Young University Advanced Combustion Engineering Research Center. The industrial and governmental members, in alphabetical order were: Advanced Fuel Research, Babcock and Wilcox, Chevron Research Co. Combustion Engineering Co., Consolidation Coal Co., Convex Computer Corp., Corning Glass Works, Dow Chemical U.S.A., Electric Power Research Institute, Empire State Electric Energy Research Corp., Foster Wheeler Development Co., Gas Research Institute, General Electric Corp., General Motors Corp., Idaho National Engineering Laboratory, International Fuel Cells, Morgantown Energy Tech. Center, Pittsburgh Energy Tech. Center, Pyropower Corp., Questar Development Corp., Shell Development Co., Southern California Edison Co., Tennessee Valley Authority, The National Science Foundation, The State of Utah, TRW, Inc. and Utah Power and Light Co. Neither the United States nor the United States Department of Energy, sponsoring U.S. industrial organizations, Brigham Young University nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by tradename, mark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by any of these agencies. The view and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government, The Electric Power Research Institute or any agency thereof.

PREFACE

Every effort has been made to produce a computer code which will converge to a solution under as wide a variety of input conditions as possible. First elements of this code have been operating at Brigham Young University since 1977, with improvements having been made continuously since that time. Hundreds of predictions have been made with the code; however, the complex nature of the physical processes being modeled results in a numerical computer program that is sensitive to input conditions. Users are cautioned that arbitrary sets of input parameters will not necessarily produce converged solutions. A thorough understanding of the model equations and the numerical solution technique will give the user a better understanding of how to adjust appropriate numerical parameters to obtain a converged solution. 87-PCGC-2 is still considered to be a "specialist useable" code.

This code has been developed to apply to a variety of reacting and non-reacting flows, including pulverized coal combustion and coal gasification. Gasification can be interpreted as fuel-rich combustion, with little or no differences in the basic governing processes. Recent extensions have included

the ability to predict liquid droplet systems and solid-liquid slurry systems, with most applications being coal-water mixture combustion and gasification.

Key improvements and changes in the code include the following: 1) generalized, two-dimensional, axisymmetric geometry; 2) multiple inlets; 3) liquid droplet and solid-liquid slurry feeds; 4) improved radiation heat transfer model; 5) improved energy equation option and 6) variable coal heat capacity. In order to differentiate among various versions of the code, the version associated with this user's manual is referred to as 87-PCGC-2, the "87" indicating the year of release. The code is referred to herein as simply PCGC-2.

ABSTRACT

A two-dimensional, steady-state model for describing a variety of reactive and non-reactive flows, including pulverized coal combustion and gasification, is presented. Recent code revisions and additions are described. The model, referred to as 87-PCGC-2, is applicable to cylindrical axi-symmetric systems. Turbulence is accounted for in both the fluid mechanics equations and the combustion scheme. Radiation from gases, walls, and particles is taken into account using either a flux method or discrete ordinates method. The particle phase is modeled in a Lagrangian framework, such that mean paths of particle groups are followed. Several multi-step coal devolatilization schemes are included along with a heterogeneous reaction scheme that allows for both diffusion and chemical reaction. Major gas-phase reactions are modeled assuming local instantaneous equilibrium, and thus the reaction rates are limited by the turbulent rate of mixing. A NO_x finite rate chemistry submodel is included which integrates chemical kinetics and the statistics of the turbulence. The gas phase is described by elliptic partial differential equations that are solved by an iterative line-by-line technique. Under-relaxation is used to achieve numerical stability. The generalized nature of the model allows for calculation of isothermal fluid mechanics/gaseous combustion, droplet combustion, particulate combustion and various mixtures of the above, including combustion of coal-water and coal-oil slurries. Both combustion and gasification environments are permissible. User information and theory are presented, along with sample problems.

ACKNOWLEDGEMENT

This document is the revised User's Manual for the improved computer model for Pulverized Coal Gasification and Combustion in Two-Dimensions (87-PCGC-2). The code is so named in order to differentiate it from the earlier version, PCGC-2, and because it was completed in 1987. Work on this code was originally initiated under contracts from the U.S. Department of Energy and the Electric Power Research Institute in December of 1974. Research and development on this technology has continued since that time.

Work during 1982 through 1984 was supported by the U.S. Department of Energy, Morgantown Energy Technology Center, Morgantown, West Virginia, under Contract No. DE-AC21-81MC-16518 with Mr. Gary R. Friggens and subsequently Dr. Holmes A. Webb, Jr., and then Dr. Lily Herskovits as Technical Project Officers; Grant No. DE-FG22-80PC-30306 with Mr. James Hickerson as Technical Project Officer; and Contract No. DE-AC21-80MC-14368 with Mr. Kenneth Markel as Technical Project Officer; The Electric Power Research Institute, Palo Alto, California, under Contract No. RP-364-3 with Mr. John Dimmer as Contract Officer. Work during the period from 1985 to April 30, 1987 was sponsored in part by the U.S. Department of Energy, Morgantown Energy Technology Center under Contract No. DE-AC21-85MC-22059. Mr. Gary Friggens was the DOE technical project officer until the summer of 1986 when Mr. Leland E. Paulson became the technical project officer for DOE. Work from 1985 to the publication of this User's Manual was also sponsored by Technical Associates and Affiliates of the University's Advanced Combustion Engineering Research Center who were in alphabetical order: Advanced Fuel Research, Babcock and Wilcox, Chevron Research Co. Combustion Engineering Co., Consolidation Coal Co., Convex Computer Corp., Corning Glass Works, Dow Chemical U.S.A., Electric Power Research Institute, Empire State Electric Energy Research Corp., Foster Wheeler Development Co., Gas Research Institute, General Electric Corp., General Motors Corp., Idaho National Engineering Laboratory, International Fuel Cells, Morgantown Energy Tech. Center, Pittsburgh Energy Tech. Center, Pyropower Corp., Questar Development Corp., Shell Development Co., Southern California Edison Co., Tennessee Valley Authority, The National Science Foundation, The State of Utah, TRW, Inc. and Utah Power and Light Co. Financial cost sharing from the Research Division of Brigham Young University for development of this code during the entire period of development is gratefully acknowledged.

The work was accomplished under the direction of Professor L. Douglas Smoot, project director and Professor Philip J. Smith, senior investigator. Dr. B. Scott Brewster, Research Associate, and Dr. A.S. Jamaluddin contributed significantly to this User's Manual. Two graduate students who made particularly significant contributions to the User's Manual reported here were Larry Baxter and Joseph Smith. Other graduate students who contributed were Knute Christensen and Richard Boardman. Earlier contributors included Dr. Thomas H. Fletcher, Dr. Scott C. Hill and Dr. David G. Sloan, all former graduate students, and Dr. David T. Pratt, now with Aerojet General, and Dr. John J. Wormeck, now at the University of Utah. Michael R. King, Lynda Richmond and Linda Ward provided technician, typing and drafting services.

TABLE OF CONTENTS

DISCLAIMER.....	ii
PREFACE.....	ii
ABSTRACT.....	iii
ACKNOWLEDGEMENT.....	iv
LIST OF FIGURES.....	vii
LIST OF TABLES.....	x

PART ONE: MODEL FORMULATION AND SOLUTION

CHAPTER

I.	INTRODUCTION.....	2
	A. Code Description.....	2
	B. Code Development.....	2
	C. Code Improvements and Revisions.....	3
	D. Limitations.....	4
	E. Document Format.....	4
	F. Code Availability and Training.....	4
II.	THEORETICAL MODEL DEVELOPMENT.....	6
	A. Model Basis.....	6
	B. Differential Equation Sets.....	9
	C. Gas-Phase Fluid Mechanics.....	11
	D. Turbulence Model.....	13
	E. Particle Phase Mechanics.....	16
	F. Gas Phase Reactions.....	20
	G. Particle Phase Reactions.....	31
	H. Radiation.....	42
	I. Nitrogen Oxide (NO) Model.....	56
III.	SOLUTION TECHNIQUE.....	64
	A. Approach.....	64
	B. Finite Difference Scheme.....	69
	C. Boundary Conditions.....	110
	D. Generalized Geometry.....	114
	E. Additional Inlets.....	121
	F. Gas Phase Properties.....	126
	G. Radiation.....	127
	H. Integration of Particle Equations.....	128
	I. Particle-Gas Coupling.....	135
	J. Nitrogen Oxide Model.....	137

PART TWO: CODE USERS MANUAL

IV.	USER GUIDE.....	142
	A. General Description.....	142
	B. Description of Subroutines.....	144
	C. Program Input.....	153
	D. Program Output.....	161
	E. Code Operation.....	164
V.	IMPLEMENTATION GUIDE.....	172
	A. Code Files.....	172
	B. Fortran and Machine Incompatibilities.....	173

VI.	SAMPLE PROBLEMS.....	175
A.	Methane Combustion Case (METH).....	175
B.	Coal Combustion Case (ASAYSUB).....	175
C.	High-Pressure Coal Gasification Case (UTAZ45).....	181
D.	Coal-Water Mixture Combustion Case (CWM).....	181
	NOMENCLATURE.....	188
	REFERENCES.....	195
	APPENDICES	
A.	Help File for Input File Editing Program (PCEDIT).....	203
B.	Description of Subroutines.....	206
C.	Description of Input Data.....	217
D.	Command (SCRIPT) Files for VAX/VMS and UNIX Operating Systems.....	236
E.	Use (MAKE) Files for Program Maintenance.....	246
F.	Methane Combustion Case.....	258
G.	Pulverized Coal Combustion Case.....	263
H.	High-Pressure Coal Gasification Case.....	301
I.	Coal-Water Mixture Combustion Case.....	307

LIST OF FIGURES

<u>Figure</u>	<u>Page</u>
1. Two-dimensional reactor schematic.....	7
2. Schematic of submodels in PCGC-2.....	8
3. Schematic of coal particle, illustrating constituents and reaction processes.....	33
4. Directional intensities reaching a volume element.....	46
5. The direction cosines.....	47
6. The absorption, scattering and extinction efficiencies of char particles at a wavelength of $2\text{ }\mu\text{m}$ and refractive index of $1.93 [1 - i(0.53)]$	54
7. Information flow for PCGC-2.....	65
8. Sample grid pattern for PCGC-2.....	67
9. The boomerang-shaped structure enclosing the points of definition of u , v , p , and ϕ corresponding to FORTRAN index I , J	73
10. Illustration of the grid symbols for a computational cell.....	74
11. FORTRAN symbols for p -cell.....	75
12. FORTRAN symbols for u -cell.....	76
13. FORTRAN symbols for v -cell.....	77
14. Illustration of the main cell finite-difference grid showing the node point labeling.....	79
15. A typical u -cell showing adjacent velocities.....	93
16. A typical v -cell showing adjacent velocities.....	94
17. A typical main boundary cell.....	106
18. Sample reactor configurations possible with modified PCGC-2....	116
19. Example of saw-tooth representation of reactor wall.....	117
20. Arbitrary grid cell showing location of X , R , I and J	117
21. Arbitrary U -cell showing locations of cells affected by intrusion at (I,J)	120

22.	Arbitrary V-cell showing locations of cells affected by intrusion at (K,J).....	120
23.	Example of feed stream configurations.....	123
24.	Axial grid locations for west wall inlets.....	124
25.	Radial grid locations for north wall inlets.....	124
26.	Predicted particle trajectory map showing non-rebounding wall collisions.....	132
27.	Predicted particle trajectory map showing recirculation of particles.....	133
28.	Predicted particle trajectory map showing case where $\hat{v}_{pd}$ was artificially set to 0.....	134
29.	Information flow for nitrogen oxide model.....	140
30.	Subroutines called by the main program.....	145
31.	Subroutines called by COALØ (initialization for Particle Reactions submodel).....	146
32.	Subroutines called by TABLE (physical properties table generation algorithm).....	147
33.	Subroutines called by PROPS (gas physical properties calculation).....	149
34.	CALC subroutines called by the main program (Gas Fluid Mechanics and Reactions submodels).....	150
35.	Subroutines called by EOLP (Particle Dispersion and Reactions submodels).....	151
36.	Information flow diagram for combined Eulerian-Lagrangian particle model.....	152
37.	Subroutines called by FLUX (Radiation submodel).....	154
38.	Subroutines called by NOXMN (Pollutants submodel).....	155
39.	Convergence of pulverized coal combustion sample problem.....	180
40.	Schematic diagram of high pressure entrained gasifier.....	182
41.	Predicted centerline temperature profiles for high pressure (~5 atm) gasification of Utah bituminous coal at heat loss factors of 0.0 (adiabatic), 0.30, and 0.45.....	184

42.	CO, CO ₂ and H ₂ radial profiles of PCGC-2 predictions and experimental data (Azuhata et al., 1986), for high pressure gasification of Utah bituminous coal.....	185
43.	Contour map of measured nitrogen oxide concentrations (Brown, 1985) for high pressure (~5 atm) gasification of a Utah bituminous coal.....	186
44.	Contour map of theoretical nitrogen oxide concentrations for high pressure (~5 atm) gasification of a Utah bituminous coal with a reactor heat loss factor of 0.30.....	186
45.	Contour map of theoretical nitrogen oxide concentrations for high pressure (~5 atm) gasification of a Utah bituminous coal with a reactor heat loss factor of 0.45.....	186

LIST OF TABLES

<u>Table</u>	<u>Page</u>
1. Gas Phase Differential Equations.....	10
2. Turbulence Model Constants.....	15
3. Turbulent Combustion Model Constants.....	23
4. Parameters for Gaussian Probability Density Function.....	25
5. Outline of Output from PCGC-2 Calculation.....	36
6. PCGC-2 Differential Equation Set I.....	39
7. PCGC-2 Differential Equation Set II.....	40
8. Devolatilization Rate Expressions and Parameters for Use in PCGC-2.....	42
9. Coefficients for Char Reactions with O ₂ , CO ₂ and H ₂ O.....	44
10. The S ₂ Quadrature for Axisymmetric Cylindrical Closures.....	49
11. The S ₄ Quadrature for Axisymmetric Cylindrical Enclosures.....	49
12. Coefficients for Flux Sums.....	53
13. Kinetic Parameters Used in the Nitrogen Pollutant Submodel.....	58
14. Equation Set for Nitrogen Oxide Submodel in Turbulent, Coal- Laden Systems.....	63
15. PCGC-2 Boundary Conditions.....	115
16. Use of FORTRAN Logical Input Variables INRDGD and INTRUS.....	122
17. Finite Difference for the Radiation Flux Sums.....	129
18. Finite Difference Equation for $\theta = \bar{n}_j$	138
19. Boundary Conditions for $\bar{n}_j$	139
20. Summary of Input for PCGC-2.....	143
21. Input Data.....	157
22. Program Output Control.....	162
23. Outline of Output from PCGC-2 Calculation.....	163
24. PCGC-2 Output Files.....	165

25.	Parameters for Methane Combustion Case.....	176
26.	Parameters for Pulverized Coal Combustion Case.....	177
27.	Parameters for High Pressure Coal Gasification Case.....	183
28.	Parameters for Coal-Water Mixture Case.....	187

PART ONE
MODEL FORMULATION AND SOLUTION

CHAPTER I. INTRODUCTION

A. CODE DESCRIPTION

This manual presents the details of the improved and revised two-dimensional computer code, referred to as 87-PCGC-2 (Pulverized Coal Gasification and Combustion: 2-Dimensional), which describes a variety of reacting and non-reacting flows, including pulverized coal combustion and gasification. It can also describe the combustion of gaseous diffusion flames, liquid sprays, coal slurries, isothermal two-phase fluid mechanics, and other oxidation/reduction reaction chambers. The scheme is based on an Eulerian framework for the gas phase and a Lagrangian framework for the particle phase. The approach emphasizes the turbulent fluid mechanics and the turbulent combustion processes in a turbulent flame. Most gas-phase reactions are assumed to be mixing-limited, so that gaseous combustion is modeled with a statistical probability density function based on the mixture fraction. A two-equation ($k-\epsilon$) turbulence model is used for closure. The particle phase includes the effects of aerodynamic particle drag and turbulent particle dispersion. Particle droplet reactions are considered to be slow with respect to the gas-phase turbulence time scale. Rate processes for liquid vaporization, coal devolatilization, and heterogeneous reaction of coal particles are included, based on time-mean gaseous properties. Particle and gas radiation are incorporated using either a six-flux or a discrete ordinates method. Anisotropic and multiple scattering are included.

The development of this code is based on the general equations of change together with extensive independent results from experimental observations. There are still many unresolved questions regarding the turbulent fluid mechanics, gas phase reactions, and coal reactions. An attempt has been made to formulate a general reaction scheme that can accommodate results of future measurements and improved kinetic parameters.

The description that follows applies to entrained-flow, pulverized-coal reaction processes, where particles are small ($<150\text{ }\mu\text{m}$) and heating rates are high ($10^3\text{-}10^6\text{ K s}^{-1}$). This treatment would not necessarily apply to fixed- or fluidized-bed processes without modification.

B. CODE DEVELOPMENT

Formulation, numerical solution and evaluation of 87-PCGC-2 or just PCGC-2, as it is commonly called herein, has been completed over the past several years. Development has reached a point where the code is being applied to systems of practical interest. However, appropriate use of this comprehensive code requires a thorough understanding of the basic code foundations and operation. Our experience suggests that a person with a technical degree and strong technical background requires six months to a year (full time) to effectively understand and use the code. Results can be obtained faster with the guidance of more experienced users.

C. CODE IMPROVEMENTS AND REVISIONS

The 1987 release of PCGC-2 contains several improvements and revisions over the previous (1985) release, including generalized geometry, additional inlets, droplet or slurry feeds (coal-water mixtures), improved radiation heat transfer, improved solution of the energy equation and variable coal heat capacity. These improvements are described below.

The new geometry feature allows for truly arbitrary axisymmetric geometry. Previously, the reactor diameter was required to remain constant outside of a quarl region at the inlet, and internal surfaces (e.g. bluff objects in the interior of the flow domain) were not allowed. The 1987 release of PCGC-2 allows for both varying diameter and bluff objects. Of course, since geometry is axisymmetric, bluff objects must be modeled as ring-shaped structures in three-dimensional space. The new geometry is discussed in more detail in Section III.D of this users manual.

Additional inlets beyond the primary and secondary is another new feature. These inlets may be located anywhere along the west or north walls. Because of the 2-D formulation, additional inlets on the north wall are modeled as slits that extend all the way around the outer wall. Gas composition for the additional inlets must be identical to that of the primary or secondary streams, as only a single mixture fraction is used for tracking inlet gas mixing (see Section II.F., Gas Phase Reactions). This feature is described in Section III.E.

The ability to simulate combustion of liquids and slurry (e.g. coal-water mixtures) is another major improvement. At present, this application is limited to cases where the primary and secondary (if present) streams are of identical composition. This capability is described in Chapters II and III, and an example problem is included in Appendix F and described in Section VI.D.

A new flux method for solving the radiation equations has been implemented. The new method is based on discrete ordinates and accounts for coupling between the directional fluxes. In addition, corrections have been added which account for the broadening effect of pressure on gas emissivity and the spectral overlap of the emissivities of carbon dioxide and water vapor.

Recently, Merrick (1983) developed a model for the heat capacity of coal and char as a function of composition and temperature. The variation in heat capacity with these parameters has been shown to have significant impact on particle temperature histories and ultimate yield (with a two-step devolatilization model) (Brewster et al., 1987), and the Merrick formulation has been programmed as an additional option (Brewster et al., 1987). The theoretical formulation is discussed in Section II.G.2, and the use of the option is explained in Section II.C.

The option for solving the energy equation for non-adiabatic reactors has been significantly improved. Convergence continues to be difficult to achieve, however, unless gas-to-particle convective heat transfer is ignored. Fortunately, this term is insignificant in most cases. Use of the improved energy equation option is described in Section VI.B.

D. LIMITATIONS

The following assumptions are basic to PCGC-2.

- The flowfield, geometry, and body forces (gravity) are axisymmetric.
- The flow is subsonic (dilatation is ignored). The maximum Mach number should be less than about 0.3.
- Chemical reaction rates are limited by turbulent mixing and not by kinetics (with the exception of nitrogen oxides).
- Particles are dispersed in the gas phase, and particle interactions are ignored.

These assumptions are discussed in Chapter II.

The submodels dealing with turbulence issues are the most tenuous. Specifically, the turbulent flowfield submodel ($k-\epsilon$), turbulent particle dispersion, and turbulence-chemistry interactions, are not yet capable of producing accurate results in all applications.

Other limitations, at least for coal combustion, are in the reactivity parameters specified for the particles. These parameters are specified in the input data files and, while the reaction rates are modeled accurately for a given set of coefficients, the coefficients are not well characterized for the high temperatures and heating rates typical of coal combustors. The uncertainty of these parameters can have a significant impact on the predicted results.

E. DOCUMENT FORMAT

This users manual is organized in two parts. Part One documents the theory (Chapter II) and solution of the model equations (Chapter III). An understanding of the theoretical foundations of the code is prerequisite to its correct application, and potential users should study this material carefully. Part Two describes the use of the code (Chapter IV), gives suggestions regarding its implementation on computer systems (Chapter V), and discusses several sample problems illustrating code application (Chapter VI). Chapters V and VI constitute new additions to the users manual and reflect our interest in facilitating its use by other researchers and engineers. However, it must be recognized that PCGC-2 is still very much a "user-specialist" code requiring a significant amount of experience beyond simple theoretical understanding for efficient management and use. Laboratories interested in extensive use of PCGC-2 should plan on committing a technical person full-time for approximately six months to a year to learn the code. Training is available as described below.

F. CODE AVAILABILITY AND TRAINING

The 1987 version of PCGC-2 was funded partly by this grant and partly by the Advanced Combustion Engineering Research Center (ACERC) and is subject to

ACERC policy on the distribution of computer software. The code will be made available to Industrial Associates of ACERC on January 1, 1988, to Industrial Affiliates on January 1, 1989, and to other U.S. organizations on January 1, 1990. Foreign organizations not belonging to ACERC may inquire about code availability after January 1, 1990, and universities interested in cooperative development may inquire anytime.

Organizations wishing to obtain the code should contact

Dr. B. Scott Brewster
Combustion Laboratory, 280 CB
Brigham Young University
Provo, Utah 84602
(801) 378-6240
TELEX 706448

Please use the complete address as given above in any TELEX communications. The source code and sample problems are available on magnetic tape. The code was originally developed to run on VAX/VMS computer systems, but has recently been implemented on Convex/C-1 and Sun 3/260 computers with the Berkeley 4.3 Unix operating system. The code is not guaranteed to run on any particular computer system, however, and potential users should plan on making modifications, particularly if their system is not one of the above. The extent of the required modifications varies with each installation.

Training in the use of the code is also available through the BYU Combustion Computations Laboratory (CCL). This training is best accomplished on an individual basis. Interested scientists and engineers are encouraged to visit the laboratory for a short period (4-6 weeks) during which time they will be assigned to two graduate students who will assist them in learning how to use the code and apply it to a problem of interest. All travel and living expenses during this period will be the responsibility of the visiting scientist/engineer*. On-campus housing may be available, especially during the non-academic (summer) months. BYU will provide office space and computer resources and assist in making suitable housing arrangements.

*Industrial Associate trainees can request partial financial support from ACERC for their visit to the center.

CHAPTER II. THEORETICAL MODEL DEVELOPMENT

A. MODEL BASIS

The mathematical modeling of turbulent combustion and gasification has been recognized as a difficult problem not only due to the numerical challenges associated with solving the differential equation set but also the challenges of physically describing the important chemical and physical processes, such as chemistry-turbulence interactions, turbulent particle dispersion, particle reactions, etc. PCGC-2 uses currently available mathematical technology to combine knowledge of fluid mechanics with a reasonable approach to the reaction processes. Care has been taken to maintain the scope of the simplifying approximations on an equivalent level.

The present version of PCGC-2 is applicable to non-reacting flow systems, gaseous diffusion flames, pulverized coal-fired combustion, entrained flow-gasification, droplet combustion, and slurry combustion or gasification (including coal-water mixtures) in axisymmetric coordinates. Variations in the properties are considered only in the axial and radial directions. Symmetry is assumed in the angular direction. A schematic of a typical reactor modeled by PCGC-2 is shown in Figure 1 (Smith, 1979; Thurgood, 1979). This particular cylindrical reactor is coaxial, with coal entering the reactor in the central (primary) stream and the majority of the oxidizer entering in the outer (secondary) stream or annulus. The code has been generalized to include multiple inlets that can be located along any of the walls and to include arbitrary shapes within the axi-symmetric assumption. Typical pulverized coal particles range in size from two micrometers (microns) to one hundred fifty micrometers. Fuel droplets can reach several hundred micrometers. The model predicts the mean gas field properties for axisymmetric, steady-state, turbulent flames (i.e., local velocity, temperature, density, and species composition). Particle properties are also computed, such as coal burnout, particle or droplet velocity and temperature, and coal/droplet component composition. Figure 2 illustrates the various submodels incorporated into PCGC-2.

The gas phase is assumed to be a turbulent, reacting continuum field that can be described locally by general conservation equations. The flow is assumed to be time-steady. Gas properties (i.e., density, temperature, species composition) are assumed to fluctuate randomly according to a probability density function (PDF) characteristic of the turbulence. Gas-phase body forces are neglected. The gas is assumed to be Newtonian and dilatation is neglected.

The gas field is treated in an Eulerian framework. Turbulence is modeled by breaking the variables into fluctuating and time-mean components in the conventional manner (Hinze, 1967; Tennekes and Lumley, 1972). The two-equation $k-\epsilon$ model is used for closure (Launder and Spalding, 1972). PCGC-2 is coded to handle either Reynolds- or Favre-averaging. The effect of particles on the gas-phase turbulence is modeled with an empirical correlation. Gas-phase reactions are assumed to be limited by mixing rates for major species and not by kinetics; gaseous properties are calculated assuming local instantaneous equilibrium. For non-equilibrium reactions, such as occur in methane flames or in coal gasifiers, partial (frozen) equilibrium can be

Figure 1. Two-dimensional reactor schematic.

Figure 2. Schematic of submodels in PCGC-2.

used to describe mixing-limited reactions. Work is currently underway to incorporate general non-equilibrium chemical reactions, particularly for CO/CO₂ (Colson, 1988).

The pulverized coal flame radiation field is a multi-component, non-uniform, emitting, absorbing, scattering gas-particle system (Smith et al., 1981). The coal particles cause anisotropic and multiple scattering. The flame may be surrounded by non-uniform, emitting, reflecting, absorbing surfaces. Optical coefficients for the gas, walls, and particles are difficult to obtain in flames (Sarofim and Hottel, 1978) and PCGC-2 uses the recommendations of Varma and Pratt (1978) to calculate the optical coefficients necessary for a pulverized coal flame. An Eulerian framework is used to model the radiation, which facilitates incorporation of radiation properties into gas-phase equations. The Lagrangian particle field does not mesh completely with the Eulerian radiation equations, since a bulk particle density is difficult to obtain from Lagrangian systems.

The particle phase is not considered a continuum as is the gas phase (Smith et al., 1981; Fletcher, 1980). Different particles at the same location may exhibit different properties due to their different histories. In PCGC-2, Lagrangian treatment of the particles is performed, representing the particle field as a series of mean trajectories. Particle properties can be obtained along the mean trajectories by integration of the governing particle equations. The effect of turbulent fluctuations on the trajectories of the particles is treated in a mixed Eulerian-Lagrangian framework. The effect of turbulent fluctuations in the gas phase on particle reaction rates is ignored.

PCGC-2 assumes that the off-gas from the coal is of constant elemental composition. The particle reaction submodel is discussed by Smith (Smith, 1979) (see also Smoot and Pratt, 1979; Fletcher, 1983). Particles are defined to consist of liquid coal, char, and ash. Ash is inert by definition; volatile mineral matter is considered as part of the volatile matter of the coal. Coal reaction rates are characterized by multiple parallel reaction rates with fixed activation energies. Coal particle swelling is accounted for empirically. The particles are assumed to be isothermal. The parameters which describe the coal reaction rates are part of the input to the code. Work is currently underway to incorporate effects of variable coal offgas composition and to predict the coal particle reaction process based on coal functional group composition (Brewster et al., 1987).

B. DIFFERENTIAL EQUATION SETS

All of the gas-phase equations are Eulerian, steady-state, second-order, non-linear, elliptical partial differential equations. Each of these may be conveniently cast into one finite difference form, so that only one solution technique is required. Table 1 contains a summary of this form for all of the gas phase equations. Note that the particles are accounted for only by appropriate particle source terms of mass (S_p^m), momentum (S_p^u and S_p^v), and enthalpy (S_p^h). These terms represent the addition of mass, momentum, and energy to the gas phase from the particles. The source terms are found along a particle trajectory by taking the difference in the particle properties on each side of a computational cell and dividing by the cell volume (see Chapter III).

TABLE 1
GAS PHASE DIFFERENTIAL EQUATIONS

$$\frac{\partial}{\partial x} (\bar{\rho} \tilde{u} \phi) + \frac{1}{r} \frac{\partial}{\partial r} (r \bar{\rho} \tilde{v} \phi) - \frac{\partial}{\partial x} \left(\Gamma_{\phi} \frac{\partial \phi}{\partial x} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left(r \Gamma_{\phi} \frac{\partial \phi}{\partial r} \right) = S_{\phi}$$

ϕ	Γ_{ϕ}	S_{ϕ}
1	0	S_p^m
$\tilde{u}$	μ_e	$-\frac{\partial \bar{p}}{\partial x} + \frac{\partial}{\partial x} (\mu_e \frac{\partial \tilde{u}}{\partial x}) + \frac{1}{r} \frac{\partial}{\partial r} (r \mu_e \frac{\partial \tilde{v}}{\partial r}) + S_p^u + \tilde{u} S_p^m$
$\tilde{v}$	μ_e	$-\frac{\partial \bar{p}}{\partial r} + \frac{\partial}{\partial x} (\mu_e \frac{\partial \tilde{u}}{\partial r}) + \frac{1}{r} \frac{\partial}{\partial r} (r \mu_e \frac{\partial \tilde{v}}{\partial r}) - 2 \mu_e \tilde{v} / r^2 + \frac{\bar{\rho}}{r} \tilde{w} \tilde{w} + S_p^v + \tilde{v} S_p^m$
$\tilde{w}$	μ_e	$-\rho \tilde{w} \tilde{w} / r - (\tilde{w} / r^2) \frac{\partial}{\partial r} (r \mu_e)$
k	μ_e / σ_k	$\phi - \bar{\rho} \epsilon$
ϵ	$\mu_e / \sigma_{\epsilon}$	$(\epsilon / k) [C_1 \phi - C_2 \bar{\rho} \epsilon]$
$\tilde{f}_p$	μ_e / σ_f	S_p^f
g_f	μ_e / σ_g	$C_{g1} \mu_e / \sigma_g [(\frac{\partial \tilde{f}}{\partial x})^2 + (\frac{\partial \tilde{f}}{\partial r})^2] - C_{g2} \bar{\rho} \epsilon g_f / k$
$\tilde{n}$	μ_e / σ_n	S_p^n
g_n	μ_e / σ_g	$C_{g1} \mu_e / \sigma_g [(\frac{\partial \tilde{n}}{\partial x})^2 + (\frac{\partial \tilde{n}}{\partial r})^2] - C_{g2} \bar{\rho} \epsilon g_n / k$
$\tilde{h}$	μ_e / σ_h	$q' r g + \tilde{u} \frac{\partial \bar{p}}{\partial x} + \tilde{v} \frac{\partial \bar{p}}{\partial r} + S_p^h + \tilde{h} S_p^m$

where $\phi = \mu_e \{ 2 [(\frac{\partial \tilde{u}}{\partial x})^2 + (\frac{\partial \tilde{v}}{\partial r})^2 + (\frac{\tilde{v}}{r})^2] + [\frac{\partial \tilde{u}}{\partial r} + \frac{\partial \tilde{v}}{\partial x}]^2 + [r \frac{\partial}{\partial r} (\frac{\tilde{w}}{r})]^2 + (\frac{\partial \tilde{w}}{\partial x})^2 \}$

$$\mu_e = \mu^t + \mu^l$$

$$\mu^t = C_{\mu} \bar{\rho} k^2 / \epsilon$$

$$S_p^m = S_p^f + S_p^n$$

The following sections describe each of the equations in Table 1 in more detail. The equations for the radiation field and the particle number-density field do not fit the form of the gas-phase equations and are discussed separately. The method used to solve these equations is discussed in Chapter III

C. GAS-PHASE FLUID MECHANICS

The instantaneous gas-phase equations of continuity and momentum (Bird et al., 1960) are presented here with the particle reaction source terms (Smoot and Pratt, 1979). Equations for turbulence properties, mixture fractions, and energy can be similarly derived. The equations of continuity and motion are:

$$\frac{D\rho}{Dt} = -\rho(\vec{v} \cdot \vec{v}) + S_p^m \quad (1)$$

$$\rho \frac{D\vec{v}}{Dt} = -\vec{v}p - \vec{v} \cdot \vec{\tau} + \rho \vec{g} + S_p^v \quad (2)$$

where D/Dt is the substantial derivative. The S_p terms represent the coupling between the gas phase and the particle phase, i.e. the particle source/sink terms. All variables are defined in the Nomenclature.

The equations are reduced with the following simplifications: 1) cylindrical coordinates, 2) 2-dimensional axi-symmetric geometry, 3) no body forces, 4) steady-state, and 5) Newtonian fluid. Equations 1 and 2 become:

$$\frac{\partial}{\partial x}(\rho u) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v) = S_p^m \quad (3)$$

$$\begin{aligned} & \frac{\partial}{\partial x}(\rho u u) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v u) - \frac{\partial}{\partial x}(\mu \frac{\partial u}{\partial x}) - \frac{1}{r} \frac{\partial}{\partial r}(\mu r \frac{\partial u}{\partial r}) \\ &= -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x}(\mu \frac{\partial u}{\partial x}) + \frac{1}{r} \frac{\partial}{\partial r}(\mu r \frac{\partial v}{\partial x}) - \frac{\partial}{\partial x}(\frac{2}{3} \mu \text{div } \vec{v}) + S_p^u + u_{pg} S_p^m \end{aligned} \quad (4)$$

$$\begin{aligned} & \frac{\partial}{\partial x}(\rho u v) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v v) - \frac{\partial}{\partial x}(\mu \frac{\partial v}{\partial x}) - \frac{1}{r} \frac{\partial}{\partial r}(\mu r \frac{\partial v}{\partial r}) \\ &= -\frac{\partial p}{\partial r} + \frac{\partial}{\partial x}(\mu \frac{\partial u}{\partial r}) + \frac{1}{r} \frac{\partial}{\partial r}(\mu r \frac{\partial v}{\partial r}) - 2\mu v/r^2 \\ & - \frac{1}{r} \frac{\partial}{\partial r}(\frac{2}{3} \mu r \text{div } \vec{v}) + \frac{2\mu}{3r} \text{div } \vec{v} + S_p^v + v_{pg} S_p^m \end{aligned} \quad (5)$$

$$\begin{aligned} & \frac{\partial}{\partial x} (\rho u w) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho v w) - \frac{\partial}{\partial x} \left(\mu \frac{\partial w}{\partial x} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left(\mu r \frac{\partial w}{\partial r} \right) \\ & = -\rho v w / r - (w / r^2) \frac{\partial}{\partial r} (r \mu) \end{aligned} \quad (6)$$

One more approximation is made before arriving at the equations used in PCGC-2. The $\text{div } \vec{v}$ term in Eqs. 4 and 5 are associated with the dilatation of the fluid. These terms describe the volume change of a fluid element due to expansion or compression. For perfectly incompressible fluids, the equation of continuity can be used to prove that those terms are identically zero. For a compressible fluid, the effect is minimal at low velocities (less than 0.25 Mach No.) and is often neglected (Bird et al., 1960; Smoot and Pratt, 1979). This convention is also followed in PCGC-2.

It is useful to understand the significance of each term in the equation set. The first two terms in the equation of continuity (Equation 3) represent the net rate of mass addition to the volume element by convection from the axial and radial components respectively. The S_p^m term represents the net rate of mass addition per unit volume due to particle reaction. The first two terms in the momentum equations (Equations 4, 5 and 6) are the convection terms. They represent the net rate of convected momentum to the volume element attributed to the axial and radial components. Equation 4 describes the momentum contributed by the axial component of the velocity, Eq. 5 describes that contributed by the radial component, and Eq. 6 describes that contributed by the tangential component. The third and fourth terms in each of these equations may conveniently be thought of as the corresponding diffusion terms. When turbulence is modeled using Reynold's stresses, they are not strictly molecular diffusion terms because of the contribution to the momentum due to turbulent transfer. The diffusion appearance of second-order derivatives makes it natural to refer to them in this way. The first term on the right hand side of the axial and radial momentum equations represents the pressure force on the volume element. All other terms on the right-hand side of these equations are considered source or sink terms, representing other sources or sinks of momentum. The S_p^u and S_p^v terms represent the aerodynamic drag effects of the particles on the axial and radial components of momentum. The $u_{pg} S_p^m$ and $v_{pg} S_p^m$ terms represent the momentum exchange due to particle mass efflux. In this version of the code, u_{pg} and v_{pg} are assumed to be equal to the gas velocity and S_p^w and $w_{pg} S_p^m$ are neglected. These assumptions will be relaxed in future versions of the code. The reasons for these physical meanings for each term are more apparent because each differential equation is cast into the standard form of Table 1. The numerical method for solving these equations is discussed in Chapter III.

Equations 3-6 must be solved for u , v , w , and p . Historically, the pressure term caused numerical solution difficulties, and thus a transformation was used to change the four variables and four partial differential equations into two partial differential equations and two variables, namely, the stream function and vorticity. The pressure term was then eliminated. This approach had difficulties with defining the physical boundary conditions. The numerical approach discussed in Chapter III obviates the difficulties with the pressure term, and thus the primitive variable formulation (u , v , w , p) is solved in PCGC-2.

The Eulerian equation set, along with the appropriate boundary conditions (see Section III.C), is sufficient to permit solution for the flow field, provided that the density and viscosity are known everywhere in the field. In an isothermal, constant-density fluid, these variables are known apriori. However, in the combustion system of interest, these variables are position dependent. It is through these terms alone that coupling of the combustion model to the fluid mechanics model occurs. This subject is discussed later in this chapter. Also, the problems of time-averaging change the equation set somewhat. This is the topic of the next section.

D. TURBULENCE MODEL

1. The Closure Problem

In laminar flows, velocity gradients are sufficiently mild that the fluid can dynamically adjust to imposed shear stresses through molecular (viscous) forces. When imposed shear forces are too great for the fluid to adjust through molecular processes, the fluid is "torn" into largely coherent regions (turbulent eddies), which can rotate and thus relieve the shear forces caused by the imposed velocity differences. A review of turbulence and its associated closure problem can be found in Tennekes and Lumley (1972), and for applications to coal combustion modeling, in Smoot and Smith (1985). A particularly pertinent review of turbulence models and their applications to swirling flow is given by Sloan, et al. (1986).

2. k-ε Turbulence Model used in PCGC-2

PCGC-2 uses the approach to this closure problem credited to Boussinesq (1877) which is derived by analogy to the laminar Newtonian viscosity. It is assumed that

$$\overline{u'v'} = -\nu_g^t \left(\frac{\partial \bar{u}}{\partial r} + \frac{\partial \bar{v}}{\partial x} \right) \quad (7)$$

where ν_g^t is the turbulent kinematic eddy viscosity. The correlation of fluctuating variables is thus expressed in terms of the mean field variables. Although Eq. 7 is convenient, it does not have a sound theoretical basis. However, this approach has been widely used in turbulent gaseous systems, and is therefore applied in PCGC-2 for lack of a better model (Smith, 1979; Tennekes and Lumley, 1972; Pratt, 1976). A review of the accuracy of the approach in these applications with comparisons to more sophisticated approaches is given by Sloan, et al. (1986). The turbulence closure model used in PCGC-2 (Launder and Spalding, 1972) relates the turbulent kinetic energy (k) and its rate of dissipation (ε) by:

$$\nu_g^t = C_\mu k^2 / \epsilon \quad (8)$$

where:

$$k = (\overline{u'^2} + \overline{v'^2} + \overline{w'^2})/2 \quad (9)$$

Transport equations for k and ϵ can be derived from basic principles (Launder and Spalding, 1972), although some terms must be modeled empirically. The k and ϵ equations used in PCGC-2 are:

$$\begin{aligned} & \frac{\partial}{\partial x}(\overline{\rho u k}) + \frac{1}{r} \frac{\partial}{\partial r}(r \overline{\rho v k}) - \frac{\partial}{\partial x} \left(\frac{\mu_e \partial k}{\sigma_k \partial x} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\mu_e \partial k}{\sigma_k \partial r} \right) \\ &= \mu_e \left(2 \left[\left(\frac{\partial \tilde{u}}{\partial x} \right)^2 + \left(\frac{\partial \tilde{v}}{\partial r} \right)^2 + \left(\frac{\tilde{v}}{r} \right)^2 \right] + \left(\frac{\partial \tilde{u}}{\partial r} + \frac{\partial \tilde{v}}{\partial x} \right)^2 + \right. \\ & \left. \left[r \frac{\partial}{\partial r} \left(\frac{\tilde{w}}{r} \right) \right]^2 + \left(\frac{\partial \tilde{w}}{\partial x} \right)^2 \right) - \overline{\rho \epsilon} \end{aligned} \quad (10)$$

$$\begin{aligned} & \frac{\partial}{\partial x}(\overline{\rho u \epsilon}) + \frac{1}{r} \frac{\partial}{\partial r}(r \overline{\rho v \epsilon}) - \frac{\partial}{\partial x} \left(\frac{\mu_e \partial \epsilon}{\sigma_\epsilon \partial x} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\mu_e \partial \epsilon}{\sigma_\epsilon \partial r} \right) \\ &= (\epsilon C_1 / k) \mu_e \left(2 \left[\left(\frac{\partial \tilde{u}}{\partial x} \right)^2 + \left(\frac{\partial \tilde{v}}{\partial r} \right)^2 + \left(\frac{\tilde{v}}{r} \right)^2 \right] + \left(\frac{\partial \tilde{u}}{\partial r} + \frac{\partial \tilde{v}}{\partial x} \right)^2 + \right. \\ & \left. \left[r \frac{\partial}{\partial r} \left(\frac{\tilde{w}}{r} \right) \right]^2 + \left(\frac{\partial \tilde{w}}{\partial x} \right)^2 \right) - \epsilon^2 C_2 \overline{\rho} / k \end{aligned} \quad (11)$$

where:

$$\mu_e = \mu^l + \mu^t \quad (12)$$

and:

$$\mu^t = \overline{\rho} \nu_g^t \quad (13)$$

The constants C_μ , C_1 , C_2 , σ_k , and σ_ϵ are "universal" constants and have been optimized by comparison with experimental observations of both isothermal and reacting flows (Kahlil et al., 1975). The recommended values of these constants are found in Table 2. The k - ϵ model is the most popular method for turbulent closure for both gaseous and particle-laden systems (Bilger, 1974; Spalding, 1975; Smoot and Smith, 1987). Models which account for combustion-generated turbulence, coherent structures, and gas-particle interaction (Bilger, 1976; Spalding, 1975) are needed.

Melville and Bray (1979) note that the presence of particles has only a slight effect on the gas-phase turbulence. They suggest a correlation using the ratio of the mean particle bulk density to the mean gas density, as follows:

TABLE 2
TURBULENCE MODEL CONSTANTS

<u>Constant</u>	<u>Value</u>
C_μ	0.09
C_1	1.44
C_2	1.92
σ_k	0.9
σ_ϵ	1.22
κ	0.42

$$v_{g \text{ particles}}^t = v_{g \text{ no part.}}^t (1 + [\bar{\rho}_b / \bar{\rho}_g])^{-.5} \quad (14)$$

According to this equation, the amount of turbulence decreases as the bulk particle density increases. PCGC-2 is coded to allow for this empirical correction of gas-phase turbulence due to particles. The correction is limited to a minimum value of 0.95.

E. PARTICLE PHASE MECHANICS

1. Background

A distinguishing feature among pulverized coal models is the treatment of the dispersed particle phase. In large-scale furnaces there are large recirculation zones. Swirling inlet flows can also have a major influence on the particle motion. Gas molecules tend to equilibrate locally. However, particles exist locally with different properties due to the varying history of each particle.

The approach used in PCGC-2 is based on the PSI-CELL technique of Crowe, et al. (1977). Care is taken to account for all modes of gas-particle coupling. The method does not account for particle-particle interactions and thus would not be applicable to highly loaded, dense-phase flow. It is intended to be applied to dispersed-flow systems. The model is based on calculating the trajectories or paths of representative particles through the gas phase (continuum) field in a Lagrangian fashion. These particles are used to calculate sources of mass, momentum, and energy to the gas phase. These source terms were introduced in the previous section. Crowe, et al. (1977) discuss the basic concept, the derivation of the gas and particle equations, and calculation of the source terms. Briefly, mean particle velocities, trajectories, temperatures, and compositions are obtained by integrating representative equations for the mean motion, energy, and component continuity for an ensemble of particles in the gas flow field. Total momentum, energy, and mass of the particle cloud are recorded on crossing cell boundaries. The net difference in the particle properties between leaving and entering any given cell then provides the particle source terms for the gas flow equations. While the mean location of the particle ensemble is being tracked, the statistical spatial distribution about this mean is currently modelled only by a delta function at the mean. Work is currently underway to include the variance (Baxter, 1987).

2. Particle Momentum Equation

The particle momentum equation for a single particle in the Lagrangian framework is given by:

$$\alpha_j d(\vec{v}_j)/dt = \vec{f}_j + \alpha_j \vec{g} \quad (15)$$

The reaction rate term is accounted for by assuming the particle mass leaves the particle with equal mass and velocity in all directions. The drag term ($\vec{f}_p$) is related to the difference in gas and particle velocities by:

$$\vec{f}_j = \Gamma_d (\vec{v}_g - \vec{v}_j) \quad (16)$$

where Γ_d is some time constant based on the drag coefficient (C_d), as shown below:

$$\Gamma_d = A_j \rho_g C_d \|\vec{v}_j - \vec{v}_g\|/2 \quad (17)$$

For spherical particles, the following correlation is suggested for the drag coefficient (Wallis, 1969):

$$C_{do} = (24/Re) (1 + 0.15Re^{0.687}) \quad (18)$$

It has been shown that high particle reaction rates can alter the drag coefficient (Bird et al., 1960). The relationship used in PCGC-2 is that suggested by Bailey, et al. (1970):

$$C_d = C_{do}/(1 + B_m) \quad (19)$$

$$B_m = \sum r_i/k_i \quad (20)$$

where B_m is the particle blowing parameter for mass transfer, which will be discussed in Section II.G.2.

In a turbulent system, the equation of motion for an individual particle becomes more complicated. The approach taken to account for turbulence in Eq. 15 is to decompose the particle velocity into convective and diffusive components:

$$\vec{v}_j = \vec{v}_{jc} + \vec{v}_{jd} \quad (21)$$

The convective component of velocity ($\vec{v}_{jc}$) is defined as the velocity that would arise in the absence of turbulence, or the ballistic velocity based on the mean gas velocity. Therefore, Eq. 15 is used to find $\vec{v}_{jc}$ along a trajectory by numerical integration. The diffusive component of velocity ($\vec{v}_{jd}$) is added to account for the turbulence effects on particle motion.

In the Lagrangian framework, the diffusive velocity $\vec{v}_{jd}$ is modeled using the mean particle bulk density gradient:

$$\vec{v}_{jd} \bar{\rho}_b = -r_j \vec{v}_{jb} \quad (22)$$

Equation 22 can be viewed as a particle diffusivity equation, since the left-hand side can be thought of as a turbulent mass flux (relative to the convective velocity):

$$\vec{j}_j = (\vec{v}_j - \vec{v}_{jc}) \bar{\rho}_{jb} = \vec{v}_{jd} \bar{\rho}_{jb} \quad (23)$$

Equation 22 now defines the transport coefficient r_j as a turbulent particle diffusivity, which can also be expressed as:

$$r_j = D_j^t = v_j^t / \sigma_j^t \quad (24)$$

where D_j^t is the turbulent particle diffusivity, v_j^t is the turbulent particle kinematic viscosity, and σ_j^t is the turbulent particle Schmidt number. Much research is currently being conducted by the scientific community on how to obtain the turbulent particle kinematic viscosity (v_j^t).

An expression for v_j^t should account for particle size, so that larger particles are not affected by the turbulence as much as are smaller particles. The v_j^t expression should also include some term to account for the level of turbulence intensity. The model selected for use in PCGC-2 is that of Melville and Bray (1979), which relates v_j^t to v_g^t as follows:

$$v_j^t = v_g^t (1 + [t_j/t^t])^{-1} \quad (25)$$

The particle relaxation time (t_j) is related to the Stokesian particle drag (Melville and Bray, 1979; Longwell and Weiss, 1980; Lockwood et al., 1980; Lilly, 1973) by:

$$t_j = \alpha_j / (3\pi\mu_g d_j) \quad (26)$$

The turbulence time scale (t^t) is related to the local turbulence by:

$$t^t = v_g^t / (\overline{u_g'^2}) \quad (27)$$

Assuming isotropic turbulence ($\overline{u_g'^2} = 2/3 k$) and substituting Eq. 8 for v_g^t , Eq. 27 becomes

$$t^t = \frac{3 C_\mu k}{2\epsilon} \quad (28)$$

The value of the turbulent particle Schmidt number σ_j^t is not well characterized. Comparisons of predictions to data can be used to empirically determine this parameter. Best results were obtained by Fletcher (1983) using $\sigma_j^t = 0.35$. This value compares well with the results of Lilly (1973), where $\sigma_j^t = 0.34$, but not as well with the results of Melville and Bray (1979), who recommended a value of 0.7.

Several other particle dispersion models are also found in the current literature. Lockwood, et al. (1980) used an empirical approach to get v_{pd} from u'^2 and v'^2 . Longwell and Weiss (1980) considered that the ratio of particle eddy diffusivity to gas eddy diffusivity followed a sinusoidal pattern involving t_j and t^t . Lilly (1973) gives evidence that v_j^t/v_g^t decreases as t_j/t^t increases, especially for small particles (6 to 16 μm). Lilly's results are surprising, since the larger particles were more dispersed than the smaller particles. The model of Melville and Bray (1979) was selected here because it seemed to be more complete than the other models and is applicable to the size range of interest (10 to 100 μm).

3. Bulk Particle Density

The bulk particle density is needed to calculate the radiation field (discussed later) and to calculate particle velocities (Eq. 22). However, the Eulerian bulk particle density field cannot be calculated directly from the Lagrangian particle trajectory information. Methods used for obtaining this gradient by counting particles and smoothing Lagrangian density information have not been completely acceptable. The bulk particle mass, and number densities are related as follows:

$$\bar{\rho}_b = \alpha_j \bar{n}_j \quad (29)$$

The number density ($\bar{n}_j$) is easier to calculate than the mass density ($\bar{\rho}_b$) because the number of particles represented by each trajectory is constant throughout the computational domain. The mass density changes due to particle reaction. Equation 22 then becomes:

$$\vec{v}_{jd} \bar{n}_j = r_j \vec{\nabla} \bar{n}_j \quad (30)$$

Equation 30 is thought to approximate $\vec{v}_{jd}$ just as well as Eq. 22. However, $\bar{n}_j$ cannot be calculated from the Lagrangian particle-phase information, and can only be approximated using the Eulerian gas-phase information. The Eulerian equation of continuity for the particle number density in turbulent flow (steady-state) is:

$$\frac{\partial}{\partial x}(\bar{u}_j \bar{n}_j) + \frac{1}{r} \frac{\partial}{\partial r}(r \bar{v}_j \bar{n}_j) - \frac{\partial}{\partial x}(\Gamma_j \frac{\partial \bar{n}_j}{\partial x}) - \frac{1}{r} \frac{\partial}{\partial r}(r \Gamma_j \frac{\partial \bar{n}_j}{\partial r}) = 0 \quad (31)$$

The diffusion coefficient (Γ_j) in Eq. 31 is the same as in Eq. 24, and can be approximated on an Eulerian basis assuming an average size for the particle as it reacts. This equation, however, requires the Eulerian particle velocity field for its solution. For the purposes of Eq. 31 the gas-phase velocity components are used to approximate u_j and v_j . With the small particles of interest to pulverized coal conversion processes, the particle and gas velocities are similar. Reynolds numbers for the particles relative to the gas are often less than 0.01. This approximation is only used for the purposes of Eq. 31, since the Lagrangian solution yields the particle velocity including the effects of particle drag.

F. GAS PHASE REACTIONS

1. The Turbulent Reaction Rate

The importance of properly accounting for the turbulent interactions with the combustion chemistry in diffusion flames cannot be overemphasized (Bilger, 1974). In writing conservation equations for individual species in turbulent reacting systems, time-averaging is required as has been shown earlier. The instantaneous form of these equations can be found in several sources (Bird et al., 1960; Smoot and Pratt, 1979; Williams, 1965). All of these species conservation equations contain reaction rate terms of the form

$$r_i = m_i m_j \rho^2 A \exp(-E/RT) \quad (32)$$

Proper time averaging of such terms is accomplished by decomposing the instantaneous variables into their main and fluctuating components giving rise to terms of the form:

$$\begin{aligned} \bar{r}_i = \overline{m_i m_j \rho^2 A \exp(-E/RT)} = \bar{\rho}^2 \bar{m}_i \bar{m}_j A \exp(E/R\bar{T}) \left\{ 1 + \frac{\overline{\rho'^2}}{\bar{\rho}^2} + \frac{\overline{m_i' m_j'}}{\bar{m}_i \bar{m}_j} \right. \\ \left. + \frac{2\overline{\rho' m_i'}}{\bar{\rho} \bar{m}_i} + 2\frac{\overline{\rho' m_j'}}{\bar{\rho} \bar{m}_j} + \frac{E}{R\bar{T}} \left[\frac{\overline{m_i' T'}}{\bar{m}_i \bar{T}} + \frac{\overline{m_j' T'}}{\bar{m}_j \bar{T}} + \left(\frac{E}{2R\bar{T}} - 1 \right) \frac{\overline{T'^2}}{\bar{T}^2} \right] + \dots \right\} \quad (33) \end{aligned}$$

The other terms which appear, involve triple correlations of the fluctuating variables. It is to be remembered that for any realistic reaction scheme, scores of these equations must necessarily appear.

Historically, two approaches have been used to solve this problem. At one extreme, complex finite rate chemistry is considered but turbulent mixing is disregarded. Bowman (1975) and Caretto (1976) reviewed this literature. At the other extreme, turbulent mixing is treated in detail as described earlier, but local instantaneous (infinite rate) chemistry is assumed. Bilger (1974) reviewed this literature. Very few attempts have been made to combine finite rate chemistry and detailed turbulent mixing. Borghi (1974) applied turbulent chemical reaction rate calculations to a CO-containing plume. He introduced the concept of the contact index. Spalding (1978) proposed a combined Eulerian and Lagrangian formulation. Even with these difficulties, in many situations simplified combustion models can predict gaseous turbulent combustion processes with acceptable engineering accuracy (Spalding, 1978; Gosman et al., 1978; Libby, 1976; Spalding, 1971). Each of these references suggests different forms of a combustion model. Simplifications are usually made by assigning properties to the bulk fuel and oxidizer streams.

2. The Mixture Fraction

In gas phase diffusion flames, the fuel and oxidizer are initially separated in different streams. They enter the reactor in separate eddies which must be intimately contacted on a molecular level before reaction can occur. The assumption is then made that this micromixing process is rate-limiting, not the kinetic process. This allows the chemistry to be computed from equilibrium considerations. Only one differential equation is required to describe the degree of "mixedness" or "unmixedness" at a point, a great simplification as compared to the immense system of equations described above for the kinetic scheme.

For cases where there are two identifiable streams or states that have uniform properties, it is convenient to describe a conservative scalar f , the mixture fraction:

$$f = \frac{M_p}{M_p + M_s} = \begin{array}{l} \text{mass fraction of fluid atoms} \\ \text{originating in primary stream} \end{array} \quad (34)$$

The advantage of the mixture fraction approach lies in its ability to calculate any conserved scalar (s) from the local value of f :

$$s = fs_p + (1 - f)s_s \quad (35)$$

The following sections develop an approach to comprehensive calculations which use the concept of mixture fractions. The application of this concept requires that the turbulent diffusivity of all gas phase species be equal and that their boundary conditions be the same. These properties, taken together, constitute what is sometimes called Crocco similarity (Smith, 1979). The mixture fraction approach greatly reduces the number of conserved scalars required to describe a combustion system. An example of a conserved scalar is the mass fraction of a given element.

3. Scalar Transport

The differential equation for the transport of a scalar variable is shown here in its Favre-averaged form:

$$\frac{\partial}{\partial x}(\bar{\rho} \tilde{u} \tilde{f}) + \frac{1}{r} \frac{\partial}{\partial r}(r \bar{\rho} \tilde{v} \tilde{f}) - \frac{\partial}{\partial x} \left(\frac{\mu_e}{\sigma_f} \frac{\partial \tilde{f}}{\partial x} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{r \mu_e}{\sigma_f} \frac{\partial \tilde{f}}{\partial r} \right) = 0 \quad (36)$$

The solution of this equation, together with the fluid mechanics model, will prescribe the mean fluid values for the flow and the mixing, provided the appropriate mean density is available. The advantage of knowing $\tilde{f}$ is that with the aid of a probability density function (PDF) for f , the time mean values may be found for any arbitrary value β which is only a function of f .

$$\beta = \alpha_p \beta_p + \alpha_s \beta_s + \int_0^1 \beta(f) \bar{P}(f) df \quad (37)$$

The mean of the distribution of the mixture fraction (first moment about the origin) is given by Eq. 36. The variance (second moment about the mean, or the mean square fluctuation) of the mixture fraction is defined as:

$$g_f = \overline{(f - \bar{f})^2} = \frac{1}{T} \int_0^T [f(t) - \bar{f}]^2 dt \quad (38)$$

where T is large as compared to the time scale of the local turbulence. Launder and Spalding (1972) show how a transport equation for g_f can be derived and appropriate terms modeled in a manner analagous to, and consistent with the other two equations in the k - ϵ turbulence model. The resulting equation is:

$$\begin{aligned} & \frac{\partial}{\partial x}(\bar{\rho} \tilde{u} g_f) + \frac{1}{r} \frac{\partial}{\partial r}(r \bar{\rho} \tilde{v} g_f) - \frac{\partial}{\partial x} \left(\frac{\mu_e}{\sigma_g} \frac{\partial g_f}{\partial x} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{r \mu_e}{\sigma_g} \frac{\partial g_f}{\partial r} \right) \\ & = C_{g1} \mu_e / \sigma_g \left[\left(\frac{\partial \tilde{f}}{\partial x} \right)^2 + \left(\frac{\partial \tilde{f}}{\partial r} \right)^2 \right] - C_{g2} \frac{\bar{\rho} \epsilon g}{k} \end{aligned} \quad (39)$$

Appropriate constants for the combustion submodel, introduced by Eqs. 36 and 39, are given in Table 3.

Besides $\tilde{f}$ and g_f , the PDF shape is needed. In regions of small g_f the shape of the PDF makes little difference. The PDF shape is determined from experimentally observed fluctuations in coal flames. Smith (1979), for example, used a top-hat (uniform) distribution, while forms of the Gaussian distribution and the Beta distribution have also been used. Kent and Bilger (1977) used a "clipped" Gaussian distribution which accounts for intermittency, and noted significant sensitivity of the predictions to the form of the PDF used, particularly with respect to nitric oxide concentrations. Other

TABLE 3
TURBULENT COMBUSTION MODEL CONSTANTS

<u>Constant</u>	<u>Value</u>
C_{g1}	2.8
C_{g2}	1.92
σ_f	0.9
σ_g	0.9
σ_{ht}	0.9
σ_h^*	0.8
E^*	9.793

*These constants arise from boundary conditions

references pertaining to PDF shape are found in Smith (1979), Fletcher (1980), Kuo (1986), Lockwood and Naguib (1975), and Kent and Bilger (1976). PCGC-2 is presently coded to use the clipped Gaussian distribution, (i.e. adjusted for intermittency) similar to that used in the last two references. The parameters needed to calculate this Gaussian PDF are found in Table 4.

4. Chemical Equilibrium

In a combustor which is assumed locally adiabatic (no gas radiation, external heat loss, or compressible heating/cooling), the standard enthalpy is a conserved scalar, and thus with the assumption of equal diffusivities, the instantaneous local enthalpy h may be calculated directly from f :

$$h = fh_p + (1 - f) h_s \quad (40)$$

If the local turbulent diffusivities are equal, the elemental mass fractions (b_k) are also conserved scalars and are given by:

$$b_k = fb_{kp} + (1 - f)b_{ks} \quad (41)$$

Equations 40 and 41 are not dependent on the assumption of chemical equilibrium but only on the equality of diffusivities, and in the case of Eq. 40, on the assumption of adiabatic operation. These assumptions comprise what is called Crocco similarity (Smith, 1979). For non-adiabatic operation, the energy equation (discussed later) must be solved.

If local instantaneous equilibrium is assumed (micromixing is limiting rather than chemical kinetics), all thermodynamic properties can be obtained. For a Gibbs free energy reduction scheme, the required parameters are the energy level, pressure, and elemental composition. The equilibrium properties are then functions of f alone:

$$T = T(b_k, h) = T[b_k(f), h(f)] = T(f) \quad (42)$$

$$\rho = \rho(b_k, h) = \rho[b_k(f), h(f)] = \rho(f) \quad (43)$$

$$y_i = y_i(b_k, h) = y_i[b_k(f), h(f)] = y_i(f) \quad (44)$$

The turbulent flow mean compositions and other properties are obtained by weighting with the PDF of f , as in Eq. 37:

$$\tilde{y}_i = \alpha_p y_{ip} + \alpha_s y_{is} + \int_{0+}^1 y_i(f) P(f) df \quad (45)$$

TABLE 4
PARAMETERS FOR GAUSSIAN PROBABILITY DENSITY FUNCTION

$$P(\phi) = (2\pi G_\phi)^{-1/2} \exp(-Z_\phi^2/2)$$

$$\alpha = (2\pi)^{-1/2} \int_L^U \exp(-Z_\phi^2/2) dZ_\phi$$

Intermittency	ϕ	U	L	Z_ϕ
α_p	f	∞	$(1-F)/\sqrt{G_f}$	$(f-F)/\sqrt{G_f}$
α_s	f	$-F/\sqrt{G_f}$	$-\infty$	$(f-F)/\sqrt{G_f}$
α_c	η	∞	$(1-H)/\sqrt{G_\eta}$	$(\eta-H)/\sqrt{G_\eta}$
α_I	η	$-H/\sqrt{G_\eta}$	$-\infty$	$(\eta-H)/\sqrt{G_\eta}$

where F and G_f come from:

$$\tilde{f} = \alpha_p + (1/\sqrt{2\pi G_f}) \int_{0+}^{1-} f \exp[-(f-F)^2/2G_f] df$$

$$f = \alpha_p - (\tilde{f})^2 + (1/\sqrt{2\pi G_f}) \int_{0+}^{1-} f^2 \exp[-(f-F)^2/2G_f] df$$

and where H and G_η come from:

$$\tilde{\eta} = \alpha_c + (1/\sqrt{2\pi G_\eta}) \int_{0+}^{1-} \eta \exp[-(\eta-H)^2/2G_\eta] d\eta$$

$$g_\eta = \alpha_c - (\tilde{\eta})^2 + (1/\sqrt{2\pi G_\eta}) \int_{0+}^{1-} \eta^2 \exp[-(\eta-H)^2/2G_\eta] d\eta$$

$$\tilde{\rho} = \alpha_p \rho_p + \alpha_s \rho_s + \int_{0+}^{1-} \rho(f) P(f) df \quad (46)$$

$$\tilde{T} = \alpha_p T_p + \alpha_s T_s + \int_{0+}^{1-} T(f) P(f) df \quad (47)$$

This approach to find the mean properties is dependent on the enthalpy (h) and the element mass fractions (b_k) being functions only of the mixture fraction (f). When heat losses (due to radiation, external heat loss, or compression/expansion) are significant, then Crocco similarity must be abandoned for the conservation equation in h (discussed later). In this situation, Eqs. 42 through 44 are no longer valid, and in general, the properties become functions of both f and h.

$$\beta = \beta(b_k, h) = \beta[b_k(f), h] = \beta(f, h) \quad (48)$$

Favre-averaged properties are obtained by convolution with a joint PDF:

$$\tilde{\beta} = \int_h \int_f \beta(f, h) P(f, h) df dh \quad (49)$$

This equation is valid for adiabatic operation as well, in which case the enthalpy is a function of f alone, and Eq. 49 reduces to Eq. 37.

The problem of obtaining $P(f, h)$ is greatly simplified by partitioning the enthalpy into: 1) the energy which would be convected if there were no external heat losses or gains (h_f), and 2) the residual energy due to the non-adiabatic boundary condition (h_r).

$$h = h_f + h_r \quad (50)$$

$$h = [f h_p + (1 - f) h_s] + h_r \quad (51)$$

In practice, the residual enthalpy can be calculated directly from the known field values of h and f and from the inlet conditions:

$$\tilde{h}_r = \tilde{h} - \tilde{f} h_p - (1 - \tilde{f}) h_s \quad (52)$$

Finally, it is assumed that the effects of the fluctuations of h_r are small compared with the effects of the fluctuations of h_f as implied by Eq. 52.

$$h'_r = 0 \quad (53)$$

Thus

$$\tilde{h}_r = h_r \quad (54)$$

This means that the fluctuations are correlated by the single variable f as before

$$\tilde{\beta} = \alpha_p \beta_p + \alpha_s \beta_s + \int_{0+}^{1-} \beta(f, h_r) P(f) df \quad (55)$$

where h_r is constant with respect to the fluctuations in f . Since h_r will be small relative to h_f , this approximation is thought to be reasonable. Without the above assumption, it would be necessary to include transport equations for both h and the mean square fluctuation of h_r . In addition, Eq. 55 would need to be convoluted over the joint probability density function $P(f, h_r)$.

A special case arises if it is assumed that the heat loss from the reactor is uniform throughout the reactor. The amount of sensible heat in the reactor is

$$Q_s = \int_{T_{ref}}^{T_a} C_{pd} T \quad (56)$$

where T_a is the adiabatic gas temperature and T_{ref} is the inlet gas temperature (ambient). The heat loss factor (γ) is defined to be the fraction of the total sensible heat lost from the reactor:

$$\gamma = \frac{h_a - h}{Q_s} \quad (57)$$

where h_a is the adiabatic enthalpy calculated from Eq. 40. The enthalpy can now be calculated as a function of the heat loss:

$$h = h_a - \gamma Q_s \quad (58)$$

Equation 58 maintains Crocco similarity while allowing for an approximation to non-adiabatic operation.

5. Reacting Particles

The gas model development to this point has assumed that no particles are present. When reacting particles are accounted for, it is convenient to define a new progress variable " η " (similar to f) which describes the mass fraction of gas originating from the burning coal. This progress variable is called the coal-gas mixture fraction, and is defined as shown below:

$$\eta = \frac{M_c}{M_p + M_s + M_c} = \begin{array}{l} \text{mass fraction of fluid atoms} \\ \text{originating from the coal} \end{array} \quad (59)$$

If the only source of fuel for the combustion or gasification system of interest is from the coal particle or droplets themselves, and if all of the remaining transporting fluid is composed of the same fluid with the same energy level, then η is the only required progress variable. Such is the case for practical combustors where the coal particles are transported with air in the primary stream, and the secondary stream is composed of air at the same temperature as the primary stream. In such systems the primary and secondary streams have exactly the same composition and energy level. In this limiting case the coal gas mixture fraction (η) is adequate to describe the progress of mixing in the chemical field since the components of the gas can be broken into only two parts, namely the coal offgas and the inlet gas.

A more general approach is adopted in PCGC-2. A mixture fraction is included to allow primary carrier gas fluid different than the secondary gas in either composition and/or enthalpy level. Alternatively, the mixture fraction may be used to track vaporized liquid, which evolves at a different rate and has a different composition and heating value than the coal offgas. In either case, the gas phase must be broken into three components: 1) mass of gas originating from the primary or liquid fuel, 2) gas originating from the secondary, and 3) the coal offgas. A minimum of two progress variables are required to describe the gas field at any one point in this approach. The variable η is used to describe the mass fraction of coal offgas. In addition, the mixture fraction f provides the information regarding the amount of primary carrier gas fluid or liquid fuel. Whether the variable f is used to track the mixing of the primary and secondary streams or the mixing of vaporized liquid in the combustion gases, there is a significant advantage in defining it as a mass ratio rather than a mass fraction. That is

$$f = \dot{m}_p / (\dot{m}_p + \dot{m}_s) \quad (60a)$$

or, in the case of slurry combustion,

$$f = \frac{\dot{m}_l}{\dot{m}_l + \dot{m}_{(p+s)}} \quad (60b)$$

In this case f , is not the local mass fraction of gas originating from the primary stream or liquid fuel but instead is the mass fraction of this quantity in the local mixture of primary plus secondary or vaporized liquid plus inlet gas. Since the mixture fraction f contains only information of the intermixing of the primary and secondary gas streams, or inlet gas with vaporized liquid, it is somewhat insensitive to local fluctuations of η , and thus much more independent of η than is the local mass fraction of primary fluid or liquid fuel. This statistical independence is useful in calculating the local chemical composition. Thus, f and η can be considered statistically independent to a first-order approximation.

Although f , as defined in Eq. 60, is a useful quantity for the calculational procedure, the local mass fraction of primary fluid or vaporized liquid is also an important parameter. This quantity is defined as f_p :

$$f_p = \dot{m}_p / (\dot{m}_p + \dot{m}_s + \dot{m}_c) \quad (61a)$$

$$\text{or } f_p = \dot{m}_l / (\dot{m}_l + \dot{m}_{p+s} + \dot{m}_c) \quad (61b)$$

where f_p is the conserved scalar for the reacting particle or droplet-laden system. The variable f as defined in Eq. 60 is not a conserved scalar in reacting, particle-laden systems. The importance of f_p is obvious from this conservative principle. Its mean value can be calculated from a Favre-averaged ($\tilde{f}_p$) conservation equation which includes convection and turbulent diffusion terms. There is no source term for the $\tilde{f}_p$ equation when f_p is defined as in Eq. 61a. When f_p is defined by Eq. (61b), the source term is given by the mass of vaporizing liquid. From these definitions, the relationship between f and f_p is:

$$f = f_p / (1 - \eta) \quad (62)$$

The progress variables f and η are useful quantities for partitioning the characteristics of the gas field. In order to obtain the mean chemical properties temperature, density, composition, etc. of the gas field, we must understand the statistical distribution of these variables due to the presence of the turbulent fluid mechanics (i.e. probability density function). In addition, each of the three components (coal offgas, primary carrier gas and secondary gas or vapor) can react chemically to form new products.

In coal combustion/gasification systems, $\tilde{f}$ can be obtained from a nonconservative (i.e., with a source term) transport equation. Alternatively, f_p can be calculated from a conservative transport equation and f obtained through the relationship shown in Eq. 62. Of course, Eq. 62 relates the instantaneous f and f_p variables. But if f_p can be considered statistically independent of η , then the relationship also holds true in the mean:

$$\tilde{f} = \tilde{f}_p / (1 - \tilde{\eta}) \quad (63)$$

The assumption of Crocco similarity applies there as well as in the case of gaseous diffusion flames. With the above assumptions, any local property that is a function of f and η can be calculated directly.

$$\beta = \beta_c \eta + (1 - \eta)[f\beta_p + (1 - f)\beta_s] \quad (64)$$

The subscript c stands for pure coal off gas. Time-mean gas properties (i.e., species composition, density, and temperature) can be obtained for any values of η and f by convolution over a joint probability density function:

$$\tilde{\beta} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \beta(\eta, f) P(\eta, f) d\eta df \quad (65)$$

Note that Eq. 65 is analagous to Eq. 37. Assuming η and f are independent quantities, the joint probability density function, $P(\eta, f)$, can be separated:

$$P(\eta, f) = P(\eta) P(f) \quad (66)$$

Intermittency can occur for both η and f , and must be handled carefully (Fletcher, 1980). Intermediate steps to the final formulation are shown for completeness. By substituting Eq. 66 into 65 and expanding:

$$\tilde{\beta} = \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} P(f) \beta(\eta, f) df \right] P(\eta) d\eta \quad (67)$$

$$\tilde{\beta} = \int_{-\infty}^{\infty} [\alpha_p \beta(\eta, 1) + \alpha_s \beta(\eta, 0) + \int_{0+}^{1-} P(f) \beta(\eta, f) df] P(\eta) d\eta \quad (68)$$

Finally:

$$\begin{aligned} \tilde{\beta}(\eta, f) = & \alpha_c \beta_c + \alpha_I [\alpha_p \beta_p + \alpha_s \beta_s + \int_{0+}^{1-} P(f) \beta(0, f) df] \\ & + \alpha_p \int_{0+}^{1-} P(\eta) \beta(\eta, 1) d\eta + \alpha_s \int_{0+}^{1+} P(\eta) \beta(\eta, 0) d\eta \\ & + \int_{0+}^{1-} \int_{0+}^{1-} P(\eta) P(f) \beta(\eta, f) d\eta df \end{aligned} \quad (69)$$

The subscript I represents pure inlet gas from both the primary and secondary streams. Equations for $\tilde{\eta}$ and $\tilde{g}_\eta$ are necessary to obtain the PDF, and are derived in a manner which is analagous to the equations for f and g_f :

$$\frac{\partial}{\partial x} (\overline{\rho u \eta}) + \frac{1}{r} \frac{\partial}{\partial r} (r \overline{\rho v \eta}) - \frac{\partial}{\partial x} \left(\frac{\mu_e}{\sigma_\eta} \frac{\partial \tilde{\eta}}{\partial x} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\mu_e}{\sigma_\eta} \frac{\partial \tilde{\eta}}{\partial r} \right) = S_p^\eta \quad (70)$$

$$\begin{aligned} & \frac{\partial}{\partial x} (\overline{\rho u g_\eta}) + \frac{1}{r} \frac{\partial}{\partial r} (r \overline{\rho v g_\eta}) - \frac{\partial}{\partial x} \left(\frac{\mu_e}{\sigma_g} \frac{\partial g_\eta}{\partial x} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\mu_e}{\sigma_g} \frac{\partial g_\eta}{\partial r} \right) \\ & = C_{g1} \mu_e / \sigma_g \left[\left(\frac{\partial \tilde{\eta}}{\partial x} \right)^2 + \left(\frac{\partial \tilde{\eta}}{\partial r} \right)^2 \right] - C_{g2} \bar{\rho} \epsilon g_\eta / k \end{aligned} \quad (71)$$

For lack of better constants, the "universal" constants from Table 3 (i.e., C_{g1} , C_{g2} , etc.) are used in Eqs. 70 and 71. These constants are semi-empirical, and need to be investigated further. The S_p^n term in Eq. 70 represents the local mass addition to the gas phase from coal reactions (one component of the total particle mass source term).

When the adiabatic assumption is relaxed, the enthalpy must be calculated from a transport equation. Gas properties will then be functions of n , f , and h , so that (n, f) in Eq. 65 must be replaced by (n, f, h) . Equation 65 must also be convoluted with $P(h)$ if fluctuations in h are important (Smith, 1979). The gas-phase energy conservation equation is listed here for completeness:

$$\begin{aligned} \frac{\partial}{\partial x}(\overline{\rho u h}) + \frac{1}{r} \frac{\partial}{\partial r}(r \overline{\rho v h}) - \frac{\partial}{\partial x} \left(\frac{\mu_e}{\sigma_h} \frac{\partial \tilde{h}}{\partial x} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\mu_e}{\sigma_h} \frac{\partial \tilde{h}}{\partial r} \right) \\ = q'_{rg} + \tilde{u} \frac{\partial \bar{p}}{\partial x} + \tilde{v} \frac{\partial \bar{p}}{\partial r} + S_p^h + \tilde{h}_{pg} S_p^m \end{aligned} \quad (72)$$

The q'_{rg} term represents the net volumetric radiative heat transfer due to gas-phase radiation. The S_p^h term represents the volumetric energy change due to the particle reactions. The $\tilde{h}_{pg} S_p^m$ term represents the addition of enthalpy associated with the addition of coal off gas. The other terms on the right-hand side of Eq. 72 come from the overall gas continuity equation.

Formally, the gas phase properties are a function of the elemental composition, the total enthalpy and the local pressure. The enthalpy fluctuations due to the presence of the particles can be accounted for by partitioning the total gas enthalpy into the contributions by n , by f , and by the residual enthalpy contributions.

To this point the elemental composition of the coal off gas has been assumed constant. This assumption could be relaxed, and each reaction involved (i.e., high activation energy pyrolysis, heterogeneous oxidation, etc.) could produce different gaseous elemental compositions by defining a new n_m for each reaction. In this case, n_m would be a local mass ratio of gas originating from the m^{th} reaction, defined in such a way as to preserve (if possible) their statistical independence. The instantaneous local gaseous properties would then be obtained from f , n_1 , n_2 , . . . n_m . Intermittency of each mixture fraction would need to be properly included as before. The added complexity in solving transport equations for each new n_m and for each new g_n , and then convolving the instantaneous properties over the probability density functions of all mixture fractions would significantly increase computational time and storage. The approximations involved in the statistical model would then probably nullify any advantage achieved by way of increased flexibility in specification of the coal off gas composition unless n fluctuations were ignored.

G. PARTICLE PHASE REACTIONS

This section presents the details of single coal particle model reactions that occur in pulverized coal combustion and gasification processes. The description of coal reaction processes includes vaporization, devolatilization, char oxidation, and gas-particle interchange. The resulting model describes the response of a coal particle to its thermal, chemical, and physical environment.

Development of an analytical treatment of pulverized coal-char behavior in reacting systems is based largely on independent experimental observations and kinetic parameters deduced from these observations. Since there are still unresolved questions regarding the kinetics of coal reactions, an attempt has been made to formulate a general reaction scheme that can accommodate results of future measurements and improved kinetic parameters.

The description that follows applies to pulverized coal reaction processes, where particles are small ($<150 \mu\text{m}$) and heating rates are high ($10^3 - 10^6 \text{ K s}^{-1}$). The treatment is intended for application to pulverized-coal furnaces and entrained-coal gasifiers and would not necessarily apply to fixed or fluidized-bed processes without modification.

1. Particle Continuity Equations

The coal particle droplet is considered to consist of four components: liquid, coal, char, and ash. Ash is defined as that part of the coal particle that is inert in the combustion scheme. Char is the residue left in the coal particle when the volatile products are released plus that portion of the particle which cannot undergo devolatilization.

The process by which each particle reacts is schematically presented in Figure 3. The reacting particle is assumed to be composed of specified amounts of liquid raw coal, char, and ash. The continuity equations for each coal component are listed below for the j^{th} particle size:

$$d\alpha_{wj}/dt = r_{wj} \quad (73)$$

$$d\alpha_{cj}/dt = r_{cj} \quad (74)$$

$$d\alpha_{hj}/dt = r_{hj} \quad (75)$$

$$d\alpha_{aj}/dt = 0 \quad (76)$$

The liquid vaporizes in accordance with classical expressions.

Figure 3. Schematic of coal particle, illustrating constituents and reaction processes.

The vaporization rate is modeled such that it can be controlled by either heat or mass transfer. In practice, the vaporization rate is nearly always controlled by the heat transfer rate. The mass transfer driving force, i.e., the difference between the vapor concentration at the particle surface and that in the bulk gas has a larger impact on the droplet/particle temperature difference than on the vaporization rate.

The fraction of the surface area covered with liquid is specified in the case of a slurry droplet. The raw coal, or the dry, ash-free portion of the coal, undergoes devolatilization to volatiles and char by one or more reactions (M in total number) of the form:

The volatiles react further in the gas phase. The char reacts heterogeneously, after diffusion of the reactant (i.e., O_2 , CO_2 , H_2O , H_2) to the particle surface, by one or more reactions (L in total number) of the form:

ϕ_L is the stoichiometric coefficient (moles carbon required per mole of oxidizer). Values of ϕ_L usually assumed for O_2 , CO_2 , H_2O , and H_2 , are 2.0, 1.0, 1.0, and 0.5, respectively. Hence, CO is usually assumed to be the primary product of char oxidation by oxygen rather than CO_2 . The oxidation reactions are assumed to be first-order with respect to the oxidizer concentration.

An overview of this coal submodel is presented in the following sections and further detail is given in Smoot and Pratt (1979), Smith (1979), Fletcher (1980), Smoot and Smith (1985) and Baxter (1987). The differential equations for the Lagrangian trajectories of each particle are those for continuity (Eqs. 73-76), momentum (Eqs. 15, 21-28), and energy (Eq. 80 in the next section).

2. Particle Energy Equation

The particle energy conservation equation in the lagrangian form is:

$$d(\alpha_j h_j)/dt = Q_{rj} - Q_j - r_j h_{jg} \quad (80)$$

where h_{jg} is the enthalpy of the coal offgas and accounts for heats of reaction, Q_{rj} represents the net radiation to the particle, and Q_j represents convection and conduction from the particle to the gas phase. The third term on the right represents the enthalpy lost to the gas phase by transfer of mass due to particle reaction. The heat of reaction is given to the particle. Note that the radiative and convective heat transfer have opposite signs. That is, if both are heating the particle, radiation is positive and

convection is negative. This is a consequence of sign conventions used in other portions of the code dealing with heat transfer.

Physical Properties. This section discusses the equations proposed to obtain the particle and gas phase properties needed for the particle reaction model. The gas phase properties discussed are necessary in order to incorporate diffusion limitations on particle reaction rates. These properties are not determined from the statistical PDF approach since incorporation of turbulent fluctuating effects on such physical properties is not justifiable.

Equations 82 through 88 of Table 5 show the calculation procedures used for the gas phase properties. These approximations are discussed by Smith (1979) and Baxter (1987) and may be found in standard text books on transport properties (e.g., Bird et al., 1960). The physical characteristics of the j^{th} particle type are calculated with Eqs. 81, 89, and 90. During vaporization, slurry droplets maintain diameters which are essentially equal to their original diameter (see Baxter, 1987, for discussion). Fuel oil droplets decrease in diameter with density kept constant (see Eq. 91 below). The particle is allowed to swell linearly with the extent of devolatilization as shown in Eq. 89. The swelling coefficient γ must be specified. This swelling during devolatilization is an experimentally observed phenomenon (Anson et al., 1971). The average particle diameter increase is often on the order of 10 percent (Smoot and Horton, 1978) for highly volatile bituminous coals.

Two possible options regarding the diameter of the char residue have been suggested. After devolatilization, the particle could be envisioned as a porous sphere where reaction takes place mainly within the pores themselves. As char combustion proceeds, the particle diameter can be taken to remain relatively constant, but with variable density until breakup or complete burnout of the fuel. Alternatively, the particle may be perceived to react mostly on the surface and thus burn out as a shrinking particle at constant density:

$$d_j = [6\alpha_j / \pi \rho_{\alpha j}]^{1/3} \quad (91)$$

where $\rho_{\alpha j}$ is the solid density of the j^{th} particle type after complete devolatilization (i.e., when $\alpha_{cj} = 0$). Both options are included. The external particle surface area is given by Eq. 90. Equation 91 is also recommended for fuel oil combustion.

Particle heat capacity is either entered as a polynomial or calculated according to the suggestions of Merrick (1983). The latter is the suggested form. The predicted particle temperature and reaction rates change substantially with changing heat capacity (see Baxter, 1987). The model of Merrick is selected by zeroing all coefficients for the heat capacity in the data file.

Merrick suggested the following function for the heat capacity of coal:

$$c_v = \left(\frac{R}{a}\right) \left[g_1 \left(\frac{380}{T}\right) - 2g_1 \left(\frac{1800}{T}\right)\right] \quad (92)$$

TABLE 5

PHYSICAL PROPERTIES FOR PARTICLE MODEL

No.	Type	Equation
81	Particle heat capacity	$C_{pj} = (\alpha_{wj}C_{pwj} + \alpha_{hj}C_{phj} + \alpha_{cj}C_{pcj} + \alpha_{aj}C_{paj})/\alpha_j$
82	Gas species conductivity	$k_i = [C_{pi} + (5R/4M_i)]\mu_i$
83	Gas mixture conductivity	$k_g = \sum_i [X_i k_i / \sum_k X_k \phi_{ik}]$
84	Gas species viscosity	$\mu_i = 2.67 \times 10^{-6} (M_i T_g)^{1/2} / \sigma_i^2 \Omega_\mu$
85	Interaction parameter	$\phi_{ik} = (1/\epsilon)^{1/2} [1 + (M_i/M_k)]^{1/2} [1 + (\mu_i/\mu_k)^{1/2} (M_k M_i)^{1/4}]^2$
86	Gas mixture viscosity	$\mu_g = \sum_i [X_i \mu_i / \sum_k X_k \phi_{ik}]$
87	Species diffusivity	$D_{ik} = 1.83 \times 10^{-12} T_g^{3/2} [(1/M_k) + (1/M_i)]^{1/2} / p \sigma_{ik}^2 \Omega_d$
88	Mixture diffusivity	$D_{im} = (1 - X_i) / \sum_{i \neq k} (X_k / D_{ik})$
89	Particle diameter	$d_j = d_{j0} [1 + (\alpha_{cjo} - \alpha_{cj})/\alpha_{cjo}]$ (swelling during devolatilization) $d_j = d_{j0}$ (during coal slurry vaporization) $d_j = \text{constant or } \rho_j = \text{constant during oxidation, depending on input parameters}$
90	Particle surface area	$A_j = \pi d_j^2$

where R is the universal gas constant (8314.4 J/kg-mol/K), a is the average atomic weight of the coal or char (kg/kg-mol), T is temperature (K), and g_1 is the following function:

$$g_1(z) = \frac{e^z}{\left[\frac{(e^z-1)}{z}\right]^2} \quad (93)$$

The average atomic weight of the coal is given by

$$a = \left[\sum_i^n y_i / \mu_i \right]^{-1} \quad (94)$$

where y_i is the mass fraction of element i, μ is the atomic weight of element i, and n is the number of elements in the organic portion of the coal. Merrick compared his heat capacity model with experimental data and found agreement within about 10% in the temperature range of 0-300°C and coal ranks ranging from 15-35% volatile matter. Graphite and char heat capacities were correlated within 5% between 0 and 800°C. The heat capacity of ash is taken as

$$c_v = 593.3 + 0.586 T \quad (95)$$

where T is in K. Predicted particle temperatures can differ by as much as 500 K depending on the choice of heat capacity models used (Baxter, 1987).

The equilibrium mole fraction of liquid at the temperature, T, of the droplet is calculated from the Clapeyron equation and Raoult's law:

$$x_\ell = \frac{P(T_1)}{P_{tot}} \exp \left[\int_{T_1}^T \frac{\int_{T_0}^{T'} \Delta C_p dT'' + \Delta h(T_0)}{RT'^2} dT' \right] \quad (96)$$

ΔC_p is the difference in the vapor and liquid heat capacities, and $\Delta h(T_0)$ is the difference in specific enthalpies at the specified temperature T_0 . All quantities needed for this equation are input variables. An option for an Antoine equation is also included.

The actual mole fraction of the vaporizing liquid at the surface of the droplet/particle is not equal to the equilibrium value but is a function of it. The actual interface conditions are discussed in detail by Baxter (1987). A simplified version of the techniques Baxter discusses has been incorporated in the code. If the droplet temperature is greater than or equal to its boiling temperature, the vaporization rate is given by an equation which does not depend on the surface concentration. The heat of vaporization as a function of temperature is calculated according to the numerator of Eq. 96. Baxter (1987) discusses the details of these calculations more fully.

Convective and Conductive Heat Transfer. The particle energy is computed from the Lagrangian differential equation of energy shown in Eq. 80. Auxiliary relationships needed to describe the heat transfer processes are shown in Table 6.

The temperature of the particle is obtained by integrating Eq. 80 formally with the definition of C_{pj} given in Eq. 81 and h_{fj}^0 in Eq. 109. The resulting nonlinear equation is solved with a combined bisection-regula falsi technique as discussed in Baxter (1987).

Equation 98 of Table 6 represents the heat transfer rate for a single particle between the j^{th} particle and the gas phase. The Nu_{jg} term represents the mean conductive Nusselt number for heat transfer from spheres without the presence of particle blowing. The term enclosed between brackets is the blowing correction. Smith (1979) discusses the derivation of this term based on classical film theory as well as introducing other approximate correction forms. A reasonable expression for Nu_{jg} is given in Eq. 99 (Kreith, 1973). The blowing transpiration parameter for heat transfer (B_j) is given in Eq. 100. The relationship of this parameter to that for mass transfer is also discussed by Smith (1979). The definitions of Re_{jg} and Pr_g are given in Eqs. 101 and 102. The resulting Q_j is required for the particle differential energy equation (Eq. 80).

Equations 103 through 106 show how the enthalpy of each of the particle constituents is calculated for use in the particle enthalpy calculation (Eq. 97). The functional form of the heat capacity correlation depends on input parameters, as discussed earlier. The enthalpy of the volatile matter from each of the M devolatilization reactions is calculated from an energy balance as shown in Eq. 107. The enthalpy of the particle products for use in Eq. 80 is shown in Eq. 108. The first three terms in Eq. 108 represent the enthalpy of coal volatiles, oxidized char, and slurry liquid, respectively, assuming negligible heat of reaction for the devolatilization and char oxidation reactions and negligible heat of vaporization for the slurry liquid. The last three terms (multiplied by ζ) represent the heats of reaction for devolatilization and char oxidation and the heat of vaporization of the slurry liquid, respectively, a fraction (ζ) of which is added to the product gas enthalpy. Since heats of reaction and vaporization are negative when heat is given off (exothermic) ζ represents the fraction of these heats which is given to the particle phase. When ζ equals one, the heats of reaction and vaporization are given entirely to the particle phase. When ζ equals zero, they are given entirely to the gas phase. The proper value of ζ is thought to be 1.0 (Baxter, 1987).

3. Particle Reactions

This section discusses each of the reactions involved in the reaction model of the j^{th} particle classification. The rate expression for each is presented and the effects of oxidizer diffusion and high rates of mass transfer or particle blowing are incorporated. As presented schematically in Figure 3, the three overall mass loss processes for each particle are vaporization, devolatilization, and heterogeneous reaction. The corresponding equations are shown in Table 7. The model allows one vaporization reaction, M devolatilization reactions, and L char oxidation reactions of the form shown in Eq. 79 per particle type. Each of these reaction sets will be discussed in

TABLE 6
CONVECTIVE AND CONDUCTIVE HEAT TRANSFER FOR PARTICLE MODEL

No.	Type	Equation
97	Particle enthalpy	$h_j = (\alpha_{wj}h_{wj} + \alpha_{cj}h_{cj} + \alpha_{hj}h_{hj} + \alpha_{aj}h_{aj})/\alpha_j$
98	Particle-gas heat transfer	$Q_j = Nu_{jg}\pi[B_j/(\exp B_j - 1)]k_g(T_j - T_g)d_j$
99	Nusselt No.	$Nu_{jg} = 2.0 + 0.65 (Re_{jg})^{1/2}(Pr_g)^{1/3}$
100	Transpiration parameter	$B_j = r_j C_{pg}/2\pi d_j k_g$
101	Reynolds No.	$Re_{jg} = d_j \vec{v}_g - \vec{v}_j \rho_g / \mu_g$
102	Prandtl No.	$Pr_g = (C_{pg}\mu_g/k_g)$
103	Liquid enthalpy	$h_{wj} = h_{fwj}^0 + \int_{298}^{T_j} C_{pwj} dT_j$
104	Raw coal enthalpy	$h_{cj} = h_{fcj}^0 + \int_{298}^{T_j} C_{pcj} dT_j$
105	Char enthalpy	$h_{hj} = h_{fhj}^0 + \int_{298}^{T_j} C_{phj} dT_j$
106	Ash enthalpy	$h_{aj} = h_{faj}^0 + \int_{298}^{T_j} C_{paj} dT_j$
107	Volatiles enthalpy	$h_{vjm} = [h_{cj} - h_{hj} (1 - Y_{jm})]/Y_{jm}$
108	Total particle product gas enthalpy	$h_{jg} = [\sum_m r_{vjm} h_{vjm} + h_{hj} \sum_\ell r_{hj\ell} + r_{wj} h_{wj} + \zeta(\sum_m r_{vjm} h_{g_{vjm}}) + \sum_\ell r_{hj\ell} h_{g_{hj\ell}} + r_{wj} h_{vw}]/r_j$
109	Particle heat of formation	$h_{fj}^0 = (\alpha_{wj}h_{fwj}^0 + \alpha_{hj}h_{fhj}^0 + \alpha_{cj}h_{fcj}^0 + \alpha_{aj}h_{faj}^0)/\alpha_j$

TABLE 7
PARTICLE REACTIONS FOR PARTICLE MODEL

No.	Type	Equation
110	Liquid vaporization rate	non-boiling $r_{wj} = [S_f A_j k_{jw} \rho_g (x_{wjs} - x_{wb}) + x_{wjs} (\sum_m S_f r_{vjm})] / (1.0 - x_{wjs})$
111	Same as 110	boiling $r_{wj} = [-Q_j + Q_{rj} + r_{cj} (h_{jg} - h_{cj}) \zeta + r_{hj} \zeta (h_{jg} - h_{hj})] / \zeta (h_{jg} - h_{wj})$
112	Particle reaction rate to gas phase	$r_j = \sum_\ell r_{hj\ell} + \sum_m r_{vjm} + r_{wj}$
113	Net char reaction rate	$r_{hj} = \sum_m r_{hjm} - \sum_\ell r_{hj\ell}$
114	Oxidizer-char reaction rate	$r_{hj\ell} = A_j^2 M_{hj} M_g \phi_\ell k_{cj\ell} k_{j\ell} \zeta_j C_{o\ell} C_g / [M_g A_j C_g (\zeta_j k_{j\ell} + k_{cj\ell}) + r_j]$
115	Kinetic char reaction rate coefficient	$k_{j\ell} = A_{j\ell} T_j^m \exp(-E_{j\ell}/RT_j)$
116	Transpiration parameters for mass transfer	$B_{ji} = r_j / 2\pi D_{im} \rho_g d_j$
117	Mass transfer coefficient	$k_{ji} = Sh_{jg} D_{im} B_{ji} / [d_j (\exp(B_{ji}) - 1)]$
118	Total coal reaction rate	$r_{cj} = \sum_m -r_{cjm} = -[\sum_m r_{hjm} + r_{vjm}]$
119	Volatile production rate	$r_{vjm} = k_{mj} Y_{mj} \alpha_{cj}$
120	Char production rate	$r_{hjm} = r_{vjm} (1 - Y_{mj}) / Y_{mj}$
121	Coal kinetic rate coefficient	$k_{mj} = A_{mj} \exp(-E_{mj}/RT_j)$

turn. The total reaction rate of the j^{th} particle classification per unit reactor volume is then the sum of each of these reactions, $(1 + L + M)$ in total number, as shown in Eq. 111.

The equations for the vaporization reactions are shown in Table 7. Vaporization is controlled by either heat transfer or mass transfer. The vaporization rate for non-boiling liquid (Eq. 110) is the sum of diffusive and convective components. k_w in the diffusion term is the mass transfer coefficient uncorrected for mass transfer. w is the mass transfer correction factor. S_f is the fraction of the particle surface area over which evaporation is taking place. The contribution of oxidizer-char reactions to the total mass flux from the particle has been neglected in the correction term because char oxidation is not usually important during slurry liquid vaporization. Baxter (1987) found that slurry droplets, often are not predicted to boil unless the local gas phase mass fraction of slurry liquid (e.g. water) reaches a high value. However, the vaporization rate is normally heat-transfer-limited.

The devolatilization reaction of Eq. 78 for the j^{th} particle is that proposed by Ubhayakar, et al. (1976). The kinetic rate of production of volatiles from the m^{th} reaction is given in Eq. 119, where the reaction rate constant is given in Eq. 121. Diffusional effects only become important when the volatiles repolymerize or condense prior to diffusion into the gas phase. Eq. 119 is used because of uncertainties in the repolymerization rate coefficients, the nature of the volatiles diffusion process, and because techniques and models used to correlate existing pyrolysis data most often have taken forms like Eq. 119.

The recommended rate constants for devolatilization are shown in Table 8. The chosen two-step mechanism of Ubhayakar, et al. (1976) is a reasonable compromise between a simple one-step mechanism (e.g., Godridge and Read, 1976), which would not account for the effect of particle history on volatiles yield, and a more complex, multistep mechanism (e.g., Lowe et al., 1979) which would increase computational time, and where rates and processes remain uncertain. Baxter (1987) performed a detailed analysis of these coefficients and provided the results tabulated here. The rates of Ubhayakar have been most often used in the past. Further analysis of rate coefficients with results not shown in Table 8 are given by Baxter (1987).

In accordance with Eq. 78, the devolatilization of the raw coal can produce char. A simple mass balance results in the rate of formation of char from the j^{th} particle type from the m^{th} reaction as shown in Eq. 120. Finally, the net rate of disappearance of the raw coal in the j^{th} particle class may be obtained by summing over all M devolatilization reactions. The rate of raw coal disappearance is the rate of char plus volatiles formation according to Eq. 78 and as shown in Eq. 118.

Char is assumed to react heterogeneously with gaseous oxidizers that diffuse to the particle surface from the bulk gas phase. Two rate-limiting steps are considered for this process: 1) gas phase diffusion and 2) heterogeneous reaction. The combined reaction rate is given in Eq. 114. In this form of the equation, the surface reaction has been assumed to be first-order in the surface concentration of the oxidizer. The Arrhenius expression for the rate constant is given in Eq. 115. Following the recommendations of

TABLE 8

DEVOLATILIZATION RATE EXPRESSIONS AND PARAMETERS FOR JSE IN PCGC-2

Single Step Reactions

Rank	Reference	ω_c^0 (DAF) ⁺	ω_h^0 (DAF) ⁺	Y	A (s ⁻¹)	E (J/kmol)
Lignit	Solomon, et al., 1986	[0.4]	1 - ω_i^0	1.0	4.3 x 10 ¹⁴	2.29 x 10 ⁸
	Kobayashi, et al., 1977	[0.7]	"	"	6.6 x 10 ⁴	1.05 x 10 ⁸
	Anthony, et al., 1976	[0.4]	"	"	2.83 x 10 ²	4.64 x 10 ⁷
	Truelove & Jamaluddin, 1986	[0.4]	"	"	6.2 x 10 ³	4.64 x 10 ⁷
Bituminous	Solomon, et al., 1986	[0.4]	1 - ω_i^0	1.0	4.3 x 10 ¹⁴	2.29 x 10 ⁸
	Kobayashi, et al., 1977	[0.7]	"	"	6.6 x 10 ⁴	1.05 x 10 ⁸
	Anthony, et al., 1976	[0.4]	"	"	7.1 x 10 ²	4.94 x 10 ⁷
	Truelove & Jamaluddin, 1986	[0.4]	"	"	2.0 x 10 ⁴	4.94 x 10 ⁷
	Wiser, et al., 1964	[0.5]	"	"	4.8 x 10 ¹	6.27 x 10 ⁷
	Badzioch & Hawksley, 1970	[0.4]	"	"	1.14 x 10 ⁵	7.45 x 10 ⁷
	Badzioch & Hawksley, 1970	[0.4]	"	"	3.12 x 10 ⁵	7.45 x 10 ⁷

Two Step Model

Rank	Reference	Reaction	ω_c^0 (DAF)	ω_h^0 (DAF)	Y _i	A _i (s ⁻¹)	E _i (J/kmol)
Lignite	Kobayashi, et al., 1977	1	1.0	1 - ω_i^0	0.3	2.0 x 10 ⁵	1.05 x 10 ⁸
		2	"	"	1.0	1.3 x 10 ⁷	1.67 x 10 ⁸
Bituminous	Kobayashi, et al., 1977	1	"	"	0.3	2.0 x 10 ⁵	1.05 x 10 ⁸
		2	"	"	1.0	1.3 x 10 ⁷	1.67 x 10 ⁸
	* Ubhayakar, et al., 1977	1	"	"	0.4	3.7 x 10 ⁵	7.36 x 10 ⁷
		2	"	"	0.8	1.5 x 10 ¹³	2.51 x 10 ⁸

*Most commonly used parameters if no data are available.

Baxter (1987), values of the experimental constants are shown in Table 9. Baxter (1987) showed substantial increase in accuracy of predictions when statistically sound methods of data analysis were used. The parameters from these analyses are also listed in Table 9. The mass transfer coefficient, which is also required, must be corrected for particle blowing or high rates of mass transfer. The mass transfer coefficient without blowing may be calculated from an empirical correlation for the Sherwood Number such as (Bird et al., 1960):

$$Sh_{jg} = \frac{k_{ji} d_j}{D_{im}} = 2.0 + 0.6 (Re_{jg})^{1/2} (Sc)^{1/3} \quad (122)$$

where the Schmidt Number is $(\mu_g / \rho_g D_{im})$, and the Reynolds Number is based on the difference in velocity between the particle and gas phases. If the Reynolds number is zero, this expression reduces to the theoretical value of 2.0 for molecular diffusion. The resulting expression for k_{CO} , corrected for particle blowing, is given in Eq. 117. In this case, the blowing parameter is that for mass transfer (Eq. 116).

Since char is being formed by each of the M devolatilization reactions and depleted by each of the L oxidation reactions, the net rate of char reaction is given in Eq. 113. Further, since the heterogeneous reaction is zero order with respect to the char concentration, heterogeneous ignition is permitted. The ignition phenomenon of the coal is not limited to devolatilization. Heterogeneous surface ignition is possible even if devolatilization has not been initiated.

H. RADIATION

1. Background

Radiative transfer becomes increasingly important as the furnace dimensions are increased, and in a typical coal-fired furnace environment, radiation includes contributions from both particulates (coal/char, ash and soot) and the gas phase (mainly CO_2 and H_2O). The accuracy of the radiation calculation depends on a combination of the accuracy of the calculation method, and the degree of certainty with which the radiative properties of the medium and surrounding walls are known. The radiative properties of the particulates depend on their concentration, size distribution, and complex refractive indices; those of the gases depend on their temperature, partial pressures and the optical thickness of the enclosure. Considerable uncertainties exist, in particular, regarding the size and concentration of soot, and the refractive index of ash. A recent study (Jamaluddin and Smith, 1987) of the sensitivity of predicted radiation fluxes to variations in the inputs indicated that these predictions are most sensitive to the particle concentration and size distribution, while the effect of the absorption and scattering efficiencies of the particles are rather insignificant. As for the gas phase radiation, emissivity data (Sarofim and Hottel, 1978) are known with more certainty than the local variations in gas temperature and species concentrations.

TABLE 9.

COEFFICIENTS FOR CHAF. REACTION WITH O₂, CO₂, AND H₂O

$$\frac{d\alpha_h}{dt} = AT^n \exp(-E/RT) \text{ [oxidizer]}$$

Oxidizer	Rank	Reference	n	A (m/K ⁿ s)	E (J/kmol)	
O ₂	*	all ranks	Baxter, 1987	1.0	2.30	9.29 x 10 ⁷
		all ranks	Field, et. al., 1967	1.0	0.30	1.49 x 10 ⁸
		hv Bituminous A	Baxter, 1987	1.0	1.03	7.49 x 10 ⁷
		hv Bituminous C	"	1.0	0.479	5.25 x 10 ⁷
		Subbituminous C	"	1.0	10.4	9.31 x 10 ⁷
		hv Bituminous A	Goetz, et. al., 1982	1.0	2.25	8.52 x 10 ⁷
		hv Bituminous C	"	1.0	2.02	7.18 x 10 ⁷
		Subbituminous C	"	1.0	4.96	8.36 x 10 ⁷
CO ₂		Lignite	Baxter, 1987	1.0	3.419	1.30 x 10 ⁸
		hv Bituminous A	"	1.0	1160.0	2.59 x 10 ⁸
		hv Bituminous C	"	1.0	4890.0	2.60 x 10 ⁸
		Subbituminous C	"	1.0	6188.0	2.40 x 10 ⁸
		Lignite	Goetz, et al., 1982	1.0	45.0	1.65 x 10 ⁸
		hv Bituminous A	"	1.0	95.14	2.25 x 10 ⁸
		hv Bituminous C	"	1.0	88.5	2.36 x 10 ⁸
		Subbituminous C	"	1.0	70.95	1.78 x 10 ⁸
		Graphite	Mayers, 1934	1.0	4.40	1.62 x 10 ⁸
		Graphite	Mayers, 1934	1.0	1.33	1.47 x 10 ⁸
		Lignite	Otto, et al., 1979	1.0	4.26 x 10 ⁴	3.16 x 10 ⁸
	Lignite	"	1.0	208	2.40 x 10 ⁸	

*Recommended good estimate for high rank coals if no data are available.

Radiative heat transfer models of gas- or oil-fired (Field et al., 1967; Bueters et al., 1974), and pulverized coal-fired furnaces (Lowe et al., 1974) have been reported using zone and flux methods with simple empirical assumptions for flow characteristics, temperatures, heat release rates, and gas composition. Recent radiation modeling has focused on the more efficient but less fundamental flux methods.

The flux methods commonly used are the four-flux type (Gosman and Lockwood, 1973; Lowes et al., 1973; DeMarco and Lockwood, 1975; Varma, 1979). Most of these models suffer from a lack of coupling between the directional fluxes. The discrete ordinates method (an extension of the flux method) corrects this defect, and still offers an equation form which is amenable to numerical methods consistent with the fluid mechanics. The consequences of the lack of effective coupling between the directional fluxes on the predictions of the radiation models has been demonstrated earlier (Jamaluddin and Smith, 1986). PCGC-2 uses either the Varma axisymmetric six-flux method (VFM), or the discrete ordinates method (DOM).

2. Formulation

Radiation calculations are based on an energy balance for a beam of radiation passing through a volume element (see Fig. 4) containing an absorbing-emitting-scattering medium:

$$\begin{aligned} & (\mu_m/r) [\partial(rI_m)/\partial r] - (1/r) [\partial(\eta_m I_m)/\partial \psi] + \epsilon_m (\partial I_m/\partial z) \\ & = - (k_a + k_s) I_m + k_a I_b + \frac{k_s}{4\pi} \int_{4\pi} P(\Omega, \Omega') I_m d\Omega' \end{aligned} \quad (123)$$

The left side of Eq. 123 represents the gradients of intensity in the direction of propagation, and the right side represents, respectively, the attenuation of intensity due to absorption and out-scattering, and the contribution to the directional intensity due to emission by the medium, and in-scattering. $P(\Omega, \Omega')$ is a probability density function, formally known as the phase function, which determines the distribution of the scattered intensity. Eq. 123 is better known as the radiation transport equation. The quantities μ_m , η_m and ϵ_m represent the direction cosines for the direction Ω , and are expressed as (see Fig. 5)

$$\mu_m = \sin\theta \cos\psi, \quad \eta_m = \sin\theta \sin\psi, \quad \epsilon_m = \cos\theta \quad (124)$$

The flux methods (including the discrete ordinates method) solve Eq. 123 in a number of pre-determined directions. The number of directions, N_m , depends on the order of the approximation. In the discrete ordinates method, this is given by $N_m = n(n+2)$ (Carlson and Lathrop, 1968), where n represents the order of the discrete ordinates approximation (the number of values for the direction cosines considered within the range ± 1.0). The angular integral is evaluated using numerical quadrature. Each direction Ω_m is pictured as a point on the surface of a unit sphere with which a surface area w_m is associated. w_m can be viewed as the angular quadrature weight, with the requirement that

Figure 4. Directional intensities reaching a volume element. (a) S_2 (b) S_4 .

Figure 5. The direction cosines.

$$\sum_m w_m = 4\pi \quad (125)$$

In the conventional flux methods (e.g., VFM), the quadrature weight is assumed to be uniform for all directions. In the VFM this is assigned a value of $4\pi/6$. In the discrete ordinates method, the entire quadrature scheme (i.e., the direction cosines and the weights) is obtained using the "moment matching" technique of Carlson and Lathrop (1968). The quadrature schemes for the S_2 and S_4 discrete ordinates, where the radiation transport equation is solved in 4 and 12 directions, respectively ($N_m/2$ directions required due to axial symmetry), are reported in Tables 10 and 11 (Truelove, 1976, 1978). These direction cosines establish a coupling between the directional intensities. In the orthogonal flux methods (like the VFM), the directions chosen to solve the radiative transport equation coincide with the coordinate directions, and therefore the coupling between the directional intensities is lost (for every direction, one of the direction cosines has a value of unity, while the other two are zeroes).

Considering the surrounding surfaces to be diffusely emitting-reflecting, the boundary conditions for the above equation are

$$\begin{aligned} \text{at } r = R : I_m &= \epsilon_w I_{bw} + (1 - \epsilon_w) \frac{q_r^+}{\pi} \quad ; \quad \mu_m < 0 \\ \text{at } r = 0 : I_m &= I_{m'}, \mu_{m'} = \mu_m \\ \text{at } z = 0 : I_m &= \epsilon_w I_{bw} + (1 - \epsilon_w) \frac{q_z^-}{\pi} \quad ; \quad \epsilon_m > 0 \\ \text{at } z = L : I_m &= \epsilon_w I_{bw} + (1 - \epsilon_w) \frac{q_z^+}{\pi} \quad ; \quad \epsilon_m < 0 \end{aligned} \quad (126)$$

with the hemispherical fluxes given by

$$\begin{aligned} q_r^+ &= \sum_m w_m \mu_m I_m \quad ; \quad \mu_m > 0 \\ q_r^- &= \sum_m w_m |\mu_m| I_m \quad ; \quad \mu_m < 0 \\ q_z^+ &= \sum_m w_m \epsilon_m I_m \quad ; \quad \epsilon_m > 0 \\ q_z^- &= \sum_m w_m |\epsilon_m| I_m \quad ; \quad \epsilon_m < 0 \end{aligned} \quad (127)$$

In the VFM, these fluxes are obtained as

$$q^+ = (F + q)/2$$

TABLE 10
THE S_2 QUADRATURE FOR AXISYMMETRIC CYLINDRICAL ENCLOSURES

m	μ	η	ξ	w_m
1	-0.5	0.7071	-0.5	π
2	0.5	0.7071	-0.5	π
3	-0.5	0.7071	0.5	π
4	0.5	0.7071	0.5	π

TABLE 11
THE S_4 QUADRATURE FOR AXISYMMETRIC CYLINDRICAL ENCLOSURES

m	μ	η	ξ	w_m
1	-0.2959	0.2959	-0.9082	$\pi/3$
2	0.2959	0.2959	-0.9082	$\pi/3$
3	-0.9082	0.2959	-0.2959	$\pi/3$
4	-0.2959	0.9082	-0.2959	$\pi/3$
5	0.2959	0.9082	-0.2959	$\pi/3$
6	0.9082	0.2959	-0.2959	$\pi/3$
7	-0.9082	0.2959	0.2959	$\pi/3$
8	-0.2959	0.9082	0.2959	$\pi/3$
9	0.2959	0.9082	0.2959	$\pi/3$
10	0.9082	0.2959	0.2959	$\pi/3$
11	-0.2959	0.2959	0.9082	$\pi/3$
12	0.2959	0.2959	0.9082	$\pi/3$

$$q^- = (F - q)/2 \quad (128)$$

the flux-sums and the net fluxes being those from the previous iteration.

Assuming scatter to be linearly anisotropic, the phase function may be represented by

$$P(\underline{\Omega}, \underline{\Omega}') = 1 + a_0 \cos \phi \quad (129)$$

where ϕ is the angle between the incident and the scattered intensities, and a_0 is an asymmetry factor with a value between +1.0 and -1.0. In terms of the direction cosines, $P(\underline{\Omega}, \underline{\Omega}')$ can be written as

$$P(\underline{\Omega}, \underline{\Omega}') = 1 + a_0 (\mu_m \mu_{m'} + \xi_m \xi_{m'}) \quad (130)$$

In the VFM, the directional contributions due to scattering are evaluated as

$$\begin{aligned} \bar{f} &= 2\pi \int_0^{\pi/2} P(\underline{\Omega}, \underline{\Omega}') \sin \phi \cos^2 \phi d\phi \\ \bar{b} &= 2\pi \int_{\pi/2}^{\pi} P(\underline{\Omega}, \underline{\Omega}') \cos^2 \phi \sin \phi d\phi \\ \bar{s} &= (1 - \bar{f} - \bar{b})/4 \end{aligned} \quad (131)$$

where $\bar{f}$, $\bar{b}$ and $\bar{s}$ are the forward-, backward-, and side-scattered components.

The angular derivative term in Eq. 123 is evaluated using a direct-differencing technique (Carlson and Lathrop (1968)). Using this technique, the second term on the left hand side of Eq. 123 can be re-written as

$$(1/r)[\partial(\eta_m I_m)/\partial\psi] = (1/r)[(\alpha_{m+1/2} I_{m+1/2} - \alpha_{m-1/2} I_{m-1/2})/w_m] \quad (132)$$

The directions $m \pm 1/2$ define the edges of the angular range of w_m , the two terms representing, respectively, the flow out of and into the angular range. A direct relationship between α_m and w_m can be drawn on the basis of isotropic radiation

$$\alpha_{m+1/2} - \alpha_{m-1/2} = w_m \mu_m \quad (133)$$

The α 's are chosen so that the radiation intensity is only redistributive in the azimuthal direction (i.e., no net transfer). In the Varma method this is achieved by letting $dI_{\psi}^+/d\psi = dI_{\psi}^-/d\psi = 0.0$, which eliminates two of the six first-order equations of intensity distribution and reduces them to algebraic form.

3. Working Equations

The working equations for DOM and VFM are quite different, and deserve separate discussion.

Discrete Ordinates Method (DOM). Multiplying both sides of Eq. 123 by $2\pi r dr dz$, and integrating over the volume element (Fig. 4), we obtain

$$\begin{aligned} \mu_m (A_{i+1} I_{i+1} - A_i I_i) - (A_{i+1} - A_i) [(\alpha_{m+1/2} I_{m+1/2} - \alpha_{m-1/2} I_{m-1/2}) / w_m] \\ + \xi_m (B_{j+1} I_{j+1} - B_j I_j) = - (k_a + k_s) V_p I_m + k_a V_p I_b \\ + \frac{k_s V_p}{r \pi} \sum_m [1 + a_0 (\mu_m \mu_m' + \xi_m \xi_m')] w_m \end{aligned} \quad (134)$$

The intensities I_{i+1} , I_{j+1} and $I_{m+1/2}$ can be expressed in terms of the discrete intensities I_i , I_j and $I_{m-1/2}$ using central differencing:

$$I_i + I_{i+1} = I_j + I_{j+1} = I_{m-1/2} + I_{m+1/2} = 2I_m \quad (135)$$

I_m , the intensity at the center of the volume element can therefore be evaluated as

$$I_m = \frac{\mu_m A I_i + \beta_m I_{m-1/2} + \xi_m B I_j + V_p (k_a I_b + k_s I_s)}{\mu_m A - \beta_m + \xi_m B + V_p (k_a + k_s)} \quad (136)$$

where

$$A = A_i + A_{i+1}$$

$$B = B_j + B_{j+1}$$

$$\beta_m = - (\alpha_{m+1/2} + \alpha_{m-1/2}) (A_{i+1} - A_i) / w_m$$

$$I_s = \sum_m w_m I_m \left[\frac{1 + a_0 (\mu_m \mu_m' + \xi_m \xi_m')}{4\pi} \right]$$

Eq. 134 is strictly applicable to the case where both μ_m and ξ_m are positive. For other combinations of μ_m and ξ_m , the equation changes.

Varma Six-Flux Method. The four first-order equations for the r- and x-directed intensities are combined into two second-order equations following the approach of Gosman and Lockwood (1973). The radiation flux sum and the net radiation are defined as

$$F = q^+ + q^- \quad (137)$$

$$q = q^+ - q^- \quad (138)$$

Combining each pair of radiation flux equations results in an expression of the following form (for the x-component):

$$q_x = - r_x (dF_x/dx) \quad (139)$$

where

$$r_x = [k_a + k_s (1 - \bar{b} - \bar{f})]^{-1}$$

Adding each pair, and combining with Eq. 139, the following equation for the x-component results

$$- \frac{d}{dx} (r_x \frac{dF_x}{dx}) = (c_1 + c_2) F_x + 2c_3 F_r + 2c_4 E_b \quad (140)$$

The corresponding equations for the r and ψ component are

$$(1/r) \frac{d}{dr} [r F_r] = (c_1 + c_2) F_r + 2c_3 F_x + 2c_4 E_b \quad (141)$$

$$F_\theta = 2 c_5 (F_x + F_r) + 2c_6 E_b \quad (142)$$

The necessary coefficients are defined in Table 12. The extinction coefficient and the albedo of scatter are given by

$$k_t = k_a + k_s \quad (143)$$

$$w_0 = k_s / k_t \quad (144)$$

4. Radiative Properties

To carry out the above calculations, information is needed on the absorption and scattering cross sections for the particulates, as well as the scattering phase functions. These can be calculated using Mie theory (Mie, 1908) if the particle size, the wavelength of the radiation, and the complex refractive index of the particle are known. Sample results from such calculations, using a published program (Dave, 1968), are presented in Figure 6 for size parameters ($\pi d_p / \lambda$) in the range of 0-100. In this figure, the refractive index of char is taken as 1.93 (1.0-0.53i) at a wavelength of 2 μm .

TABLE 12
COEFFICIENTS FOR FLUX SUMS

$$C_1 = -K_t(1 - \omega_0 f) + K_t [2\omega_0^2 s^2 / (1 - \omega_0 f - \omega_0 b)]$$

$$C_2 = K_t \omega_0 b + K_t [2\omega_0^2 s^2 / (1 - \omega_0 f - \omega_0 b)]$$

$$C_3 = K_t \omega_0 s + K_t [2\omega_0^2 s^2 / (1 - \omega_0 f - \omega_0 b)]$$

$$C_4 = K_t [(1 - \omega_0)/6] \{1 + [2\omega_0 s / (1 - \omega_0 f - \omega_0 b)]\}$$

$$C_5 = \omega_0 s / (1 - \omega_0 f - \omega_0 b)$$

$$C_6 = (1 - \omega_0) / [6(1 - \omega_0 f - \omega_0 b)]$$

Figure 6. The absorption, scattering, and extinction efficiencies of char particles at wavelength of 2 μm and refractive index of 1.93 $[1 - i(0.53)]$.

Optical properties of coal are not well characterized (Solomon et al., 1986; Brewster and Kunitomo, 1984; Baxter et al., 1987). The absorption and scattering efficiencies depend strongly on these properties. Once the absorption and scattering efficiencies are known from Mie theory, the absorption and scattering coefficients of the particulates can be evaluated as

$$k_{ap} = \sum_j k_{aj} = \sum_j (\pi/4) Q_a \bar{n}_j d_j^2 \quad (145)$$

$$k_{sp} = \sum_j k_{sj} = \sum_j (\pi/4) Q_s \bar{n}_j d_j^2 \quad (146)$$

Soot particles absorb, but do not scatter radiation significantly due to their microscopic size. Soot radiation is not considered in PCGC-2 at this stage.

The absorption coefficients for the gases are evaluated from gas emissivity data:

$$k_{ag} = (1/\ell) [\ln (1-\epsilon_g)] \quad (147a)$$

where

$$\epsilon_g = C_{CO_2} \epsilon_{CO_2} + C_{H_2O} \epsilon_{H_2O} - \Delta\epsilon \quad (147b)$$

and the mean beam length (a single overall value used in PCGC-2 is given by

$$\ell = 3.5 (V_F/A_F) \quad (148)$$

C_{CO_2} and C_{H_2O} represent the pressure corrections to the gas emissivities, and $\Delta\epsilon$ represents the spectral overlap correction. The gas emissivity data are taken from Hottel and Sarofim (1967) and Siegel and Howell (1981). The overall absorption coefficient for the volume can therefore be obtained as

$$k_a = k_{ap} + k_{ag} \quad (149)$$

and the total heat absorption by the volume zone as

$$q_r = k_a (F_x + F_r + F_\psi - E_b) \quad (150)$$

out of which a fraction $g_{rg} = (k_{ag}/k_a)q_r$ is absorbed by the gas phase, and the remainder $q_{rp} = (k_{ap}/k_a)q_r$ is absorbed by the particle phase within the volume zone. q_r is the radiation source term due to the particulates in the Eulerian

equation of energy. Conversion of the source term from Eulerian to Lagrangian coordinates is done through the particle number density

$$q_{rp} = Q_{rp} n_j \quad (151)$$

1. NITROGEN OXIDE (NO) MODEL

1. Background

The kinetic model for NO formation in coal systems must contain sufficient detail to adequately describe the process. It must also be limited to sufficiently few reactions to allow for coupling with the turbulent mixing process. The kinetic model and method of calculating the time-mean reaction rates in the turbulent system are discussed. The approach used for calculating each reaction rate is dependent on the relative time scales of reaction and turbulent fluctuation.

2. NO Formation Mechanism

The literature on NO pollutant formation shows several comprehensive reaction sets used to describe the net rate of NO formation in various types of flames (Heap et al., 1977; Saliman and Hanson, 1980). These reaction sets give insight into the formidable task involved in a detailed kinetic description of the NO formation process.

The coal combustion process usually takes place in a turbulent environment, and calculation of the net NO formation rate must be coupled with the turbulent mixing process. This is not presently feasible with a detailed kinetic mechanism. A practical kinetic mechanism must use a "minimum" set of reactions to approximate the essential features of the NO formation process.

This section provides a discussion of the essential features of NO formation in coal systems, and a proposed kinetic mechanism to describe this process.

Nitrogen Evolution. Coal contains 1-2 percent nitrogen by weight. This nitrogen is released to the gas phase during the coal combustion process. Approximately half of the nitrogen is released during devolatilization and half during char oxidation. Nitrogen is assumed to evolve at a rate equal to the total coal weight loss (Smoot, 1980). Thus the amount of nitrogen released from the coal is calculated directly from the source of particle mass added to the gas phase (S_p^n). A specified fraction of the nitrogen evolved from the coal is assumed to evolve as HCN or instantaneously convert to HCN in the gas phase. This assumption is based on several studies (Chen et al., 1980; and Heap et al., 1978) and simplifies the prediction of fuel NO to a mechanism which is initiated by decay of HCN in the gas phase. The amount of HCN formed from devolatilized nitrogen is given by

$$w_0 = \zeta \omega_N S_p^n / M_N \quad (152)$$

where ω_N is the mass fraction of nitrogen in the coal, S_p^n is the local source of particle mass given to the gas from the particle reactions, and M_N is the molecular weight of nitrogen. ζ is a constant used to specify the percentage of coal nitrogen initially converted to HCN. Since devolatilization is rapid (5-20 msec), about half of the nitrogen is evolved at the same location in the reactor.

Homogeneous NO Reactions. Once the coal particle begins to devolatilize, the gaseous constituents react homogeneously in the gas phase. In this phase, NO can be formed by three separate reaction processes classified as: thermal NO, prompt NO, and fuel NO.

Thermal NO is formed by oxidation of atmospheric molecular nitrogen, and its formation is highly dependent on temperature and equivalence ratio. Consequently, NO formation by this mechanism is significantly reduced in fuel-rich systems and at temperatures below 1600-1800 K. As a result of the low temperatures and the locally fuel-rich nature of pulverized coal flames (which lack oxygen atoms), thermal NO is not considered a significant source of NO in coal flames.

Prompt NO is formed by hydrocarbon fragments (resulting from the devolatilization process) attacking molecular nitrogen near the reaction zone of the flame. Since prompt NO formation requires a hydrocarbon to initiate the attack on the molecular nitrogen, prompt NO formation is more prevalent in fuel-rich flames. Prompt NO formation occurs in coal flames, but since coal generally contains 1-2% nitrogen, prompt NO is likely to be overshadowed by fuel NO. It is estimated that prompt NO typically accounts for less than 5% of the total NO formed. Neither thermal nor prompt NO are currently modeled by PCGC-2. Work is underway, however to incorporate thermal NO and to extend the model to fuel-rich flames, sulfur species and capture by sorbents (Solomon et al., 1987).

Fuel NO formed in the gas phase results from oxidation of the nitrogen constituents devolatilized from the coal, and generally accounts for 70-90% of the total NO formed. A specified fraction of the devolatilized nitrogen is assumed to evolve as HCN or instantaneously convert to HCN in the gas phase. The HCN can then react homogeneously to either NO or N_2 , depending on the amount of oxidizer present. Global reaction rates have been reported by DeSoete (1975) to describe the reactions of HCN. These measurements were made with the addition of C_2N_2 to $C_2H_4/O_2/Ar$ flat, premixed, laminar flames, and apply to both fuel-rich and fuel-lean conditions.

The global reaction rates measured by DeSoete (1975) are:

$$w_1 = A_1 X_{HCN} X_{O_2}^b \exp(-E_1/RT) \quad (153)$$

$$w_2 = A_2 X_{HCN} X_{NO} \exp(-E_2/RT) \quad (154)$$

where the rate parameters are shown in Table 13. The order of reaction in Eq. 153 varies according to the O_2 mole fraction (DeSoete, 1975; Hill, 1983). The

TABLE 13
KINETIC PARAMETERS USED IN THE NITROGEN POLLUTANT SUBMODEL

<u>Reaction</u>	<u>Pre-exponential Factor</u>	<u>Activation Energy J (kmol⁻¹)</u>
w ₁ (Eq. 153)	1.0 x 10 ¹¹ s ⁻¹	2.8 x 10 ⁸
w ₂ (Eq. 154)	3.0 10 ¹² s ⁻¹	2.5 x 10 ⁸
w ₃ (Eq. 155)	4.1 x 10 ⁻⁴ kmol N ⁻¹ s ⁻¹	1.5 x 10 ⁸

order is zero for O_2 mole fractions greater than 1.8×10^4 ppm and unity for mole fractions of O_2 less than 2500 ppm. These global reactions of DeSoete are used to describe the homogeneous NO formation and decay processes in the NO pollutant model.

Heterogeneous NO Reactions. NO can also be reduced by interaction with the char particles. The rate of heterogeneous NO reduction is given by Levy et al. (1981):

$$w_3 = A_3 \exp(-E_3/RT) A_E p_{NO}(\gamma) \quad (155)$$

A_E is the external surface area of the char in m^2/gm and p_{NO} is the partial pressure of NO in atmospheres while RT is in kcal/mole. The parameter γ is used to include the change in the external area of the char particles due to swelling and fracturing during the reaction process. This rate was measured in an electrically-heated laminar flow furnace for the temperature range of 1250 to 1750 K. Size-graded, pulverized Montana lignite char particles were used to measure the rate of heterogeneous NO reduction.

Reaction Sequence. In summary, the NO model reaction sequence is depicted as:

This sequence of reactions can be represented schematically as:

The kinetic parameters used for the reactions in the NO model are summarized in Table 13. These are taken, with some modification, from the work of DeSoete (1975).

The major assumptions of the NO pollutant model are:

1. Nitrogen is evolved at a rate equal to the rate of coal weight loss.

2. A specified fraction (usually unity) of the nitrogen which leaves the coal is converted instantaneously to HCN in the gas phase.
3. Thermal and prompt NO formation are neglected; only fuel NO is considered.
4. Homogeneous NO decay proceeds by decay of the HCN formed from coal devolatilization. The kinetic rates measured by DeSoete (1975) are used to describe this process.
5. Heterogeneous NO formation is modeled by the same procedure as is homogeneous NO formation. Heterogeneous NO reduction by char is modeled using the rates measured by Levy, et al. (1981).

3. Calculation of Time-mean Reaction Rates

The Favre-averaged species continuity equations can be used to calculate the Favre-mean mass fractions of the nitrogen pollutants (NO and HCN) throughout a turbulent coal reactor. Favre-averaging and the form of these equations have been discussed previously. Solution of these equations requires calculation of time-mean, net formation rates ($\bar{W}_i$) for these species. These net formation rates are given by the difference between the time-mean formation rate and the time-mean depletion rate for each species as determined from the kinetic mechanism outlined in the previous section. The procedure requires consideration of the relative time scales of each reaction and the time scale of the turbulent fluctuations.

Homogeneous Reactions. The reactions of DeSoete shown previously describe the homogeneous decay of HCN and the homogeneous formation and decay of NO. These reactions have a typical time scale on the order of one millisecond. The integral time scale of turbulence is around ten milliseconds. Since these time scales are nearly the same order of magnitude, the effects of the turbulent fluctuations on the reaction rates cannot be ignored.

For kinetically limited reactions, the extent of reaction (π) can be defined to measure the reaction progress. For example, for the global reaction for oxidation of cyanide described by Eq. 157 (rate expressed in Eq. 154), the extent of reaction measures how much of the fuel nitrogen (represented by HCN) is converted to NO via this reaction. If Y_{NO}^f represents the local mass fraction of NO that would be formed if all fuel nitrogen reacted completely to NO through this reaction then:

$$\pi = \frac{Y_{NO}}{Y_{NO}^f} \quad (160)$$

The local concentration of each species is a function of the mixing variables (η , f), the chemical enthalpy (h) and the local extent of reaction (π) for all reactions in which that species is involved. Since pollutant concentrations will not affect the temperature field, the reaction rates (Lowry, 1963; Field et al., 1967; Bueters et al., 1974) of Eqs. 153-155 are functions of only these same variables. Bilger (1978) determined experimentally that, for a broad region in a hydrogen/air diffusion flame, the molecular species composition is only a function of the mixture fraction. Fenimore and Fraenkel

(1981) reported the same finding for thermal NO concentrations in laminar, gaseous, diffusion flames. These data suggest that for each unique mixing time scale there may exist a unique reaction time scale. This interdependence of extent of reaction with mixing is not necessarily expected on a theoretical basis, but is only suggested by these experimental data.

From these observations it is concluded that it may not be necessary to include the effects of the turbulent fluctuations on the extent of reaction. In the current version of PCGC-2, the temporal fluctuations in the extent of reaction are assumed to be small. The extent of reaction for each of the three pollutant reactions is defined as:

$$Y_i = \pi_i Y_i^f \quad (161)$$

where Y_i^f is the fully-reacted mass fraction of species i . Since each π is taken to be constant, it can also be obtained from the mean properties:

$$\pi_i = \bar{Y}_i / \bar{Y}_i^f \quad (162)$$

The mean reaction rates $\bar{w}_i$ are then obtained by convolution of each π over the probability density functions of the mixture fractions.

Heterogeneous Reactions. The heterogeneous reactions of NO are much slower than the homogeneous reactions. The time scale for the heterogeneous reduction of NO is on the order of one second. Since the heterogeneous reactions are slow compared to the turbulence time scale, calculation of the heterogeneous time-mean reaction rates is greatly simplified. The time-mean reaction rate for heterogeneous NO decay can be calculated from Eq. 155 using time-mean properties, and thus ignoring the effects of the turbulent fluctuations on T , A_E , and P_{NO} .

Once the Favre-mean mass fraction fields for NO and HCN are found by solving the species continuity equation, the O_2 mass fraction field can be obtained by a mass balance:

$$\tilde{Y}_{O_2} = \tilde{Y}_{O_2}^0 - \tilde{Y}_{NO} M_{O_2} / M_{NO} \quad (163)$$

$\tilde{Y}_{O_2}^0$ represents the O_2 mass fraction prior to calculation of the pollutant concentrations, and $\tilde{Y}_{O_2}$ represents the O_2 mass fraction after calculation of the pollutant concentrations. The procedure assumes that the pollutant species do not significantly affect the major species concentrations. This assumption should be valid because of the low level of the pollutant species relative to the major species. In regions of very low oxygen concentration, the oxygen concentration may require updating following calculation of the pollutant species.

Time-Mean Net Formation Rates. The time-mean concentrations for the nitrogen pollutant species are obtained by solution of the species continuity equation. Solution of the species continuity equation requires calculation of the time-mean net formation rate for the individual species. The time-mean net formation rates for NO and HCN are the difference between the time-mean formation rate and the time-mean depletion rate for these species. The time-mean net formation rates for NO and HCN are shown below:

$$\bar{w}_{\text{NO}} = (\bar{w}_1 - \bar{w}_2 - \bar{w}_3)M_{\text{NO}} \quad (164)$$

$$\bar{w}_{\text{HCN}} = (\bar{w}_0 - \bar{w}_1 - \bar{w}_2)M_{\text{HCN}} \quad (165)$$

The w_i 's are the time-mean formation and depletion rates discussed previously. All of the equations to be solved for the desired Favre-mean mass fraction are summarized in Table 14.

TABLE 14

EQUATION SET FOR NITROGEN OXIDE SUBMODEL IN TURBULENT,
COAL-LADEN SYSTEMS

Description	Equation
166 Rate of Nitrogen Release from the Coal	$\bar{w}_0 = \zeta \omega_N S_p^\eta / M_N$
167 Instantaneous Reaction Rate Terms	$w_1 = \rho(A_1) X_{\text{HCN}} X_{\text{O}_2}^b \exp(-E_1/RT) / M_m$
	$w_2 = \rho(A_2) X_{\text{HCN}} X_{\text{NO}} \exp(-E_2/RT) / M_m$
168 NO-Char Reduction Reaction	$\bar{w}_3 = \alpha_p \tilde{n}_p (A_3) A_{E\text{PNO}} \tilde{p}_{\text{NO}} \exp(-E_3/RT) \gamma$
169 Species Continuity for i - NO, HCN	$\begin{aligned} \bar{\rho} \tilde{u}(\partial \tilde{Y}_i / \partial x) + \bar{\rho} \tilde{v}(\partial \tilde{Y}_i / \partial r) - (\partial / \partial x)(\Gamma_Y \partial \tilde{Y}_i / \partial x) \\ - (1/r) (\partial / \partial r)(r \tilde{r}_Y \partial \tilde{Y}_i / \partial r) = \bar{w}_i \end{aligned}$
170 Instantaneous Mass Fractions	$Y_i = \pi_i Y_i^f$
171 Mean Reaction Rate Term by Convolution over Probability Density Functions	$\bar{w}_i = \bar{\rho} \int_f \int_n [w_i(f, n) / \rho(f, n)] P(f) P(n) df dn$
172 Deviation from Fully Reacted Mass Fractions	$\pi_i = (\tilde{Y}_i / Y_i^f)$
173 Mass balance for O_2	$\tilde{Y}_{\text{O}_2} = \tilde{Y}_{\text{O}_2}^0 - \tilde{Y}_{\text{NO}} M_{\text{O}_2} / M_{\text{NO}}$
174 Overall Mean Reaction Rates for Each Species	$\bar{w}_{\text{NO}} = (\bar{w}_1 - \bar{w}_2 - \bar{w}_3) M_{\text{NO}}$
	$\bar{w}_{\text{HCN}} = (\bar{w}_0 - \bar{w}_1 - \bar{w}_2) M_{\text{HCN}}$

CHAPTER III. SOLUTION TECHNIQUE

A. APPROACH

An information flow diagram for PCGC-2 is shown in Figure 7. The basic approach is to decouple the gas and particle equations using the particle source terms as tear variables. After initializing the flow field and geometric quantities, the gas variables are first solved for an assumed set of source terms. After converging the gas phase, the gas properties are updated, the Eulerian particle number density fields are calculated, and the radiation field is solved. The Lagrangian particle trajectories are then solved one at a time. New values of the source terms are calculated from particle mass, enthalpy, and velocity, when trajectories cross cell boundaries. Based on the previously guessed values of the source terms and the newly calculated values, an improved guess of the source terms is made, the gas phase reconverged, the particle trajectories recalculated, and so forth, until overall convergence of both phases is achieved. An option is also provided (INEACH = T) for solving the gas and particle phases simultaneously, in semi-coupled form, rather than in nested form as described above. The approaches for solving the gas and particle phases are discussed in more detail below.

1. Gas Phase

All of the gas phase equations are Eulerian, steady-state, second order, non-linear, elliptical partial differential equations. All of the gas phase equations are conveniently cast into one finite difference form, so that only one solution technique is required. Table 1 (Chapter II) contains a summary of this form for all of the gas phase equations.

The gas field is solved using a line-by-line technique; a tri-diagonal algorithm is used to solve the finite difference equations along a line using appropriate boundary conditions. PCGC-2 is coded to calculate the gas field line-by-line in either direction, or else in alternate directions. The tri-diagonal algorithm is solved iteratively for a specific variable until convergence is achieved. These iterations on a specific variable are termed "micro-iterations"; generally only three micro-iterations are necessary to obtain convergence for each variable. Each variable in Table 1 is solved in succession, starting with u and ending with h (if needed). A "macro-iteration" is completed after the complete set of variables has been calculated once (Steps 2 and 3 in Figure 7). Between 200 and 1000 macro-iterations are required to completely converge the gas phase (Steps 2-4 in Figure 7; this comprises one "gas-phase iteration").

The particles are accounted for only by appropriate particle source terms of mass (S_p^m), momentum (S_p^u and S_p^v), and enthalpy (S_p^h). These terms represent the addition of mass, momentum, and energy to the gas phase by the particles. The source terms are found along a particle trajectory by taking the difference in the particle properties on each side of a computational cell and dividing by the cell volume.

Roache (1976) presents a good review of techniques for solving fluid dynamics problems. The particular fluid flow problem solved by PCGC-2 consists of a recirculating fluid, and this type of problem has been heavily

Figure 7. Information flow for PCGC-2.

investigated by researchers at Imperial College. A method similar to the TEACH technique (Gosman and Pun, 1973) developed at Imperial College is used in PCGC-2 to solve the gas equations in the primitive variables. This technique is an iterative, steady-state, finite difference approach, and is widely used (Lockwood et al., 1980; Smith, 1979; Smoot and Pratt, 1979). Recently, finite element methods have been applied successfully to fluid flow problems (Gallagher et al., 1975). These methods have some strong advantages, particularly pertaining to arbitrary boundary shapes, but they are still in a developing stage and have not been applied extensively to compressible recirculating flows.

Each of the differential equations must be cast in finite difference form and solved over some appropriate grid spacing. A series of grid lines running orthogonally to the coordinate directions define at their intersection, node points, where the values of the dependent variables are usually identified. Roache (1976) has reviewed application of the flow equations to various possible mesh systems and shows that in the (u, v, p) formulation, the variables u and v are most conveniently and accurately evaluated with node points lying on the boundary and with p and ρ being placed at one-half grid spacing off the boundary. This staggered-mesh system is shown in Figure 8 as it is applied in PCGC-2. The grid spacing may be non-uniform, with grid points concentrated in areas of steep gradients. This spacing increases the convergence rate and accuracy of the computations. PCGC-2 locates all faces midway between node points. Arithmetic averaging is used to obtain property values at mesh boundaries between node points. Throughout PCGC-2, the distance between nodes is stored and used in the differencing scheme. Completely arbitrary grid spacing is thus permitted.

It has already been mentioned that special difficulties arise in the primitive variable approach in that the momentum equations contain the pressure gradient terms, yet pressure does not explicitly appear in the continuity equation. Roache (1976) used the Los Alamos Marker and Cell (MAC) method for solving this problem. Patankar (1975, 1980) developed a semi-implicit method for pressure-linked equations (SIMPLE). PCGC-2 has been coded to include both the SIMPLE and revised SIMPLE (SIMPLER) algorithms. A brief outline of the technique is presented here. More complete derivations may be found in the next section.

Figure 8 shows a typical computational cell. Attention is focused on the node point P and its nearest neighbors (N, S, E, W). The pressure, along with other variables, is calculated for these nodes. The velocity components associated with this node point are calculated at cell faces as shown. This staggered grid helps in writing the mass conservation equation for a cell since the velocities at the cell faces are needed in the convection terms. In addition, the difference of pressure between two adjacent nodes is used to derive the velocity component for the point midway between them.

When the momentum equations are cast in finite difference form (discussed in the next section) the unknown pressure terms will appear. At this point, the true pressure $\bar{p}$ is decomposed into a best estimate p^* and a pressure correction term $\bar{p}^C$.

$$\bar{p} = \bar{p}^* + \bar{p}^C \quad (175)$$

Figure 8. Sample grid pattern for PCGC-2.

With the help of this decomposition of the true pressure and the two momentum difference equations, expressions may be found for two velocity components in terms of starred velocity components and pressure-correction variables (p^C).

The continuity equation permits closure of the problem. By writing it in finite difference form and substituting the velocity equation in terms of $\bar{p}^C$, a finite difference equation for the pressure correction is formed. In other words, the continuity equation is written in terms of the unknown pressure corrections of Eq. 175.

The overall iterative solution procedure for the SIMPLE algorithm is:

1. Begin with the best available initial guess for all variables including pressure ($\bar{p}^*$).
2. Calculate auxiliary variables such as density, temperature, etc., from the associated combustion model.
3. Solve the momentum difference equations for the starred velocity field.
4. Solve the pressure correction form of the continuity equation for $\bar{p}_C$.
5. Calculate the pressure (from Eq. 175) and corrected velocities.
6. Solve the difference equations for all other associated variables (i.e., k , ϵ , T , g_f , n , g_n , h).
7. With the new updated variables, return to Step 2 and continue iteration until convergence is achieved.

The overall iterative solution procedure for the SIMPLER algorithm is similar to the procedure for the SIMPLE algorithm (as shown above). The continuity equation is used in connection with the momentum equations to formulate an equation for pressure ($\bar{p}$) instead of the pressure correction ($\bar{p}_C$). The iterative scheme is discussed later in the text.

2. Particle Phase

The particle source-in-cell (PSI-CELL) technique of Crowe and coworkers (1977) has been followed directly to account for the Lagrangian particle field in the Eulerian gas field. The procedure is outlined below:

1. The Eulerian gas field is solved without particles using the above algorithm.
2. The radiation field is solved using the flux method.
3. The Lagrangian particle field is solved with a representative number of trajectories and the particle source term field is calculated.
4. The gas field is solved with the updated particle source term field.

5. Step 2 is repeated and iteration continued until overall convergence is achieved.

The PSI-CELL technique is very efficient with respect to storage and computational time required. The only significant storage requirement is for the particle source term field. Steps 2 through 4 represent one "particle iteration" (Steps 7 through 11 in Figure 7). Convergence is achieved when the gas phase does not change significantly between particle iterations.

B. FINITE DIFFERENCE SCHEME

The majority of this section was taken directly from Wormeck (1976) with the author's permission. Modifications to the original material have been made where appropriate.

1. Introduction

This section presents the basic fluid flow solution procedure. This derivation brings to light various questions and possible alternative routes to take. The pressure is usually the variable giving the most trouble and can be eliminated by cross-differentiation of the momentum equations and introducing vorticity ξ as a dependent variable. The two velocity components are then removed by defining the stream function ψ . The resultant (ψ, ξ) system requires two equations to be solved for the unknown vorticity and stream function. If the flow is compressible, then the pressure must be recovered by the usual technique of integrating one of the momentum equations, after which the density can be updated by an equation of state.

The (ψ, ξ) system has been developed and published by Gosman, et al. (1969), but because of difficulties with boundary conditions, failure for many compressible flows, and not being readily extendable to three-dimensional flows, the method was abandoned in favor of a new algorithm (Gosman and Pun, 1973) which solves the flow equations in the primitive variables. The latter method is discussed in this section.

2. Differential Equations

The gas-phase equation set has been presented in Table 1, illustrating that the equations can be cast into one standard form. The presentation in this section will focus on this general form and on deviations from this form for the momentum equations due to the staggered grid. The continuity and momentum equations are presented here in their customary form as in Bird, et al. (1960) with particle source terms:

$$\text{MASS (continuity): } \frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v}) = S_p^m \quad (176)$$

$$\text{MOMENTUM: } \rho \frac{D\vec{v}}{Dt} = -\vec{\nabla} p - \vec{\nabla} \cdot \bar{\tau} + \rho \vec{g} + \vec{\nabla}_{pg} S_p^m + S_p^{\vec{v}} \quad (177)$$

where D/Dt is the substantive derivative, and $\bar{\tau}$ is the stress tensor. The S_p terms are the source terms due to the particle phase. After the complete

derivation, an analysis will be performed to modify the finite-difference equations such that total mass is conserved.

Neglecting body forces, this system of equations can be expanded in terms of cylindrical coordinates for steady, axi-symmetric flows as (Gosman et al., 1969):

$$\text{CONTINUITY: } \frac{\partial}{\partial x} (\rho u) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho v) = S_p^m \quad (178)$$

U-MOMENTUM (direction x):

$$\begin{aligned} & \frac{\partial}{\partial x} (\rho u u) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho u v) - \frac{\partial}{\partial x} (\mu \frac{\partial u}{\partial x}) - \frac{1}{r} \frac{\partial}{\partial r} (\mu r \frac{\partial u}{\partial r}) \\ &= - \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} (\mu \frac{\partial u}{\partial x}) + \frac{1}{r} \frac{\partial}{\partial r} (\mu r \frac{\partial v}{\partial x}) - \frac{\partial}{\partial x} (\frac{2}{3} \mu \text{div } \vec{v}) + u_{pg} S_p^m + S_p^u \end{aligned} \quad (179)$$

V-MOMENTUM (direction r):

$$\begin{aligned} & \frac{\partial}{\partial x} (\rho u v) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho v v) - \frac{\partial}{\partial x} (\mu \frac{\partial v}{\partial x}) - \frac{1}{r} \frac{\partial}{\partial r} (\mu r \frac{\partial v}{\partial r}) = - \frac{\partial p}{\partial r} + \frac{\partial}{\partial x} (\mu \frac{\partial u}{\partial r}) \\ &+ \frac{1}{r} \frac{\partial}{\partial r} (\mu r \frac{\partial v}{\partial r}) - \frac{2 \mu v}{r^2} - \frac{1}{r} \frac{\partial}{\partial r} (\frac{2}{3} \mu r \text{div } \vec{v}) + \frac{2}{3} \frac{\mu \text{div } \vec{v}}{r} + \frac{\rho w w}{r} + v_{pg} S_p^m + r S_p^v \end{aligned} \quad (180)$$

W-MOMENTUM (tangential direction)

$$\begin{aligned} & \frac{\partial}{\partial x} (\rho u w) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho v w) - \frac{\partial}{\partial x} (\mu \frac{\partial w}{\partial x}) - \frac{1}{r} \frac{\partial}{\partial r} (\mu r \frac{\partial w}{\partial r}) = - \frac{\rho v w}{r} \\ & - \frac{1}{r^2} \frac{\partial}{\partial r} r^3 \mu \frac{\partial w}{\partial r} + w_{pg} S_p^m + S_p^w \end{aligned} \quad (181)$$

All of the above equations can be cast into a standard form:

$$\text{div} (\rho \vec{v} \phi) - \text{div} (\Gamma \text{grad } \phi) = S \quad (182)$$

where ϕ is taken as the dependent variable, Γ as the exchange coefficient relating the force with the flux in the transport law for ϕ , and S as the source term that includes all terms not contained in the first two terms. The first term is generally referred to as the convection term while the second term is the diffusion term. Writing Eq. 182 in cylindrical two-dimensional coordinates,

$$\frac{1}{r} \left[\frac{\partial}{\partial x} (r \rho u \phi) + \frac{\partial}{\partial r} (r \rho v \phi) \right] - \frac{1}{r} \left[\frac{\partial}{\partial x} (r \Gamma \frac{\partial \phi}{\partial x}) + \frac{\partial}{\partial r} (r \Gamma \frac{\partial \phi}{\partial r}) \right] = S \quad (183)$$

The corresponding terms in Eqs. 178 to 181 are easily identified.

Note that the diffusion terms are simply the divergence of a gradient and that any other form of a transport law must be contained in the source term. In particular, the $(\partial/\partial r)[2\mu r(\partial v/\partial r)]$ term in the second momentum equation has been split, with half of it becoming the second diffusion term in Eq. 180 while the remainder becomes the third source term on the right. This is required for success of the method; the reasoning will follow once the two modifications for correcting mass conservation are developed below.

Therefore our equation system becomes

CONTINUITY ($\phi = 1$):

$$\frac{\partial}{\partial x}(\rho u) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v) = S_p^m \quad (184)$$

U-MOMENTUM ($\phi = u$):

$$\frac{\partial}{\partial x}(\rho u u) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho u v) - \frac{\partial}{\partial x}(\mu \frac{\partial u}{\partial x}) - \frac{1}{r} \frac{\partial}{\partial r}(r \mu \frac{\partial u}{\partial r}) = -\frac{\partial p}{\partial x} + S^u \quad (185)$$

V-MOMENTUM ($\phi = v$):

$$\frac{\partial}{\partial x}(\rho u v) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v v) - \frac{\partial}{\partial x}(\mu \frac{\partial v}{\partial x}) - \frac{1}{r} \frac{\partial}{\partial r}(r \mu \frac{\partial v}{\partial r}) = -\frac{\partial p}{\partial r} + S^v \quad (186)$$

W-MOMENTUM ($\phi = w$):

$$\frac{\partial}{\partial r}(\rho u w) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v w) - \frac{\partial}{\partial x}(\mu \frac{\partial w}{\partial x}) - \frac{1}{r} \frac{\partial}{\partial r}(r \mu \frac{\partial w}{\partial r}) = S^w \quad (187)$$

where the three source terms are given by:

$$S^u = \frac{\partial}{\partial x}(\mu \frac{\partial u}{\partial x}) + \frac{1}{r} \frac{\partial}{\partial r}(r \mu \frac{\partial v}{\partial x}) - \frac{\partial}{\partial x}(\frac{2}{3} \mu \text{div } \vec{v}) + u_{pg} S_p^m + r S_p^u \quad (188)$$

$$S^v = \frac{\partial}{\partial x}(\mu \frac{\partial u}{\partial r}) + \frac{1}{r} \frac{\partial}{\partial r}(r \mu \frac{\partial v}{\partial r}) - \frac{2\mu v}{r^2} - \frac{1}{r} \frac{\partial}{\partial r}(\frac{2}{3} r \mu \text{div } \vec{v}) + \frac{2}{3} \frac{\mu \text{div } \vec{v}}{r} + \frac{\rho w w}{r} + v_{pg} S_p^m + S_p^v \quad (189)$$

$$S^w = -\frac{\rho v w}{r} - \frac{1}{r^2} \frac{\partial}{\partial r} r^3 \mu \frac{\partial w}{\partial r} + w_{pg} S_p^m + S_p^w \quad (190)$$

The $\text{div } \vec{v}$ term is always dropped in the TEACH program. The effect of particle mass source terms on tangential momentum is ignored in this version of the code.

3. Finite-Difference Equations

There are four methods of deriving finite-difference equations from the differential equations. These include Taylor series expansions, polynomial fitting, integral methods, and the control volume approach. The approach taken here is to use the integral technique as in Gosman, et al. (1969).

Grid. Before integrating the standard equations over the flow domain, a satisfactory grid is required. The boundaries of the flow domain are made to coincide with one of the constant coordinate directions, with only the Cartesian and cylindrical geometries considered.

A series of grid lines orthogonal to the coordinate directions define (at their intersections) node points where the values of the dependent variables will usually be identified. TEACH incorporates non-uniform spacing between these grid points to obtain higher resolution (and therefore accuracy) in regions where the flow gradients are expected to be severe, but does not utilize the more numerically accurate coordinate-stretching transformations; e.g., exponential stretch.

The choice of mesh system depends on whether the node points are to lie on the flow boundary or one-half grid spacing away from it. Roache (1976) derives and compares all of the flow equations in these various mesh systems and shows that in the (u, v, p) formulation, the variables u and v are most conveniently and accurately evaluated in the mesh system with node points lying on the boundary, while p and ρ are most conveniently and accurately evaluated when node values are one-half grid spacing off the walls. The use of a hybrid- or staggered-mesh system thus suggests itself.

A staggered grid is used as shown in Figure 9, where a boomerang-shaped structure has been drawn to emphasize the field positions of the dependent variables u , v , p , and ϕ (a general variable) that correspond to FORTRAN indices I and J .

It should be noted that the flow domain is a continuous field which has been discretized by a mesh to perform a numerical analysis. All dependent variables and fluid properties are stored in two-dimensional FORTRAN arrays and all grid coordinates and distances are stored in one-dimensional arrays. Referencing a variable requires consideration of the field location specified by subscripts and its representation in the computer code.

The various computational cells are centered at the point of definition of the variable of interest and extend halfway to the four adjacent (in two-dimensional) neighboring node points. Thus we speak of the p -cell (main cell), u -cell and v -cell. The practice in TEACH is to name the node point of interest as P and the neighboring nodes as the four points of a compass.

The mathematical description is illustrated in Figure 10, where the absence of a subscript on these compass points signifies the main cell and addition of u or v superscripts implies the u - or v -cell respectively. Figures 11-13 illustrate the FORTRAN description of these three computational cells. Note how the velocity cells "overlap" the grid lines when the grid spacing is non-uniform.

Figure 9. The boomerang-shaped structure enclosing the points of definition of u , v , ρ , and ϕ corresponding to FORTRAN index I, J.

Figure 10. illustration of the grid symbols for a computational cell.

Figure 11. FORTRAN symbols for p-cell.

Figure 13. FORTRAN symbols for v-cell.

Three computational cells are associated with each node point. The node points are specified by the FORTRAN indices I and J. The main cell center is denoted by subscript p and is located at (x_p, r_p) (FORTRAN symbols X(I) and R(J)). The u-cell center has the same radial location as the p-cell and is referenced mathematically by subscript p and superscript u. It is located at x_p^u, r_p in the mathematical developments and in FORTRAN by coordinates [XU(I), R(J)]. With the v-cell, the center has the same x location as the main cell, but the radial coordinate is r_p^v [RV(J)]. Thus Figure 11 is a template which, when centered on grid location X(I), R(J), references the main cell (no superscripts). Adding a superscript u to the symbols will describe the field if node P is moved to the center of the u-cell at coordinates XU(I), R(J). Similarly, the v-cell notation is shown by moving Figure 11 to the center of the v-cell [X(I), RV(J)] and addition of the v superscript to all variables.

A location can be referenced in several ways; for example, consider the center of the west face of the main cell. A variable ϕ is referenced there mathematically by either ϕ_w or ϕ_p and approximately (exactly in a uniform grid) by ϕ_{nw}^v . In the derivation of the finite-difference equations which will follow, these different notations will be utilized to reference the same position. When writing the computer code, the best available FORTRAN variables are employed.

Use of the staggered grid also has the convenient feature that velocity is defined at the locations where it is needed in the convective terms. Pressure is defined so as to make it easy to compute the pressure gradients in the two momentum equations.

4. Integration of the Standard Equation

The standard equation (Eq. 183) will be developed first, followed by the momentum equations and the equation for pressure.

General Finite-Difference Equation (ϕ -Equation). Figure 14 displays a typical internal main cell where the ϕ -equation (Eq. 183) can be integrated over the volume obtained by rotating the area, represented by the dotted lines, about the symmetry axis to give:

$$\int_{x_w}^{x_e} \int_{r_s}^{r_n} \int_0^1 \left[\frac{\partial}{\partial x} (\rho u r \phi) + \frac{\partial}{\partial r} (\rho v r \phi) - \frac{\partial}{\partial x} (r \Gamma \frac{\partial \phi}{\partial x}) - \frac{\partial}{\partial r} (r \Gamma \frac{\partial \phi}{\partial r}) - r S \phi \right] dx dr d\xi_3 = 0 \quad (191)$$

where the third coordinate, ξ_3 , has the integration limits of 0 and 1 radians for convenience instead of 0 to 2π radians, because of assumed axial symmetry (i.e., the final overall equation is divided by 2π).

Considering the first convection term in Eq. 191

Figure 14. Illustration of the main cell finite-difference grid showing the node point labeling.

$$\int_{x_w}^{x_e} \int_{r_s}^r \int_0^1 \frac{\partial}{\partial x} (\rho u r \phi) dx dr d\xi_3 \quad (192)$$

and noting that all properties are uniform in the third direction, we can perform exact two integrations giving

$$\int_{r_s}^r [\rho u r \phi]_w^e dr \quad (193)$$

where e and w indicate that the expression is to be evaluated at the east and west faces, respectively. The derivation to this point is exact. Factoring r from the integrand, and applying the mean-value theorem

$$\int_{r_s}^r [\rho u r \phi]_w^e dr = \int_{r_s}^r [\rho u \phi]_w^e r dr = \int_{r_s}^r \{ [\rho u \phi]_e - [\rho u \phi]_w \} r dr \quad (194)$$

$$= \{ [\overline{\rho u \phi}]_e - [\overline{\rho u \phi}]_w \} 1/2 (r_n^2 - r_s^2) \quad (195)$$

where the subscript stands for evaluation at that particular face. The right-hand side of Equation 195 may be rewritten as

$$\{ [\overline{\rho u \phi}]_e - [\overline{\rho u \phi}]_w \} A_{ew} \quad (196)$$

where A_{ew} , the area of the east or west face of the cell, is given by

$$A_{ew} = \int_{r_s}^r \int_0^1 r dr d\xi_3 = \frac{1}{2} (r_n^2 - r_s^2) \quad (197)$$

or

$$A_{ew} = \frac{1}{2} (r_n - r_s) (r_n + r_s) = r_{ap} (r_n - r_s) \quad (198)$$

where

$$r_{ap} = (r_n + r_s)/2 \quad (199)$$

For arbitrary grid spacing, r_{ap} is not the same as r_p . Thus r_{ap} is stored throughout the entire calculational domain.

In the staggered grid system, the u velocities are defined at the cell boundaries where they are required ($u_e = u_E$, $u_w = u_P$) and the first convection term now becomes

$$\rho_e \phi_e u_E A_{ew} - \rho_w \phi_w u_p A_{ew} \quad (200)$$

We can define convection coefficients as

$$C_E = \rho_e u_E A_{ew} \quad (201)$$

$$C_W = \rho_w u_p A_{ew} \quad (202)$$

which gives the mass flowrate through the face corresponding to the subscript.

Both ρ and ϕ are defined at the main grid nodes and some sort of interpolation is needed to determine their values at the faces midway between node points. The practice typically employed is to linearly interpolate dependent variables and use simple averaging for fluid properties, thus:

$$\rho_e = \frac{1}{2}(\rho_p + \rho_E), \quad \rho_w = \frac{1}{2}(\rho_W + \rho_p) \quad (203)$$

and

$$P < \phi < E \quad \phi = (1 - f_E)\phi_p + f_E\phi_E, \quad f_E = \frac{x - x_p}{x_E - x_p} \quad (204)$$

$$W < \phi < P \quad \phi = (1 - f_W)\phi_W + f_W\phi_p, \quad f_W = \frac{x - x_W}{x_p - x_W} \quad (205)$$

$$P < \phi < N \quad \phi = (1 - f_N)\phi_p + f_N\phi_N, \quad f_N = \frac{r - r_p}{r_N - r_p} \quad (206)$$

$$S < \phi < P \quad \phi = (1 - f_S)\phi_S + f_S\phi_p, \quad f_S = \frac{r - r_S}{r_p - r_S} \quad (207)$$

Since PCGC-2 always employs cell faces halfway between node points, this interpolation is identical to simple averaging, even for non-uniform grid spacing since the f 's are always equal to 0.5. Using these relationships, with all f 's set equal to 0.5, the convection coefficients become

$$C_E = \frac{1}{2}(\rho_p + \rho_E) u_E A_{ew} \quad (208)$$

$$C_W = \frac{1}{2}(\rho_p + \rho_W) u_p A_{ew} \quad (209)$$

The first convection term in the ϕ -equation (Eq. 191) then becomes (upon substitution)

$$C_E f_E \phi_E - C_W (1 - f_W) \phi_W + [C_E (1 - f_E) - C_W f_W] \phi_P \quad (210)$$

Similarly, the second convection term in Eq. 191 is

$$\int_{x_W}^{x_e} \int_{r_S}^{r_n} \int_0^1 \frac{\partial}{\partial r} (\rho v r \phi) dx dr d\xi_3 \quad (211)$$

Again, two exact integrations can be performed to give

$$\int_{x_W}^{x_e} [\rho v r \phi]_S^n dx \quad (212)$$

From the mean-value theorem this term becomes

$$\{[\rho v \phi]_n r_n - [\rho v \phi]_S r_S\} (x_e - x_W) \quad (213)$$

In terms of the geometric quantities

$$A_n = r_n (x_e - x_W) \quad (214)$$

$$A_S = r_S (x_e - x_W) \quad (215)$$

the convection coefficients are defined as:

$$C_N = \rho_n v_n A_n = \frac{1}{2} (\rho_N + \rho_P) v_N A_n \quad (216)$$

$$C_S = \rho_S v_S A_S = \frac{1}{2} (\rho_S + \rho_P) v_P A_S \quad (217)$$

The final form of the second convection term of the ϕ -equation becomes:

$$C_N f_N \phi_N - C_S (1 - f_S) \phi_S + [C_N (1 - f_N) - C_S f_S] \phi_P \quad (218)$$

Considering the diffusion terms in Eq. 191 separately, we have:

$$\int_{x_W}^{x_e} \int_{r_S}^{r_n} \int_0^1 \left[-\frac{\partial}{\partial x} \left(r \Gamma \frac{\partial \phi}{\partial x} \right) - \frac{\partial}{\partial r} \left(r \Gamma \frac{\partial \phi}{\partial r} \right) \right] dx dr d\xi_3 \quad (219)$$

and integrating twice gives:

$$- \int_{r_s}^{r_n} [r \Gamma \frac{\partial \phi}{\partial x}]_w^e dr - \int_{x_w}^{x_e} [r \Gamma \frac{\partial \phi}{\partial r}]_s^n dx \quad (220)$$

Using the same technique as presented for the convection terms, these last integrals can be evaluated as:

$$- \Gamma_e (\frac{\partial \phi}{\partial x})_e r_{ap} (r_n - r_s) + \Gamma_w (\frac{\partial \phi}{\partial x})_w r_{ap} (r_n - r_s) \quad (221)$$

$$- \Gamma_n (\frac{\partial \phi}{\partial r})_n r_n (x_e - x_w) + \Gamma_s (\frac{\partial \phi}{\partial r})_s r_s (x_e - x_w) \quad (222)$$

As expected, the same geometric quantities appear as in the convection terms; substituting Eqs. 200, 214, and 215 yields:

$$- \Gamma_e (\frac{\partial \phi}{\partial x})_e A_{ew} + \Gamma_w (\frac{\partial \phi}{\partial x})_w A_{ew} - \Gamma_n (\frac{\partial \phi}{\partial r})_n A_n + \Gamma_s (\frac{\partial \phi}{\partial r})_s A_s \quad (223)$$

The derivatives at the four faces must be expressed in terms of variables at the main node points. Employing central differences (which are second-order accurate) (Dave, 1968) gives:

$$\begin{aligned} & - \Gamma_e (\frac{\phi_E - \phi_P}{\delta x_{PE}}) A_{ew} + \Gamma_w (\frac{\phi_P - \phi_W}{\delta x_{PW}}) A_{ew} \\ & - \Gamma_n (\frac{\phi_N - \phi_P}{\delta y_{NP}}) A_n + \Gamma_s (\frac{\phi_P - \phi_S}{\delta y_{PS}}) A_s \end{aligned} \quad (224)$$

Where the δx and δy stand for coordinate distance between the node points indicated by their corresponding subscripts.

Diffusion coefficients can be defined and calculated as:

$$D_E = \Gamma_e \frac{A_{ew}}{\delta x_{PE}} = (\frac{\Gamma_P + \Gamma_E}{2}) (\frac{A_{ew}}{\delta x_{PE}}) \quad (225)$$

$$D_W = \Gamma_w \frac{A_{ew}}{\delta x_{PW}} = (\frac{\Gamma_P + \Gamma_W}{2}) (\frac{A_{ew}}{\delta x_{PW}}) \quad (226)$$

$$D_N = \Gamma_n \frac{A_n}{\delta y_{NP}} = (\frac{\Gamma_P + \Gamma_N}{2}) (\frac{A_n}{\delta y_{NP}}) \quad (227)$$

$$D_S = r_s \frac{A_s}{\delta y_{PS}} = \left(\frac{r_P + r_S}{2} \right) \left(\frac{A_s}{\delta y_{PS}} \right) \quad (228)$$

Thus the diffusion terms can be expressed as

$$-D_E (\phi_E - \phi_P) + D_W (\phi_P - \phi_W) - D_N (\phi_N - \phi_P) + D_S (\phi_P - \phi_S) \quad (229)$$

Note the similarity with a control-volume formulation: the exchange coefficients and geometric quantities are contained in the diffusion coefficients D , while the difference in ϕ , which drives the diffusion, is explicitly shown with the correct sign (ϕ enters the cell when the ϕ -difference is negative).

Finally, we are left with the source terms in Eq. 191,

$$\int_{x_w}^{x_e} \int_{r_s}^{r_n} \int_0^1 r S^\phi dx dr d\xi_3 \quad (230)$$

One of the major reasons for the success of the TEACH formulation is the linearization of this source term. Thus

$$\int_{x_w}^{x_e} \int_{r_s}^{r_n} \int_0^1 r S^\phi dx dr d\xi_3 = S_U^\phi + S_P^\phi \phi_P \quad (231)$$

which defines two source term coefficients, S_U^ϕ and S_P^ϕ . If the source term happens to be nonlinear in terms of the dependent variable, ϕ , the technique calls for ϕ_P to be factored from the expression (if possible) and to appear with the S_P^ϕ coefficient in Eq. 231. Thus, ϕ appears implicitly while the remaining factored expression involving ϕ_P will be considered as known (explicit, based on previous values) and lumped together in the S_U^ϕ coefficient of Eq. 231. Furthermore, as shown below in Section III.B.7 S_P^ϕ must be negative to guarantee stable convergence.

In general, S^ϕ will be a function of all the dependent variables and other fluid properties as well as various types of derivatives involving these quantities. When integrating this source term, the value prevailing at the cell center will be used for all quantities. Any derivatives will be evaluated by central differencing. Therefore, the source term is considered constant, and:

$$\int_{x_w}^{x_e} \int_{r_s}^{r_n} \int_0^1 r S^\phi dx dr d\xi_3 = S^\phi (\Delta V) = S_U^\phi + S_P^\phi \phi_P \quad (232)$$

where ΔV is the volume of the cell.

Upon substitution of these newly defined coefficients, the general ϕ -equation becomes

$$\begin{aligned}
& [C_E f_E - D_E] \phi_E - [C_W (1 - f_W) + D_W] \phi_W + [C_N f_N - D_N] \phi_N - [C_S (1 - f_S) \\
& + D_S] \phi_S + [C_E (1 - f_E) + D_E - C_W f_W + D_W + C_N (1 - f_N) + D_N \\
& - C_S f_S + D_S] \phi_P = S_U + S_P \phi_P
\end{aligned} \tag{233}$$

Adding and subtracting $C_E - C_W + C_N - C_S$ from the bracket preceding ϕ_P and rearranging to obtain common expressions yields:

$$\begin{aligned}
& [(C_E - C_W + C_N - C_S) + D_W + (1 - f_W) C_W + D_E - f_E C_E \\
& + D_S + (1 - f_S) C_S + D_N - f_N C_N] \phi_P \\
& = [D_W + (1 - f_W) C_W] \phi_W + [D_E - f_E C_E] \phi_E + [D_S + (1 - f_S) C_S] \phi_S \\
& + [D_N - f_N C_N] \phi_N + S_U + S_P \phi_P
\end{aligned} \tag{234}$$

It is convenient to define new total coefficients to replace these common expressions:

$$A_E = D_E - f_E C_E \tag{235}$$

$$A_W = D_W + (1 - f_W) C_W \tag{236}$$

$$A_N = D_N - f_N C_N \tag{237}$$

$$A_S = D_S + (1 - f_S) C_S \tag{238}$$

The A 's with the single subscript are not area coefficients, but convection/diffusion coefficients. In terms of these total coefficients, the finite-difference form of the ϕ -equation becomes

$$\begin{aligned}
& [C_E - C_W + C_N - C_S + A_E + A_W + A_N + A_S] \phi_P \\
& = A_E \phi_E + A_W \phi_W + A_N \phi_N + A_S \phi_S + S_U + S_P \phi_P
\end{aligned} \tag{239}$$

5. First Modification (Stability)

Checking to see if mass is conserved, we can express the continuity equation in finite-difference form as follows. From Eq. 184

$$\int_{x_w}^{x_e} \int_{r_s}^{r_n} \int_0^1 \left[\frac{\partial}{\partial x} (r \rho u) + \frac{\partial}{\partial r} (r \rho v) - r S_p^m \right] dx dr d\xi_3 = 0 \quad (240)$$

or

$$\int_{r_s}^{r_n} [r \rho u]_w^e dr + \int_{x_w}^{x_e} [r \rho v]_s^n dx = S_p^m (\Delta V) \quad (241)$$

and in terms of convection coefficients,

$$C_E - C_W + C_N - C_S - S_p^m (\Delta V) = \dot{M}_{net} \quad (242)$$

At steady-state, $\dot{M}_{net}$ should equal zero in a converged solution. During the course of iterating to obtain a converged solution, the quantity $(C_E - C_W + C_N - C_S - S_p^m (\Delta V))$ will not in general vanish. In addition, a situation may arise where all of the total coefficients (A's) are zero, thus causing the finite-difference ϕ -equation (Eq. 239) to become singular. Therefore, we cannot allow this grouping of convection coefficients on the LHS of Eq. 239 to become equal to zero. From the definitions of these coefficients (Eqs. 235-238), if $\dot{M}_{net}$ is positive, then mass is being lost in the cell and a mass flow rate of $C_E - C_W + C_N - C_S - S_p^m (\Delta V)$ is carrying the property ϕ out of the cell. Under such conditions, it is reasonable to set $\dot{M}_{net}$ to zero and to include an additional term corresponding to the mass flow rate $C_E - C_W + C_N - C_S - S_p^m (\Delta V)$ carrying the (old) property (ϕ_p^{old}) with it. The other possibility (of $\dot{M}_{net}$ being negative) implies accumulation of mass in the cell, with ϕ being transported from the neighboring cells. Since Eq. 239 predicts this, no modification is necessary. Combining this modification into the source coefficients, Eq. 239 becomes

$$[A_E + A_W + A_N + A_S] \phi_p = A_E \phi_E + A_W \phi_W + A_N \phi_N + A_S \phi_S + S_U + S_p \phi_p \quad (243)$$

with

$$S_U = \max \{ C_E - C_W + C_N - C_S - S_p^m (\Delta V), 0 \} \phi_p^{old} + S_U^{rest} \quad (244)$$

$$S_p = -\max \{ C_E - C_W + C_N - C_S - S_p^m (\Delta V), 0 \} + S_p^{rest} - S_p^m (\Delta V) \quad (245)$$

where

$$\phi_p^{old} = \text{old or known value of } \phi \text{ at node P} \quad (246)$$

$$S_U^{\text{rest}}, S_p^{\text{rest}} = \text{source coefficients of the original equation as given by Eq. 232 times the volume of the cell} \quad (247)$$

This modification will ensure that the finite-difference equation will behave reasonably when the mass flow rates for the control volume do not satisfy continuity.

Equation 243 can be written more compactly by introducing a subscript d for the four directions (E, W, N, S), and combining the coefficients of the ϕ_p term:

$$[(\sum_d A_d) - S_p] \phi_p = \sum_d A_d \phi_d + S_U \quad (248)$$

where S_U and S_p are given by Eqs. 243 and 244. In the actual computer code, another coefficient is defined as

$$A_p = \sum_d A_d - S_p \quad (249)$$

and the standard equation form which TEACH solves is expressed as

$$A_p \phi_p = \sum_d A_d \phi_d + S_U \quad (250)$$

6. Second Modification (Improved Differencing Scheme)

Thus far the derivation resulting in Eq. 250 has used central differencing for all terms. Because of non-linearities in the transport equations, central differencing is not exact. For problems in computational fluid mechanics with large convection terms (i.e. cell Reynolds numbers greater than 2) central differencing causes problems in some locations (Roache, 1976; Patankar, 1980).

A simple one-dimensional analysis can be performed, for which a known exact solution exists (Wormeck, 1976; Patankar, 1980). It can be concluded from such an analysis that central differencing is preferable for small cell Reynolds numbers, and upwind differencing is performed for large values, but neither is satisfactory for all Reynolds numbers. Equation 250 is therefore modified to conform to these non-linearities while at the same time conserving mass. This approach is discussed in more detail by Patankar (1980). Questions and modifications concerning stability and convergence rates will be discussed in the next section.

The technique employed by PCGC-2 alters the differencing scheme depending on the local value of the cell Reynolds Number (Re). For example for a west face we note that:

$$G_w A_w = (\rho u A)_w = C_w \quad (251)$$

$$Re_w = \left(\frac{\rho u \delta}{\mu} \right)_w = \left(\frac{\rho u A}{\mu \delta} \right)_w = \frac{C_w}{D_w} \quad (252)$$

Therefore, the local cell Reynolds number is a measure of the relative magnitude of convection and diffusion. When convection terms are very small relative to diffusion terms (small Re), then central differencing is preferred. However, when convection terms are large relative to diffusion terms (large Re) then upwind differencing is preferred. In middle regions of Re , some combination is preferred. PCGC-2 has been coded to use either 1) hybrid differencing or 2) power-law differencing.

The mathematical representation of the alternate schemes is as follows. The total coefficients for each direction are rewritten as:

$$A_N = \Omega_N + \max(0, -C_N) \quad (253)$$

$$A_S = \Omega_S + \max(0, C_S) \quad (254)$$

$$A_E = \Omega_E + \max(0, -C_E) \quad (255)$$

$$A_W = \Omega_W + \max(0, C_W) \quad (256)$$

where Ω depends on the differencing scheme used. For upwind differencing:

$$\Omega_d = D_d \quad (257)$$

For central differencing:

$$\Omega_d = D_d - 0.5|C_d| \quad (258)$$

For hybrid differencing:

$$\Omega_d = \max[0, (D_d - 0.5|C_d|)] \quad (259)$$

For power-law differencing:

$$\Omega_d = \max\{0, D_d[(D_d - 0.1|C_d|)/D_d]^5\} \quad (260)$$

The difference between the various differencing schemes can be summarized as follows: in upwind differencing, the finite difference is taken in the

direction from which the velocity vector is arriving. Central differencing has already been discussed. Hybrid differencing uses upwind differencing when cell Reynolds Numbers are larger than 2 or less than -2 and central differencing when $-2 < Re < 2$. Power-law differencing uses the fifth order power law expression for $-10 < Re < 10$ and upwind differencing outside this range. For both power-law and hybrid differencing, the appropriate differencing is applied to convection terms. Diffusion terms are ignored for high Reynolds numbers (pure upwind differencing). These advanced differencing options allow for greater accuracy with less grid resolution than is permissible with central differencing. The power-law scheme is recommended in all cases.

7. Convergence Test

The finite-difference equations will now be analyzed for convergence criteria. Writing Eq. 250 as

$$\phi_p = \sum_d A'_d \phi_d + S'_U \quad (261)$$

where $A'_d = A_d/A_p$ and $S'_U = S_U/A_p$, we have a system of linear algebraic equations of the form

$$x_i = \sum_{j, i \neq j} (a_{ij} x_j) + b_i \quad (262)$$

From the theory of linear equations (Gosman et al., 1969; Patankar and Spalding, 1970) if the a_{ij} and b_i are constants, the sufficient conditions for convergence are:

$$\sum_{j, i \neq j} |a_{ij}| \begin{cases} < 1 \text{ for all } i \\ < 1 \text{ for at least one } i \end{cases} \quad (263)$$

Since A'_d and S'_U in Eq. 261 are not constant, the criteria in Eq. 263 do not apply exactly. However, as an approximation, we may expect convergence if

$$\sum_d \frac{A_d}{A_d - S_p} \begin{cases} < 1 \text{ for all } i \\ < 1 \text{ for at least one } i \end{cases} \quad (264)$$

which implies that S_p must be less than zero. The S_p term is the source term involving the dependent variable implicitly (based on new value). Therefore, to insure a negative value for S_p , if any source term containing the dependent variable is positive, the old value of ϕ must be used and the term combined this term with the S_U quantity (i.e., appearing explicitly).

Since the coefficients are not constant, convergence is not guaranteed by Eq. 263 but is reasonably assured if $S_p < 0$. If divergence is encountered, under-relaxation may be used as discussed later. PCGC-2 generally converges if the source terms are linear or mildly nonlinear. Highly nonlinear source terms may not converge or require very small (0.1-0.3) under-relaxation factors.

8. Solution of the Finite-Difference Equations (TDMA)

PCGC-2 has a large system of linear algebraic finite-difference equations to solve, and vast numbers of techniques are available (Carnahan, 1969) to solve this system of equations. Roache (1976) presents some of the more popular methods to solve the fluid flow type of equation systems.

Matrix inversion and other direct techniques are out of the question because of the large number of equations involved, and therefore iterative methods must be employed. The formulation of Gosman, et al. (1969) in terms of vorticity and stream function utilized a Gauss-Seidel algorithm, which is a point-by-point method. The equations are solved one at a time, passing from node point to node point throughout the flow field. New values of the variables are used as soon as they become available, and the complete flow field is solved for each dependent variable before going to the next dependent variable.

The technique used in PCGC-2 is to solve simultaneously a line of node points in a so-called line-by-line method. This line-by-line technique is implemented in a very efficient numbered scheme, the Tri-Diagonal Matrix Algorithm (TDMA). The equations are of the form:

$$D_i \phi_i = A_i \phi_{i+1} + B_i \phi_{i-1} + C_i \quad (265)$$

where $i=2, N-1$ and the values of the constant coefficients A_i , B_i , C_i , and D_i are given for $i=2, N-1$ together with the boundary values ϕ_1 and ϕ_N . The procedure calls for rewriting Eq. 265 as:

$$\phi_i = A'_i \phi_{i+1} + C'_i \quad (276)$$

and obtaining a solution by successive substitution, starting with $i=N-1$ and working backwards to $i=2$. The transformed coefficients A'_i and C'_i are given by the recurrence relations:

$$A'_i = \frac{A_i}{D_i - B_i A'_{i-1}} \quad (267)$$

$$B'_i = \frac{C_i + C'_{i-1} B_i}{D_i - B_i A'_{i-1}} \quad (268)$$

with the starting values of $A'_1 = 0$ and $C'_1 = \phi_1$.

The TDMA can be implemented to solve Equation 250 by considering the equations for all the control volumes along a grid line with the last or best estimates for the values of ϕ along the two neighboring grid lines, and hence constructing an equation set which can be solved by the TDMA. In this manner,

we can first traverse along all the grid lines in, say, the x direction; then, using this solution as the best estimate, go over lines in the r direction.

For the r-direction sweep, Eq. 250 is written as:

$$A_P \phi_P' = A_N \phi_N' + A_S \phi_S' + (A_E \phi_E + A_W \phi_W + S_U) \quad (269)$$

where the term in the parentheses is considered known and TDMA can be applied. The superscript ' denotes the values obtained from this first phase of solution, while the second phase, the x-direction sweep is the solution of:

$$A_P \phi_P'' = A_E \phi_E'' + A_W \phi_W'' + (A_N \phi_N' + A_S \phi_S' + S_U) \quad (270)$$

in a similar manner.

It must be remembered that the TDMA is an iterative solution technique to solve the finite-difference equations, the coefficients of which are only tentative and require updating to account for the changes in the values of the variables. The number of sweeps needed for an accurate solution of the finite-difference equations before the coefficients are recalculated is arbitrary and problem-dependent. Typically, 2 or 3 sweeps are used for each variable except particle number density, in which case five sweeps are typically used.

9. Final Form

The final form of the ϕ -finite-difference equation in PCGC-2 is:

$$A_P \phi_P = A_E \phi_E + A_W \phi_W + A_N \phi_N + A_S \phi_S + S_U \quad (271)$$

where

$$A_P = A_E + A_W + A_N + A_S - S_P \quad (272)$$

$$A_E = \Omega_E + \max(0, -C_E) \quad (273)$$

$$A_W = \Omega_W + \max(0, C_W) \quad (274)$$

$$A_N = \Omega_N + \max(0, -C_N) \quad (275)$$

$$A_S = \Omega_S + \max(0, C_S) \quad (276)$$

$$\Omega_d^* = [0, D_d[(D_d - 0.1|C_d|)/D_d]^5] \quad d = E, W, N, \text{ or } S \quad (277)$$

$$D_E = 1/2 (\Gamma_P + \Gamma_E) (A_{ew}) / \delta x_{PE} \quad (278)$$

$$D_W = 1/2 (\Gamma_P - \Gamma_W) (A_{ew}) / \delta x_{PW} \quad (279)$$

$$D_N = 1/2 (\Gamma_P + \Gamma_N) (A_n) / \delta r_{NP} \quad (280)$$

$$D_S = 1/2 (\Gamma_P + \Gamma_S) (A_s) / \delta r_{PS} \quad (281)$$

$$C_E = 1/2 (\rho_P + \rho_E) (A_{ew}) u_E \quad (282)$$

$$C_W = 1/2 (\rho_P + \rho_W) (A_{ew}) u_P \quad (283)$$

$$C_N = 1/2 (\rho_P + \rho_N) (A_n) v_N \quad (284)$$

$$C_S = 1/2 (\rho_P + \rho_S) (A_s) v_P \quad (285)$$

$$S_U = \max \{C_E - C_W + C_N - C_S - S_p^m(\Delta V), 0\} \phi_p^{old} + (S_U^{rest}) (vol) \quad (286)$$

$$S_p = -\max \{C_E - C_W + C_N - C_S - S_p^m(\Delta V), 0\} + (S_p^{rest}) (vol) - S_p^m(\Delta V) \quad (287)$$

$$S_U^{rest} + S_p^{rest} \phi_p = S^\phi \quad (288)$$

and the grid definition implies that all the f's are equal to 0.5.

10. Finite-Difference Form of the Momentum Equation

The finite-difference form of the momentum equation closely resembles Eq. 271 for the general ϕ -equation, with two exceptions. First, as mentioned previously, a staggered velocity grid is employed (see Figures 15 and 16) for the definition of the velocity components, and therefore control volumes centered at these velocity locations are defined which are different from those for the other dependent variables. Secondly, the pressure gradient term, which may be regarded as a source of momentum, is treated in a special manner, and the geometric coefficient which relates a velocity component to

Figure 15. A typical u-cell showing adjacent velocities. Other symbols define the location of the control volume over which the first momentum equation is integrated.

Figure 16. A typical v-cell showing adjacent velocities. Other symbols define the location of the control volume over which the second momentum equation is integrated.

the pressure difference between the adjacent nodes is stored for use in the pressure equation.

If the pressure distribution were known, the momentum equations (Eq. 185-187) would be uncoupled from the continuity equation (Eq. 184) and could be solved in a straightforward manner. Unfortunately, the pressures are not known in advance.

PCGC-2 employs both the SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) and SIMPLER (SIMPLE-Revised) algorithms as developed by Patankar and Spalding (1970, 1972) and Patankar (1980). In these techniques, the pressure distribution is guessed (i.e., assumed known) and denoted by p^* . The solution of the momentum equations for the two velocity components that correspond with this guessed (or "starred") pressure field becomes the "starred" velocity field. Corrections are then made to the "starred" pressure field so as to bring the velocity field into conformity with the continuity equation.

u-Equation. From Eq. 185, the u-equation is:

$$\frac{\partial}{\partial x}(r\rho uu) + \frac{\partial}{\partial r}(r\rho uv) - \frac{\partial}{\partial x}(r\mu \frac{\partial u}{\partial x}) - \frac{\partial}{\partial r}(r\mu \frac{\partial u}{\partial r}) = -r \frac{\partial p}{\partial x} + rS^u \quad (289)$$

where the source term is given by Eq. 188. The convection and diffusion terms are identical to the ϕ -equation with $\phi = u$ and $\Gamma = \mu$, and hence the derivation of the finite-difference equations is similar to the ϕ -equation, but the integration is performed over the u-control volume, which is staggered from the main ϕ -cell. The pressure term is handled explicitly. Figure 15 shows a typical u-cell, and the superscript u means that reference to this u-cell is being made instead of to the main control volume.

Integrating Eq. 295 over the u-cell in the same way as the ϕ -equation was integrated over the main or p-cell, the first convection term becomes:

$$\int_{x_w^u}^{x_e^u} \int_{r_s^u}^{r_n^u} \int_0^1 \frac{\partial}{\partial x}(r\rho uu) dx dr d\xi_3 \quad (290)$$

or

$$(\rho uu)_e^u A_{ew}^u - (\rho uu)_w^u A_{ew}^u \quad (291)$$

A problem arises here as to which way to expand the density and velocity. For example, one method would be to linearly interpolate the velocities and simply average the density. Another method would be to linearly interpolate the product $\rho u = G$ as well as the remaining u . The former method results in:

$$\rho_e^u (u_e^u)^2 = \rho_p[(1 - f_E^u) u_p + f_E^u u_E] \quad (292)$$

and, for $f_E^u = 1/2$, the east face convection term is:

$$1/2 A_{ew}^u (\rho_p) (u_p + u_E) \quad (293)$$

The latter method yields

$$(\rho u)_e^u u_e^u = [(1 - f_E^u) (\rho u)_p + f_E^u (\rho u)_E] [(1 - f_E^u) u_p + f_E^u u_E] \quad (294)$$

requiring the densities midway between their points of definition. By averaging them and taking $f_E^u = 1/2$, the convection through the east face is given by:

$$1/2 A_{ew}^u \left[\left(\frac{\rho_E + \rho_p}{2} \right) u_E + \left(\frac{\rho_p + \rho_W}{2} \right) u_p \right] \quad (295)$$

The second convection term integrates to

$$(\rho v u)_n^u A_n^u - (\rho v u)_s^u A_s^u \quad (296)$$

where the ρv products are linearly interpolated between the points of definition of the v velocities as:

$$(\rho v)_n^u = (1 - f_W^u) \left(\frac{\rho_W + \rho_{NW}}{2} \right) v_{NW} + f_W^u \left(\frac{\rho_N + \rho_p}{2} \right) v_N \quad (297)$$

$$(\rho v)_s^u = (1 - f_W^u) \left(\frac{\rho_W + \rho_{SW}}{2} \right) v_W + f_W^u \left(\frac{\rho_S + \rho_p}{2} \right) v_p \quad (298)$$

where

$$f_W^u = \frac{x_p^u - x_W}{x_p - x_W} \quad (299)$$

PCGC-2 defines the velocities midway between the main node points at cell faces ($f_W^u = 1/2$), and the four u -equation convection coefficients are:

$$C_E^u = 1/4 [(\rho_p + \rho_E) u_E + (\rho_p + \rho_W) u_p] A_{ew}^u \quad (300)$$

$$C_W^u = 1/4 [(\rho_p + \rho_W) u_p + (\rho_W - \rho_{WW}) u_W] A_{ew}^u \quad (301)$$

$$C_N^u = 1/4[(\rho_p + \rho_N) v_N + (\rho_W + \rho_{NW}) v_{NW}] A_n^u \quad (302)$$

$$C_S^u = 1/4[(\rho_p + \rho_S) v_p + (\rho_W + \rho_{SW}) v_W] A_s^u \quad (303)$$

where-

$$\rho_{WW} = \rho_{i-2,j} \quad (304)$$

The diffusion terms for the u-equation are defined as:

$$D_E^u = \mu_e^u A_{ew}^u / \delta x_{EP}^u \quad (305)$$

$$D_W^u = \mu_w^u A_{ew}^u / \delta x_{PW}^u \quad (306)$$

$$D_N^u = \mu_n^u A_n^u / \delta y_{NP} \quad (307)$$

$$D_S^u = \mu_s^u A_s^u / \delta y_{PS} \quad (308)$$

where the viscosities are interpolated as:

$$\mu_e^u = \mu_p \quad (309)$$

$$\mu_w^u \approx \mu_W \quad (310)$$

$$\mu_n^u = 1/4 (\mu_{NW} + \mu_N + \mu_W + \mu_p) \quad (311)$$

$$\mu_s^u = 1/4 (\mu_W + \mu_p + \mu_{SW} + \mu_S) \quad (312)$$

Considering the pressure term in Eq. 185

$$\int_{x_w^u}^{x_e^u} \int_{r_s^u}^{r_n^u} \int_0^1 (-r \frac{\partial p}{\partial x}) dx dr d\xi_3 \quad (313)$$

and integrating twice yields:

$$-\int_{x_w^u}^{x_e^u} \{1/2 (r_n^u)^2 - (r_s^u)^2 (\frac{\partial p}{\partial x})\} dx \quad (314)$$

or

$$-1/2 (r_n^u - r_s^u) (r_n^u + r_s^u) [p] \begin{matrix} x_e^u \\ x_w^u \end{matrix} \quad (315)$$

$$\text{and since } r_p = 1/2 (r_n^u + r_s^u) \quad (316)$$

$$A_{ew}^u (-p_e^u + p_w^u) \quad (317)$$

where these pressures are approximately (exactly only for uniform grids) defined at their required locations to give:

$$A_{pw_u} (p_w - p_p) \quad (318)$$

Since the leading coefficient will be needed in the pressure equation, it is stored as a new area coefficient, $D^u = g_c A_{ew}^u$. The expression

$$D^u (p_w - p_p) \quad (319)$$

will be incorporated into the S_u term. The gravitational constant, g_c , has been added since pressure has force dimensions.

Evaluating the source terms the same way, the final u-equation is

$$A_p u_p = \sum_d A_d u_d + D^u (p_w - p_p) + S_u \quad (320)$$

where:

$$A_p = \sum_d (A_d) - S_p \quad (321)$$

$$A_d = \Omega_d + \max (0, -C_d) \text{ for } d = E \text{ or } N \quad (322)$$

$$A_d = \Omega_d + \max (0, C_d) \text{ for } d = W \text{ or } S \quad (323)$$

$$\Omega_d^* = \max \{0, D_d [(D_d - 0.1 |C_d|) / D_d]^5\} \quad (324)$$

*This Ω_d is for power-law differencing. If hybrid differencing is used $\Omega_d = \max [0, (D_d - 0.5 |C_d|)]$.

$$S_U = \max \{C_E - C_W + C_N + C_S - S_p^m(\nabla V), 0\} u_p + S_U^{rest} (vol) \quad (325)$$

$$S_p = -\max \{C_E - C_W + C_N - C_S - S_p^m(\nabla V), 0\} + (S_p^{rest} (vol) - S_p^m(\nabla V)) \quad (326)$$

and C_d and D_d are given by Eqs. 300 to 308.

v and w Equations. Following a similar procedure, the second momentum equation, Eq. 186 can be expressed as:

$$A_p v_p = \sum_d A_d v_d + S_U \quad (327)$$

where the total coefficients are defined in the usual manner, but S_U is given as:

$$S_U = \max \{C_E - C_W + C_N - C_S - S_p^m(\nabla V), 0\} v_p + D_v(p_s - p_p) + (S_U^{rest} (vol)) \quad (328)$$

The v-equation convection coefficients are:

$$C_E = 1/4 [(\rho_p + \rho_E) u_E + (\rho_S + \rho_{SE}) u_{SE}] \quad (329)$$

$$C_W = 1/4 [(\rho_p + \rho_W) u_p + (\rho_S + \rho_{SW}) u_S] \quad (330)$$

$$C_N = 1/4 [(\rho_p + \rho_N) v_N + (\rho_p + \rho_S) v_p] \quad (331)$$

$$C_S = 1/4 [(\rho_p + \rho_S) v_p + (\rho_S + \rho_{SS}) v_S] \quad (332)$$

The diffusion coefficients are given by:

$$D_E = (\mu_e^v) A_{ew}^v / \delta x_{EP} \quad (333)$$

$$D_W = (\mu_w^v) A_{ew}^v / \delta x_{PW} \quad (334)$$

$$D_N = (\mu_p) A_n^v / \delta y_{NP}^v \quad (335)$$

$$D_S = (\mu_s) A_s^v / \delta y_{PS}^v \quad (336)$$

Figure 16 shows a typical v control volume and notation. Similar results can be obtained for the tangential momentum equation.

11. Pressure Correction Equation (Continuity)

The next task in the SIMPLE or SIMPLER algorithms is to correct the starred pressure and velocity fields such that the continuity equation is satisfied. The two finite-difference momentum equations are from Eqs. 320 and 327:

$$A_p^u u_p = \sum_d A_d^u u_d + D^u (p_W - p_p) + S_U^u \quad (337)$$

$$A_p^v v_p = \sum_d A_d^v v_d + D^v (p_S - p_p) + S_U^v \quad (338)$$

Lacking knowledge of the pressure distribution, the pressures in the above momentum equations are guessed (denoted by a star superscript) to allow the computation of the two velocity components u^* and v^* corresponding to the p^* distribution. The true pressure is

$$p = p^* + p' \quad (339)$$

where p' is the pressure correction which, when summed with the guessed pressure, will give the correct pressure.

The SIMPLE algorithm utilizes the continuity equation to determine the pressure corrections. The equations expressing the true velocities in terms of the guessed velocities and pressure corrections are developed below. Substituting the guessed pressures in Eqs. 337 and 338 yields:

$$A_p^u u_p^* = \sum_d A_d^u u_d^* + D^u (p_W^* - p_p^*) + S_U^u \quad (340)$$

$$A_p^v v_p^* = \sum_d A_d^v v_d^* + D^v (p_S^* - p_p^*) + S_U^v \quad (341)$$

These equations are solved for the "starred" velocity fields. Subtracting the corresponding Eqs. 340 and 341 from Eqs. 337 and 338 and substituting the pressure corrections, we have:

$$A_p^u (u_p - u_p^*) = \sum_d A_d^u (u_d - u_d^*) + D^u (p_W' - p_p') \quad (342)$$

$$A_p^v (v_p - v_p^*) = \sum_d A_d^v (v_d - v_d^*) + D^v (p_S' - p_p') \quad (343)$$

which gives the true velocities as:

$$u_p = u_p^* + \frac{D_p^u}{A_p^u} (p_W' - p_p') + \sum_d \frac{A_d^u}{A_p^u} (u_d - u_d^*) \quad (344)$$

$$v_p = v_p^* + \frac{D_p^v}{A_p^v} (p_S' - p_p') + \sum_d \frac{A_d^v}{A_p^v} (v_d - v_d^*) \quad (345)$$

A similar derivation applied to the neighboring nodes leads to

$$u_E = u_E^* + \left(\frac{D_p^u}{A_p^u}\right)_E (p_p' - p_E') + \sum_{d_E} \left(\frac{A_d^u}{A_p^u}\right)_E (u_d - u_d^*) \quad (346)$$

$$v_N = v_N^* + \left(\frac{D_p^v}{A_p^v}\right)_N (p_p' - p_N') + \sum_{d_N} \left(\frac{A_d^v}{A_p^v}\right)_N (v_d - v_d^*) \quad (347)$$

where the new subscript refers to the total coefficients at the node point.

From Eq. 239, the finite-difference form of the continuity equation is

$$\rho_e u_E A_e - \rho_w u_p A_w + \rho_n v_N A_n - \rho_s v_p A_s - S_p^m(\Delta V) = 0 \quad (348)$$

In the so-called incompressible pressure correction equation, the density does not depend on pressure; this derivation follows.

Equation 350 calls for substitution of Eqs. 344 to 347 for the velocities, but the last term in each of these equations is lengthy and complicated, so that it will be dropped to give the true velocities as:

$$u_p = u_p^* + D_p^u (p_W' - p_p') \quad (349)$$

$$v_p = v_p^* + D_p^v (p_S' - p_p') \quad (350)$$

$$u_E = u_E^* + D_E^u (p_p' - p_E') \quad (351)$$

$$v_N = v_N^* + D_N^v (p_p' - p_N') \quad (352)$$

where the new pressure coefficients include the corresponding A_p terms. Now substituting these velocities, the continuity equation becomes:

$$[\rho_e A_e D_E^u + \rho_w A_w D_P^u + \rho_n A_n D_N^v + \rho_s A_s D_P^v] p_P' = (\rho_e A_e D_E^u) p_E' + (\rho_w A_w D_P^u) p_W' +$$

$$(\rho_n A_n D_N^v) p_N' + (\rho_s A_s D_P^v) p_S' - \rho_e A_e u_E^* + \rho_w A_w u_P^* - \rho_n A_n v_N^* + \rho_s A_s v_P^* + S_p^m(\Delta V) \quad (353)$$

This equation allows the pressure corrections to be determined from known quantities, and furthermore has a similar form to the standard finite-difference equation. Defining the following pressure-correction coefficients:

$$A_E = \rho_e A_e D_E^u \quad (354)$$

$$A_W = \rho_w A_w D_P^u \quad (355)$$

$$A_N = \rho_n A_n D_N^v \quad (356)$$

$$A_S = \rho_s A_s D_P^v \quad (357)$$

$$S_U = -\rho_e A_e u_E^* + \rho_w A_w u_P^* - \rho_n A_n v_N^* + \rho_s A_s v_P^* + S_p^m(\Delta V) \quad (358)$$

the pressure-correction equation becomes simply:

$$(\sum_d A_d) p_P' = \sum_d A_d p_d' + S_U \quad (359)$$

which can be solved by the TDMA. Note that no hybrid differencing is required.

The quantity S_U defined above is the net mass source resulting from the starred velocity field which in general does not satisfy continuity. The aim of the pressure correction equation is to reduce this mass source to zero; indeed, by monitoring this quantity, the extent of convergence is known, with complete convergence of PCGC-2 occurring when the sum of these pressure source terms throughout the flow domain is less than some input tolerance (typically 0.001-0.0001).

After resolving the pressure correction equation by the TDMA, the correct pressure and velocities are given by

$$p = p^* + p' \quad (360)$$

$$u_p = u_p^* + D_u (p_W' - p_P') \quad (361)$$

$$v_p = v_p^* + D_v (p_S' - p_p') \quad (362)$$

It should be pointed out that the pressure correction equation calculates just the corrections to the pressure field; and in a converged solution these corrections vanish, and therefore the dropping of the last terms in the momentum equations, to arrive at Eqs. 349 to 353, has no effect on the accuracy of the solution. Also, it must be noted that under-relaxation is required (~ 0.5) so that only a portion of these corrections are added at one time.

The SIMPLER (SIMPLE-Revised) algorithm was developed by Patanker (1980) to allow faster convergence than the SIMPLE algorithm. Solving Equations 337 and 338 for u_p and v_p yields:

$$u_p = [\sum_d A_d^u u_d + D_p^u (p_W - p_p) + S_U^u] / A_p^u \quad (363)$$

$$v_p = [\sum_d A_d^v v_d + D_p^v (p_S - p_p) + S_U^v] / A_p^v \quad (364)$$

Pseudo-velocities ($\hat{u}_p, \hat{v}_p$) are defined to simplify Eqs. 363 and 364:

$$\hat{u}_p = (\sum_d A_d^u u_d + S_U^u) / A_p^u \quad (365)$$

$$\hat{v}_p = (\sum_d A_d^v v_d + S_U^v) / A_p^v \quad (366)$$

Similar equations are easily derived for $\hat{u}_E$ and $\hat{v}_N$. Using Eqs. 365 and 366, Eqs. 363 and 364 are reduced to:

$$u_p = \hat{u}_p + D_p^u (p_W - p_p) \quad (367)$$

$$v_p = \hat{v}_p + D_p^v (p_S - p_p) \quad (368)$$

Eqs. 367 and 368 are very similar to Eqs. 349 and 350. Substituting the velocities from Eqs. 357 and 368 into the continuity equation yields an equation similar to Eq. 359, except that the pseudovelocities are used instead of the starred velocities:

$$(\sum_d A_d) p_p = \sum_d A_d p_d + S_u^p \quad (369)$$

where the A 's are given by Eqs. 354-357, and S_u^p is defined by:

$$S_U^p = -\rho_e A_e \hat{u}_E + \rho_w A_w \hat{u}_P - \rho_n A_n \hat{v}_N + \rho_s A_s \hat{v}_P + S_p^m(\nabla V) \quad (370)$$

The SIMPLER algorithm is summarized below (see Patankar, 1980):

1. Start with a guessed velocity field.
2. Calculate the coefficients for the axial and radial momentum equations and then calculate the pseudo-velocities from Equations 365 and 366 using the guessed velocity field.
3. Calculate the pressure coefficients and solve for the pressure field using Eq. 369.
4. Treating this pressure field as p^* , solve for the starred velocity field using the starred momentum equations.
5. Solve the pressure correction equation (Eq. 359) to get p' .
6. Correct the starred velocity field using Eqs. 349-350, but do not correct the pressure field.
7. Solve the other conservation equations as necessary (w , k , ϵ , f , η , etc.).
8. Return to Step 2 and repeat as necessary.

Fletcher (1983) showed that the SIMPLER algorithm converged in nearly half the time required by the SIMPLE algorithm. It should be pointed out that Eq. 370 is not a continuity equation like Eq. 359, and hence S_U^p should not necessarily vanish when convergence is achieved. Also, it must be noted that best results are achieved when under-relaxation is not used for either the pressure (Eq. 369) or the pressure correction (Eq. 359) when the SIMPLER algorithm is used. The SIMPLER algorithm makes it possible to use much larger values for all other under-relaxation factors in the model (i.e. less under-relaxation). Typical values are 0.7 instead of 0.5.

12. Under-Relaxation

The solution of the finite-difference equations in the form of Eq. 369 generally diverges unless the iterative corrections are under-relaxed. The conventional practice in computational fluid dynamics is to under-relax the dependent variables to avoid numerical instabilities. However, based on considerable experience, under-relaxation in this code is accomplished by under-relaxing the source terms.

If f_{UR} is the under-relaxation factor, then the two source terms become (in FORTRAN replacement notation)

$$A_p = A_p / f_{UR} \quad (371)$$

and

$$S_U = S_U + (1 - f_{UR}) \phi_P^{old} A_P / f_{UR} \quad (372)$$

where ϕ_P^{old} is the known value of ϕ computed during the previous iteration.

These modifications are performed before solution of the finite-difference equations by TDMA. All dependent variables are relaxed by this method, where the under-relaxation factor can be different for each variable. In the pressure-correction equation (Eq. 359), the pressure coefficients can also be under-relaxed:

$$D^U = (D^U) f_{UR}^U / A_P^U \quad (373)$$

$$D^V = (D^V) f_{UR}^V / A_P^V \quad (374)$$

It may also be required to under-relax the fluid properties if they change rapidly as is the case with viscosity in turbulent flow and the density in compressible flow. If $\phi^{(n)}$ is the value of the property used in iteration $n+1$, and $\phi^{(n+1)}$ is the value computed in the $n+1^{st}$ iteration, the value used in the $n+1^{st}$ iteration is computed from

$$\phi = f_{UR} \phi^{(n+1)} + (1 - f_{UR}) \phi^{(n)} \quad (375)$$

The values of the under-relaxation factors must be between zero and one, and for computational efficiency, should be the largest value allowing a stable solution. The optimum values of the under-relaxation factors are problem dependent. Should divergence occur, smaller values may be required.

13. Boundary Conditions

There exist an infinite number of solutions to the governing equations, and only the boundary conditions distinguish one solution from another. Thus, the boundary conditions play an important role. Roache (1976) gives an excellent presentation of many types of boundary conditions occurring in fluid dynamic calculations and discusses their effects on numerical stability and accuracy.

In PCGC-2 all boundaries coincide with the control volume sides as illustrated in Figure 17. The implementation of the boundary conditions in the numerical procedure is accomplished by modifying the finite-difference equations for the boundary cells:

$$(\sum_d A_d - S_p) \phi_P = A_E \phi_E + A_W \phi_W + A_N \phi_N + A_S \phi_S + S_U \quad (376)$$

The four total coefficients (A's) and the two source term coefficients S_U and S_p in Eq. 376 are altered in such a way that the boundary conditions are

Figure 17. A typical main boundary cell.

satisfied. This technique, generally referred to as "breaking the link," is illustrated by rewriting Eq. 376 as

$$A_E (\phi_P - \phi_E) + A_W (\phi_P - \phi_W) + A_N (\phi_P - \phi_N) + A_S (\phi_P - \phi_S) = S_U + S_P \phi_P \quad (377)$$

It may be seen that ϕ may be considered as being "linked" to its four neighbors. Equation 377 is correct for interior cells; for boundary cells, the appropriate total coefficients (A's) must be set to zero, and the correct conditions of convection and diffusion at the boundary included by modifying the two source terms. Thus the procedure calls for specifying the boundary conditions as linear functions of the dependent variable. All three types of boundary conditions for elliptic equations are permissible, and will be discussed in turn.

Dirichlet conditions, or prescribed values of the function, are inserted by calculating the correct convection and diffusion coefficients based on the prescribed values of the dependent variable on the boundary, and using the hybrid differencing scheme to obtain a new total coefficient $A^{(new)}$.

Hence:

$$A_d^{(new)} = 0 \quad (378)$$

$$D_d = \Gamma_B A_B / \delta_{BP} \quad (379)$$

$$C_d = \rho_B \text{vel}_B A_B \quad (380)$$

$$A_d^{(new)} = \text{HYBRID} [C_d, D_d] \quad (381)$$

$$S_U^{(new)} = S_U^{(old)} + A_d^{(new)} \phi_B \quad (382)$$

$$S_P^{(new)} = S_P^{(old)} - A_d^{(new)} \quad (383)$$

where the subscript B refers to the conditions at the boundary located at a distance of δ_{BP} from the cell center in the d direction, ϕ_B is the prescribed boundary value, A_B is the area of the control volume on the boundary, and C_d and D_d are the convection and diffusion coefficients at the control volume face on the boundary. If the velocity at the boundary, vel_B , is zero (as in the case of a solid wall), then Eqs. 378-383 reduce to:

$$A_d^{(new)} = 0 \quad (384)$$

$$S_U^{(new)} = S_U^{(old)} + \left(\frac{\Gamma_B A_B}{\delta_{BP}} \right) \phi_B \quad (385)$$

$$S_P^{(new)} = S_P^{(old)} - \left(\frac{\Gamma_B A_B}{\delta_{BP}} \right) \quad (386)$$

where A_B is the area of the bounding face.

For Neumann conditions, for which the normal derivative of the function is specified, the usual "links" to all the adjacent exterior cells are broken by setting to zero the appropriate A 's and inserting the prescribed boundary fluxes, as follows:

$$S_U^{(new)} = S_U^{(old)} + (c \frac{\partial \phi}{\partial n})_B A_B \quad (387)$$

$$S_P^{(new)} = S_P^{(old)} \quad (388)$$

where $(c \frac{\partial \phi}{\partial n})_B$ is the specified flux at the boundary.

The third type of boundary condition is the mixed or Robbin's type with the linear combination of the function value and normal gradient specified (for example in a convection heat transfer calculation). Consider heat conduction occurring from node W in Figure 17 to the boundary where convection takes place with a heat transfer coefficient α . Then the required boundary condition (for steady state) is:

$$q = \alpha A_W (T_B - T_P) = k_B A_W \frac{T_W - T_B}{\delta_{WB}} \quad (389)$$

where k_B is the conductivity of the conducting media, T_B is the boundary temperature, and δ_{WB} is the distance between node W and the boundary. The boundary temperature can be eliminated in Eq. 389 to give:

$$q = \frac{T_W - T_P}{\frac{1}{\alpha A_W} + \frac{k_B A_W}{\delta_{WB}}} \quad (390)$$

and the two source terms become:

$$S_U^{T(new)} = S_U^{T(old)} + T_W / R_T \quad (391)$$

$$S_P^{T(new)} = S_P^{T(old)} - R_T^{-1} \quad (392)$$

where

$$R_T = \frac{1}{\alpha A_w} + \frac{k_B A_w}{\delta_{WB}} \quad (393)$$

Normally PCGC-2 iterates on a rectangular domain (being controlled by FORTRAN do-loops) and if this domain contains node points which are outside the flow field domain, either the computer code can be altered to skip these nodes or the following technique can be employed to fix the value of ϕ at the node:

$$S_U = (\gamma \phi_p) \quad (394)$$

$$S_P = (-\gamma) \quad (395)$$

where γ is a large number (10^{30}) and ϕ_p is the value desired at the node point. Boundary conditions must be inserted for each boundary cell.

14. Numerical Diffusion

The hybrid differencing scheme introduces numerical errors in the convection terms of order $O(\Delta x)$ when upwind differencing is used and $O(\Delta x^2)$ when central differencing is used. Roache (1976) notes that when upwind differencing is used, the error introduced from the finite-difference approximation can be viewed as an artificial numerical diffusion. This numerical diffusion is a function of the Courant number:

$$C_x = u \Delta t / \Delta x \quad (396)$$

Roache (1976) says that if $C_x = 1$, the numerical diffusion terms will be identically zero, meaning that the finite-difference approximation is exact. The errors introduced by upwind differencing should be investigated by using a different finite-differencing scheme. Central-differencing, however, is thought to be unstable for elliptical partial differential equations (Roache, 1976).

Several authors (Leonard, 1979; Castro, 1978; Raithby, 1976; Argarwal, 1981; Leschiziner, 1980; Lillington, 1978) have developed methods to eliminate numerical diffusion in simple flow systems. Leschiziner (1980) showed that significant numerical diffusion arose in predictions where convection dominated physical diffusion and where there was a streamline-to-grid skewness. His predictions were made when the streamlines were at a 45-degree angle to the grid. Lillington (1978) reported significant numerical diffusion when gradients existed normal to the streamlines in the dependent variable and source terms. He also noted that higher-order differencing schemes could have poor convergence in some elliptical flow regimes. Raithby (1976) found that numerical diffusion was significant only when the source terms take a certain form and if the streamlines were skew to the grid. Leonard (1979) showed

predictions where significant numerical diffusion occurred when streamlines were at an 18-degree angle to the grid. Leonard and co-workers also argued that their scheme allows larger grid spacing since it was more accurate.

Fletcher (1983) incorporated the method of Leonard (1979) into PCGC-2 to determine the effect of numerical diffusion in typical PCGC-2 predictions. The basis for the differencing scheme of Leonard (1979) is a second-order interpolation scheme for the values for the variable of interest (ϕ) at the cell wall. The predictions made using Leonard's higher-order differencing scheme required 10 to 15 times the computational time required for the prediction made using upwind differencing. The results for the non-reacting flow system indicated that numerical diffusion does not seriously affect PCGC-2 predictions, and that the hybrid differencing prediction is sufficiently accurate for this particular flow system. However, it is important to note that this observation was made for only a single computation, and was not achieved in a reacting or particle-laden system.

The negligible effect of numerical diffusion is somewhat surprising, since the streamlines in the recirculation zone of the reactor were definitely skew to the grid. Roache (1976) states that if the grid size is small enough, the effects of numerical diffusion will not be significant. He also says that a free outflow boundary condition (such as that used in PCGC-2) tends to reduce upstream error in elliptical systems.

In light of these results, the effects of numerical diffusion in PCGC-2 predictions for this particular geometry (namely the BYU Combustor) are thought to be of secondary importance. The higher-order differencing algorithm of Leonard (1979) was not used in PCGC-2 for any other predictions. Other higher-order differencing methods should not be used unless they are first demonstrated for reacting flows.

C. BOUNDARY CONDITIONS

A discussion of the numerical approach used in PCGC-2 is not complete without a discussion of the boundary conditions for all of the equations used. Each variable must have a boundary condition specified at each of the boundaries for elliptic equations. Symmetry conditions are imposed along the centerline, while other types of boundary conditions must be specified at the reactor walls, inlets, and exits.

1. Inlet Streams

The inlet mass flow rate is used to set the inlet velocities, with assumed parallel injection ($v_{pri} = v_{sec} = 0$). This gives a Dirichlet condition for u and v . Turbulence intensities must be specified for the inlet streams in order to get Dirichlet boundary conditions for k . Turbulence intensities are defined as follows:

$$I = \left[\overline{(u')^2} + \overline{(v')^2} \right]^{1/2} / [\overline{u^2} + \overline{v^2}]^{1/2} = [2k]^{1/2} / \|\vec{v}\| \quad (397)$$

where $\|\vec{v}\|$ is the magnitude of vector $\vec{v}$. Since $\bar{u}$ and $\bar{v}$ are known in the inlet streams, k is specified when I is set. The dissipation level (ϵ) must be estimated at the inlet from empirical correlations (Syed and Sturgess, 1980):

$$\epsilon = C_{\mu} k^{1.5} / (.03 D_e) \quad (398)$$

where D_e is the effective inlet diameter. The mixture fraction is known by definition in each of the inlet streams, and the mixture fraction fluctuations (g_f) are assumed zero in the inlet streams. The coal is not allowed to react in the inlet streams, so that η and g_{η} are both zero at the inlet boundary.

PCGC-2 is coded to allow user-specified inlet profiles of u, v, w, f, k , and ϵ in both the primary and/or secondary streams. Theoretical or experimental velocity profiles can be used. Theoretical inlet velocity profiles are calculated according to Bird, et al. (1960). The inlet velocity profile is normalized to match continuity with the specified inlet mass flowrate.

2. Centerline

Symmetry conditions are imposed at the centerline on all variables meaning that the radial component of the gradient of any variable is zero ($\frac{\partial \phi}{\partial r} = 0$) at the centerline. This specifies a Neumann condition at the axis or symmetry for all variables. The only exception to this rule is the radial radiation flux (F_r). The quantity (rF_r) is assumed zero along the centerline.

3. Outlet Stream

The radial component of the velocity ($\tilde{v}$) is set to zero at the reactor exit, while the axial component (u) is adjusted to satisfy over-all continuity with the inlet gas mass flow rates. The outlet values of f and η are set to force continuity with the inlet particle mass droplet flow rate. It is assumed that all of the other variables have smooth axial profiles at each radial location near the reactor exit. The outlet condition for these variables is extrapolated from the computational cells just upstream of the reactor exit.

4. Walls

The wall boundary conditions are of special interest. Of course, it would be possible to use parabolic boundary layer equations and solve them all the way to the wall; however to reduce computer storage and run times, it is convenient to bridge over the wall region. The Van Driest hypothesis on turbulent flow near a wall is used to derive wall functions which are consistent with the logarithmic law of the wall. Launder and Spalding (1972) outline the derivation and Patankar and Spalding (1970) give more details. In this way the dependent variables at the wall are linked to those in the logarithmic region (also see Khalil et al., 1975). For the velocity component normal to the wall in question, a Neumann condition is used and the gradient is set equal to zero (i.e., $\partial v / \partial r = 0$ for the north wall). For the component

of velocity parallel to the wall in question, a no-slip boundary condition is assumed. A Dirichlet condition is imposed and the velocity component is set equal to zero (i.e., $u = 0$ for the north wall; however, in this near-wall region, the fully developed turbulent exchange coefficient is not valid, and an exchange coefficient (effective turbulent viscosity) is calculated from the logarithmic law of the wall as given below and derived by Launder and Spalding (1972) (for a north wall, u velocity):

$$\Gamma_u = \mu_e = \tau_w \Delta r / \Delta u = \tau_w \Delta r / u_p = \frac{\rho C_\mu^{1/4} k^{1/2} \kappa \Delta r}{\ln[EC_\mu^{1/4} k^{1/2} \Delta r \rho / \mu]} \quad (399)$$

When the reactor is non-adiabatic and convective/conductive heat losses must be considered, a Neumann condition is specified for the enthalpy (h). The normal derivative is calculated from a universal temperature profile in the logarithmic region for the near-wall turbulence (for the north wall)

$$\Gamma \frac{\partial h}{\partial r} = -(\Gamma \partial h / \partial r)_w - (C_p \Gamma \partial T / \partial r)_w = q_w \quad (400)$$

$$q_w = (T_p - T_w)(\rho C_\mu^{1/4} k^{1/2}) [/\sigma_{h,t} \{ P + \frac{1}{\kappa} \ln[EC_\mu^{1/4} k^{1/2} \rho / \mu] \}] [C_{pmix}] \quad (401)$$

where P is the extra resistance to heat transfer that arises due to the difference in σ_h and $\sigma_{h,t}$. Jayatilleke (1969) gives the following correlation for P

$$P = 9.24 [(\sigma_h / \sigma_{h,t})^{3/4} - 1] \quad (402)$$

where $\sigma_{h,t} = 0.9$. Equation 402 was found to cause numerical instability in PCGC-2, apparently due to some nodes being too close to the wall. Rather than sacrifice the accuracy of the bulk flow solution by moving all nodes farther away from the wall, a constant value of unity is used for P . No instability is caused when P is non-negative. For $\sigma_h = 0.8$, the available data (Jayatilleke, 1969) are extremely scattered, and P ranges from -8 to +23. The value predicted by Equation 402 is -0.78, however the correlation is thought to be inaccurate at the low value of σ_h due to the scatter in the data. Therefore, a constant value of unity is reasonable. The quantity $(\Gamma \partial h / \partial r)_w$ is the total turbulent flux of enthalpy to or from the wall and is the quantity needed by the numerical scheme for the Neumann condition.

At the walls, the normal derivative of the turbulent energy is zero:

$$\frac{\partial k}{\partial x_i} = 0 \quad (403)$$

However, the production of turbulent kinetic energy (P) and the dissipation (ϵ) near the walls require modification. Near a wall in axi-symmetric, polar-cylindrical coordinates,

$$P_W = - \overline{u'_x u'_x} \frac{\partial \bar{u}_x}{\partial x} - \overline{u'_r u'_r} \frac{\partial (r \bar{u}_r)}{\partial r} + \frac{\tau_w}{\rho} \left(\frac{\partial \bar{u}_x}{\partial r} + \frac{\partial \bar{u}_r}{\partial x} \right) \quad (404)$$

When the wall is parallel to the u_x direction, $\partial \bar{u}_r / \partial x = 0$. For a wall perpendicular to u_x , $\partial \bar{u}_x / \partial x = 0$. An extension of Eq. 404 to include axisymmetric, swirling flows is discussed by Lilley and Rhode (1982).

The wall shear stress (τ_w) can be estimated from turbulent Couette flow near a wall. The modified log-law is used:

$$u^+ = \frac{1}{\kappa} \ln(Ey^+) \quad (405)$$

where

$$y^+ = y \rho (C_\mu^{1/2} k)^{1/2} / \mu \quad (406)$$

and

$$u^+ = \bar{u} / \sqrt{\tau_w / \rho} \quad (407)$$

Thus, the wall shear stress can be calculated directly:

$$\tau_w = \bar{u} \kappa (C_\mu^{1/2} k)^{1/2} \rho / \ln[E \Delta r (C_\mu^{1/2} k)^{1/2} \rho / \mu] \quad (408)$$

Equation 408 is substituted into Eq. 393 for the production of turbulent energy near a wall (P_w).

The dissipation rate at solid boundaries is harder to evaluate. In this case, it is suggested that the last node point in the flow field near a wall be set according to the following mixing length approximation.

$$\ell_m = \kappa \Delta y_i \quad (409)$$

where κ is a mixing length constant ($= 0.42$) and Δy_i is the distance from the wall:

$$\epsilon = \frac{C_\mu^{3/4} k^{3/2}}{\kappa \Delta y_i} \quad (410)$$

The dissipation in the k-equation can also be altered accordingly. The wall boundary conditions on $\bar{\epsilon}$, $\bar{\eta}$, and $\bar{\theta}$ are simply Neumann conditions of zero normal derivative ($\partial \phi / \partial r = 0$, or $\partial \phi / \partial x = 0$).

5. Summary

15. A summary of the boundary conditions for each variable is found in Table

D. GENERALIZED GEOMETRY

The principal purpose of this section is to describe the treatment of axi-symmetric combustors with non-uniform cross-sections. Modern pulverized combustors and gasifiers and CWM combustors cannot always be represented in two-dimensions using a cylindrical reactor vessel. Some reactors incorporate radiation baffles, "wasp waists", exit constrictions, and other extensions of the wall into the flow field. When modeling reactors, the boundary conditions must be modified to account for these flow field "intrusions." PCGC-2 allows for generalized wall boundary conditions. Figure 18 shows sample reactor configurations that are possible with the code.

1. Approach

Eulerian gas phase equations are steady-state, yielding an elliptic system of partial differential equations. Such systems require boundary conditions at every boundary surrounding the flow domain. In a two-dimensional, axi-symmetric framework, boundary conditions are set at the inlets, along the centerline, along the exit, and along the walls. Cell faces are labeled like the directions of a compass (north, south, east, west) for ease of description. The flow chambers are generally modeled with inlets in the west wall, the centerline along the south boundary, and the exit along the east boundary, as if the reactor were horizontal.

Gas phase equations are transformed into algebraic form using power-law finite differencing (Patankar, 1980). A staggered grid is used in the finite difference approach, with velocities stored at cell faces and other variables (e.g. density, mixture fraction) stored at cell centers. Figure 8 showed a sample grid used for PCGC-2 calculations.

Table 15 shows typical boundary conditions used in PCGC-2 for the main gas field variables. In this formulation, any deviation from the cylinder wall is termed an "intrusion" into the flow field. All intrusions must be symmetrical around the centerline of the reactor. For example, a triangular exit constriction is modeled as a cone when rotated around the centerline.

Intrusions are allowed in any part of the computational domain, and need not be connected to the outer wall in this formulation. The only restriction to this geometric formulation is that each grid cell is rectangular (in two dimensions), and not triangular. This means that any smooth intrusions must be modeled in a saw-tooth manner, as shown in Figure 19. In the limit, if grid spacing is small, smooth intrusions can be accurately modeled. However, computational time and memory requirements generally limit the fineness of the grid.

TABLE 15
PCGC-2 BOUNDARY CONDITIONS

	$\tilde{u}$	$\tilde{v}$	$\tilde{w}$	$\tilde{k}$	$\tilde{\epsilon}$	g_f, g_n	$\tilde{h}$	$\tilde{f}$	$\tilde{n}$
Primary jet	uniform at u_p , or profile	0, or profile	0, or profile	from primary turbulence intensity	from empirical correlations	0	uniform at h_p	specified in input data	0
Secondary jet	uniform at u_s , or profile	uniform at v_s , or profile	0, or profile	from secondary turbulence intensity	from empirical correlations	0	uniform at h_s	specified in input data	0
Symmetry axis	$\tilde{u}_{i,1} = \tilde{u}_{i,2}$	0	0, or $\tilde{w}_{i,1} = \tilde{w}_{i,2}$	$k_{i,1} = k_{i,2}$	$\epsilon_{i,1} = \epsilon_{i,2}$	$g_{i,1} = g_{i,2}$	$\tilde{h}_{i,1} = \tilde{h}_{i,2}$	$\tilde{f}_{i,1} = \tilde{f}_{i,2}$	$\tilde{n}_{i,j} = \tilde{n}_{i,2}$
North wall	τ_w from wall function	0	τ_w from wall function	Near the wall values from wall	Near the wall values from length	$g_{i,j} = g_{i,j-1}$	q_w from wall function	$\tilde{f}_{i,j} = \tilde{f}_{i,j-1}$	$\tilde{n}_{i,j} = \tilde{n}_{i,j-1}$
South wall	τ_w from wall function	0	τ_w from wall function	Near the wall values from wall function	Near the wall values from length scale	$g_{i,j} = g_{i,j+1}$	q_w from wall function	$\tilde{f}_{i,j} = \tilde{f}_{i,j+1}$	$\tilde{n}_{i,j} = \tilde{n}_{i,j+1}$
West wall	0	τ_w from wall function	τ_w from wall function	function	scale	$g_{i,j} = g_{i+1,j}$	q_w from wall function	$\tilde{f}_{i,j} = \tilde{f}_{i+1,j}$	$\tilde{n}_{i,j} = \tilde{n}_{i+1,j}$
East wall	0	τ_w from wall function	τ_w from wall function	Near the wall values from wall function	Near the wall values from length scale	$g_{i,j} = g_{i-1,j}$	q_w from wall function	$\tilde{f}_{i,j} = \tilde{f}_{i-1,j}$	$\tilde{n}_{i,j} = \tilde{n}_{i-1,j}$
Outlet	$\tilde{u}_{i,j} = \tilde{u}_{i-1,j}$	0	$\tilde{w}_{ij} = \tilde{w}_{i-1,j}$	quadratic extrapolation	quadratic extrapolation	quadratic extrapolation	quadratic extrapolation	quadratic extrapolation	quadratic extrapolation

NOTE: Saying $\phi_{i,1} = \phi_{i,2}$, etc., is the differencing scheme for $(\partial\phi/\partial n) = 0$.

Figure 18. Sample reactor configurations possible with modified PCGC-2.
 (■ are intrusions)

Figure 19. Example of saw-tooth representation of reactor wall.

Figure 20. Arbitrary grid cell showing location of X, R, I and J.

2. Numerical Method

An arbitrary grid cell is pictured in Figure 20 along with the eight adjacent cells. The center cell has location $X(I)$ and $R(J)$, and the surrounding cells are therefore described in terms of $I+1$, $I-1$, $J+1$, and $J-1$. The array $INTR(I,J)$ is defined to be 1 if the cell is an intrusion (wall) and 0 if the cell is part of the flow field. The value of $INTR(I,J)$ is checked at each cell in the computational domain to see where the intrusions are located. When an intrusion is located, the boundary conditions of the surrounding cells are adjusted accordingly.

Suppose that cell (I,J) is an intrusion and that we are solving the mixture fraction (f) equation. The value of $F(I,J)$ is set to zero as follows:

$$SU(I,J) = 0 \quad (411)$$

$$SP(I,J) = -1.0 \times 10^{30} \quad (412)$$

Table 15 indicates that boundary conditions are satisfied for the f equation by setting the gradient at the wall to zero. For the f equation, this is done by setting the appropriate "A" coefficient (i.e. AE , AW , AN , or AS) to zero in the neighboring cell. For example, the north neighbor cell $(I,J+1)$ to an intrusion at (I,J) must have the south boundary modified so that

$$AS(I,J+1) = 0 \quad (413)$$

Similarly, the other neighbor cells to an intrusion are modified as follows:

$$AN(I,J-1) = 0 \quad (414)$$

$$AE(I+1,J) = 0 \quad (415)$$

$$AW(I-1,J) = 0 \quad (416)$$

If a neighboring cell is also an intrusion, the boundary between the cells is not modified at all, since Eqns. 411 and 412 negate the effect of the A coefficients.

Intrusions are used to describe the reactor walls as well as intrusions into the main flow field. When modifying the boundary conditions around the cells at the outer wall, care is taken not to exceed the dimensions of the arrays. For example at the north wall (I,NJ) , the north neighbor cell is not used and hence is not modified.

All P-cell variables ($w, k, \epsilon, g_f, g_n, h, f, n, p, pp$) are adjusted for intrusions as described above using the boundary conditions from Table 15 and the north, south, east and west neighboring cells. However, since a staggered grid is used, u and v are defined on the faces of the P-cells. Intrusions are also

defined on the P-cells, which complicates the boundary conditions for u and v (U-cells and V-cells).

Figure 21 shows an intrusion with the u velocity locations at the neighboring cells. Both $U(I,J)$ and $U(I+1,J)$ are zero because they are located on the edge of the intrusion. The S_u and S_p terms are modified as shown in Eqns. 411 and 412 for these two cells. The east and west neighbor cell boundary conditions for the u velocity are set as follows:

$$AE(I-1,J) = 0 \quad (417)$$

$$AW(I+2,J) = 0 \quad (418)$$

For a single cell intrusion, u velocity boundary conditions must also be applied to the northeast, northwest, southeast, and southwest neighboring u cells. These boundaries are located at the corners of the intrusion, and hence have characteristics of both boundary cells and free flow field cells. Khalil et al. (1975) suggest some type of averaging for the corner cells so that "inclined" walls can be modeled. The approach here is to treat the corner cells as if they were bounded by the wall along the entire cell boundary. The northeast $(I+1,J+1)$ and northwest $(I,J+1)$ U-cells therefore have south wall boundary conditions (see Table 15), and the southeast $(I+1,J-1)$ and southwest $(I,J-1)$ U-cells have north wall boundary conditions. In the course of development, these corner cells were also treated as free-flow field cells, but results did not merit the use of this approach.

Figure 22 shows an arbitrary V-cell with the location of the six neighboring V-cells. The v at the north and south edges of the intrusions are set to zero for (I,J) and $(I,J+1)$. The north and south neighbor cell boundary conditions simply become:

$$AN(I,J-1) = 0 \quad (419)$$

$$AS(I,J+2) = 0 \quad (420)$$

The northeast $(I+1,J+1)$ and southeast $(I+1,J)$ V-cells have west wall boundary conditions based on the logarithmic wall function (see Table 15) and the northwest $(I-1,J+1)$ and southwest $(I-1,J)$ V-cells have east wall boundary conditions.

3. Input and Output for Intrusions

The location of the intrusions in the flow field are read from the grid data file (also used to read in the locations of grid points). A sample grid data file is shown in Appendix G. A two-dimensional array of X's and O's is found at the bottom of the grid data file; the X's represent intrusions and walls and the O's represent the free flow field. This two-dimensional array is also used to govern the location of the additional inlets, as described in the next section. Each location in this two-dimensional array represents a

Figure 21. Arbitrary U-cell showing locations of cells affected by intrusion at (I,J) .

Figure 22. Arbitrary V-cell showing locations of cells affected by intrusion at (I,J) .

single computational cell, and the x-y coordinates of the cells are given at the top of the grid file.

There are two logical parameters that govern the use of the intrusions in the flow field: INRDGD and INTRUS. Table 16 shows how these two variables affect the code operation. When starting from scratch (without a restart), setting both variables to .FALSE. will allow the code to generate a new grid data file which can then be modified to allow for intrusions. The modified grid data file will then be used with both variables .TRUE. in order to read the data file and look for intrusions.

E. ADDITIONAL INLETS

The principal purpose of this section is to describe the formulation which permits multiple feed streams at arbitrary locations along the combustor boundaries. One primary stream with droplet/particles and/or gas located symmetrically about the centerline, one secondary stream, and up to three additional gaseous feed streams in either the north or west walls of the reactor vessel are allowed. Figure 23 shows sample feed stream configurations possible with the code. Since this is a 2-D, axi-symmetric formulation, all geometries must be rotated around the centerline. A north wall inlet, therefore, is really modeled as a slit all the way around the outer reactor wall.

1. Approach

Table 15 showed boundary conditions used for the primary and secondary streams. Additional inlets along the west wall have similar boundary conditions, except for the inlet gas mixture fraction f . As discussed previously in the approach to gas phase chemistry, only two mixing variables are solved. This allows definition of three independent sources of mass to the gas phase. Inlet compositions and temperatures for all inlet streams must be a function of the two mixing variables. Since one mixing variable n is generally used to account for coal off-gas, the inlets are usually specified with the remaining mixing variable f . For example, some inlets may contain high temperature air while others contain low-temperature air. The three sources of mass would then be 1) coal off-gas, 2) high-temperature air, and 3) low temperature air. The mixture fraction would be the flow ratio of high-temperature air to total inlet air, and the f value for each inlet stream would determine the mixture of air entering the reactor from that stream. For CWM computations all inlets are regarded as having the same composition and energy level and $\bar{f}$ is the mass addition of water into the gas phase from the droplets.

The staggered grid used in PCGC-2 makes the determination of inlet velocities different from P-cell variables. For west wall inlets, grid node $I=1$ is a false boundary used to establish velocities. Figure 24 shows a west wall inlet with 3 different guides in the axial direction. The velocity $U(1,J)$ is specified by knowing the inlet mass flow rate, density, and cross sectional area (in FORTRAN variables):

TABLE 16
USE OF FORTRAN LOGICAL INPUT VARIABLES
INRDGD AND INTRUS

<u>INRDGD</u>	<u>INTRUS</u>	<u>Reads New X's & Y's</u>	<u>Reads New Intrusions</u>	<u>Allows (INQRL = T)</u>	<u>Writes Out New Grid File (GRDOUT = T)</u>
T	T	yes	yes	yes	yes
T	F	yes	no	yes	yes
*F	*T	no	no	yes	yes
F	F	no	no	yes	yes

*Use of these variables not recommended with these values.

Figure 23. Example feed stream configurations.

Figure 24. Axial grid locations for west wall inlets.

Figure 25. Radial grid locations for north wall inlets.

$$U(1,J) = \dot{m}_{\text{cell}} / \text{RHO}(1,J) / A_{\text{cell}} \quad (421)$$

The velocity at $U(2,J)$ is different than $U(1,J)$ due to a change in density, but continuity yields the following equation:

$$U(1,J) * \text{RHO}(1,J) = U(2,J) * [\text{RHO}(1,J) + \text{RHO}(2,J)] / 2.0 \quad (422)$$

or

$$U(2,J) = U(1,J) * \frac{\text{RHO}(1,J) * 2.0}{\text{RHO}(1,J) + \text{RHO}(2,J)} \quad (423)$$

The value of $U(2,J)$ changes at every gas phase iteration because $\text{RHO}(2,J)$ changes.

Figure 25 shows a north wall inlet with 3 different grids in the radial direction. However, the maximum dimension on the V array is NJ , so the location of $V(I,NJ+1)$ is undefined. The array, $\text{VINLT}(I)$, stores the velocities in the false boundary above the north wall. The inlet velocity at the inlet plane is then:

$$V(I,NJ) = \text{VINLT}(I) * \frac{\text{RHO}(I,NJ) * 2.0}{\text{RHO}(I,NJ) + \text{RHO}(I,NJ-1)} \quad (424)$$

Provisions are made to allow for non-parallel injection in the additional inlets, but detailed velocity profiles in each additional inlet were not incorporated. The only detailed velocity profiles allowed are in the primary and secondary streams.

All inlets must be in the outer reactor shell with paths to the main flow field. Inlets are calculated only in the false boundary along the west and north walls. No inlets are permitted in the east wall (the east reactor wall is considered an exit).

2. Input and Output for Additional Inlets

A mixture fraction for each inlet stream, including primary and secondary streams is read from the main input data file. The f value in the primary and secondary streams need not be 1.0 and 0.0. Flow rates and turbulence intensities for each inlet stream are also read from the main data file.

The locations of the primary and secondary streams are read from the main data file, but the additional inlet stream locations are specified by the grid data file. P represents a cell in the primary stream, the S represents a cell in the secondary stream, and the numbers 1,2, or 3 represent the first, second, or third additional inlets. Primary and secondary stream locations can be changed using either the main data file or the grid data file.

F. GAS PHASE PROPERTIES

In Chapter II, the theory was introduced for finding the mean turbulent properties such as species mole fraction, density, etc. The approach requires instantaneous values of the energy level (h) and the weight fraction of the elements (b_k) to be calculated from the instantaneous values of the mixture fraction and (in the case of non-adiabatic reactors) residual enthalpy. From this input, the Gibbs free energy is minimized to give the instantaneous local equilibrium properties. These properties are then convoluted over the complete probability density function with proper account for intermittency to produce the mean properties. This can be done for either Reynolds-averaging or Favre-averaging.

The largest computational portion of this algorithm is the equilibrium computations. Pratt and Wormeck (1976) have developed a code (CREK, Combustion Reaction Equilibrium and Kinetics) for either complex kinetic or equilibrium computations. This code was developed as a module for incorporation into larger fluid mechanics schemes. The approach for equilibrium computations is the same as was described in Chapter 2 of Pratt and Wormeck (1976). CREK was used as a base but was stripped of all statements pertaining to the kinetic computations. The input was also restructured to receive local element mass fractions (b_k) as required by the above approach. The resulting submodel was named CREE (Chemical Reaction Equilibrium for Elements). The FORTRAN comment statements are profuse and with reference to Pratt and Wormeck (1976), the user explanation should be more than sufficient.

Computational efficiency is enhanced significantly by constructing table search procedures for the equilibrium properties. When the equilibrium properties are functions of only two independent variables (f and n), a table is constructed listing each property as a function of f and n . The inlet and coal gas mixture fractions are physically restricted to lie between the values of 0 and 1. A table is constructed once at the beginning of the code calculations using CREE. All subsequent calls for equilibrium properties are performed by interpolation within the table. The subroutine TABLE in PCGC-2 does all the table construction and retrieval. This subroutine uses knowledge of the stoichiometric mixture fraction for each n even though intervals of f may be different.

Chapter II showed how the PDF approach is altered when the system is non-adiabatic. In this case, the equilibrium properties are a function of three variables: the mixture fraction (f), the coal gas mixture fraction (n), and the residual enthalpy (h_r). The table look-up approach is still used; however, the table is three- rather than two-dimensional. Since the three-dimensional table is quite large, it is saved from one calculation to the next.

Two types of PDF's have been used in PCGC-2; a Gaussian distribution and a top-hat or uniform distribution. The Gaussian distribution produces slightly smoother gas property profiles, but the uniform distribution requires slightly less time to obtain a converged gas-phase solution. The present version of PCGC-2 uses only the Gaussian distribution.

The convolution of gas properties with a PDF requires numerical integration (see Eq. 69). This integration is time-consuming because the particle

properties have to be either repeatedly calculated or interpolated from a table of values (Smith, 1979). The integration must be performed with a minimum of function evaluations. The method used to perform these integrations is five-point Gaussian quadrature (Abramowitz and Stegun, 1972). This method combines reasonable accuracy with a minimum number of function evaluations.

Intermittency for the Gaussian PDF is calculated as shown in Table 4. It is easily seen that the general equation for α in Table 4 is that for the area under the normal curve, which is tabulated in standard math handbooks. Tabulated values of the area under the normal curve were fitted using a cubic spline routine.

G. RADIATION

Equation 123 is solved in each direction, forming a set of N differential equations (coupled pde's in DOM, uncoupled ode's in VFM). Due to the different forms of the working equations, the solution techniques used in the DOM and VFM are also quite different.

1. Discrete Ordinates Method (DOM)

The calculation is started at the top right-hand corner of the computational domain using the boundary conditions (Eq. 125). The boundary condition on the axis is based on the conservation of flux (i.e., a reflective boundary). An initial estimate of the aximuthal component of intensity, before starting with the recursive solution scheme, is obtained by solving Eq. 123 in the special direction where $\eta_m = 0.0$. The solution thus obtained is assigned a zero weight. The directions of traverse are chosen so that the values of the direction cosines gradually increase, a change in the sign of the direction cosine signifying a reversal in the corresponding direction of integration.

The solution to the discrete ordinates equations must be obtained iteratively, as the calculated intensities enter the boundary conditions and the in-scattering term (Eq. 123). Once the intensity at a cell-center is known (from Eq. 136), the intensity at the downstream surface of the volume element can be obtained by extrapolation using Eq. 135. However, the central differencing scheme used in Eq. 135 often results in negative intensities (particularly in the presence of steep gradients, or where spatial resolution is not high enough). Such negative intensities are impossible on physical grounds, and may be avoided using a combination of central and upwind differencing (Truelove, 1978):

$$I_{i+1} = (1 + f) I_m - f I_i, \text{ etc. ;} \quad \begin{array}{l} 0 < f < 1.0 \\ \mu_m, \xi_m > 0 \end{array} \quad (425)$$

where $f = 1.0$ yields central differencing, and $f = 0.0$ yields pure upwind differencing. If negative intensities are encountered during calculations, f is gradually decreased from its initial value of 1.0 till the negativity is

removed. For $f = 0.0$, the intensity is always non-negative, and special directions are not required to initiate the recursive solution.

In the case of a scattering medium, an approximate solution is first obtained without the in- and out-scattering terms. The scattering terms are then included as a perturbation to the approximate solution to obtain the final, converged solution for the absorbing-emitting-scattering case.

2. Varma Flux Method

The two ordinary differential equations (Eqs. 140 and 141) are cast into finite difference form as shown in Table 17. The 'C' coefficients are defined in Table 12. These equations are solved using a line-by-line technique as in the gas phase. The tri-diagonal matrix algorithm (TDMA) gives an exact solution on each line. The radiation calculations generally converge quickly, and do not take much computational time relative to the gas-phase calculations. Axial symmetry is used for the centerline boundary condition, and the wall boundary conditions (see Eq. 122) are treated in the same way as those for the gas-phase calculations.

H. INTEGRATION OF PARTICLE EQUATIONS

1. Approach

The particle source-in-cell (PSI-CELL) technique of Crowe and coworkers (1977) has been followed directly to account for the Lagrangian particle field in the Eulerian gas field. The procedure is outlined below:

1. The Eulerian gas field is solved without particles as described earlier.
2. The radiation field is solved using the flux method, as described earlier.
3. The Lagrangian particle field is solved with a representative number of trajectories and the particle source term field is calculated.
4. The gas field is solved with the updated particle source term field.
5. Step 2 is repeated and iteration continued until over-all convergence is achieved.

The PSI-CELL technique is very efficient with respect to storage and computational time required. The only significant storage requirement is for the particle source term field. Steps 2 through 4 represent one "particle iteration" (Steps 7 through 11 in Figure 7). Convergence is achieved when the gas field does not change between particle iterations.

The Lagrangian particle equation of motion (Eq. 15) is integrated once analytically to save computational time. The x-component of the equation can be written as

TABLE 17
FINITE DIFFERENCE FOR THE RADIATION FLUX SUMS

ϕ	Equation
F_x	$A_p^x \phi_p = A_E \phi_E + A_W \phi_W + S_U^x$
F_r	$A_p^r \phi_p = A_N \phi_N + A_S \phi_S + S_U^r$
	$A_p^x = A_E + A_W - S_p^x$
	$A_p^r = A_N + A_S - S_p^r$
	$A_E = 1/2(r_p + r_E)/(\delta x_{pE})$
	$A_W = 1/2(r_W + r_p)/(\delta x_{pW})$
	$A_N = 1/2(r_p + r_N)/(\delta r_{pN})$
	$A_S = 1/2(r_S + r_p)/(\delta r_{pS})$
	$S_U^x = 2(C_3 F_r + C_4 I_b)(SEW)$
	$S_U^r = 2r(C_3 F_x + C_4 I_b)(SNS)$
	$S_p^x = (C_2 + C_1)(SEW)$
	$S_p^r = (C_2 + C_1)(SNS)$

$$\frac{du_j}{dt} = \frac{r_d (u_g - u_j)}{\alpha_j} + g \quad (426)$$

where the gravitational force term assumes the reactor is vertical and down-fired. Substituting Eq. 17 for T_d and rearranging, Eq. 426 becomes

$$\frac{du_j}{dt} = \frac{C_d Re}{24 t_j} (u_g - u_j) + g \quad (427)$$

where C_d is given by Eqs. 18-20, Re is given by

$$Re = \frac{\rho_g \parallel \vec{v}_j - \vec{v}_g \parallel d_j}{\mu_g} \quad (428)$$

and t_p is given by Eq. 26. Taking u_g and $C_d Re/t_j$ constant, Eq. 427 may be integrated to obtain

$$\ln \left[\frac{A(u_g - u_j^{new}) + g}{A(u_g - u_j^{old}) + g} \right] = -A(\Delta t) \quad (429)$$

where $A = C_d Re/24t_j$. Equation 429 may be solved for u_j^{new} to obtain

$$u_j^{new} = u_g - (u_g - u_j^{old})e^{-A(\Delta t)} + \frac{g}{A} (1 - e^{-A(\Delta t)}) \quad (430)$$

A similar treatment of the r-component of Eq. 15 leads to

$$v_j^{new} = v_g - (v_g - v_j^{old})e^{-A(\Delta t)} \quad (431)$$

where the gravitational force term is missing because of the assumed orientation of the reactor. Equations 430 and 431 are integrated by the simple Euler method to obtain particle position as a function of time.

The simple Euler's method was found satisfactory for calculating the particle trajectory, but unsatisfactory for integrating the particle continuity (Eqs. 73-77) and energy (Eq. 80) equation; hence, the modified Euler's method is used to integrate the latter. The step-size for the integration scheme must be small enough so that the particle does not cross more than one cell boundary between function evaluations. Step sizes must be small in regions of rapid coal reaction in order to achieve numerical accuracy, but large enough in all regions to be numerically efficient. PCGC-2 uses a self-adjusting step-size control based on the difference between the predictor and corrector of the modified Euler's method.

The diffusive component of particle velocity is determined from Eq. 30:

$$\vec{v}_{jd} = - r_j \frac{\vec{v} \cdot \bar{n}_j}{\bar{n}_j} \quad (432)$$

In practice, $\vec{v} \cdot \bar{n}_j$ is difficult to calculate on the computer, because $\bar{n}_j$ is a large number. The calculation becomes inaccurate because of computer roundoff and taking the difference of two large numbers. To overcome this computer limitation, $\vec{v} \cdot \bar{n}_j$ is calculated as follows:

$$\vec{v} \cdot \bar{n}_j = \bar{n}_j \vec{v} \cdot (\ln \bar{n}_j) \quad (433)$$

Equation 432 then becomes

$$\vec{v}_{jd} = - r_j \vec{v} \cdot (\ln \bar{n}_j) \quad (434)$$

When a particle collides with the wall, the particle is allowed to 1) stick to the wall (in which case the particle trajectory calculation stops), or 2) bounce off the wall. Figure 26 shows particles that collide with the wall in a non-rebounding manner. This particle-wall collision behavior can easily be modified to rebounding collisions, if desired, by changing options in subroutine PSICT.

Figure 27 shows PCGC-2 predictions of particle recirculation. The particles are arbitrarily allowed to exit from the recirculation zone by setting the diffusion velocity to zero after three loops, if such a situation occurs. The particle then follows the mean flow of the gas in the recirculation zone near the wall. The recirculating particle finally travels along the west wall until it is entrained by the mean flow of the secondary stream and is carried to the reactor exit. Figure 28 shows that there is no particle dispersion when the diffusion velocity ($\vec{v}_{pd}$) is not accounted for. In other words, according to these predictions, particles are dispersed principally by the turbulent fluctuations of the gas.

2. Stiffness

Problems with stability occur in the integration of the energy equation when the integrand changes slowly. In such areas, oscillations in the energy level occur that generally increase in amplitude until solution is no longer feasible (these are called numerically "stiff" equations). When the integrand begins to change slowly, a numerical approximation is made in which the left-hand side and 3rd term on the right-hand side of Eq. 80 are set to zero and the particle properties are solved with an algebraic equation for the temperature:

$$T_{pj} = T_g + Q_{rp} / (Nu_j \pi k_g d_j) \quad (435)$$

Figure 26. Predicted particle trajectory map showing non-rebounding wall collisions.

Figure 27. Predicted particle trajectory map showing recirculation of particles.

Figure 28. Predicted particle trajectory map showing case where $\vec{v}_{pd}$ was artificially set to 0.

This equation can also be viewed from a physical standpoint. In downstream regions of the reactor, temperature gradients are small and radiation is the main cause of differences between gas and particle temperatures.

The particle energy stiffness assumption was validated by comparison with a prediction using very small step sizes. This stiffness assumption greatly decreases computational time for each trajectory without significant loss of accuracy. Care is taken to de-dimensionalize the criteria for employing the stiffness assumption in PCGC-2, in order to simplify manipulation by the user. Smith (1979) found that the errors introduced in 1-DICOG from the stiffness assumption are negligible, and that significant computational time is saved because larger integration steps can then be taken. The same conclusions are found true of the particle energy equation in PCGC-2 (Fletcher, 1980).

3. Particle Temperature

The particle temperature depends on its composition and enthalpy. All of the components of the particle, i.e. composition and enthalpy, are predicted as independent quantities. At each time step, these properties are used to solve for particle temperature. Because there are several options in the code for expressing the particle heat capacity and its dependence on temperature, an efficient and robust algorithm is used which is based on a combination of bisection and regula-falsi techniques. This algorithm assumes the particle temperature is bounded by 275 K and 1.4 times the gas temperature.

4. Particle Reactions

Calculation of the particle reaction rates and heat fluxes is iterative. Oxidizer-char reaction rates (Eq. 114) depend on the char mass transfer coefficient (Eq. 117) which, in turn, depends on the transpiration parameter for mass transfer (Eq. 116) and the reaction rate. The transpiration parameter and mass transfer coefficient are calculated using assumed reaction rates, and the reactions are then iterated on until converged. Under-relaxation is used to make the calculation more stable.

I. PARTICLE-GAS COUPLING

1. Particle Source Terms

The Eulerian gas phase equations are coupled to the Lagrangian particle phase equations through particle source terms ($S_p^m, S_p^u, S_p^v, S_p^h$). The particle field is modeled as a set of discrete trajectories, where each trajectory represents a number of particles of uniform particle size and starting location in the primary jet. It is assumed that the particle number flowrate (n_{ij}) along a trajectory is constant, so that n_{ij} may be calculated from the initial mass flow rate of particles ($\dot{m}_{p0}$), the appropriate initial mass fractions representing particle size and location, and the initial particle mass (α_{ji0}). The particle number flow rate of the i^{th} particle size and the j^{th} starting location is calculated from the input conditions as follows:

$$\dot{n}_{ij} = \dot{m}_{jo} X_{io} Y_{jo} / \alpha_{jio} \quad (436)$$

where X_{io} is the mass fraction of particles of the i th particle size and Y_{jo} is the mass fraction of the j th starting location.

The particle mass source (S_{pm}) to the gas phase is the change in mass of all particles that traverse the particular cell of interest. For the k^{th} cell, this change is represented by:

$$(\Delta \dot{m}_{pij})_{kcell} = \dot{n}_{ij} [(\alpha_{pij})_{out} - (\alpha_{pij})_{in}]_{kcell} \quad (437)$$

The mass source term is taken to be negative when the particle loses mass in order to fit the gas-phase sign convention. The mass source term is calculated from:

$$(S_p^m)_{kcell} = [(\sum_i \sum_j \Delta \dot{m}_{pij})/V]_{kcell} \quad (438)$$

The particle momentum source term (S_p^u) for the u component of momentum is similarly derived:

$$(S_p^u)_{kcell} = (\frac{1}{V} \sum_i \sum_j \dot{n}_{ij} [(u_{pij} \alpha_{pij})_{out} - (u_{pij} \alpha_{pij})_{in}])_{kcell} \quad (439)$$

The equation for S_p^v is similar to that for S_p^u :

$$(S_p^v)_{kcell} = (\frac{1}{V} \sum_i \sum_j \dot{n}_{ij} [(v_{pij} \alpha_{pij})_{out} - (v_{pij} \alpha_{pij})_{in}])_{kcell} \quad (440)$$

The particle energy source term (S_p^h) represents the energy given to the gas-phase by the particles. The heat generated from the coal reactions is given to the gas phase simply by giving the mass and enthalpy of the reacted portion of the coal to the gas phase. The heat of coal reaction does not enter into the equation for S_p^h unless this heat of reaction is partitioned between the gas and particle phases. The S_p^h equation also includes a term to account for radiation between the gas and the particles. The radiation level Q_{rp} must be multiplied by the time change across the cell. The equation for S_p^h is:

$$(S_p^h)_{kcell} = (\frac{1}{V} \sum_i \sum_j \dot{n}_{ij} [(h_{pij} \alpha_{pij} - t Q_{rp})_{out} - (h_{pij} \alpha_{pij} - t Q_{rp})_{in}])_{kcell} \quad (441)$$

where t is the elapsed time along the integrated particle trajectory. It should be realized that this equation includes the effects of chemical reaction.

It has been found that the particle mass source terms sometimes introduce instabilities into the program especially during the first few gas-phase iterations. Therefore, the source terms are under-relaxed according to Eq. 375. A value of 0.5-0.7 is typically recommended for the under-relaxation factor.

2. Particle Number Density

The bulk particle number density couples the particle field with the gas field in two ways: turbulent particle dispersion, and radiation coupling between the phases. This is evident in Eqs. 29, 30, and 123. The equation for n_j is found in Chapter II (Eq. 31). This equation does not fit the general form of the gas phase equations in Table 1 due to the missing density (ρ). As was noted in the earlier discussion of Eq. 31, the u_j and v_j terms are replaced by u_g and v_g :

$$\frac{\partial}{\partial x}(r\tilde{u}_g\bar{n}_j) + \frac{\partial}{\partial r}(r\tilde{v}_g\bar{n}_j) - \frac{\partial}{\partial x}(r\Gamma_j\frac{\partial\bar{n}_j}{\partial x}) - \frac{\partial}{\partial r}(r\Gamma_j\frac{\partial\bar{n}_j}{\partial r}) = 0 \quad (442)$$

This equation is cast into finite difference form in a manner analogous to the other gas phase variables. Differences occur in the definition of the convection coefficients (C's) and in the two modifications. The resulting finite difference equation is shown in Table 18. This equation is solved using the TDMA.

In the calculation of Γ_j from Eqs. 24 to 28, the ratio α_j/d_j is required. In PCGC-2 this ratio is evaluated at the reactor inlet (α_{j0}/d_{j0}) and assumed constant. The boundary conditions for Eq. 442 are shown in Table 19.

J. NITROGEN OXIDE MODEL

The equations in the NO_x model are similar in form to the Eulerian gas-phase equations, and use the same solution technique as described previously. The equations have been summarized in Table 14. The major difference in solution of the equations in the NO model is the calculation of the overall reaction rates in the species continuity equations for NO and HCN. The procedure used to calculate these reaction rates in the NO model has been described previously.

The equations for the pollutant species are decoupled from the coal combustion model since the small pollutant levels will not significantly affect the velocity, density, or temperature fields. However, the equations for the pollutant species are coupled with each other since the pollutant reaction rates are a function of the other pollutant concentrations. The equations are solved following convergence of the coal combustion model. The solution procedure is illustrated in Figure 29.

TABLE 18

FINITE DIFFERENCE EQUATION FOR $\theta = \bar{n}j$

$$A_P \theta_P = A_E \theta_E + A_W \theta_W + A_N \theta_N + A_S \theta_S + S_u$$

where

$$A_P = A_E + A_W + A_N + A_S - S_p$$

$$A_E = D_E^* - (1/2) C_E$$

$$A_W = D_E^* + (1/2) C_W$$

$$A_N = D_N^* - (1/2) C_N$$

$$A_S = D_S^* + (1/2) C_S$$

$$D_d^* = \max [D_d, (-C_d/2), (C_d/2)] \text{ where } d = E, W, N, \text{ or } S$$

$$D_E = (\Gamma_{\phi P} + \Gamma_{\phi E}) (A_{ew}) / (2\delta x_{PE})$$

$$D_W = (\Gamma_{\phi P} + \Gamma_{\phi W}) (A_{ew}) / (2\delta x_{PW})$$

$$D_N = (\Gamma_{\phi P} + \Gamma_{\phi N}) (A_n) / (2\delta r_{PN})$$

$$D_S = (\Gamma_{\phi P} + \Gamma_{\phi S}) (A_s) / (2\delta r_{PS})$$

$$C_E = (A_{ew}) (u_E)$$

$$C_W = (A_{ew}) (u_P)$$

$$C_N = (A_n) (v_N)$$

$$C_S = (A_s) (v_P)$$

$$S_u = -\min [(C_E - C_W + C_N - C_S), 0] \phi_p^{\text{old}}$$

$$S_p = -\max [(C_E - C_W + C_N - C_S), 0]$$

TABLE 19
BOUNDARY CONDITIONS FOR $\bar{n}_j$

Inlet: primary: $\bar{n}_j = \bar{n}_{j0}$
 secondary: $\bar{n}_j = 0$

Side walls: $\frac{d}{dx}(\bar{n}_j) = 0$

Top wall: $\frac{d}{dr}(\bar{n}_j) = 0$

Symmetry Axis: $\frac{d}{dr}(n_j) = 0$

Outlet: Quadratic upstream extrapolation

Figure 29. Information flow for nitrogen oxide model.

PART TWO
CODE USER'S MANUAL

CHAPTER IV. USER GUIDE

A. GENERAL DESCRIPTION

PCGC-2 was developed on a VAX/11-750 computer with VMS operating system. The syntax of the code should be compatible with most FORTRAN 77 compilers with minor changes. Plotting or graphics routines are not distributed with the code. However, graphics is very important for understanding the code's voluminous output of data, and a recommendation for a graphics package is made below. Intermediate computational values of all variables can be printed out into restart files, so that computations need not start from scratch each time. Approximately 1 Megabyte of disk space is required for the FORTRAN listing. Two megabytes of real memory are required for running the code.

All input data to PCGC-2 are in SI units with the exception of angles, which are in degrees. The essential input is summarized in Table 20. All working variables within the program are either dimensionless or in SI units. Units associated with all variables are given in the nomenclature. A program (PCEDIT) has been developed to edit the input files. PCEDIT is a terminal interactive program. The help file for PCEDIT is included in Appendix A; directions are self-explanatory. PCEDIT uses VAX-specific FORTRAN features to perform tasks which are not possible in standard FORTRAN 77. Therefore, it may not work properly on other computers without modification.

CPU run time varies widely according to the particular simulation and the machine. Fifteen CPU-hours is typical for simulation of simple pulverized-coal combustion with a VAX/11-750. Five hours is typical on a VAX-8600 or Convex C-1. Ten hours is typical for a SUN 3/260.

The importance of graphics in examining the voluminous output data of PCGC-2 cannot be overestimated. We have selected the UNIRAS graphics software for use in our laboratory and recommend UNIRAS to all PCGC-2 users. UNIRAS was selected after a rather extensive investigation of available commercial graphics packages because of the ease of use and extensive color capability. The UNIMAP package of UNIRAS is sufficient for most applications. PCGC-2 users wishing to obtain UNIRAS software should contact Bob Wiley, P.E.; Senior Sales Representative; UNIRAS, Inc.; 21601 Devonshire Street, Suite 108; Chatsworth, CA 91311; Telephone (818) 407-1711. Please mention that your intended use of the software is with the BYU combustion software.

The 1987 version of PCGC-2 is available for license from Brigham Young University as of January 1, 1988, to Technical Associates of the Advanced Combustion Engineering Research Center (ACERC). It will be available to Technical Affiliates of ACERC after a one-year delay, and to non-member U.S. industrial organizations after two years. Foreign non-member organizations may inquire about availability after two years and U.S. universities may inquire anytime. A magnetic tape containing the FORTRAN source code and sample problems, a copy of this users manual, and consultation by telephone during the first 90 days to assist with initial code implementation and use are provided. Users may receive assistance beyond the first 90 days by joining a users group. A one-week short course on coal combustion and gasification modeling is also offered periodically, based on demand, and on-site

TABLE 20
SUMMARY OF INPUT FOR PCGC-2

Geometry

Primary tube diameter (m)
Secondary tube diameter (m)
Chamber diameter (m)
Chamber length (m)
Additional¹ inlets, location and sizes

Feed Rates

Primary gas (kg/s)
Secondary gas (kg/s)
Coal in primary² (kg/s)
Additional inlet #1 (kg/s)
Additional inlet #2 (kg/s), etc.

Inlet Gas Properties

Primary swirl number
Primary turbulence intensity (% or m/s)
Primary temperature (K)
Primary mole fractions of all species

Secondary swirl number
Secondary turbulence intensity (% or m/s)
Secondary temperature (K)
Secondary mole fractions of all species
Turbulence intensity, temperature and composition
for additional inlets³

Reactor Parameters

Reactor pressure (N/sq m)
Wall temperatures (K)

Particle Parameters

Particle solid density (kg/cu m)
Mass mean particle diameter and distribution
of particle sizes (m)
Coal composition (≠ proximate analysis) (%)
raw coal
char
ash
water
Coal elemental analysis (daf, %)

¹Up to 3 additional inlets are allowed.

²Particles are not allowed in the secondary or additional inlets.

³Some restrictions apply to temperature and composition of additional inlets.

training is available anytime on an individual basis. Information concerning licensing of PCGC-2, the users group, and training may be obtained by writing or phoning Dr. B. Scott Brewster, 45 CTB, Brigham Young University, Provo, Utah 84602 (801) 378-6240.

B. DESCRIPTION OF SUBROUTINES

An overall information flow diagram of PCGC-2 was given in Figure 7. A tree diagram of the structure of the program showing the actual computer routines is given in Figures 30-37. The calling routines are on the left, and the called routines are on the right. The routines are generally given in the order in which they are called, however each called routine is shown only once for a given calling routine. Not shown in the figures are calls to a program named CPUTIM, which are used to keep track of execution time for various portions of the program. The calls to CPUTIM are very numerous and would clutter the figures if shown. Entry points are shown with the name of the routine in parentheses. A detailed description of the routines is given in Appendix B.

The main program is PCGC-2, and the routines it calls are shown in Figures 30 and 34. INFLOW reads the input data for the inlet streams. GRID generates the numerical grid. GRMAP modifies the numerical grid if a grid datafile is being used and writes a new grid datafile. GRDGRF writes a schematic showing the grid locations in the output file. CREEO reads the reactant composition data and thermochemical datafile. INIT initializes arrays used in the code.

PSICTO, COALO, FLUXO, and NOXMNO read input data and perform initial calculations for the particle trajectory calculations, particle reaction scheme, radiation submodel, and pollutant submodel, respectively. Routines called by COALO are shown in Figure 31 (Step 1 of Figure 7). Other input data are read primarily by the main program and by the driver program for the nitrogen oxide submodel (NOXMN).

TABLE is the driver program for generating the table of equilibrium gas properties for lookup. Routines called by TABLE are shown in Figure 32. TBLF, TBLFE, TBLFEH, and TBLFH generate tables of equilibrium properties as functions of f only; both f and n ; f , n , and h_p ; and both f and h_p ; respectively. These four tables correspond to adiabatic, gas only; adiabatic, gas and reacting particles; non-adiabatic, gas and reacting particles; and non-adiabatic, gas only; respectively. All four table generators call CREE to calculate the equilibrium properties. TBLFE and TBLFEH provide for table restart (TBLRSTFE and TBLFEHRST).

PROFIL reads input data and sets the boundary values for the gas inlet streams. PRINT is a routine that is called frequently to print values of field variables to the output file. RESRT reads and writes gas-phase restart files. Particle phase restart files are read and written by the main program. FLINT initializes the flow field variables and calculates the gas density field. EULINT is an entry in PSICTO that calculates the particle number flowrate for each particle trajectory.

Figure 30. Subroutines called by the main program.

Figure 31. Subroutines called by COAL0 (initialization for Particle Reactions submodel).

Figure 32. Subroutines called by TABLE (physical properties table generation algorithm).

PROPS calculates the time-mean gas properties, incorporating the effects of turbulence. Routines called by PROPS are shown in Figure 33. FGABL is a routine that provides the upper and lower limits of the clipped Gaussian probability density function from a table of precalculated values. CREE may be utilized to calculate equilibrium gas properties when residual enthalpy falls outside the table limits. UPDATE is an entry point in TABLE that calls the appropriate entry point in TBLF, TBLFE, TBLFEH, or TBLFH, to retrieve the needed gas properties.

STREAM calculates the velocity streamlines for plotting. PLTWRT writes plotting files.

The CALC routines calculate the flowfield variables such as velocities, turbulence properties, mixture fractions, and pressure, at each node throughout the flowfield (Step 2 of Figure 7). These routines are shown in Figure 34. Each CALC routine calls an entry point in PROMOD to modify the coefficients and source terms in the appropriate finite difference equation in order to account for the boundary conditions as described in Section III.B.13. LISOLV is the solver that uses the TDMA algorithm as described in Section III.B.8.

PROG monitors the progress of the calculation toward convergence by recording the values of the variables at a specified location for each iteration.

EOLP is the driver program for the particle calculations. Routines called by EOLP are shown in Figure 35. CALCNJ solves the Eulerian particle density equation using the TDMA (LISOLV). CALACJ, CALAHJ, and PSOLVP solve the Eulerian particle calculations. Although the pure Eulerian approach for solving the particle phase has been programmed into PCGC-2, it is not yet operational. FLUX is the driver program for the radiation submodel. BVALIN is an entry point in BPROPS that inserts reasonable values into boundary intrusions in order to allow for 2-D interpolation of gas properties. PSICT solves the particle trajectories using the Particle-Source-In-Cell of Crowe and coworkers (1977) and calculates the particle source terms. COAL1 calculates the gas properties. COAL2 calculates the particle reaction rates, and PSOLVE solves the particle continuity equations. PSOLVS is a special solver that is used when the particle enthalpy equation goes stiff (after burnout it essentially complete). BVALOUT is an entry in BPROPS that substitutes the original values of properties back into the boundary intrusions after the particle trajectory calculations are complete.

An information flow diagram for the combined Eulerian-Lagrangian particle model is shown in Figure 36. CALCNJ first calculates the Eulerian number density field for each particle size. The Eulerian number density is needed by the FLUX routines for calculating the radiation fluxes and by the PSI-CELL routine for calculating the turbulent diffusion component of particle velocity as given by Eq. 434. PSICT solves the particle momentum equations for each trajectory, keeps track of particle position and properties as a function of time, and calculates the appropriate source terms for each cell. PSICT also interpolates Eulerian properties (total radiation flux, gas density, and gas temperature) across cells to be used in the particle calculations. COAL1 uses the local gas temperature to calculate gas viscosity, gas thermal conductivity, species diffusivities, gas thermal heat capacity, and Prandtl

Figure 33. Subroutines called by PROPS (gas physical properties calculation).

Figure 34. CALC subroutines called by the main program. (Gas Fluid Mechanics and Reactions submodels.)

Figure 35. Subroutines called by EOLP (Particle Dispersion and Reactions submodels).

Figure 36. Information flow diagram for combined Eulerian-Lagrangian particle model.

number. COAL2 uses this information to calculate the component reaction rates, convection and radiation heat transfer rates, volatiles enthalpy, and particle temperature. Particle diameter (or density if completely devolatilized and constant-density option is chosen) is also calculated by COAL2 and used by PSICT in solving the momentum equations. PSOLVE uses the particle reaction rates, heat transfer rates, particle temperature, and volatiles enthalpy to solve the particle continuity equations and provide the mass of each particle component at each time step. The final product of the particle model is the source terms which are returned to the gas phase.

Routines called by FLUX are shown in Figure 37. RADCOF calculates the gas emissivity and absorption and scattering coefficients for either the Varma six-flux (VFM) or discrete ordinates (DOM) model. EIC02 and EIH2O calculate the emissivity contributions for carbon dioxide and water vapor, respectively. DISORD solves the radiation equations using the DOM model. RESULT prints a summary of the results of the DOM calculations in the output file. SETUP calculates the coefficients for the VFM model. FLUXX, FLUXR, and FLUXT solve the VFM model equations for the axial, radial, and tangential directions, respectively. The equation for the tangential direction is algebraic due to the axial symmetry and does not utilize the TDMA solver (LISOLV).

NOXMN is the driver program for the pollutant submodel. Routines called by NOXMN are shown in Figure 38. RATE calculates the time-mean reaction rates for the nitrogen oxide reactions, incorporating the effects of turbulence on the homogeneous reaction rates, analogous to the manner in which PROPS incorporates the effects of turbulence on the time-mean gas properties. CALCNO and CALHCN calculate the field values for nitrogen oxide and hydrogen cyanide concentration, using the TDMA algorithm (LISOLV), analogous to the other CALC routines which solve the field variables for the gas phase. CALO2 adjusts the time-mean mass fraction of oxygen throughout the flowfield following the pollutant reactions.

C. PROGRAM INPUT

At least three input files are required by PCGC-2: the main data file (PCGCIN), the thermodynamic properties data file (THERMO), and the inlet profile data file (INLET). Other data files may also be required. For example, if the individual grid locations are to be specified (INRDGD = T in the main data file) a grid data file (GRID) is needed. If the calculation is being restarted from the results of a previous calculation (INRST = T and/or INPRST = T in the main data file), restart files are needed for the gas (INOUT) and/or particles (PARSOU).

The data contained in the three required input files are shown in Table 21 and are briefly described below. The data are given in the actual order in which they are read by the program, and are divided into seventeen groups according to function. Also shown in Table 21 are the calling routine and required format. A detailed description of the input data is given in Appendix C.

Figure 37. Subroutines called by FLUX (Radiation submodel).

Figure 38. Subroutines called by NOXMN (Pollutants submodel).

Group 1 in Table 21 contains comment statements that are printed out as a header at the beginning of the main output (PCGCOT) and log files. Any number of comment statements may be included in the header.

Group 2 contains program control information, including which field variables are to be calculated, and numerical parameters for degree of under-relaxation, convergence criteria, etc. The reactor geometry, enthalpy bounds for the physical properties table, reactor heat loss, wall temperatures, and gas viscosity and pressure are also specified in Group 2.

Group 3 describes the flowrate, composition (in terms of the reactant streams described below), swirl, and turbulence intensity of each of the gas inlet streams. Up to three additional inlets (in addition to primary and secondary) may be included, but they must all be described in terms of the reactant streams specified below.

Data in Groups 1, 2, and 3 are all contained in the main input file, PCGCIN. For Groups 4 and 5, only the first data item, i.e. the keywords ELEM and THER, are contained in file PCGCIN. The remaining data in these groups are contained in the THERMO file. Group 4 gives the molecular weight and valence of each of the elements. The order in which the elements are listed is the order in which they are treated in the program calculations. Group 5 gives the elemental composition, heat of formation, temperature ranges, and heat capacity coefficients for each of the molecular species.

Group 6 describes the reactant streams that are used to specify the inlet stream compositions and temperatures. Only two reactant streams are allowed. The inlet streams are specified as a mixture of the two reactant streams. Usually, the first reactant stream is used to specify the primary gas, and the second reactant stream is used to specify the secondary and any additional inlets. However, any inlet may also be specified as any mixture of both reactant streams using the input variable FFLOW in Group 3.

Group 7 gives information about the particles, including the number of particle trajectories (up to 10), number of particle sizes (up to 20), the particle loading in the primary stream, particle density, starting location of the trajectories, initial particle velocity and temperature, initial particle size distribution, particle Prandtl number, and information controlling the particle phase calculations, such as maximum number of particle iterations.

Groups 8, 9, 10 and 11 give information about the solids composition and reactions. Group 8 contains any number of comment cards which are reprinted in the output file. Group 9 specifies the number of reactions and numerical control parameters. Group 10 gives kinetic parameters for each of the devolatilization and char oxidation reactions, as well as the particle composition and heat capacity data. Group 11 gives the Lennard-Jones parameters for predicting the transport properties of the gas species. Group 12 specifies the oxidizing species and stoichiometry for the heterogeneous reactions.

Group 13 gives information for the radiation submodel, including the method of solving the governing equations (Varma six-flux or discrete ordinates), whether to include gas emissivities and corrections, maximum number of iterations, and absorption and scattering cross-sections.

TABLE 21

INPUT DATA

<u>Group</u>	<u>Calling Routine</u>	<u>Data File¹</u>	<u>Line</u>	<u>Data Items</u>	<u>Format</u>
1	MAIN	PCGCIN	1	NSAY	*
			2	SAY(I)...SAY(18)	18A4
			NSAY+1	SAY	.
2	MAIN	PCGCIN	1	INRST, INCALF, INCREK, INCALH, INCALG	8L5
			2	IPSICT, INPRST, INEACH, INCLET, INCLGE	.
			3	INCALN, INCURF, LEULP, INTFRZ, INSIMP	.
			4	INCNOX, POLLUT, INQRL, INCSWP, INCSWS	.
			5	INNOZZ, INFYOU, LTBUG, GRDOUT, INPROG	.
			6	INCFP, INRAD, INRDGD, INTRUS, MAGHJER	.
			7	URFU, URFV, URFW, URFH	*
			8	URFE, URFK, URFF, URFG, URFVIS	*
			9	URFDEN, URFETA, URFGET, URFNJ, URFPP, URF	*
			10	DIAP, DIAS, DIACH	*
			11	NDIA (REAL), THICK	*
			12	MAXIT, INDPRI, INDRST	*
			13	NJINP, NJINS, NIWOQ	*
			14	AL1, EPSX, NL, EPSI, EPSD	*
			15	HRMIN, HRMAX, HLOSS	*
			16	NIINQ, QHA, QLX	*
			17	TBN, TBW, TBE	*
			18	VISCOS, PRES	*
			19	SORMAX, SORMIN	*
3	INFLOW	PCGCIN	1	STRING	A5
			2	FLOW(I), FFLOW(I), SWIRLN(I), TINFLO(I) I=1, NINLET	*
4	CREEP	PCGCIN THERMO	1	ELEM	A4
			2	ATOM(1, NLM), ATOM(2, NLM), ATOM(3, NLM)	A2, 7X, 2F10.6
			3	repeat card 3-2 for each element(nlm) BLANK LINE	A4
5	CREEP	PCGCIN THERMO	1	THER	A4
			2	DATA(1), DATA(2), DATA(3)	3A4, 6X
				DT1, DT2, AT(1), B(1)	2A3, A2, F3.0
				AT(2), B(2), AT(3), B(3)	2(A2, F3.0)
				AT(4), B(4), PHASE	A2, F3.0, A1
				TLOW, THIGH	2F10.3
				IDON(1), IDON(2), IDON(3), IDON(4)	4I3
				NCD	I3
			3	Z(1, 1, NS), Z(2, 1, NS), Z(3, 1, NS)	3E15.8
				Z(4, 1, NS), Z(5, 1, NS), NCD	2E15.8, I5

TABLE 21 (Continued)

<u>Group</u>	<u>Calling Routine</u>	<u>Data File¹</u>	<u>Line</u>	<u>Data Items</u>	<u>Format</u>
			4	Z(6,1,NS),Z(7,1,NS),Z(1,2,NS) Z(2,2,NS),Z(3,2,NS),NCD	3E15.8 2E15.8,I5
			5	Z(4,2,NS),Z(5,2,NS),Z(6,2,NS) Z(7,2,NS),NCD	3E15.8 E15.8,I5
				repeat lines 4-3 to 4-5 for each specie to be considered	
			6	BLANK LINE	A4
6	CREEØ	PCGCIN	1	REAC	A4
			2	TMP	*
			3	AT(1),B(1),...,AT(4),D(4),	4(A2,F7.5)
			3	ASUB(1),ASUB(2),PECWT,	2A4,1X,F7.5
			3	MULE,PHASE	A1,9X,A1
				Repeat card 5-3 for each species in reactant stream	
			4	BLANK LINE	A4
				Repeat group 5 once the primary and secondary stream, respectively	
7	PSICTØ	PCGCIN	1	NSL,NPS	*
			2	PLOADP,PDEN	*
			3	YPS(ISL),ISL=1,5	*
			4	YPS(ISI),ISI=6,NSL	*
			5	UPLAG(IPS),IPS=1,NPS	*
			6	SPRANG(ISL),ISL=1,5	*
			7	SPRANG(ISI),ISI=6,NSL	*
			8	TLAG(IPS),IPS=1,NPS	*
			9	PD(IPS),IPS=1,3	*
			10	PD(IPS),IPS=4,NPS	*
			11	PMF(IPS),IPS=1,NPS	*
			12	LPBUG,LYPS,LPARTP,LPARTS,LPBOTH	5L5
			13	LSPM,LSPU,LSPV,LSPH	5L5
			14	YPSH,YPSL	*
			15	MAXITP,MINITP,IGASV	*
			16	PRK(IPS),IPS=1,NPS	*
8	COALØ	PCGCIN	1	NCARD	*
			2	COMENT(1,1),...,COMENT(1,14)...	14A4
			2	COMENT(2,1),...,COMENT(2,14)...	
			2	COMENT(NCARD,1),...,COMMENT(NCARD,14)	
9	COALØ	PCGCIN	1	INCOAL	L5
			2	NCRXN,NHRXN,NPROP,IEUCK,KEQ,NSHRNK	*
			3	DELTPJ,DELRRJ,GAMMA,URFPM	*

TABLE 21 (Continued)

<u>Group</u>	<u>Calling Routine</u>	<u>Data File¹</u>	<u>Line</u>	<u>Data Items</u>	<u>Format</u>
10	COALØ	PCGCIN	1	XI(1)	*
			2	HCO(1),HHO(1),HAO(1)	*
			3	HWO(1),TNBP	*
			4	OMEGAC(1),OMEGAH(1),OMEGAA(1)	*
			5	OMEGAW(1)	*
			6	AMJ(1,1),EMJ(1,1),YY(1,1)	*
			7	HGV(1,1)	*
				Repeat line 9-6 and 9-7 for each raw coal reaction up to a total of NCRXN	
			8	ALJ(1,1),EL(1,1),EMM(1,1)	*
			9	HGH(1,1)	*
11	COALØ	THERMO		Repeat line 9-8 and 9-9 for each char reaction up to a total of NHRXN	
			10	CCP(1,1,1),CCP(1,1,2),CCP(1,1,3)	*
				CCP(1,2,1),...	*
				...CCP(1,4,3)	*
				WIC(1,1),WIC(1,2),...WIC(1,NLM)	*
				Group 9 parameters are used for all particles	
12	COALØ	PCGCIN	1	SLRCMP(I),I=1,3	A4
			2	OXYD(1),OXYD(2)...OXYD(NHRXN)	5A4
13	FLUXØ	PCGCIN	3	PHIL(1),PHIL(2),...PHIL(NHRXN)	*
			1	LDISO,LGASE,LEMCOR,MAXITR	3L5,2X,I10
			2	QAB(1),QAB(2),...QAB(NPS)	*
			3	QSC(1),QSC(2),...QSC(NPS)	*
			4	EMW,TOUT	*
14	PROFIL	INLET	5	AØ,AF	*
			1	UPDAT,KOPUP,USDAT,KOPUS	2(1X,L1,1X,I3)
			1	UPD(N),KOPU(N),N=1,NINLET	3(1X,L1,1X,I3)
			2	VPDAT,KOPVP,VSDAT,KOPVS	2(1X,L1,1X,I3)
			2	VPD(N),KOPV(N),N=1,NINLET	3(1X,L1,1X,I3)
			3	WPDAT,KOPWP,WSDAT,KOPWS	2(1X,L1,1X,I3)
			3	WPD(N),KOPW(N),N=1,NINLET	3(1X,L1,1X,I3)
			4	TIPDAT,KOPTTEP,TISDAT,KOPTES2	2(1X,L1,1X,I3)
			4	TIPD(N),KOPTE(N),N=1,NINLE	3(1X,L1,1X,I3)
			5	EDPDAT,KOPEDP,EDSDAT,KOPED	2(1X,L1,1X,I3)
			5	EDPD(N),KOPED(N),N=1,NINLET	3(1X,L1,1X,I3)

TABLE 21 (Continued)

<u>Group</u>	<u>Calling Routine</u>	<u>Data File¹</u>	<u>Line</u>	<u>Data Items</u>	<u>Format</u>
15	PROFIL	INLET	1	PLS,SLS	*
			2	NSFORM,ALPHA0	*
			3	RP,RS1,RS2	*
			4	UIN(1),VIN(1),WIN(1),TURBIN(1)	*
			4	EDIN(1),RIN(1)	*
				Repeat line 4 for entire profile defined by an arbitrary number of radial locations	
16	NOXMN	PCGCIN	1	NSAYNX	*
			2	SAYNX(1),SAYNX(2),...SAYNX(18)	18A4
			NSAYNX+1	SAYNX(1),SAYNX(2),...SAYNX(18)	18A4
17	NOXMN	PCGCIN	1	A1,A2,A3	*
			2	EACT1,EACT2,EACT3	*
			3	PRNOX,PRHCN,FCTNO,FCTHCN,YHCNPR,YHCNS	*
			4	MXITNX,ITYNX,INDPNX	*
			5	XIANOX,ZEDA,MAXRES	*
			6	IRSTNX,IPLTNX,INHTNX	3L5

-
1. Indicates data file where information is found.
 2. If case uses restart file for particles (INPRST = TRUE), it is read in prior to reading data group 6.

Groups 14 and 15 contain data for calculating (theoretical) or reading (experimental) profile data for velocity, turbulence intensity, and eddy dissipation for the primary and secondary inlets. These data are contained in the inlet profile data file.

Groups 16 and 17 contain input data for the pollutant submodel. Group 16 contains comment statements. Group 17 contains the kinetic, numerical, and program control parameters.

As explained above, several optional data files may be included as input to PCGC-2. These include: 1) a file containing information which describes the grid geometry (assigned logical name GRIDS in the Fortran subroutine GRMAP), 2) files used as initial guesses based on previous calculations for the gas phase (assigned logical name INOUT in the Fortran subroutine RESTRT) and for the particle phase (assigned logical name PARSOU in the Fortran program PCGC2), and 3) a file consisting of the equilibrium table (assigned logical name TBLRST in the Fortran subroutines TBLRSTFE and TBLRSTFEH) used in calculating gas properties (temperature, density, etc.) as functions of the progress variables f , η , and h_r .^{*} Each of the data files are accessed in VAX/VMS Fortran using an OPEN statement. Some use the IOSTAT qualifier to insure proper operation. IOSTAT is assumed equal to 0 if the open command is successful.

D. PROGRAM OUTPUT

Program output is contained in the main output (PCGCOT) and log (for batch runs) files. The quantity of output in the main output file is controlled by the relative values of INDPRI and MAXIT as shown in Table 22. Three options are available: Output can be a) turned completely off, b) restricted to the beginning and end of the calculation, or c) printed periodically during program execution. Option (a) is used most commonly, since the output file can get rather large and cumbersome otherwise, and graphics are usually used to examine code results.

Table 23 presents an outline of the output file produced during a PCGC-2 computation. All of the input parameters (i.e. thermodynamic properties, flowrates, particle size information, coal reaction rate information, and radiation information) and many parameters calculated from them are written to the output file early during execution (Options B and C). Also, the initial values for each scalar field (i.e. gas temperature, velocities, pressure, etc.) used for initialization are written to the output file. During the iteration process, values of each critical field variable are printed for each node point in the computational grid (Option c). The y (or r) values of the grid are found at the right-hand side of the array, and the axial location (x) is found along the bottom of the grid printout. Since the sample grid is too long to be printed in one block, it is "wrapped around" in three segments. The index values for the node point (I and J) are also printed out. Other gas

^{*}An option is provided (INCALH = F) for assuming a locally adiabatic reactor, in which case h is not independent of f and η .

TABLE 22
PROGRAM OUTPUT CONTROL

<u>INDPRI</u>	<u>Output</u>
a) < or > MAXIT	None
b) = MAXIT	Input summary, initial values of field variables, final values of field variable.
c) > 0 and < MAXIT	Same as b) plus intermediate output of field variables every INDPRI iterations.

TABLE 23

OUTLINE OF OUTPUT FROM PCGC-2 CALCULATION

I. INPUT DATA FOR COMPUTATION

- a) Comment lines describing calculation
- b) Elements considered
- c) Thermodynamic data required to predict equilibrium properties
- d) Inlet stream information
- e) Particle property information
- f) Particle reaction information
- g) Radiation information
- h) Reactor parameters
- i) Computational grid information
- j) Initial scalar fields (i.e. velocity, mixture fraction, etc.)

II. GAS-PHASE ITERATION INFORMATION (see note below)

- a) Normalized residual source sums

III. PARTICLE ITERATION INFORMATION

- a) Time/position information for Lagrangian particle trajectories
- b) Axial mixing-cup coal burnout

IV. FINAL OUTPUT

- a) All scalar fields
- b) Summary of CPU time requirements

Note: Residual terms are printed for either INDRST iterations or until gas phase convergence is obtained. On gas phase convergence, the field variables are printed and the computation proceeds in the particle phase until convergence. After each Lagrangian particle calculation is completed, computation returns to the gas phase at which time the field variables are computed with the updated particle source terms. If the difference between the most recent calculated field variables and those calculated at the end of the last gas phase iteration is less than SORMIN the calculation is complete. Otherwise, computation continues in the gas phase. If the gas phase converges in fewer than MINITP iterations, the calculation is considered complete. Otherwise, computation returns to the particle phase after gas phase convergence, and the process is repeated. On overall convergence, the field variables are written to the output file along with a summary of the time required.

properties are printed only upon convergence or after other normal termination (Options b and c).

The particle trajectory information is printed out each 10 trajectory time steps as the calculations proceed. Among other things, the output shows the location of the particle (XP and YP), the time step of integration (DT), the elapsed residence time along the particle trajectory (TIME), the particle gas temperatures (TMPG), the mass of liquid, raw coal, char, ash, and total mass of the particle normalized by the original particle mass (WFRAC, CFRAC, HFRAC, AFRAC, TFRAC, respectively). This information is given for each of the particle trajectories (ISL = initial starting location, and IPS = initial particle size).

In addition to the main output file, several other files contain program results. These are summarized in Table 24. Standard Fortran 77 commands were used, where possible, to manipulate these files. However, several of the files (e.g. PRGRSS and PLOT3) use a VAX extension (Associate Variable) in directing output to selected portions of the files.

E. CODE OPERATION

PCGC-2 is a "user-specialist" code that requires familiarity with the theory and structure of the code in order to be used correctly and efficiently. This section gives several hints for new users. A thorough understanding of the problem physics and numerical assumptions is essential.

1. Editor

When setting up a new problem for simulation, it is easiest to start by editing input files from a previous simulation, since much of the information will remain unchanged. Several sample input files are supplied on tape with the program for this purpose. The new user may find the input file editor (PCEDIT) to be useful, since it steps through most of the input variables one at a time and allows the user to either keep the same value or change it. A brief description of each variable is given in PCEDIT as it is presented. PCEDIT uses several VAX-specific Fortran features which are not available in standard Fortran 77 and may not work on other computers without modification.

2. Restart

Unless the user has a converged or partially converged solution of a similar problem with identical geometry, he will probably want to start his problem from "scratch." To do so, the logical variables that will cause the code to try to "restart" from a guessed solution (INRST, INPRST, and IRSTNX) must be set equal to F in the main input file. This will not prevent the code from writing restart files for future restarts, since writing to restart files is automatic at a frequency specified by the variable INDRST. A value of 50 is recommended. Subsequent runs for the same case can be restarted from a previously converged solution by setting the above logical variables equal to T in the input file. The restart feature is useful when small changes are made for the same case and geometry. If the changes are large or the geometry changes, the restart option should not be used.

TABLE 24
PCGC-2 OUTPUT FILES

<u>File</u>	<u>Type</u>	<u>Description</u>
PCGCOT	Text	Main output file.
PARSOU	Binary	Particle source terms for restart (INPRST = T).
GASPLT	Binary	Eulerian gas properties and particle density for plotting.
POLPLT	Binary	Pollutant data for plotting.
INOUT	Binary	Eulerian gas properties for plotting.
RSNXIO	Binary	Pollutant data for restart (IRSTNX = T).
PPLLOT1	Text	No records for each trajectory in PPLLOT2 and pointers to trajectories in PPLLOT3.
PPLLOT2	Text	Particle coordinate residence time, and time increment for plotting. Also contains centerline burnout and mixture fraction data.
PPLLOT3	Text	Particle coordinates, composition, temperature, and gas temperature for plotting.
TBLRST	Binary	Gas property data.
PRGRSS	Text	Residual source sums and gas properties at a selected point in the reactor for monitoring progress toward convergence.

3. Particle and Gas Iterations

The maximum number of particle iterations is controlled by the parameter MAXITP. It typically takes 5-15 particle iterations to converge a PCGC-2 calculation from scratch. The maximum number of gas iterations is controlled by the parameter MAXIT. A typical value of MAXIT is 1000.

4. Gas Convergence

The code has the capability of completely converging the gas phase for every calculation of the particle phase, which is the normal approach, or of calculating the particle phase every 5 iterations of the gas phase. The latter approach is used when INEACH is set to T. and may be useful in cases where the gas and particles are highly coupled. In all cases, convergence of the gas phase is controlled by the value of SORMAX. Overall convergence is controlled by SORMIN.

An efficient approach to obtaining a solution is as follows. Obtain an approximate solution by selecting large values for SORMAX and SORMIN, 1.0 and 2.5 respectively, for example. Systematically reduce both parameters, converging the case between each change. For example, after a case is converged with SORMAX = 1.0 and SORMIN = 2.5, change the parameters to 0.1 and 0.5, respectively. Then change them to 0.01 and 0.10, respectively. This is usually sufficient for most cases. If detailed analysis of trace species is desired, both may be reduced further. It is usually desirable to solve the NO_x model only after the main code is converged to the desired level.

5. Gaseous Combustion (No Particles)

For gaseous combustion (no particles), the following control variables should be turned off (set equal to F): INCLET, INCLGE, IPSICT, INPRST and INCALN. This will prevent the calculation of the coal gas mixture fraction and its variance, particle trajectories, and particle Eulerian density. In addition, the input data for the particle phase (data groups 7-12) should be removed. The pollutant submodel should not be solved since thermal NO formation is not currently considered.

6. Coal Particle Combustion

In most combustion simulations, both the primary and secondary gas streams are composed of air and are therefore identical in composition. If the gas streams were also identical in temperature, it would be unnecessary to calculate the gas mixture fraction (controlled by INCALF) or its variance (INCLG). However, the secondary stream is usually preheated, and in this case it may be important to calculate the gas mixture fraction. However, the turbulent fluctuations can often be ignored, even though there is a difference in temperature. Of course, the coal-gas mixture fraction (controlled by INCLET) and its variance (controlled by INCLGE) must always be calculated when reacting coal particles are present.

7. Energy Equation

If a locally adiabatic solution is desired, the calculation of enthalpy can be turned off with the logical INCALH. Otherwise, the energy equation is

explicitly solved subject to the given temperature boundary conditions (TBN, TBW, and TBE).

If the energy equation is to be solved, upper (HRMAX) and lower (HRMIN) bounds for residual enthalpy (see Section III) must be given. These bounds are for the equilibrium table. They represent a percentage of the fully mixed enthalpy. It is recommended that the table debug flag (LTBUG) be turned on when generating a new table. This will stop execution after table generation so that the results of the table generation calculations can be reviewed before the actual simulation begins. If failures in the equilibrium algorithm occur during table generation, messages will appear in both the output and log files. It is normal to obtain a few failures during table generation if the energy equation is being solved, due to the equilibrium algorithm attempting to perform calculations at conditions corresponding to a temperature of less than 0 K. If convergence error(s) occur during table generation, the area(s) of the table in which the failure(s) occurred should be checked to see if they are of physical importance. If not, calculations can proceed without serious error. Without a "good" equilibrium table, it is impossible to obtain good simulation results.

It is difficult to state a priori what the values of HRMIN and HRMAX should be, since they are dependent on the problem. If they are too narrow, the simulation will require table lookup values that are outside the range of the table. In such cases, the limiting table value for the same stoichiometry will be assumed unless the variable INOCRE is turned off in the main calling program. In the latter case, an equilibrium calculation will be performed each time table values are required outside the range of the table.

Whenever table values are needed by the program outside the range of the table, the residual enthalpy is reset to the table limiting value for the particular values of f and n , and a counter (NCREE) is incremented. NCREE is printed in the log and output files, and therefore represents the number of times (for a given gas-phase iteration) the residual enthalpy was outside the table limits. For an unconstrained solution, NCREE should be equal to zero at the solution. The narrower the table limits, the fewer the number of table failures, but the larger the value of NCREE. Therefore, by trial-and-error, values of HRMIN and HRMAX must be determined that provide as narrow a range of residual enthalpy as possible, without resulting in any calls to CREE (NCREE = 0) at the solution. In the past, it was recommended that the user start with a relatively narrow range (e.g. HRMIN = -100, HRMAX = 50), and expand as necessary. The value of HRMIN is the most critical and the most difficult to determine, as it is the limit that results in table failures when the true solution corresponds to a temperature less than absolute zero. Recently, an iterative scheme was developed that will automatically adjust the table enthalpy limits to achieve a value of zero for NCREE, and the initial limits are not as critical as long as they are reasonable. It is better to start with limits that are too wide rather than too narrow. Values of -10, +100 are recommended.

After generating an acceptable table as defined above, LTBUG should be turned off to allow the combustion calculation to proceed using the table that was generated previously. A new table will then be generated only when a variable that affects the table generation is altered. If for some reason the user desires to regenerate the table, even though no variable affecting the

table generation has been altered, he must delete the file containing the previous table.

Inclusion of the source term due to gas-to-particle convective heat transfer in the energy equation is controlled by the flag LSPH. This flag is usually set equal to F when the energy equation is solved, because the calculation will usually be unstable when this term is included. The term is relatively unimportant in most cases.

8. Radiation

In the 1987 version of PCGC-2, the Discrete Ordinates Radiation Submodel has been included as an option. This option can be chosen by setting the logical 'LDISO' equal to true in the main data-file. Gas-phase radiation is included if 'LGASE' is set to true; otherwise only radiation due to the particulates (excluding soot) is considered. The gas phase radiation is calculated in two ways: if 'LEMCOR' is set true, the calculation includes the corrections in gas emissivities due to species partial pressures and spectral overlap of CO₂ and H₂O emissivities, using the Hottel charts (Hottel and Sarofim, 1967); otherwise, the overall emissivity of the gas is calculated using the Hadvig (1970) plot. 'QAB' and 'QSC' are the absorption and scattering efficiencies of the particulates based on Mie theory.

The scattering phase function has been changed to linearly anisotropic in the 1987 version of the code. This has been done because it can be adjusted to account for either isotropic, or strongly forward- or backward-directed scatter. Since scatter by coal/char particles is known to be strongly forward-directed, the recommended value for a_0 , the asymmetry factor, is 1.0. The phase function used earlier in PCGC-2 was that for ash particles (Hottel and Sarofim, 1967), which represented strongly backward-directed scatter.

Finally, the user can choose a value for the differencing factor, f , in extrapolating intensities across volume elements. This parameter is contained in the main datafile. If a value of 1.0 (i.e., central differencing scheme) is chosen, and negative intensities are encountered, the radiation submodel will automatically adjust (reduce) the value of f until the negative intensities are all removed. This is expected to result in slightly more accurate predictions of the intensity field as compared with upwind differencing (i.e., $f=0.0$), but requires more computer time. It is therefore recommended that upwind differencing ($f=0.0$) be used.

9. Numerical Algorithm

Two choices of numerical algorithm for solving the gas phase are provided: SIMPLE and SIMPLER. SIMPLER (selected by INSIMP equals T) is recommended in all cases because it is more efficient. Although SIMPLER converges much faster than SIMPLE, some cases that fail to converge with SIMPLER may converge if SIMPLE is used. The use of SIMPLE requires significantly lower under-relaxation parameters, as explained below.

10. Under-relaxation

When using SIMPLER, values of 0.7-0.9 are recommended for all under-relaxation factors for the independent gas field variables except URFPP and URFP (which should be 1.0) and URFDEN (which should be 0.5-0.7). When using SIMPLE, all factors should be substantially lower (0.3-0.6). A value of 0.9 is recommended for URFH for both algorithms. Of course, these factors are problem-dependent, and the convergence rate can be increased by increasing the under-relaxation factor of variables that seem to be controlling the convergence rate, as determined by monitoring the terminal-directed output from the code. The most efficient mode of operation is for each under-relaxation parameter to be as high as possible without causing the program to oscillate or diverge. Under-relaxation factors can be altered interactively every 25 iterations by setting INCURF equal to T.

A value of 0.5-1.0 is recommended for the particle phase under-relaxation (URFPM). This parameter is applied to all of the particle source terms in the gas phase equations.

11. Maximum Number of Iterations and Generation of Output

A value of 1000 is recommended for the maximum number of iterations for the gas phase (MAXIT). The frequency of intermediate output is determined by INDPRI. A value of zero is recommended unless printed output is desired.

12. Grid

The maximum number of nodes for both axial and radial directions is forty, and in most cases, it is wise to use as many node points as possible. It is felt that a 40x40 grid may be somewhat marginal for an accurate solution in some cases, but 40x40 represents a reasonable tradeoff between accuracy and calculation time. However, neither the number of radial node points nor the number of axial node points are specified directly in the input. Rather, node locations and number of node points are determined indirectly, based on the input variables AL1, NJINP, NJINS, EPSX, NL, EPSI, EPSD, and NIINQ. The grid generation algorithm uses these parameters to generate a grid for specified reactor dimensions that spaces the grid points closely in the flame region and near the walls, where gradients are expected to be large, and less closely in regions where the gradients are expected to be small. Therefore, trial-and-error is often required to generate an acceptable grid for new geometry.

The program also allows the user to specify the grid locations directly. In this case, another input file for the grid must be created, and the variable INRDGD in the input must be set equal to T. The recommended approach is to let PCGC-2 generate a grid file (GRDOUT equals to T and INRDGD equals F) and then edit the resulting grid file that is generated. INRDGD can then be set equal to T.

13. Intrusions

The program can accommodate intrusions within the constraint of axisymmetric geometry. An intrusion is a boundary cell in the interior of the flowfield. Intrusions can be used to model converging walls or other internal structures. To define intrusions, the grid structure must be read from an

input file. Therefore, the easiest approach is to first generate a grid input file as described above, and then add intrusions at the appropriate locations by changing 0's to X's. The logical variables INTRUS and INRDGD must be equal to T to use this option.

14. Additional Inlets

Additional inlets are used in a manner similar to intrusions by altering a previously generated grid file. Up to three additional inlets may be specified by changing X's to 1's, 2's, or 3's at the appropriate boundary location on the north or west walls. The flowrate, composition (in terms of the reactant streams), swirl number, and turbulence intensity must be specified in the input file for each additional inlet. Profiles for additional inlets are assumed flat.

15. Overall Code Convergence

Overall convergence of the code is assumed when the gas phase is not changed significantly by a particle phase calculation. Two input parameters are used to determine this condition quantitatively. If the maximum residual source sum is less than SORMIN on the first iteration after a particle iteration, then overall convergence is assumed to have been achieved. A value of 0.1 is recommended. Since the gas phase is converged to the value of SORMAX each time, this means that the maximum residual source sum increased from 0.01 to 0.1 during the particle iteration if the value of SORMAX is 0.01. Even if the maximum residual source sum is greater than SORMIN (e.g. 0.1) on the first gas phase iteration after a particle phase iteration, the gas phase is considered to be unchanged and the problem therefore converged if the gas phase can reconverge to the SORMAX criterion in less than MINITP iterations. The recommended value of MINITP is 25.

16. Particle Reaction Rate Parameters

The particle reaction rate parameters (AMJ, EMJ, YY, ALJ, EL, EMM, etc.) are coal-specific. Also, the code predictions are quite sensitive to these parameters, and they need to be chosen carefully, based on experimental data for the coal-type and conditions of interest (see Tables 5 and 8 and associated discussion).

17. NO_x Model

The NO_x model is decoupled from the solution of the major species and can be executed separately, based on a previously converged solution of PCGC-2. This is accomplished by setting POLLUT equal to T.

18. Chemical Species

The chemical species considered in the equilibrium calculations are governed by the input in the THERMO file. Data for additional species not being considered can be stored by moving them to the end of the file (after the Leonard-Jones parameters).

19. Coal-Water Mixtures

Simulation of coal slurries is limited to cases where all inlet gas streams have the same composition and temperature. The gas mixture fraction variable is then used to track the evaporating moisture from the particles rather than the inlet gas mixing. In such cases, INF SOU should be set to T to include a source term in the f equation. The variable OMEGAW is used to specify the initial liquid content of the slurry. For ordinary combustion of pulverized coal, OMEGAW is set equal to zero, and the inherent moisture of the coal is added directly to the input composition and flowrate of the primary gas.

The variable INNOZZ allows specification of the primary diameter rather than the secondary diameter. This option is useful when primary diameters are small, such as when slurry nozzles are being modelled. The option can also be used to generate a grid for dry coal combustion, however.

20. Coal Heat Capacity

If all of the polynomial coefficients for any coal component (coal, char, or ash) are zero, the Merrick heat capacity model will be used for that component. Otherwise, the polynomial correlation will be used.

CHAPTER V. IMPLEMENTATION GUIDE

A. CODE FILES

This chapter discusses the implementation of PCGC-2 on VAX/VMS and UNIX operating systems. The discussion uses VAX/VMS terminology with UNIX terminology given in parentheses. The concepts that are illustrated are applicable to other computer systems as well.

A typical PCGC-2 run involves approximately 15 input and output files. File management is therefore tedious if performed manually. If PCGC-2 is going to be used frequently, it is recommended that command (script) files be developed to assist in the file management task. Depending on the available software, command (script) files can also be used to perform other useful tasks, such as recompiling portions of the program that have been edited and then relinking the program, submitting jobs to a batch queue, prompting interactively for information needed to submit the program (such as the name of the batch queue, if there is more than one), etc. Typical PCGC-2 command (script) files for VAX/VMS and UNIX are included in Appendix D.

The operation of these files is described as follows: First, filenames for the various input and output files are specified. These include the main data files (geometry and general flow conditions), inlet data file (inlet velocity flow conditions), thermo datafile (thermodynamic parameters), output datafiles (these include the formatted output file as well as those files created specifically for graphics display), and restart data files (restart files for both gas and particle phases). The command (script) file prompts the user interactively for the names of these five sets of files. Alternatively, they may be specified as parameters in the command used to invoke the command (script) file. If only a single parameter is specified, all filenames are assumed identical except for the extensions.

After determining the actual filenames to be used and/or created by the run, these files are assigned (linked) to their corresponding filenames used in PCGC-2. For example, the main data file is opened as PCGCIN in the main program. Assigning the filename that was specified above to PCGCIN allows the specified data file to be opened. The filenames that are opened by PCGC-2 are listed below.

PCGCIN	--	Main data file
THERMO	--	Thermo data file
INLET	--	Inlet data file
GRIDS	--	Grid data file
PCGCUT	--	Main output file
INOUT	--	Main restart file
RSNXIO	--	NO _x restart file
TBLRST	--	Chem. equilibrium restart file
PARSOU	--	Particle restart file
PLOT1	--	Particle plot file 1
PLOT2	--	Particle plot file 2
PLOT3	--	Particle plot file 3
GASPLT	--	Gas phase plot file

POLPLT -- Pollutants plot file
PRGRSS -- Progress file

After assigning (linking) the above file names, PCGC-2 is compiled and linked, using the most recent version of each subroutine. This step is especially important if any code development work is being done. There are some very useful utilities which automate this step on both VAX and UNIX systems (i.e. USE, MAKE files). Examples are shown in Appendix E.

After assigning (linking) the actual file names to the file names used in PCGC-2 and compiling and linking the program (if necessary), the program is executed. Instructions to access the batch queues are included in this step. After the program has finished executing, all of the assigned variables are deassigned (links broken).

B. FORTRAN AND MACHINE INCOMPATIBILITIES

PCGC-2 was developed on a VAX/11-750 computer with VMS operating system. Significant effort has been expended to make the code compatible with Fortran-77 standards. However, a few VAX Fortran extensions remain. These present potential problems when running the code on a different machine as discussed below.

1. Hollerith strings are read and stored using the A format. Four letters are stored per word in this case. Other machines may not operate this way.
2. Some of the COMMON variables in PCGC-2 have the same name as the COMMON BLOCK in which they are contained. Many compilers will not allow this. Furthermore, some compilers do not allow different variable types (character, floating-point, integer) to be contained in the same COMMON BLOCK. This is a common occurrence in PCGC-2.
3. Most of the variables used in PCGC-2 are initialized (to zero or some other number), but some are not. PCGC-2 assumes that all of the memory registers that are to be allocated for its use will be initialized to zero before execution. Most compilers normally do this automatically, or have an option to do it. If the compiler being used cannot perform this initialization of allocated memory, a significant effort may be required to insure that all variables are initialized before they are used.
4. PCGC-2 assumes that all local variables (variables unique to only one subroutine) are saved in memory for use next time that subroutine is called. Compilers which do not automatically save local variables will require the addition of a standard Fortran 77 SAVE statement to each subroutine.
5. There are instances where PCGC-2 branches into DO loops. Similarly, there are other instances where PCGC-2 branches to the last CONTINUE statement of a DO loop. This is not allowed in standard Fortran 77. The intention of these branches is that the code continue out of

the loop (the next line following the terminal statement of the loop) when it comes to the terminal statement.

6. There are a few instances where DO WHILE and ENDDO statements have been utilized. These are not standard Fortran statements, although many recent compilers have included these statements.
7. Some of the input/output files used by PCGC-2 are 'direct-access' (rather than 'sequential-access'). The direct-access feature of these files is only used for post-processing of data by graphics packages. All of the files can be changed to sequential files without changing the performance of the code. The single exception is the PRGRSS file. The purpose of this file is to print information about the code in a file that can be accessed while the code is running. Machine-specific modifications of this file may be required for it to function properly. If you are unfamiliar with this type of file you should review the Fortran manual supplied with your computer. The syntax of the READ and WRITE statements for these files can differ between compilers.
8. Before closing restart, plotting and some other sequential files, it may be necessary to REWIND them so that they will be written from the beginning the next time they are opened. Otherwise, they may be appended, defeating their purpose and consuming large amounts of memory.
9. PCGC-2 frequently calls a subroutine called CPUTIM. CPUTIM uses a VAX/VMS utility called SYS\$GETJPI, which allows PCGC-2 to monitor the amount of CPU time it uses in various subroutines. If this feature is desired, modifications should be made so that CPUTIM can access the internal timing device of the computer it is being run on. See the CPUTIM and GETCPU subroutines for the exact use of this function. If it is not needed, calls to CPUTIM can be easily commented out, or dummy variables can be passed back from CPUTIM to PCGC-2.

CHAPTER VI. SAMPLE PROBLEMS

Four sample problems are presented in this chapter: methane combustion, coal combustion, high-pressure gasification, and coal-water mixture combustion. Input data files for all cases are included in the appendices and are available on magnetic tape with the licensing of the program as explained in Chapter I. Run id's are shown in parentheses. The output files are too large to include here, but are included on the tape.

A. METHANE COMBUSTION CASE (METH)

This sample problem is the combustion of methane in oxygen. Methane is fed at room temperature in the primary stream, and oxygen is fed at room temperature in the secondary stream. Neither stream is swirled. The reactor is at atmospheric pressure and is assumed to be adiabatic, i.e. the energy equation is not solved explicitly. Important parameters for the problem are shown in Table 25, and the inlet files are contained in Appendix F.

B. PULVERIZED COAL COMBUSTION CASE (ASAYSUB)

This sample problem is the combustion of coal in air. Pulverized coal entrained in air is fed at room temperature in the primary stream. The secondary air is preheated and swirled. The reactor is at atmospheric pressure. The coal is a subbituminous coal. Other important parameters are shown in Table 26. The case uses nine chemical species and fifty particle trajectories. Input files are included in Appendix G. The thermo file is not included because it is similar to the one shown in Appendix F. The inlet data file shows how to input experimental data, in this case for turbulence intensity. A grid file is shown, which can be used to alter the node locations, add nodes (up to 40 in each direction), add intrusions, and/or add additional inlets (up to 3) as discussed in Chapters III and IV.

The VAX/VMS "log" file for this case is also included in Appendix G. Information (identifying the computation) was first printed out, followed by a figure showing the important node locations. As shown in the figure, and as also shown in the grid file in Appendix G, this problem used a 29x34 grid. Next, a header was printed out for the gas phase solution. Next, the physical properties table was generated. Because the energy equation was solved in this case (INCALH is set to T in the main data file), the table is a function of three independent variables: gas mixture fraction (f), coal gas mixture fraction (n), and residual enthalpy (h_r). A message was printed out showing the total number of times the equilibrium algorithm failed to converge during table generation. In this particular case, there were 61 failures. All of these failures correspond to points in the table where the residual enthalpy was negative and greater in magnitude than the adiabatic enthalpy for the particular f and n . As explained in Section VI.E, the mathematical solution for this situation corresponded to a temperature less than absolute zero, hence the reason for the failures. Even though there were 61 failures, this corresponds to only a relatively small region of the table, since there are a total of 858 points in the table (11 points in the n direction, 6 in the h_r direction, and 13 in the f direction). The exact points that failed to

TABLE 25
PARAMETERS FOR METHANE COMBUSTION CASE

<u>Geometry</u>	
Primary tube diameter (m)	0.016
Secondary tube diameter (m)	0.057
Chamber diameter (m)	0.203
Chamber length (m)	1.520
<u>Feed Rates</u>	
Primary gas (kg/s)	3.100E-03
Secondary gas (kg/s)	0.012
<u>Inlet Gas Properties</u>	
Primary swirl number	0.000
Primary turbulent intensity	10.0
Primary temperature (K)	298.0
Primary mole fractions:	
CH ₄	1.000
Secondary swirl number	0.000
Secondary turbulent intensity	10.0
Secondary temperature (K)	298.0
Secondary mole fractions:	
O ₂	1.000
<u>Reactor Parameters</u>	
Reactor pressure (N/sq.m)	1.013E+05
Side wall temperature (K)	1000.0

TABLE 26
PARAMETERS FOR PULVERIZED COAL COMBUSTION CASE

<u>Geometry</u>	
Primary tube diameter (m)	0.022
Secondary tube diameter (m)	0.084
Chamber diameter (m)	0.203
Chamber length (m)	1.561
<u>Feed Rates</u>	
Primary gas (kg/s)	6.228E-03
Secondary gas (kg/s)	0.019
Coal in primary (kg/s)	2.853E-03
<u>Inlet Gas Properties</u>	
Primary swirl number	0.000
Primary turbulent intensity	15.0
Primary temperature (K)	300.0
Primary mole fractions:	
AR	0.046
H ₂ O	0.035
N ₂	0.725
O ₂	0.194
Secondary swirl number	2.000
Secondary turbulent intensity	18.0
Secondary temperature (K)	589.0
Secondary mole fractions:	
AR	0.009
N ₂	0.781
O ₂	0.210
<u>Reactor Parameters</u>	
Reactor pressure (N/sq.m)	8.600E+04
Side wall temperature (K)	1000.0
<u>Particle Parameters</u>	
Particle solid density (kg/cu.m)	1340.0
Heat of formation, daf (J/kg)	5.611E+05
Mass mean particle diameter (m)*	5.025E-05
Initial analysis:	
raw coal	0.931
ash	0.069
Elemental analysis (daf):	
C	0.724
H	0.047
O	0.218
N	0.012

*Continuous distribution simulated with 5 discrete sizes.

converge, as well as the temperature for the points that did converge can be seen in the output file (not included here because of its size, but available with the program on magnetic tape).

After generating the table, the first gas phase iteration began. As shown, information was printed out for the first iteration and every 5 gas macro-iterations thereafter. This corresponds to Steps 2 and 3 in Figure 7. Residual source sums were printed out for u-velocity, v-velocity, w-velocity, mass source term, pressure, enthalpy, mixture fraction, and coal-gas mixture fraction. The maximum of these source sums was printed to the left. At the far right, is shown the number of potential calls to CREE, or the number of times equilibrium properties were needed for a value of residual enthalpy that was outside the table limits. As shown in the main input file, upper (HRMAX) and lower (HRMIN) bounds of 10.0 and -410.0 percent (for the residual enthalpy, respectively, were used initially. This means the upper bound was initially 10 percent of the total enthalpy contained in the inlet streams. Similarly, the lower bound was -410 percent of the total inlet enthalpy initially. As shown in the log file, after the first gas-phase iteration, the program automatically adjusted HRMIN from -410.0 to -40.0 and generated a new table. After the fifth iteration, it adjusted HRMIN to -240.0 and then converged the gas phase with 59 potential calls to CREE.

After the gas phase was calculated, the gas properties were updated (Step 4, Figure 7) and then the Eulerian particle density field was calculated (Step 5, Figure 7). The bulk velocity of the particles is assumed equal to that of the gas, with the particles diffusing according to the concentration gradient. This calculation is indicated in the log file by the brief header starting with "NJITER" shown following the gas phase. Residual source sums for each of the allowable five particle sizes are printed out in a manner similar to the source sums for the gas phase every five iterations. For this case, this calculation always converged in less than 5 iterations, and so only the header is shown, with no numerical information below.

After the particle density fields were calculated, the radiation field was solved (Step 6, Figure 7). In this case, the discrete ordinates method was used (LDISO = T in the main input file of Appendix G). As shown in the log file, the radiation model is solved alternately without (SCATTER ITER: 0) and with (SCATTER ITER: 1) radiation scattering by particles included. A total of seven iterations were required the first time without scattering followed by three iterations to converge with scattering. Iteration continued until the change in total net wall flux fell below a prescribed level.

After solving the gas phase, particle density, and radiation fields, the Lagrangian particle calculation was performed (Steps 7-10, Figure 7). The assumption for this case was that if particles hit the wall, they stick. The other option available in PCGC-2 is that the particles rebound off the wall at the same angle that they approached it. For each particle size and starting location, the terminating location, transit time, and number of iteration steps are shown. If the trajectory recirculated, it was so noted. Four trajectories recirculated during the first particle calculation for this case. After the particle trajectory information, a summary of the solid phase coupling was printed. This is the sum of the particle source terms for all of the gas cells for n , f , mass, u-velocity, v-velocity, and enthalpy. Since this is a coal combustion case, the values for SSPE (n) and SSPM (mass) are

identical, since the only source of mass to the gas phase is from the coal. For coal-water mixture combustion, the variable f is used to track the mixing of the moisture from the coal-water mixture droplets, and both SSPE and SSPF would be non-zero, with SSPM being the sum of both. The solid coupling for enthalpy (SSPH) is zero because the gas-particle convective source term in the energy equation is turned off (LSPH set to F), as indicated by the value of LSPH in the main data file. As explained in Chapter IV, the code is not currently stable when this term is included, and its effects can be shown to be relatively minor. Finally, the cumulative particle burnout was printed for the outlet location of the reactor. After the particle phase was calculated, the gas phase was recalculated, using the new particle source terms.

This case converged from scratch (no restart files were used) in 12 particle iterations. A total of approximately 1800 gas-phase macro-iterations were required. The progress toward convergence is plotted in Figure 39. The maximum residual source sum of the first iteration and number of iterations required to converge the gas phase are shown for each macro-iteration. The convergence criterion which finally terminated the calculation was the SORMIN criterion. After the 11th particle iteration, the maximum residual source sum for the gas phase during the first iteration was 0.092, which is less than the value of 0.1 specified for SORMIN in the main data file. The gas phase was converged one more time, followed by one more particle iteration. For the final gas phase calculation, only 17 macro-iterations, were required, which is less than the value of 25 specified for MINITP, thus satisfying the other criterion for overall convergence. Only the SORMIN criterion or the MINITP criterion need be satisfied to terminate the code, but both were satisfied in this case.

During the first macro-iteration, the gas phase was converged with 59 potential calls to CREE (residual enthalpy outside table limits). During the second macro-iteration, the gas phase was converged with 13 potential calls to CREE. During the third macro-iteration, the program automatically adjusted the table limits (regenerating the table each time) until the gas was converged with zero potential CREE calls. The bounds of the table were kept as narrow as possible while maintaining zero potential calls to CREE. During the fourth and subsequent macro-iterations, only minor adjustments of the table boundaries were occasionally needed to maintain this condition. These adjustments were performed automatically by the program.

Following the convergence of the main calculation, the NO_x model was called. Residual source sums for every two iterations as well as the pollutant levels at the outlet are shown. Finally the total CPU time is shown for the various portions of the program where the calculation took place. TPROPS represents the cumulative time spent in calculating physical properties (which in this problem was performed with the aid of an equilibrium table). Even when equilibrium values are calculated only once and stored in a table, the time required to look up and interpolate these values to perform the integrations over probability density functions is large. TEOLP is the time spent on the Lagrangian particle calculations. TTABLE is the time spent on generating the equilibrium table. TGRID is the time for generating the grid. TPRINT is the time spent writing to the output files. TCALCUP and TCALC represent the time spent in calculating the gas-phase variables. TRST is the time spent in reading and writing restart information. And finally,

Figure 39. Convergence of pulverized coal combustion sample problem.

TPLOTS is the time spent writing information for plotting. As shown, this case required nearly 35 hours on a VAX 750.

C. HIGH-PRESSURE COAL GASIFICATION CASE (UTAZ45)

This sample problem is the gasification of Utah bituminous coal in oxygen at 4.08 atmospheres in the BYU gasifier (Azuhata et al., 1986; Nichols, 1985). Figure 40 shows a schematic of the gasifier, which was operated in the down-fired mode. The injector located at the top center consists of a primary feed tube with a concentric secondary. Both coal and oxygen were fed in the primary stream. A small amount of nitrogen was fed in the secondary to simulate a nitrogen purge stream that was used to keep the visual observation window clean. Important parameters are shown in Table 27, and input files are included in Appendix H.

Three trials were made for this case, corresponding to heat loss factors of 0.0 (adiabatic), 0.30 and 0.45. Results are plotted in Figures 41-45. Figure 41 is a plot of the centerline temperature profiles for each trial. The major species are plotted against the experimental data in Figure 32 for the 0.30 heat loss factor solution. Figures 43-45 illustrate two-dimensional NO profiles for the experimental measurements and NO_x submodel predictions.

D. COAL-WATER MIXTURE COMBUSTION CASE (CWM)

This sample problem simulates the BYU coal-water mixture combustor. The primary stream consists of a slurry of coal particles in water suspended in air at room temperature. A secondary stream consisting of preheated air is swirled around the primary. Important parameters for the problem are shown in Table 28, and input files are included in Appendix I. As shown in the main input file, a mass source term must be included in the "f" equation, since f is used to track the mixing of moisture from the slurry rather than the mixing of primary and secondary gas. This was discussed in Chapter IV. Using f this way rather than adding another progress-of-mixing variable means that the mixing of primary and secondary gas cannot be tracked in PCGC-2 for coal-water mixtures. However, this is not usually a concern in coal-water mixture combustion, because both the primary and secondary gas streams are typically identical, e.g. pure air. If one wanted to model coal-water mixture gasification, with the secondary stream being pure oxygen, an additional progress variable would be required. The f equation does not normally have a source term because the total amount of gas that originated from the primary and secondary streams is fixed. However, the amount of gas that originated from the slurry water changes as the water evaporates.

Inclusion of the source term in the f equation is controlled by the logical variable INFSOU. The value of FFLOW is set to zero for both the primary and secondary inlets, meaning that the inlet gas contains none of the slurry moisture. The weight fraction of the slurry that is liquid water is specified with the variable OMEGAW. The component ID for the liquid is indicated with the variable SLRCMP (e.g. H₂O). The slurry component ID must also be present in the thermo data file.

Figure 40. Schematic diagram of high pressure entrained gasifier.

TABLE 27

PARAMETERS FOR HIGH PRESSURE COAL GASIFICATION CASE

<u>Geometry</u>	
Primary tube diameter (m)	0.013
Secondary tube diameter (m)	0.029
Chamber diameter (m)	0.200
Chamber length (m)	1.730
<u>Feed Rates</u>	
Primary gas (kg/s)	0.011
Secondary gas (kg/s)	4.170E-03
Coal in primary (kg/s)	9.011E-03
<u>Inlet Gas Properties</u>	
Primary swirl number	0.000
Primary turbulent intensity	10.0
Primary temperature (K)	367.0
Primary mole fractions:	
AR	0.132
H ₂ O	0.094
O ₂	0.774
Secondary swirl number	0.000
Secondary turbulent intensity	10.0
Secondary temperature (K)	367.0
Secondary mole fractions:	
N ₂	1.000
<u>Reactor Parameters</u>	
Reactor pressure (N/sq.m)	4.137E+05
Side wall temperature (K)	1000.0
<u>Particle Parameters</u>	
Particle solid density (kg/cu.m)	1340.0
Heat of formation, daf (J/kg)	-1.504E+06*
Mass mean particle diameter (m)	3.238E-05
Initial analysis:	
raw coal	0.839
ash	0.161
Elemental analysis (daf):	
C	0.797
H	0.063
O	0.118
N	0.017
S	0.006

*Continuous distribution simulated with 5 discrete sizes.

Figure 41. Predicted centerline temperature profiles for high pressure (~5 atm) gasification of Utah bituminous coal at heat loss factors of 0.0 (adiabatic), 0.30, and 0.45.

Figure 42. CO, CO₂, and H₂ radial profiles of PCGC-2 predictions (—) and experimental data (Azuhata et al., 1986), for high pressure gasification of Utah bituminous coal. Open symbols are measured values.

Figure 43. Contour map of measured nitrogen oxide concentrations (Brown, 1985) for high pressure (~5 atm) gasification of a Utah bituminous coal. Experimental measurements made in BYU Combustion Laboratory gasifier.

Figure 44. Contour map of theoretical nitrogen oxide concentrations for high pressure (~5 atm) gasification of a Utah bituminous coal with a reactor heat loss factor of 0.30.

Figure 45. Contour map of theoretical nitrogen oxide concentrations for high pressure (~5 atm) gasification of a Utah bituminous coal with a reactor heat loss factor of 0.45.

TABLE 28
PARAMETERS FOR COAL-WATER MIXTURE CASE

<u>Geometry</u>	
Primary tube diameter (m)	0.003
Secondary tube diameter (m)	0.145
Chamber diameter (m)	0.350
Chamber length (m)	3.000
<u>Feed Rates</u>	
Primary gas (kg/s)	4.868E-03
Secondary gas (kg/s)	0.031
Coal in primary (kg/s)	6.961E-03
<u>Inlet Gas Properties</u>	
Primary swirl number	0.000
Primary turbulent intensity	20.0
Primary temperature (K)	295.2
Primary mole fractions:	
H ₂ O (L)	1.000
Secondary swirl number	1.500
Secondary turbulent intensity	20.0
Secondary temperature (K)	688.4
Secondary mole fractions:	
AR	0.020
HE	0.020
N ₂	0.757
O ₂	0.204
<u>Reactor Parameters</u>	
Reactor pressure (N/sq.m)	8.546E+04
Side wall temperature (K)	1100.0
<u>Particle Parameters</u>	
Particle solid density (kg/cu.m)	1214.3
Heat of formation, daf (J/kg)	-2.682E+06
Mass mean particle diameter (m)*	4.600E-05
Initial analysis:	
raw coal	0.480
ash	0.080
water	0.440
Elemental analysis (daf):	
C	0.753
H	0.047
O	0.173
N	0.015
S	0.013

*Continuous distribution simulated with 5 discrete sizes.

NOMENCLATURE

<u>Symbol</u>	<u>Units</u>	<u>Definition</u>
a	---	Size parameter $\pi d/\gamma$
a_0	---	Asymmetry factor
A	varies	Pre-exponential factor
A	kg s^{-1}	Total coefficient (convection plus diffusion)
A, B	m^2	Area
b	---	Element mass fraction, back scatter, order of reaction in NO_x model
$\bar{b}, \bar{f}, \bar{g}$	---	Backward-, forward- and side-scattered components
B	---	Blowing parameter
c	varies	Variable constant
C	---	"Universal" constant
C	kg m^{-3}	Concentration
C	kg s^{-1}	Convection coefficient
C	(VFM)	Pressure-correction factor, coefficients
C_p	$\text{J kg}^{-1} \text{K}^{-1}$	Heat capacity
C_d	---	Drag coefficient
D, d	m	Diameter
D	kg s^{-1}	Numerical coefficient for diffusion
D	$\text{m}^2 \text{s}^{-1}$	Diffusivity
E	kW/m^2	Emissive power
E	J/kmol^{-1}	Activation energy
E	---	Constant in the law of the wall.
f	---	Mixture fraction, interpolation factor, forward scatter
f	N m^{-2}	Drag force
f	---	Differencing factor
f_p	---	Mixture fraction corrected for η
F	$\text{J m}^{-2} \text{s}^{-1}$	Radiation flux
F	---	Adjusted mixture fraction (in PDF)
F	kW/m^2	Radiative flux-sum
g	m s^{-2}	Gravitational acceleration
g	---	Mean square fluctuation (variance)

<u>Symbol</u>	<u>Units</u>	<u>Definition</u>
G	$\text{kg m}^{-2} \text{s}^{-1}$	Mass flux
G	---	Adjusted variance
h	J kg^{-1}	Enthalpy
hg	J kg^{-1}	Enthalpy of reaction
i	---	Imaginary ($i^2 = -1$)
I	varies	Turbulence intensity, radiation intensity
j	$\text{kg m}^{-2} \text{s}^{-1}$	Mass flux
k	$\text{m}^2 \text{s}^{-2}$	Kinetic energy of turbulence
k	varies	Constant, kinetic rate coefficient
k	$\text{J m}^{-1} \text{K}^{-1} \text{s}^{-1}$	Thermal conductivity
k_a, k_s, k_t	m	Absorption, scattering and extinction coefficients
K	---	Scattering coefficient
K	---	Absorption coefficient
l	m	Mean beam length
L	---	Lower limit
L	m	Length
M, m	---	Mass fraction of species
M	kg kmol^{-1}	Molecular weight
$\dot{m}, \dot{M}$	kg s^{-1}	Mass flow rate
M	kg	Mass of fluid atoms
n	---	Direction normal to boundary
n	---	Order of discrete ordinates approximation
n	m^{-3}	Particle number density
$\dot{n}$	s^{-1}	Particle number flow rate
N	---	Total number of directions used
Nu	---	Nusselt number
p, P	N m^{-2}	Pressure
ℓ	m	Length scale
P	---	Probability density function (PDF), phase function, P cells
P	---	Scattering phase function
Pr	---	Prandtl number
q	$\text{J m}^{-2} \text{s}^{-1}$	Heat flux

<u>Symbol</u>	<u>Units</u>	<u>Definition</u>
q	kW/m^2	Net flux
$q^\pm$	kW/m^2	Hemispherical flux
q_R	kW/m^3	Net radiative exchange for a volume element
Q	J s^{-1}	Heat flow
Q_a, Q_s	---	Absorption and scattering efficiency
Q_R	kW	Net radiative exchange for a single particle
r, R	M	Radius, radial direction
r	kg s^{-1}	Reaction rate
r, x	m	Distance along radial and axial directions
R	$\text{J kmol}^{-1} \text{K}^{-1}$	Universal gas constant
Re	---	Reynolds number
s	---	Scattering factor, conserved scalar
S	varies	Source term
Sc	---	Schmidt number
Sh	---	Sherwood number
T, t	s	Time, time period
T	K	Temperature
u	m s^{-1}	Axial velocity
U	---	Upper limit
v	m s^{-1}	Radial velocity, velocity vector
V	m^3	Volume
w	m s^{-1}	Tangential velocity
w	$\text{kgmol m}^{-3} \text{s}^{-1}$	Individual reaction rate
W	$\text{kg m}^{-3} \text{s}^{-1}$	Overall species reaction rate
w_m	sr	Angular quadrature weight
x	m	Axial position
X	---	Particle size function
X	---	Mole mass fraction
y	---	Species mole fraction, fluctuating mass fraction
Y	---	Volatiles coefficient, particle starting location fraction
Z	---	Arbitrary variable

Greek Symbols

α	---	Intermittency factor
α	kg	Mass
β	---	Intermittency
β	varies	Arbitrary property
γ	---	Heat loss factor
γ	---	Particle swelling coefficient
Γ	varies	Exchange coefficient
δ, Δ	---	Difference operator
ϵ	$\text{m}^2 \text{s}^{-1}$	Dissipation rate of turbulence energy
ϵ	---	Emissivity
ζ	---	Fraction of heat of reaction given to particle phase
ζ	---	Constant in NO_x model
ζ	---	Pore diffusion adjustment factor
ζ	---	Surface area factor
η	---	Coal gas mixture fraction
H	radians	Azimuthal direction
κ	---	Constant
λ	---	Under-relaxation factor
μ	$\text{kg m}^{-1} \text{s}^{-1}$	Dynamic viscosity
ν	$\text{m}^2 \text{s}^{-1}$	Kinematic viscosity
ξ	s^{-1}	Vorticity
ξ	---	Dimensionless coordinate of integration
π	---	Percentage perturbation
ρ	kg m^{-3}	Density
σ	---	Schmidt or Prandtl number
τ	$\text{m}^2 \text{s}^{-2}$	Shear stress
ϕ	varies	General variable
ϕ	---	Angle between incident and scattered intensities
Φ	$\text{kg m}^{-1} \text{s}^{-1}$	Dissipation function
Ψ	$\text{m}^2 \text{s}^{-1}$	Stream function
ω_0	---	Albedo for forward radiation scattering
Ω	---	Collision integral

<u>Greek Symbols</u>	<u>Units</u>	<u>Definition</u>
Ω	---	Differencing scheme coefficient
Ω, Ω'	---	Outward and inward directions of radiation
θ, ψ	---	Polar and azimuthal angles/directions
λ	m	Wavelength of radiation
ω_0	---	Albedo of scatter
μ, η, ξ	---	Direction cosines

<u>Subscripts</u>	<u>Definition</u>
a	Absorptive, ash, arbitrary
b	Black-body, bulk, boundary, backward scattering
B	Boundary
c	Cell, pure coal off-gas, convective, raw coal
d	Direction, diffusive, drag
E, e	East direction, effective
f	Mixture fraction, formation
F	Radiation flux
F	Furnace
g	Mean square fluctuations (variance), gas
g	Gas
g1, g2	Universal (found empirically)
h	Enthalpy, char
i	Gas species index, summation index
i, j	Area indices in the radial and axial directions, jth particle size
I	Pure inlet gas
j	Particle size, gas species index
k	Turbulent kinetic energy, element
l	Char reaction index
m	Devolatilization reaction index, mass, mixture
m, m'	Directions of the discrete ordinates
n	Number density
N, n	North direction

Subscripts

N	Nitrogen
o	Initial, oxidizer
P, p	Primary stream, particle, P-cell
ref	Reference
r	Reactor, radial, radiation
s	Secondary stream, scattering, south direction
S	South direction, source
t	Turbulence
T	Temperature
u	Axial velocity, u cell
U	Non-proportional part of source term
v	Radial velocity, v cell, volatiles, devolatilization
w	Wall
W, w	West direction
x, z	Axial direction
ϵ	Dissipation rate
η	Coal gas mixture fraction
θ	Azimuthal direction
μ	Viscosity
σ	Solid
ϕ	General variable
λ	Coal component
0	Initial value

Superscripts

c	Corrected
f	Frozen
h	Enthalpy
k	Turbulent kinetic energy
l	Laminar
m	Mass

DefinitionDefinition

SuperscriptsDefinition

n	Temperature coefficient
o	Standard or reference
p	P cell
r	Radial direction
t	Turbulent
T	Temperature
u	Axial velocity, u cell
v	Radial velocity, v cell
x	Axial direction
*	Guessed
→	Vector
≡	Tensor
-	Reynolds mean
~	Favre mean
'	Fluctuation, flux
ε	Dissipation of turbulent kinetic energy
η	Coal gas mixture fraction
f	f mixture fraction
μ	Viscosity
ρ	Density
φ	Arbitrary variable
±	Positive and negative directions of propagation

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APPENDIX A
HELP FILE FOR INPUT FILE EDITING PROGRAM
(PCEDIT)

THIS IS THE HELP FILE FOR THE EDITOR
FOR PCSON DATA FILES

The editor is divided into two levels. At the first level you may choose the section of data file which you want to edit, or exit the editor. If you choose a section of the data file to edit, you will enter the second level. In the second level you may choose the variable(s) you wish to edit. However, you may not (gracefully) exit the editor from the second level. If you wish to exit the editor from the second level, type NEXT, which will return you to the first level.

Note that the first level expects a single letter as a response to the prompt and does not require a <RETURN> after entering the letter. The second level requires a number of letters followed by a <RETURN>.

The appropriate commands for the each level of the editor are explained below.

FIRST LEVEL COMMANDS

When you are queued with the standard prompt:

PCGC-2:BYU >>>>

then you must respond with a choice of the section of the input data file you wish to edit. Note, no carriage return is required, simply enter the symbol. These choices are as follows:

B ::: BNDRY :: This choice will edit the inlet boundary conditions for the three components of velocity, turbulent kinetic energy, and dissipation length scale read into PCGC-2 in the subroutine named PROFILE.FOR

C ::: COALO :: This choice will edit the coal property variables read into PCGC-2 in the subroutine named COALO.FOR.

E ::: EXIT ::: This choice will allow you to exit from this editor.

H ::: HELP ::: This choice (or any other choice not listed) will type this help file.

I ::: INLET :: This choice will edit the inlet flowrates, temperatures, turbulent intensities, etc. of all inlet streams. These variables are read into PCGC-2 in the subroutine called INFLOW.FOR

M ::: MAIN ::: This choice will edit the variables read into PCGC-2 in the main routine; namely, PCGC2.FOR.

N ::: NOX ::: This choice will edit the NOx pollutant variables read into PCGC-2 in the subroutine entitled NOXPM.FOR.

T ::: THERMO :: This choice will edit the thermodynamic variables read into PCGC-2 in the subroutine entitled CREEC.FOR.

P ::: PSICT0 :: This choice will edit the particle properties that are read into PCGC-2 in the subroutine named PSICT0.FOR.

R ::: RAD ::: This choice will edit the radiation property variables read into PCGC-2 in the subroutine named FLUX0.FOR.

SECOND LEVEL COMMANDS

Once you have reached the section of the input file which you are going to edit you will receive a new prompt; the specific prompt depends on the section you are editing.

At this level you must respond to the prompt with one of the following responses followed by a carriage return:

ALL -----This will allow you to look at each of the variables in this section in turn and decide if you want to change the variable or not.
(A variable)---If you enter the name of any variable in this section the editor will look at that variable alone. A list of the variables can be found in the user's manual. If the variable is an array, do not enter the parenthesis with the variable name. The editor will cycle through all of the elements of the array.
NEXT-----This will cause the editor to leave this section of the input data and return you to the upper level with the normal prompt as noted above.
HELP -----This will type this help message again.

Values for the variables should be entered according to the following general rules.

REAL NUMBERS. Real numbers may be entered in either decimal form, such as 72.35, or exponential form, such as 7.235E1. A carriage return will leave the value of the variable unchanged.

INTEGERS. Decimal points may not be included in integer values.

LOGICAL VALUES. Appropriate responses for logical values are T and F. Anything other than a T or F will not effect the value of the logical variable.

Entering only a <RETURN> will leave the current value of the variable unchanged.

-----Good Luck-----

APPENDIX B

DESCRIPTION OF SUBROUTINES

A description of the routines used in PCGC-2 is given in this appendix. The description is organized in outline form, with called routines subordinate to the calling routines. Routines with more than one calling routine appear several times. The order is in general order of calling sequence. Each called routine is shown only once for a given calling routine, even though that calling routine may call the subordinate routine more than once. Entry points are shown with the name of the subroutine to which they belong in parentheses.

PCGC-2	1
I. INFLOW	1
II. GRID	1
III. GRMAP	1
IV. GRDGRF	1
V. CREED	1
A. HCPS	1
VI. INIT	1
A. PROFIL	1
VII. PSICT0	1
VIII. COALO	1
A. PEJ	1
B. CREE	1
C. ERATIO (SPECE)	1
D. HCPS	1
E. FSIFE	1
IX. FLUX0	1
X. NOXMN0	1
XI. TABLE	1
A. TBLF	1
B. TBLFE	2
C. TBLFEH	2
D. TBLFH	2
XII. PROFIL	3
XIII. PRINT	3
XIV. RESRT	3
XV. FLINT	3
XVI. EULINT (PSICT0)	3
XVII. PROPS	3
A. FGTabl	3
B. ERF	3
C. CREE	3
D. UPDATE (TABLE)	3
XVIII. STREAM	3
XIX. PLTWRT	3
XX. CALC Routines	3
A. CALCP	3
B. CALCU	4
C. CALCV	4
D. CALCPP	4
E. CALCW	4
F. CALCTE	4
G. CALCED	4
H. CALCH	5
I. CALCET	5
J. CALCF	5
K. CALGGE	5
L. CALCG	5
M. CALCYFU	5
XXI. PROG	5
XXII. EOLP	5
A. CALCNJ	5
B. EULINT (PSICT0)	5
C. CALACJ	5
D. CALAHJ	6
E. PSOLVP (PSOLVE)	6
F. FLUX	6
G. PRINT	6
H. BVALIN (BPROPS)	7
I. PSICT	7
J. BVALOUT (BPROPS)	7
XXIII. NOXMN	7
A. EQSPEC	7
B. FREACT (RATE)	8
C. RSTNOX	8
D. PSCRAT (RATE)	8
E. PRISUR	8
F. RATE	8
G. CALCNO	9
H. CALHCN	9
I. CALO2 (RATE)	9
J. INTGRT	9

PCGC-2

Main driver routine for PCGC-2. Reads basic input data for grid site, inlet conditions, etc. Calls all CALC subroutines for calculating gas variables, as well as PSICT and FLUX. Determines convergence criterion and stops program when converged.

I. INFLOW

Reads flowrates and properties of incoming streams.

II. GRID

Sets up numerical grid used to solve the equations.

III. GRMAP

Reads location of user-specified grid points from data file. Also writes calculated grid points into data file.

IV. GRDGRF

Makes visual output of grid for interactive program users.

V. CREE0

This is strictly an initializing routine, the sole function of which is to read, store, and process data from input files. The initial statements in CREE0 cause branching to appropriate chapters, depending on which of the key words ELEM, THER, REAC, or a blank field are encountered. Data fields must be in the order given, as element data are needed in order to catalog thermodynamic data.

A. HCPS

Auxiliary subroutine for thermochemical equilibrium computations.

VI. INIT

Initializes FORTRAN arrays for all field variables.

A. PROFIL

Reads in parameters governing inlet profiles of U (axial velocity), V (radial velocity), W (tangential velocity), TE (turbulence kinetic energy), and ED (eddy dissipation rate), and then initializes the inlet boundary.

VII. PSICT0

Reads initial particle information and initialized particle trajectory parameters.

VIII. COALO

Reads input coal parameters and sets up initial coal properties.

A. FEJ

Function for calculating vapor pressure and enthalpy of vaporization for liquid component of slurry and fuel oils.

B. CREE

This is the main controlling routine for the thermochemical equilibrium calculations (Chemically Reacting Equilibrium, from Elemental balances).

1. ERATIO (SPECE)

Calculates fuel/air equivalence ratio given atom numbers using positive and negative oxidation states (valences).

2. SPECE

Auxiliary subroutine for the CREE thermochemical equilibrium computations.

a) CALC

Auxiliary subroutine for the CREE thermochemical equilibrium computations.

b) HCPS

Auxiliary subroutine for thermochemical equilibrium computations.

3. HCPS

Auxiliary subroutine for thermochemical equilibrium computations.

C. ERATIO (SPECE)

Calculates fuel/air equivalence ratio given atom numbers using positive and negative oxidation states (valences).

D. HCPS

Auxiliary subroutine for thermochemical equilibrium computations.

E. PSIFE

Calculates stoichiometric mixture fraction (adiabatic reactor with F and ETA).

1. ERATIO (SPECE)

Calculates fuel/air equivalence ratio given atom numbers using positive and negative oxidation states (valences).

IX. FLUX0

Reads input data for radiation flux subroutines and initializes radiation parameters.

X. NOXMN0**XI. TABLE**

Sets up table of equilibrium gas properties (RHO, XMW, TG) as a function of F (inlet gas mixture fraction), ETA (coal gas mixture fraction), and/or HR (residual gas enthalpy).

A. TELF

Sets up gas equilibrium properties table as function of F (inlet gas mixture fraction) (gas only and adiabatic reactor).

1. CREE

This is the main controlling routine for the thermochemical equilibrium calculations (Chemically Reacting Equilibrium, from Elemental balances).

a) ERATIO (SPECE)

Calculates fuel/air equivalence ratio given atom numbers using positive and negative oxidation states (valences).

b) SPECE

Auxiliary subroutine for the CREE thermochemical equilibrium computations.

(1) CALC

Auxiliary subroutine for the CREE thermochemical equilibrium computations.

(2) HCPS

Auxiliary subroutine for thermochemical equilibrium computations.

c) **HCPS**

Auxiliary subroutine for thermochemical equilibrium computations.

2. FSIF

Calculates stoichiometric mixture fraction (gas only and adiabatic reactor).

a) **ERATIO (SPECE)**

Calculates fuel/air equivalence ratio given atom numbers using positive and negative oxidation states (valences).

B. TBLFE

Sets up table of equilibrium gas properties as function of F (inlet gas mixture fraction) and ETA (coal gas mixture fraction).

1. CREE

This is the main controlling routine for the thermochemical equilibrium calculations (Chemically Reacting Equilibrium, from Elemental balances).

a) **ERATIO (SPECE)**

Calculates fuel/air equivalence ratio given atom numbers using positive and negative oxidation states (valences).

b) **SPECE**

Auxiliary subroutine for the CREE thermochemical equilibrium computations.

(1) **CALC**

Auxiliary subroutine for the CREE thermochemical equilibrium computations.

(2) **HCPS**

Auxiliary subroutine for thermochemical equilibrium computations.

c) **HCPS**

Auxiliary subroutine for thermochemical equilibrium computations.

2. FRZFE

Calculates gas properties as a function of F (inlet gas mixture fraction) and ETA (coal gas mixture fraction) using frozen equilibrium scheme when the local equivalence ratio is greater than 2.0 (adiabatic reactor).

3. FSIFE

Calculates stoichiometric mixture fraction (adiabatic reactor with F and ETA).

a) **ERATIO (SPECE)**

Calculates fuel/air equivalence ratio given atom numbers using positive and negative oxidation states (valences).

4. MIXFE

For given mixture fraction (F and ETA), calculates fully mixed product without chemical reaction (adiabatic reactor).

5. TBLRSTFE

Reads and writes restart file for table of equilibrium gas properties.

a) **DIF**

Function that compares two numbers and returns their positive fractional difference.

C. TBLFEH

Sets up table of equilibrium gas properties as a function of F (inlet gas mixture fraction), ETA (coal gas mixture fraction), and HR (residual gas enthalpy).

1. CREE

This is the main controlling routine for the thermochemical equilibrium calculations (Chemically Reacting Equilibrium, from Elemental balances).

a) **ERATIO (SPECE)**

Calculates fuel/air equivalence ratio given atom numbers using positive and negative oxidation states (valences).

b) **SPECE**

Auxiliary subroutine for the CREE thermochemical equilibrium computations.

(1) **CALC**

Auxiliary subroutine for the CREE thermochemical equilibrium computations.

(2) **HCPS**

Auxiliary subroutine for thermochemical equilibrium computations.

c) **HCPS**

Auxiliary subroutine for thermochemical equilibrium computations.

2. FRZFEH

Calculates gas properties as function of F (inlet gas mixture fraction), ETA (coal gas mixture fraction), and HR (residual gas enthalpy, using frozen equilibrium scheme when the local equivalence ratio is greater than 2.0).

a) **HCPS**

Auxiliary subroutine for thermochemical equilibrium computations.

3. FSIFEH

Calculates stoichiometric mixture fraction (using F, ETA, and HR).

a) **ERATIO (SPECE)**

Calculates fuel/air equivalence ratio given atom numbers using positive and negative oxidation states (valences).

4. TBLRSTFEH

Reads and writes restart file for table of equilibrium gas properties as function of F (inlet gas mixture fraction), ETA (coal gas mixture fraction), and HR (residual gas enthalpy).

a) **DIF**

Function that compares two numbers and returns their positive fractional difference.

D. TBLFH

Sets up table of equilibrium gas properties as function of F (inlet gas mixture fraction) and HR (residual gas enthalpy) (gas only).

1. CREE

This is the main controlling routine for the thermochemical equilibrium calculations (Chemically Reacting Equilibrium, from Elemental balances).

a) ERATIO (SPECE)

Calculates fuel/air equivalence ratio given atom numbers using positive and negative oxidation states (valences).

b) SPECE

Auxiliary subroutine for the CREE thermochemical equilibrium computations.

(1) CALC

Auxiliary subroutine for the CREE thermochemical equilibrium computations.

(2) HCPS

Auxiliary subroutine for thermochemical equilibrium computations.

c) HCPS

Auxiliary subroutine for thermochemical equilibrium computations.

2. FSTFH

Calculates stoichiometric mixture fraction using F (inlet gas mixture fraction) and HR (residual gas enthalpy) (gas only).

a) ERATIO (SPECE)

Calculates fuel/air equivalence ratio given atom numbers using positive and negative oxidation states (valences).

XII. PROFIL

Reads in parameters governing inlet profiles of U (axial velocity), V (radial velocity), W (tangential velocity), TE (turbulence kinetic energy), and ED (eddy dissipation rate), and then initializes the inlet boundary.

XIII. PRINT

Prints output according to specified format.

XIV. RESRT

This subroutine does all the work necessary for reading and writing information necessary to restart a combustion calculation from a partially converged solution.

XV. FLINT

Initializes flow field so calculations can begin. Also initializes inlet densities.

XVI. EULINT (PSICTO)

Initializes Eulerian particle number density fields.

XVII. PROPS

Calculates gas-phase properties from the cardinal variables, including turbulence effects when appropriate.

A. FGTABLE

Calculates limits of normalized Gaussian PDF.

B. ERF

Calculates the area under the normal curve from a spline fit. This is used for values of intermittency in the turbulent combustion model.

C. CREE

This is the main controlling routine for the thermochemical equilibrium calculations (Chemically Reacting Equilibrium, from Elemental balances).

1. ERATIO (SPECE)

Calculates fuel/air equivalence ratio given atom numbers using positive and negative oxidation states (valences).

2. SPECE

Auxiliary subroutine for the CREE thermochemical equilibrium computations.

a) CALC

Auxiliary subroutine for the CREE thermochemical equilibrium computations.

b) HCPS

Auxiliary subroutine for thermochemical equilibrium computations.

3. HCPS

Auxiliary subroutine for thermochemical equilibrium computations.

D. UPDATE (TABLE)

Interpolates table values for gas properties.

1. UPF (TBLF)

Interpolates one-dimensional (F) gas properties table.

2. UPFE (TBLFE)

Interpolates two dimensional (F and ETA) gas properties table.

3. UPFEH (TBLFEH)

Interpolates three-dimensional (F, ETA, and H) gas properties table.

4. UPFH (TBLFH)

Interpolates two-dimensional (F and H) gas properties table.

XVIII. STREAM

Calculates stream lines from values of U (axial velocity) and V (radial velocity) for plotting purposes.

XIX. PLTWRT

Writes Eulerian output into appropriate output files. The output files can be used later for plotting.

XX. CALC Routines**A. CALCP**

Calculates coefficients for finite difference equation for P (pressure) and solves for the field values of P at each grid point (SIMPLER algorithm).

1. **AIM**
Matrix-solving routine. LISOLV is nearly always used instead of AIM.
 2. **LISOLV**
The tri-diagonal matrix solving routine (Based on Thomas Algorithm).
 3. **MODP (PROMOD)**
Modifies coefficients and source terms for boundary nodes so as to take boundary conditions into account for P (pressure).
 4. **UCOEF (CALCU)**
Calculates coefficients for finite difference equation for U (axial velocity).
 - a) **MODU (PROMOD)**
Modifies coefficients and source terms for boundary nodes so as to take boundary conditions into account for U (axial velocity).
 5. **VCOEF (CALCV)**
Calculates coefficients for finite difference equation for V (radial velocity).
 - a) **MODV (PROMOD)**
Modifies coefficients and source terms for boundary nodes so as to take boundary conditions into account for V (radial velocity).
- B. CALCU**
Solves for the field values of U (axial velocity) at each grid point.
1. **AIM**
Matrix-solving routine. LISOLV is nearly always used instead of AIM.
 2. **LISOLV**
The tri-diagonal matrix solving routine (Based on Thomas Algorithm).
 3. **MODU (PROMOD)**
Modifies coefficients and source terms for boundary nodes so as to take boundary conditions into account for U (axial velocity).
 4. **VCOEF (CALCV)**
Calculates coefficients for finite difference equation for V (radial velocity).
- C. CALCV**
Solves for the field values of V (radial velocity) at each grid point.
1. **LISOLV**
The tri-diagonal matrix solving routine (Based on Thomas Algorithm).
 2. **MODV (PROMOD)**
Modifies coefficients and source terms for boundary nodes so as to take boundary conditions into account for V (radial velocity).
- D. CALCPP**
Calculates coefficients for finite difference equation for PP (pressure correction) and solves for the values of PP at each grid point (SIMPLE algorithm).
1. **AIM**
Matrix-solving routine. LISOLV is nearly always used instead of AIM.
 2. **MODPP (PROMOD)**
Modifies coefficients and source terms for boundary nodes so as to take boundary conditions into account for PP (pressure correction).
 - a) **WALL (PROMOD)**
Handles intrusion boundary conditions for F (inlet gas mixture fraction), ETA (coal gas mixture fraction), G (variance in inlet gas mixture fraction), GETA (variance in coal gas mixture fraction), YFU, P (pressure), and PP (pressure correction).
 3. **PRINT**
Prints output according to specified format.
- E. CALCW**
Calculates coefficients for finite difference equation for W (tangential velocity) and solves for the field values of W at each grid point.
1. **LISOLV**
The tri-diagonal matrix solving routine (Based on Thomas Algorithm).
 2. **MODW (PROMOD)**
Modifies coefficients and source terms for boundary nodes so as to take boundary conditions into account for W (tangential velocity).
- F. CALOTE**
Calculates coefficients for finite difference equation for K (turbulence kinetic energy) and solves for the field values of K at each grid point.
1. **LISOLV**
The tri-diagonal matrix solving routine (Based on Thomas Algorithm).
 2. **MODTE (PROMOD)**
Modifies coefficients and source terms for boundary nodes so as to take boundary conditions into account for K (turbulence kinetic energy).
- G. CALCED**
Calculates coefficients for finite difference equation for eddy dissipation and solves for the field values of eddy dissipation at each grid point.
1. **LISOLV**
The tri-diagonal matrix solving routine (Based on Thomas Algorithm).

2. MODED (PROMOD)

Modifies coefficients and source terms for boundary nodes so as to take boundary conditions into account for eddy dissipation.

H. CALCH

Calculates coefficients for finite difference equation for H (gas enthalpy) and solves for the field values of H at each grid point.

1. LISOLV

The tri-diagonal matrix solving routine (Based on Thomas Algorithm).

2. MODH (PROMOD)

Modifies coefficients and source terms for boundary nodes so as to take boundary conditions into account for H (gas enthalpy).

I. CALCET

Calculates coefficients for finite difference equation for eta (coal gas mixture fraction) and solves for the field values of eta at each grid point.

1. MODETA (PROMOD)

Modifies coefficients and source terms for boundary nodes so as to take boundary conditions into account.

J. CALCF

Calculates coefficients for finite difference equation for f (inlet gas mixture fraction) and solves for the field values of f at each grid point.

1. LISOLV

The tri-diagonal matrix solving routine (Based on Thomas Algorithm).

2. MODF (PROMOD)

Modifies coefficients and source terms for boundary nodes so as to take boundary conditions into account.

K. CALGE

Calculates coefficients for finite difference equation GETA (variance of the coal gas mixture fraction) and solves for the field values of GETA at each grid point.

1. ETASTO (TABLE)

Calls either ETASTH or ETAST.

a) ETAST

Calculates stoichiometric ETA (coal gas mixture fraction) for adiabatic reactor.

b) ETASTH

Calculates stoichiometric ETA (coal gas mixture fraction) for non-adiabatic reactor.

2. LISOLV

The tri-diagonal matrix solving routine (Based on Thomas Algorithm).

3. MODGET (PROMOD)

Modifies coefficients and source terms for boundary nodes so as to take boundary conditions into account for GETA.

L. CALCG

Calculates coefficients for finite difference equation for G (variance of the coal gas mixture fraction) and solves for the field values of G at each grid point.

1. LISOLV

The tri-diagonal matrix solving routine (Based on Thomas Algorithm).

2. MODG (PROMOD)

Modifies coefficients and source terms for boundary nodes so as to take boundary conditions into account.

M. CALCYFU

Calculates coefficients for finite difference equation for YFU (fuel mass fraction) and solves for the field values of YFU at each grid point.

1. AIM

Matrix-solving routine. LISOLV is nearly always used instead of AIM.

2. LISOLV

The tri-diagonal matrix solving routine (Based on Thomas Algorithm).

3. MODYFU (PROMOD)

Modifies coefficients and source terms for boundary nodes so as to take boundary conditions into account for YFU (fuel mass fraction).

XXI. PROG

Writes progress file.

XXII. EOLP

Driver routine for solving Eulerian or Lagrangian particle equations. Eulerian particles are not debugged in this version of PCGC-2. The Lagrangian option is currently the only viable option.

A. CALCNJ

Calculates coefficients for finite difference equation for NJ (bulk particle number density for jth particle type) and solves for the field values of NJ at each grid point.

1. LISOLV

The tri-diagonal matrix solving routine (Based on Thomas Algorithm).

B. EULINT (PSICT0)

Initializes Eulerian particle number density fields.

C. CALACJ

Calculates coefficients for Eulerian finite difference equation for ACJ (at each grid point).

1. LISOLV

The tri-diagonal matrix solving routine (Based on Thomas Algorithm).

D. CALAHJ

Calculates coefficients for Eulerian finite difference equation for AHJ at each grid point.

1. LISOLV

The tri-diagonal matrix solving routine (Based on Thomas Algorithm).

E. PSOLVP (PSOLVE)

This subroutine is used when using an Eulerian particle solution (not currently implemented). Prepares the Eulerian data so that an appropriate coal to each of the coal subroutines can be made. Takes the resulting coal computations and stores them in Eulerian arrays. Computes the associated source terms for the gas-particle coupling.

1. COAL1

Calculates gas phase properties at a point in the reactor, such as thermal conductivity, diffusivity, and viscosity. These properties are needed in COAL2.

a) SIGMAD

Used by COAL1 for determining the value of the potential function needed for mass diffusivity as a function of the Lennard-Jones parameters and temperature.

b) SIGMAM

Used by COAL1 for determining the value of the potential function needed for viscosity and thermal conductivity as a function of the Stockmayer parameters and temperature.

(1) FIND

This is a short extrapolation subroutine used by SIGMAM.

2. COAL2

Calculates coal reaction rates and other auxiliary parameters from coal and gas properties at a point.

a) DIF

Function that compares two numbers and returns their positive fractional difference.

b) PEJ

Function for calculating vapor pressure and enthalpy of vaporization for liquid component of slurry and fuel oils.

3. COAL2S (COAL2)

Calculates coal reaction rates and other auxiliary parameters from coal and gas properties at a point. Used when particle energy equation goes stiff. Pseudo steady-state assumption is used.

F. FLUX

Main driver routine to calculate all of the radiation flux sums.

1. RADCOF

Calculates radiation coefficients.

a) EICO2

Calculates the emissivity of carbon dioxide from the Hottel charts.

(1) FIND

This is a short extrapolation subroutine used by SIGMAM.

b) EIH2O

Calculates the emissivity of water vapor from the Hottel charts.

(1) FIND

This is a short extrapolation subroutine used by SIGMAM.

2. DISORD

Calculates radiant wall heat fluxes and flux-sums to the volume elements using the discrete ordinates approximation.

3. RESULT

Writes the results of the discrete ordinates radiative heat transfer calculation to the output file.

4. SETUP

Sets up radiation coefficients for FLUX subroutines.

a) PRINT

Prints output according to specified format.

5. FLUXX

Calculates coefficients for finite difference equation for FX (axial flux sum) and solves for field values for FX at each grid point.

a) PRINT

Prints output according to specified format.

b) LISOLV

The tri-diagonal matrix solving routine (Based on Thomas Algorithm).

6. FLUXR

Calculates coefficients for finite difference equation for FR (radial flux sum) and solves for the field values for FR at each grid point.

a) PRINT

Prints output according to specified format.

b) LISOLV

The tri-diagonal matrix solving routine (Based on Thomas Algorithm).

7. FLUXT

Calculates FETA (azimuthal flux sum) at each grid point.

8. PRINT

Prints output according to specified format.

G. PRINT

Prints output according to specified format.

H. BVALIN (BPROPS)

Inserts reasonable properties into intrusions which border the flow field in order to allow for particle phase 2-D property interpolation.

I. PSICT

Interpolates gas property information for each point of the Lagrangian particle information. Integrates particle velocity to get particle trajectory, and calls PSOLVE to integrate particle continuity and energy equations. Saves particle source terms for gas phase.

1. COAL1

Calculates gas phase properties at a point in the reactor, such as thermal conductivity, diffusivity, and viscosity. These properties are needed in COAL2.

a) SIGMAD

Used by COAL1 for determining the value of the potential function needed for mass diffusivity as a function of the Lennard-Jones parameters and temperature.

b) SIGMAM

Used by COAL1 for determining the value of the potential function needed for viscosity and thermal conductivity as a function of the Stockmayer parameters and temperature.

(1) FIND

This is a short extrapolation subroutine used by SIGMAM.

2. COAL2

Calculates coal reaction rates and other auxiliary parameters from coal and gas properties at a point.

a) DIF

Function that compares two numbers and returns their positive fractional difference.

b) PEJ

Function for calculating vapor pressure and enthalpy of vaporization for liquid component of slurry and fuel oils.

3. PSOLVE

Solves particle energy and continuity equations for reacting particles.

a) COAL2

Calculates coal reaction rates and other auxiliary parameters from coal and gas properties at a point.

(1) DIF

Function that compares two numbers and returns their positive fractional difference.

(2) PEJ

Function for calculating vapor pressure and enthalpy of vaporization for liquid component of slurry and fuel oils.

b) COAL2S (COAL2)

Calculates coal reaction rates and other auxiliary parameters from coal and gas properties at a point. Used when particle energy equation goes stiff. Pseudo steady-state assumption is used.

4. PSOLVS (PSOLVE)

Solves particle energy and continuity equations for reacting particles when the particle energy equation is stiff.

a) COAL1

Calculates gas phase properties at a point in the reactor, such as thermal conductivity, diffusivity, and viscosity. These properties are needed in COAL2.

(1) SIGMAD

Used by COAL1 for determining the value of the potential function needed for mass diffusivity as a function of the Lennard-Jones parameters and temperature.

(2) SIGMAM

Used by COAL1 for determining the value of the potential function needed for viscosity and thermal conductivity as a function of the Stockmayer parameters and temperature.

(a) FIND

This is a short extrapolation subroutine used by SIGMAM.

b) COAL2

Calculates coal reaction rates and other auxiliary parameters from coal and gas properties at a point.

(1) DIF

Function that compares two numbers and returns their positive fractional difference.

(2) PEJ

Function for calculating vapor pressure and enthalpy of vaporization for liquid component of slurry and fuel oils.

J. BVALOUT (BPROPS)

Replaces boundary values with original properties.

XXIII. NOXMN

Main driver for the NO model. Reads basic input data for kinetic parameters, convergence criteria, etc. Calls all NO model subroutines, and stops program when converged.

A. EQSPEC

Calculates the equilibrium concentrations of nitrogen and oxygen by convolving over the probability density functions of f and η . This is necessary since there is a possibility that their storage arrays were replaced by other information if "AIM" was used in PCGC2.

1. FGtabl

Calculates limits of normalized Gaussian PDF.

2. ERF

Calculates the area under the normal curve from a spline fit. This is used for values of intermittency in the turbulent combustion model.

3. UPDATE (TABLE)

Interpolates table values for gas properties.

a) UPF (TBLF)

Interpolates one-dimensional (F) gas properties table.

b) UPFE (TBLFE)

Interpolates two-dimensional (F and ETA) gas properties table.

c) UPFEH (TBLFEH)

Interpolates three-dimensional (F, ETA, and H) gas properties table.

d) UPFH (TBLFH)

Interpolates two-dimensional (F and H) gas properties table.

4. CREE

This is the main controlling routine for the thermochemical equilibrium calculations (Chemically Reacting Equilibrium, from Elemental balances).

a) ERATIO (SPECE)

Calculates fuel/air equivalence ratio given atom numbers using positive and negative oxidation states (valences).

b) SPECE

Auxiliary subroutine for the CREE thermochemical equilibrium computations.

(1) CALC

Auxiliary subroutine for the CREE thermochemical equilibrium computations.

(2) HCPS

Auxiliary subroutine for thermochemical equilibrium computations.

c) HCPS

Auxiliary subroutine for thermochemical equilibrium computations.

R. FREACT (RATE)

Calculates the fully reacted species values which represent the maximum concentration that the species can achieve and occur when all the atoms possible are converted to the particular species under consideration.

C. RSTNOX

Reads and writes the necessary information for a restart file.

D. PSCRAT (RATE)

Calculates the intermittency rates.

1. B

Uses a cubic spline to find the reaction order for the homogeneous NO formation reaction based on the local oxygen concentration.

E. PRISUR

This subroutine calculates the external area for the coal particle [external area (m²)/kg of particle] to be used in the subroutine RATE for calculation of the rate of NO_x reduction by the char particles and to account for particle swelling during the course of reaction. The particle diameter has been increased by a user specified proportion and the mass of the particle is assumed to remain constant and the density is adjusted to account for the increase in diameter. These assumptions are obviously in error, since the mass of the particle is changing and the amount of swelling will be dependent on the extent of particle reaction. However, it is felt these errors will be somewhat compensating, and that the magnitude of error in the calculated area will be comparable with the error in the rate equation itself.

F. RATE

Calculates the time-mean reaction rates for the homogeneous and heterogeneous NO reactions. Incorporates the effects of the turbulent fluctuations on the kinetic reactions.

1. FGTABLE

Calculates limits of normalized Gaussian PDF.

2. ERF

Calculates the area under the normal curve from a spline fit. This is used for values of intermittency in the turbulent combustion model.

3. CREE

This is the main controlling routine for the thermochemical equilibrium calculations (Chemically Reacting Equilibrium, from Elemental balances).

a) ERATIO (SPECE)

Calculates fuel/air equivalence ratio given atom numbers using positive and negative oxidation states (valences).

b) SPECE

Auxiliary subroutine for the CREE thermochemical equilibrium computations.

(1) CALC

Auxiliary subroutine for the CREE thermochemical equilibrium computations.

(2) HCPS

Auxiliary subroutine for thermochemical equilibrium computations.

c) HCPS

Auxiliary subroutine for thermochemical equilibrium computations.

4. UPDATE (TABLE)

Interpolates table values for gas properties.

- a) **UPF (TBLF)**
Interpolates one-dimensional (F) gas properties table.
 - b) **UPFE (TBLFE)**
Interpolates two-dimensional (F and ETA) gas properties table.
 - c) **UPFEH (TBLFEH)**
Interpolates three-dimensional (F, ETA, and H) gas properties table.
 - d) **UPFH (TBLFH)**
Interpolates two-dimensional (F and H) gas properties table.
- 5. B**
Uses a cubic spline to find the reaction order for the homogeneous NO formation reaction based on the local oxygen concentration.
- G. CALCNO**
Calculates coefficients for finite difference equation for YNO (NO mass fraction), and solves for the field values of YNO at each grid point.
- 1. LISOLV**
The tri-diagonal matrix solving routine (Based on Thomas Algorithm).
- H. CALHCN**
Calculates coefficients for finite difference equation for YHCN (HCN mass fraction), and solves for the field values of YHCN at each grid point.
- 1. LISOLV**
The tri-diagonal matrix solving routine (Based on Thomas Algorithm).
- I. CALO2 (RATE)**
Calculates time-mean mass fraction for oxygen from a mass balance on oxygen using amount of nitric oxide formed as a sink for oxygen.
- J. INTGRT**
Calculates radially mixed values of NO concentration at each axial node location.

APPENDIX C
DESCRIPTION OF INPUT DATA

DESCRIPTION OF INPUT DATA
(Definitions for array subscripts are at the end of the table)

<u>Fortran Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
A ₁	real	sec ⁻¹	Pre-exponential factor for the homogeneous NO formation reaction, A ₁ .
A ₂	real	sec ⁻¹	Pre-exponential factor for the homogeneous NO reduction reaction, A ₂ .
A ₃	real	kmol N ⁻¹ s ⁻¹	Pre-exponential factor for the heterogeneous NO reduction reaction, A ₃ .
AF	real	--	A value of 0.0 will use upwind differencing to solve radiation equations in discrete ordinates model. A value of 1.0 will use central differencing. An intermediate value will use a hybrid of upwind and central.
AL1	real	m	Axial length where axial dimensions of the computational cells begin to shrink.
ALJ(J,L)	real	m s ⁻¹ K ⁻ⁿ	Pre-exponential factor for the L th char reaction for the J th particle size/type, A _{jp} .
ALPHA0	real	--	Scaling parameter for Burger's vortex.
AMJ(J,M)	real	s ⁻¹	Pre-exponential factor for the M th coal reaction for the J th particle size/type, A _{jm} .
A0	real	--	Degree of anisotropy of scattering in discrete ordinates radiation model.
ASUB(I,II)	Hollerith	--	Name of I th species, II = 1, 3.
AT(II)	Hollerith	--	Element symbols in a species name (e.g., CO ₂ has C and O).
ATOM(1,K)	Hollerith	--	Name of K th element.
ATOM(2,K)	real	kg kmol ⁻¹	Atomic mass of K th element.
ATOM(3,K)	real	--	Valence of K th element.
B(II)	real	--	Number of molecules of element 'AT' in species name (e.g., CO ₂ has 1 and 2).

<u>Fortran Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
BLANK	ASCII	--	A blank card.
CCP(J,II,N)	real	J kg ⁻¹ K ⁻¹	Quadratic heat capacity coefficients (I = 1,3) for the J th particle for: N = 1, coal component; N = 2, char component; N = 3 ash component. If all coefficients are set to 0.0, the code calculates the values based on coal composition and temperature (as explained in user's manual).
COMENT(II)	Hollerith	--	Comment words for output of particle information.
DELRRJ	real	--	Fractional change in total reaction rate that is acceptable for a converged reaction rate.
DELTA(I)	real	--	Stockmayer polar parameter of species I, δ_i .
DELTPJ	real	K	Temperature difference acceptable for convergence when calculating particle temperature from particle enthalpy.
DIACH	real	m	Diameter of reaction chamber.
DIAP	real	m	Diameter of primary duct.
DIAS	real	m	Diameter of secondary tube.
EACT1	real	J kmol ⁻¹	Activation energy for the homogeneous NO formation reaction, E_1 .
EACT2	real	J kmol ⁻¹	Activation energy for the homogeneous NO reduction reaction, E_2 .
EACT3	real	J kmol ⁻¹	Activation energy for the heterogeneous NO reduction reaction, E_3 .
EDIN(II)	real	m s	Experimental inlet turbulent kinetic energy dissipation rate at radial position RIN(II).
EDPD	logical	--	.TRUE. will use turbulent kinetic energy dissipation rate profile data from an inlet data file for additional inlets (option not presently functional in code).

<u>Fortran Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
EDPDAT	logical	--	.TRUE. will use turbulent kinetic energy dissipation rate profile data from an inlet data file for the primary tube, and calculates adjusted profiles at the inlet node points. .FALSE. will use theoretical calculations for the profile.
EDSDAT	logical	--	.TRUE. will use turbulent kinetic energy dissipation rate profile data from an inlet data file for the secondary annulus, and calculates adjusted profiles at the inlet node points. .FALSE. will use theoretical calculations for the profile
EK(I)	real	K	Stockmayer parameter for the I th species, ϵ/k .
EL(J,L)	real	J kmol ⁻¹	Activation energy for the L th char oxidation reaction for the J th particle size/type.
ELEM	Hollerith	--	Formatted line must contain the letters 'ELEM'.
EMJ(J,M)	real	J kmol ⁻¹	Activation energy for the M th devolatilization reaction for the J th particle size/type.
EMM(J,L)	real	--	Exponent on temperature in kinetic char rate expression, m.
EMW	real	--	Wall emmissivity, ϵ_w .
EPSD	real	--	Ratio of cell size decrease in radial direction.
EPSI	real	--	Ratio of cell increase in radial direction.
EPSX	real	--	Ratio of cell sites in axial direction (cf AL1).
FCTNO	real	--	Fraction of frozen NO concentrations used to initialize NO field throughout the coal reactor.

<u>Fortran Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
FCTHCN	real	--	Percentage of frozen HCN concentrations used to initialize HCN field throughout the coal reactor.
FLOW	real	kg s ⁻¹	Mass flow rate of gas in NINLET stream
FFLOW	real	--	Fraction of reactant stream 1 in NINLET stream.
GAMMA	real	--	Particle swelling parameter, γ .
GRDOUT	logical	--	.TRUE. print a (file name).grd file.
HAØ(J)	real	J kg ⁻¹	Heat of formation of the ash in the J th particle, h_{aj}^0 .
HCØ(J)	real	J kg ⁻¹	Heat of formation of the coal in the J th particle, h_{cj}^0 - can be calculated from coal heating value and ultimate analysis.
HGH(J,L)	real	J kg ⁻¹	Heat of reaction for L th char oxidation for J th particle
HGV(J,M)	real	J kg ⁻¹	Heat of reaction for M th devolitalization reaction for J th particle
HHØ(J)	real	J kg ⁻¹	Heat of formation of the char in the J th particle, h_{hj}^0
HWØ(J)	real	J kg ⁻¹	Heat of formation of the slurry liquid in the J th particle, h_{wj}^0
HLOSS	real	--	Fraction of enthalpy in excess of ambient conditions to be removed from each computational cell. Should be 0.0 if INCALH is set TRUE.
HRMAX	real	J kg ⁻¹	Gas enthalpy in subroutine TABLE highest excess.
HRMIN	real	J kg ⁻¹	Only used if INCALH is set TRUE. In as above table, lowest gas enthalpy loss.
IEUCK	integer	--	IEUCK = 1 gas thermal conductivity calculated from the Eucken equation, IEUCK = 0, gas thermal conductivity is calculated from Sage-Galloway equation.

<u>Fortran Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
IGASV	integer	--	Index for gas property interpolation during Lagrangian particle trajectory integration. If IGASV = 1 no interpolation gas properties are assumed constant in the cell; IGASV = 2, gas properties are interpolated in the axial direction; IGASV = 3, gas properties are interpolated in both axial and radial directions.
INCALF	logical	--	.TRUE. will solve the f mixture fraction equation.
INCALG	logical	--	.TRUE. will solve g_f equation.
INCALH	logical	--	.TRUE. will solve gas energy equation (presently under development for particle-laden flows).
INCALN	logical	--	.TRUE. will solve n_j equation.
INCFP	logical	--	.TRUE. will incorporate correction for particles into gas phase turbulent diffusion coefficients.
INCLET	logical	--	.TRUE. will solve η equation.
INCLGE	logical	--	.TRUE. will solve g_η equation.
INCNOX	logical	--	.TRUE. will solve NO_x equations.
INCOAL	logical	--	.TRUE. will solve coal reaction equations.
INCREK	logical	--	.TRUE. will set up gas property table.
INCSWP	logical	--	.TRUE. allows for swirl in the primary stream.
INCSWS	logical	--	.TRUE. allows for swirl in the secondary stream.
INCURF	logical	--	.TRUE. will stop program every INDRST/2 iterations, allowing user to change under-relaxation factors.
INDPNX	integer	--	Number of iterations of the NO model between intermediate printouts.

<u>Fortran Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
INDPRI	integer	--	Number of iterations in gas phase calculations between intermediate printouts.
INEACH	logical	--	.TRUE. will solve particle field equation after each 5 gas phase macro-iterations, .FALSE. will solve particle equations only upon reaching a converged gas phase solution.
INDRST	integer	--	Number of iterations between intermediate output of restart information.
INFSOU	logical	--	.TRUE. will include source term in f equation (should be TRUE for slurry and fuel oil calculations, FALSE otherwise).
INHTRX	logical	--	.TRUE. will include heterogeneous NO reduction reaction.
INNOZZ	logical	--	.TRUE. will configure computational grid for very small spacing near centerline (typically used w/nozzles or large reactors).
INPROG	logical	--	.TRUE. maintains a (filename).prg file (see text).
INPRST	logical	--	.TRUE. will use a particle restart file to begin computations and output intermediate particle restart files.
INQRL	logical	--	.TRUE. allows for a quarl at the secondary inlet.
INRAD	logical	--	.TRUE. will solve radiation equations.
INRDGD	logical	--	.TRUE. reads location of user specified grid points from data file.
INRST	logical	--	.TRUE. will use a gas restart file to begin computations and output intermediate gas phase restart files.
INSIMP	logical	--	.TRUE. uses the SIMPLER algorithm to solve velocity/pressure field. .FALSE. uses the SIMPLE algorithm.

<u>Fortran Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
INTRUS	logical	--	.TRUE. will allow intrusions in reactor.
INTRZ	logical	--	.TRUE. uses frozen equilibrium scheme for gas properties when the local equivalence ratio is greater than 2.0
IPLTNX	logical	--	.TRUE. will write files for plots from NO model calculations.
IPSICT	logical	--	.TRUE. will solve particle equations (should be TRUE for all calculations involving particles).
IRSTNO	logical	--	.TRUE. will use a restart file to begin NO model computations and output intermediate NO model restart files.
ITYNX	integer	--	Number of iterations of the NO model between intermediate typing of the residuals
KEQ	integer	--	IF KEQ = 1 the linear form of the Field (1967) char oxidation rate expression is used; if KEQ $\neq$ 1 normal Arrhenius form used (low temperature reactors (< 1400 K) should not use KEQ = 1).
KOPED	integer	--	Selection parameter which designates one of several optional equations to be used in calculating a theoretical or experimental turbulent kinetic energy dissipation rate profile for additional inlets.
KOPEDP	integer	--	Selection parameter which designates one of several optional equations to be used in calculating a theoretical or experimental turbulent kinetic energy dissipation rate profile for the primary.
KOPEDS	integer	--	Selection parameter which designates one of several optional equations to be used in calculating a theoretical or experimental turbulent kinetic energy dissipation rate profile for the secondary.

<u>Fortran Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
KOPTE	integer	--	Selection parameter which designates one of several optional equations to be used in calculating a theoretical or experimental turbulent kinetic energy profile for the additional inlets (option not functional at present).
KOPTEP	integer	--	Selection parameter which designates one of several optional equations to be used in calculating a theoretical or experimental turbulent kinetic energy profile for the primary.
KOPTES	integer	--	Selection parameter which designates one of several optional equations to be used in calculating a theoretical or experimental turbulent kinetic energy profile for the primary.
KOPUP	integer	--	Selection parameter which designates one of several optional equations to be used in calculating a theoretical or experimental axial velocity profile for the primary.
KOPUS	integer	--	Selection parameter which designates one of several optional equations to be used in calculating a theoretical or experimental axial velocity profile for the secondary.
KOPU	integer	--	Specifies the angle the flow in the North wall inlet makes with a plane perpendicular to the axis of symmetry. The value is disregarded for West wall inlets (not presently operational).
KOPV	integer	--	Specifies the angle the flow in the West wall inlet makes with the axis of symmetry. KOPV(N) is disregarded for North Wall inlets (not presently operational).
KOPVP	integer	--	Selection parameter which designates one of several optional equations to be used in calculating a theoretical or experimental radial velocity profile for the primary.

<u>Fortran Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
KOPVS	integer		Selection parameter which designates one of several optional equations to be used in calculating a theoretical or experimental radial velocity profile for the secondary.
KOPW	integer	--	Tangential component of velocity is zero for all additional inlets (not presently operational).
KOPWP	integer	--	Selection parameter which designates one of several optional equations to be used in calculating a theoretical or experimental tangential velocity profile for the primary.
KOPWS	integer	--	Selection parameter which designates one of several optional equations to be used in calculating a theoretical or experimental tangential velocity profile for the secondary.
LDISCO	logical	--	.TRUE. will solve radiation equations by discrete ordinates method.
LEMCOR	logical	--	.TRUE. will incorporate corrections for gas emissivity due to spectral overlap.
LEULP	logical	--	.TRUE. solves Eulerian particle equations instead of Lagrangian equations only, .FALSE. is the only currently viable option.
LGASE	logical	--	.TRUE. will solve for gas phase emissivity.
LPARTP	logical	--	.TRUE. allows for particles in the primary stream.
LPARTS	logical	--	.TRUE. allows for particles in the secondary stream.
LPBOTH	logical	--	.TRUE. allows for particles in both the primary and secondary streams.
LPBUG	logical	--	.TRUE. will print out debug information.

<u>Fortran Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
LSPH	logical	--	.TRUE. allows for particle energy source term.
LSPM	logical	--	.TRUE. allows for particle mass source term.
LSPU	logical	--	.TRUE. allows for particle axial velocity source term.
LSPV	logical	--	.TRUE. allows for particle radial velocity source term.
LTBUG	logical	--	.TRUE. allows debug of chemical equilibrium table.
LYPS	logical	--	.TRUE. allows user to specify particle trajectory starting locations, .FALSE. assumes uniform mass flux to calculate starting locations.
MAGHJER	logical	--	.TRUE. allows use of the Magnussen-Hjertauger (coal reaction) model.
MAXIT	integer	--	Maximum number of gas phase macro-iterations.
MAXITP	integer	--	Maximum number of particle phase iterations.
MAXITR	integer	--	Maximum number of radiation flux iterations.
MAXRES	real	--	Maximum normalized value of residual source for convergence of the NO model.
MINITP	integer	--	Minimum number of gas phase macro-iterations between particle phase iterations for convergence criterion.
MOLE	ASCII	--	Gas stream relative amount flag. When MOLE is 'M', relative amounts of reactant stream are in mole percent. Otherwise, relative amounts are taken to be mass percent.
NCARD	integer	--	Number of comment cards to follow.
NCD	integer	--	Card number.

<u>Fortran Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
NCRXN	integer	--	Number of devolatilization reactions, M.
NDIA	<u>real</u>	--	Length of reaction chamber divided by diameter of reaction chamber, L/D.
NHRXN	integer	--	Number of char oxidation reactions, L.
NIINQ	integer	--	Number of axial grid points in the quarl region.
NIWOQ	integer	--	Number of grid points in the axial direction without quarl.
NJINP	integer	--	Number of grid points in radial direction in primary stream, only used if INNOZZ is .TRUE.
NJINS	integer	--	Number of grid points in radial direction in the secondary stream.
NL	integer	--	Cell number associated with AL1.
NLM	integer	--	Number of elements (this is calculated from other input - not read in directly).
NPROP	integer	--	Number of particle integration steps before updating gas phase transport properties for particle reaction scheme.
NPS	integer	--	Number of particle sizes/types.
NSAY	integer	--	Number of comment cards to follow.
NSFORM	integer	--	Form of swirl number equation to be used.
NSHRNK	integer	--	If NSHRNK = 1 the shrinking particle model is used for char oxidation; If NSHRNK $\neq$ 1 the constant diameter model is used.
NSL	integer	--	Number of particle trajectory starting locations.
OMEGAA(J)	real	--	Initial mass fraction of ash in J th particle, ω_{aj} .

<u>Fortran Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
OMEGAC(J)	real	--	Initial mass fraction of raw coal in J^{th} particle, ω_{cj} .
OMEGAH(J)	real	--	Initial mass fraction of char in J^{th} particle, ω_{hj} .
OMEGAW(J)	real	--	Initial mass fraction of liquid in the J^{th} particle, ω_{wj} .
OXYD(L)	Hollerith	--	Species identification symbol for the oxidizer for the L^{th} char oxidation reaction.
PD(J)	real	m	Initial diameter of J^{th} particle, d_j .
PDEN	real	kg m ⁻³	Particle/droplet density.
PECWT	real	--	Relative amounts of each species in each input stream.
PHASE	ASCII	--	Phase of inlet stream species; only gases are allowed except for slurry calculations, which require one stream of liquid.
PHIL(L)	real	--	Ratio of moles of fuel (C) to moles of oxidizer in the L^{th} char oxidation reaction, ϕ_L .
PLOADP	real	--	Solids loading (mass of particles/mass of primary gas) in the primary stream.
PLS	real	m	Local length scale in primary stream.
PMF(J)	real	--	Mass fraction of J^{th} particle type.
POLLUT	logical	--	.TRUE. Solves only NO _x equations without recalculating other Eulerian variables.
PRES	real	N m ⁻²	Reactor outlet pressure.
PRHCN	real	--	Turbulent Prandtl/Schmidt number for HCN concentrations.
PRK(J)	real	--	Turbulent Prandtl/Schmidt number for J^{th} particle type, σ_j .
PRNOX	real	--	Turbulent Prandtl/Schmidt number for NO concentrations.

<u>Fortran Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
QAB	real	--	Absorption efficiency for particle radiation, Q_a .
QHA	real	degrees	Quarl half angle (with centerline).
QLX	real	m	Axial length of quarl region.
QSC	real	--	Scattering efficiency for particle radiation, Q_s .
REAC(II) (II=1-10)	Hollerith	--	Reactant card, the first four letters on the card must be 'REAC', 36 other ASCII symbols may be included for user description of the reactant stream. These symbols are simply echoed in output.
RIN(I)	real	m	Radial location of experimental inlet data point.
RP	real	m	Primary tube inside radius for experimental inlet data.
RS1	real	m	Primary tube outside radius for experimental inlet data.
RS2	real	m	Secondary tube radius for experimental inlet data.
S(I)	real	$\text{\AA}$	Stockmayer collision diameter, σ_1 .
SAY(II) (II=1-10)	Hollerith	--	Comment words for beginning of output.
SLRCMP(I)	Hollerith	--	Name of slurry component found in gas (e.g. H ₂ O) (I = 1, 2, and 3).
SLS	real	m	Local length scale in secondary stream.
SORMAX	real	--	Maximum normalized value of residual source sums for convergence of gas phase computations.
SPRANG(I)	real	--	Spray angle for initial starting location for SL points.
SORMIN	real	--	Minimum normalized value of residual source sums between particle phase iterations for overall convergence.

<u>Fortran Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
SWIRLN(I)	real	--	Inlet stream NINLET swirl number.
STRING	Character	--	Inlet card, must contain letters 'INLET'.
SWIRLS	real	--	Secondary stream swirl number.
TBE	real	K	Exit temperature for boundary condition (0.0 yields adiabatic condition).
TBN	real	K	Temperature of north boundary.
TBW	real	K	Temperature of west boundary.
THER	Hollerith	--	Thermo card, must contain the letters 'THER'.
THICK	real	m	Thickness of tube wall between primary and secondary streams.
TINFLO(I)	real	--	Turbulence intensity of inlet stream, NINLET, I.
TIPD	logical	--	.TRUE. will use turbulent intensity profile data from an inlet data file for the additional inlet tube, and calculates adjusted profiles at the inlet node points. .FALSE. will use theoretical calculations for the profile (option not functional at present).
TIPDAT	logical	--	.TRUE. will use turbulent intensity profile data from an inlet data file for the primary tube, and calculates adjusted profiles at the inlet node points. .FALSE. will use theoretical calculations for the profile.
TISDAT	logical	--	.TRUE. will use turbulent intensity profile data from an inlet data file for the secondary annulus, and calculates adjusted profiles at the inlet node points. .FALSE. will use theoretical calculations for the profile.
TLAG(J)	real	--	Ratio of inlet particle temperature to inlet gas temperature.

<u>Fortran Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
TMP	real	K	Temperature of inlet stream NSTRM if NSTRM = 1, TMP is temperature of primary gas stream; = 2, temperature of secondary gas stream.
TNBP	real	K	Normal boiling point of slurry liquid.
TOUT	real	K	Outlet gas temperature for radiation (0.0 yields adiabatic condition).
TURBIN(I)	real	(m/s)	Experimental normalized turbulent intensity at radial position RIN(I). (The unnormalized turbulent intensity will be utilized if the selection parameter KOPT* so specifies).
TLOW	real	K	Lower temperature limit of heat capacity parameters.
THIGH	real	K	Upper temperature limit of heat capacity parameters.
UIN(I)	real	m s ⁻¹	Experimental axial velocity at radial position RIN(I).
UPD	logical	--	.TRUE. will use axial velocity profile data from an inlet data file for the additional inlet tube, and calculates adjusted profiles at the inlet node points. .FALSE. will use theoretical calculations for the profile (option not functional at present).
UPDAT	logical	--	.TRUE. will use axial velocity profile data from an inlet data file for the primary tube, and calculates adjusted profiles at the inlet node points. .FALSE. will use theoretical calculations for the profile.
UPLAG(ISL)	real	--	Ratio of inlet particle velocity to inlet gas velocity.
URFDEN	real	--	Under-relaxation factor for density, λ_ρ .
URFE	real	--	Under-relaxation factor for eddy dissipation rate, λ_ϵ .

<u>Fortran Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
URFETA	real	--	Under-relaxation factor for n , λ_n .
URFF	real	--	Under-relaxation factor for f , λ_f .
URFG	real	--	Under-relaxation factor for g_f , λ_{g_f} .
URFGET	real	--	Under-relaxation for g_n , λ_{g_n} .
URFH	real	--	Under-relaxation factor for h , g_h .
URFGH	real	--	Under-relaxation factor for g_h , λ_n , λ_{gh} .
URFK	real	--	Under-relaxation factor for k , λ_k .
URFNJ	real	--	Under-relaxation factor for n_j , λ_{n_j} .
URFP	real	--	Under-relaxation factor for p , λ_p .
URFPM	real	--	Under-relaxation factor for S_p^m , $\lambda_{S_p^m}$.
URFPP	real	--	Under-relaxation factor for p' , $\lambda_{p'}$.
URFU	real	--	Under-relaxation factor for u , λ_u .
URFV	real	--	Under-relaxation factor for v , λ_v .
URFVIS	real	--	Under-relaxation factor for v^t , λ_{v^t} .
URFW	real	--	Under-relaxation factor for w , λ_w .
USDAT	logical	--	.TRUE. will use axial velocity profile data from an inlet data file for the secondary annulus, and calculates adjusted profiles at the inlet node points. .FALSE. will use theoretical calculations for the profile.
VIN(I)	real	$m\ s^{-1}$	Experimental radial velocity at radial position RIN(I).
VISCOS	real	$kg\ m^{-1}\ s^{-1}$	Approximate laminar viscosity for entire reaction chamber.
VPD	logical	--	.TRUE. will use radial velocity profile data from an inlet data file for the additional inlet tube, and calculates adjusted profiles at the inlet node points. .FALSE. will use theoretical calculations for the profile (option not presently functional).

<u>Fortran Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
VPDAT	logical	--	.TRUE. will use radial velocity profile data from an inlet data file for the primary tube, and calculates adjusted profiles at the inlet node points. .FALSE. will use theoretical calculations for the profile.
VSDAT	logical	--	.TRUE. will use radial velocity profile data from an inlet data file for the secondary annulus, and calculates adjusted profiles at the inlet node points., .FALSE. will use theoretical calculations for the profile.
WIC(J,K)	real	--	K th elemental mass fraction of J th particle size, w_{jk} , specified on a daf basis in order of elements listed in thermodynamic file.
WIN(I)	real	m s ⁻¹	Experimental tangential velocity at radial position RIN(I).
WPD	logical	--	.TRUE. will use tangential velocity profile data from an inlet data file for the additional inlet tube, and calculates adjusted profiles at the inlet node points. .FALSE. will use theoretical calculations for the profile (option not presently operational).
WPDAT	logical	--	.TRUE. will use tangential velocity profile data from an inlet data file for the primary tube, and calculates adjusted profiles at the inlet node points. .FALSE. will use theoretical calculations for the profile.
WSDAT	logical	--	.TRUE. will use tangential velocity profile data from an inlet data file for the secondary annulus, and calculates adjusted profiles at the inlet node points. .FALSE. will use theoretical calculations for the profile.
XI(J)	real	--	Surface area factor for J th particle type, ζ_j .

<u>Fortran Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
XIANOX	real	--	Fractional change in external char area used in NO model as a result of swelling and fracturing.
YHCNPR	real	--	Mass fraction of HCN in the primary stream.
YHCNS	real	--	Mass fraction of HCN in the secondary stream.
YPS(ISL)	real	m	Radial position of the ISL starting location.
YPSH	real	--	Normalized upper bound for particle starting locations (r/R).
YPSL	real	--	Normalized lower bound for particle starting locations (r/R).
YY(J,M)	real	--	Stoichiometric coefficient for J th particle with regards to M th devolatilization reaction Y _{jm} .
Z(N1,N,I)	real	--	Coefficients for I th species heat capacity equation. For N = 1, the temperature range of the heat capacity is generally 300 K - 1000 K and for N = 2, the temperature range is generally 1000 K - 5000 K (see TLOW and THIGH). In both cases.

$$\frac{h}{RT} = \left(\sum_{ii=1}^5 z_{ii} \frac{T^{(ii-1)}}{ii} \right) + \frac{Z_6}{T}$$

$$\frac{S^0}{R} = z_1 \ln T + \left(\sum_{n=2}^5 z_{ii} \frac{T^{ii-1}}{ii-1} \right) + z_7$$

ZETA	real	--	Fractional conversion of devolatilized nitrogen to HCN in the gas phase.
------	------	----	--

Index Identification

I	Species
ISL	Particle starting location
J	Particle size/type
K	Elements
L	Char reaction
M	Devolatilization reaction
N	Particle component
II	Arbitrary

APPENDIX D
COMMAND (SCRIPT) FILES FOR VAX/VMS AND
UNIX OPERATING SYSTEMS

```

$if p6 .nes. "DBG" then on control_Y then goto ctrl_exit
$on error then goto ctrl_exit
$if p1 .nes. "" then if p2 .eqs. "" then goto allsame
$count = 1
$one:
$if count .nes. 1 then goto two
$if p1 .nes. "" then goto go
$inquire p1 "_Input File"
$goto one
$two:
$if count .nes. 2 then goto three
$if p2 .nes. "" then goto go
$inquire p2 "_Thermo File"
$goto two
$three:
$if count .nes. 3 then goto four
$if p3 .nes. "" then goto go
$inquire p3 "_Inlet Profile File"
$goto three
$four:
$if count .nes. 4 then goto five
$if p4 .nes. "" then goto go
$inquire p4 "_Output File"
$goto four
$five:
$if count .nes. 5 then goto go
$if p5 .nes. "" then goto go
$inquire p5 "_Restart File"
$goto five
$go:
$count = count + 1
$if count .eq. 2 then goto two
$if count .eq. 3 then goto three
$if count .eq. 4 then goto four
$if count .eq. 5 then goto five
$goto skip
$allsame:
$if '$$locate(".",p1)' .eqs. '$$length(p1)' -
then goto next
$len = '$$locate(".",p1)'
$string := '$$extract(0, len, p1)'
$goto nexta
$next:
$string := 'p1'
$nexta:
$p2:='string'
$p3:='string'
$p4:='string'
$p5:='string'
$skip:
$dt := .dat
$tm := .thm
$ot := .out
$it := .inl
$if '$$locate(".",p1)' .eqs. '$$length(p1)' -
then p1:='p1' 'dt'
$if '$$locate(".",p2)' .eqs. '$$length(p2)' -
then p2:='p2' 'tm'
$if '$$locate(".",p3)' .eqs. '$$length(p3)' -
then p3:='p3' 'it'
$if '$$locate(".",p4)' .eqs. '$$length(p4)' -
then goto nextl
$len = '$$locate(".",p4)'
$stringl := '$$extract(0, len, p4)'

```



```

$goto oncemore
$next1:
$string1 := 'p4'
$oncemore:
$if '$locate(".",p5)' .eqs. '$length(p5)' -
  then goto next2
$len := '$locate(".",p5)'
$string2 := '$extract(0, len, p5)'
$goto finale
$next2:
$string2 := 'p5'
$finale:
$len1 := '$locate(".",p1)'
$p4 := 'string1'
$p5 := 'string2'
$out := .out
$rst := .rst
$rnz := .rnz
$tbl := .tbl
$pso := .pso
$pp1 := .pp1
$pp2 := .pp2
$pp3 := .pp3
$pbz := .pbz
$gsp := .gsp
$nxp := .nxp
$grd := .grd
$prg := .prg
$set noon
$copy 'p5' 'rst' 'p4' 'rst'
$copy 'p5' 'pso' 'p4' 'pso'
$copy 'p5' 'rnz' 'p4' 'rnz'
$copy 'p5' 'tbl' 'p4' 'tbl'
$set on
$assign 'p1' pccgin
$assign 'p2' thermo
$assign 'p3' inlet
$assign '$extract(0,len1, p1)' 'grd' grids
$assign 'p4' 'out' pccgot
$assign 'p4' 'rst' inout
$assign 'p4' 'rnz' rsnxio
$assign 'p4' 'tbl' tblrst
$assign 'p4' 'pso' parsou
$assign 'p4' 'pp1' pplot1
$assign 'p4' 'pp2' pplot2
$assign 'p4' 'pp3' pplot3
$assign 'p4' 'gsp' gasplt
$assign 'p4' 'nxp' polplt
$assign 'p4' 'prg' prgrss
$assign PCGC:pcgc2.use use_default
$USE PCGC2
$write sys$output "Running PCGC2"
$if "'$mode()'".eqs. "BATCH" then goto runit
$deassign sys$input
$terminal := 'terminalnumber'
$assign 'terminal' sys$input
$runit:
$set working_set/limit=400
$run bsb:PCGC2
$ctrl_exit:
$set noon
$deassign use_default
$deassign sys$input
$deassign pccgin

```

```
$deassign thermo  
$deassign inlet  
$deassign grids  
$deassign pcyrot  
$deassign inout  
$deassign rsnxio  
$deassign parsou  
$deassign tblrst  
$deassign pplot1  
$deassign pplot2  
$deassign pplot3  
$deassign gasplt  
$deassign polplt  
$deassign prgrss  
$set on  
$ EXIT
```

```
$assign sys$disk sys$print
$if p1 .eqs. "" then goto error
$if p2 .eqs. "" then goto error
$if p3 .eqs. "" then goto error
$if p4 .eqs. "" then goto error
$if p5 .eqs. "" then goto error
$if p6 .eqs. "" then goto error
$assign sys$command: for005
$set default 'p6'
$pcgc2 'p1' 'p2' 'p3' 'p4' 'p5'
$deassign for005
$exit
$error:
$write sys$output "Parameter error!"
$exit
```

```

$assign PCGC: PRO:
$if p1 .nes. "" then if p2 .eqs. "" then goto allsame
$one:
$if p1 .nes. "" then goto two
$inquire p1 "_Input File"
$goto one
$two:
$if p2 .nes. "" then goto three
$inquire p2 "_Thermo File"
$goto two
$three:
$if p3 .nes. "" then goto four
$inquire p3 "_Inlet Profile File"
$goto three
$four:
$if p4 .nes. "" then goto five
$inquire p4 "_Output File"
$goto four
$five:
$if p5 .nes. "" then goto eight
$inquire p5 "Restart File"
$if p5 .eqs. "" then goto five
$six:
$if p6 .nes. "" then goto seven
$inquire p6 "_Is the batch queue to be \"SLOW\" or not?"
$!goto six
$seven:
$if p7 .nes. "" then goto eight
$inquire p7 "_Submit AFTER what time of day(hh:mm:ss.s)?"
$!goto seven
$goto eight
$allsame:
$if '$$locate(".",p1)' .eqs. '$$length(p1)' -
  then goto next
$len = '$$locate(".",p1)'
$string := '$$extract(0, len, p1)'
$goto nexta
$next:
$string := 'p1'
$nexta:
$sp2:='string'
$sp3:='string'
$sp4:='string'
$sp5:='string'
$eight:
$if p6 .eqs. "" then inquire p6 "_Which batch queue? (BATCH,SLOW)"
$if p6 .eqs. "" then p6 := "sys$batch"
$if p6 .eqs. "BATCH" then p6 := "sys$batch"
$if p7 .eqs. "HOLD" then submit := submit/hold
$if p7 .eqs. "HOLD" then p7 := "TODAY"
$if p7 .eqs. "" then p7 := "TODAY"
$log := .log
$prenom := pcgc2:
$len = '$$locate(".",p4)'
$logfile:='$$extract(0,len,p4)'log'
$pb = $environment("default")
$submit PCGC:pcgc2run-
/parameters=('p1','p2','p3','p4','p5','p8'):-
/name='prenom'p1'-
/queue='p6'-
/after='p7'-
/log_file='p8'logfile'
$exit

```

```

$ ON ERROR THEN GOTO FIN
$if p1 .nes. "" then if p2 .eqs. "" then goto allsame
$count = 1
$one:
$if count .nes. 1 then goto two
$if p1 .nes. "" then goto go
$inquire p1 "_Input File"
$goto one
$two:
$if count .nes. 2 then goto three
$if p2 .nes. "" then goto go
$inquire p2 "_Thermo File"
$goto two
$three:
$if count .nes. 3 then goto four
$if p3 .nes. "" then goto go
$inquire p3 "_Inlet Profile File"
$goto three
$four:
$if count .nes. 4 then goto five
$if p4 .nes. "" then goto go
$inquire p4 "_Output File"
$goto four
$five:
$if count .nes. 5 then goto go
$if p5 .nes. "" then goto go
$inquire p5 "_Restart File"
$goto five
$go:
$count = count + 1
$if count .eq. 2 then goto two
$if count .eq. 3 then goto three
$if count .eq. 4 then goto four
$if count .eq. 5 then goto five
$goto skip
$allsame:
$if '$locate(".",p1)' .eqs. '$length(p1)' -
  then goto next
$len = '$locate(".",p1)'
$string := '$extract(0, len, p1)'
$goto nexta
$next:
$string := 'p1'
$nexta:
$p2:='string'
$p3:='string'
$p4:='string'
$p5:='string'
$skip:
$ TYPE PBUG:CBUG.MSG
$ assign pbug: hsb:
$ FOR := FOR/DEBUG/NOOPT
$ LINK := LINK/DEBUG
$ PCGC2 'p1' 'p2' 'p3' 'p4' 'p5' DBG
$ deassign hsb:
$ assign pcgc: hsb:
$ EXIT
$ FIN:
$ EXIT

```

```
#script file to run PCGC2 program interactively
set echo
# Copy restart files to output, if different from output
if ($SRNAME != $SONAME) cp $SRNAME.rst $SONAME.rst
if ($SRNAME != $SONAME) cp $SRNAME.pso $SONAME.pso
if ($SRNAME != $SONAME) cp $SRNAME.rnx $SONAME.rnx
if ($SRNAME != $SONAME) cp $SRNAME.tbl $SONAME.tbl
# Link specific input files to generic input files
ln $DNAME.dat $cwd/PCGCIN
ln $TNAME.thm $cwd/THERMO
ln $INAME.inl $cwd/INLET
if ( -e $DNAME.grd ) ln $DNAME.grd $cwd/GRIDS
if ( -e $SONAME.rst ) ln $SONAME.rst $cwd/INOUT
if ( -e $SONAME.rnx ) ln $SONAME.rnx $cwd/RSNXIO
if ( -e $SONAME.tbl ) ln $SONAME.tbl $cwd/TBLRST
if ( -e $SONAME.pso ) ln $SONAME.pso $cwd/PARSOU
# Run PCGC2
#mkmf "FFLAGS = -O2" PROGRAM=pcgc2 "SUFFIX = .INC:hF"
cd /mnt/brewster/afr
make pcgc2
back
/mnt/brewster/afr/pcgc2
control_exit:
# Remove linked generic file names. Move unlinked generic files
# to specific files.
rm $cwd/PCGCIN
rm $cwd/THERMO
rm $cwd/INLET
if ( -e $DNAME.grd ) then
    rm $cwd/GRIDS
else
    mv $cwd/GRIDS $DNAME.grd
endif
mv $cwd/PCGCOT $SONAME.out
if ( -e $SONAME.rst ) then
    rm $cwd/INOUT
else
    mv $cwd/INOUT $SONAME.rst
endif
if ( -e $SONAME.rnx ) then
    rm $cwd/RSNXIO
else
    mv $cwd/RSNXIO $SONAME.rnx
endif
if ( -e $SONAME.tbl ) then
    rm $cwd/TBLRST
else
    mv $cwd/TBLRST $SONAME.tbl
endif
if ( -e $SONAME.pso ) then
    rm $cwd/PARSOU
else
    mv $cwd/PARSOU $SONAME.pso
endif
if ( -e $cwd/PLOT1 ) mv $cwd/PLOT1 $SONAME.pp1
if ( -e $cwd/PLOT2 ) mv $cwd/PLOT2 $SONAME.pp2
```

```
if ( -e $cwd/PLOT3 ) mv $cwd/PLOT3 $SONAME.pp3
if ( -e $cwd/GASPLT ) mv $cwd/GASPLT $SONAME.gsp
if ( -e $cwd/POLPLT ) mv $cwd/POLPLT $SONAME.nxp
if ( -e $cwd/PRGRSS ) mv $cwd/PRGRSS $SONAME.prq
exit
```

```
#script file to run PCGC2 program in batch mode
set noglob
onintr control_exit
if ($1 != '') then
  if ($2 = '') then
    # all data and output file names the same
    # as first file name: read in argument list
    setenv DNAME $cwd/$1:r.dat
    setenv TNAME $cwd/$1:r.thm
    setenv INAME $cwd/$1:r.inl
    setenv ONAME $cwd/$1:r.out
    setenv RNAME $cwd/$1:r.rst
  else
    # separate file names for each file:
    # read in argument list
    setenv DNAME $cwd/$1:r.dat
    setenv TNAME $cwd/$2:r.thm
    setenv INAME $cwd/$3:r.inl
    setenv ONAME $cwd/$4:r.out
    setenv RNAME $cwd/$5:r.rst
  endif
else
  # prompt and read in each file name
  set a = ''
  set b = ''
  set c = ''
  set d = ''
  set e = ''
  one:
  echo 'Input File'
  set a = ($<)
  if ($a = '') goto one
  setenv DNAME $cwd/$a:r.dat
  two:
  echo 'Thermo File'
  set b = ($<)
  if ($b = '') goto two
  setenv TNAME $cwd/$b:r.thm
  three:
  echo 'Inlet Profile File'
  set c = ($<)
  if ($c = '') goto three
  setenv INAME $cwd/$c:r.inl
  four:
  echo 'Output File'
  set d = ($<)
  if ($d = '') goto four
  setenv ONAME $cwd/$d:r.out
  five:
  echo 'Restart File'
  set e = ($<)
  if ($e = '') goto five
  setenv RNAME $cwd/$e:r.rst
endif
echo 'Which queue? (s:short, l:long, or v:very long)'
set queue = ($<)
```

```
set oname = $ONAME
set jobname = $oname:r
#rm $jobname:t.log
submit -n $queue\
  -j PCGC2:$jobname:t\
  -o /mnt/brewster/work/$jobname:t.log\
  -r\
  /mnt/brewster/afr/pcgc2batch1.com
exit
```

```

#script file to run PCGC2 program in batch queue
set noglob
onintr control_exit
date
set dname=$DNAME
set iname=$INAME
set oname=$ONAME
set rname=$RNAME
set tname=$TNAME
if ($rname:r !~ $oname:r) cp $rname:r.rst $oname:r.rst
if ($rname:r !~ $oname:r) cp $rname:r.pso $oname:r.pso
if ($rname:r !~ $oname:r) cp $rname:r.rnx $oname:r.rnx
if ($rname:r !~ $oname:r) cp $rname:r.tbl $oname:r.tbl
# Link specific input files to generic input files
ln $DNAME $cwd/PCGCIN
ln $TNAME $cwd/THERMO
ln $INAME $cwd/INLET
if ( -e $dname:r.grd ) ln $dname:r.grd $cwd/GRIDS
if ( -e $oname:r.rst ) ln $oname:r.rst $cwd/INOUT
if ( -e $oname:r.rnx ) ln $oname:r.rnx $cwd/RSNXIO
if ( -e $oname:r.tbl ) ln $oname:r.tbl $cwd/TBLRST
if ( -e $oname:r.pso ) ln $oname:r.pso $cwd/PARSOU
# Run PCGC2
cd /mnt/brewster/afr
make pcgc2
back
echo 'Running PCGC2'
/mnt/brewster/afr/pcgc2
control_exit:
# Remove linked generic file names. Move unlinked generic files
# to specific files.
rm $cwd/PCGCIN
rm $cwd/THERMO
rm $cwd/INLET
if ( -e $dname:r.grd ) then
  rm $cwd/GRIDS
else
  mv $cwd/GRIDS $dname:r.grd
endif
mv $cwd/PCGCOT $oname
if ( -e $oname:r.rst ) then
  rm $cwd/INOUT
else
  mv $cwd/INOUT $oname:r.rst
endif
if ( -e $oname:r.rnx ) then
  rm $cwd/RSNXIO
else
  mv $cwd/RSNXIO $oname:r.rnx
endif
if ( -e $oname:r.tbl ) then
  rm $cwd/TBLRST
else
  mv $cwd/TBLRST $oname:r.tbl
endif
if ( -e $oname:r.pso ) then

```

```

  rm $cwd/PARSOU
else
  mv $cwd/PARSOU $oname:r.pso
endif
if ( -e $cwd/PLOT1 ) mv $cwd/PLOT1 $oname:r.pp1
if ( -e $cwd/PLOT2 ) mv $cwd/PLOT2 $oname:r.pp2
if ( -e $cwd/PLOT3 ) mv $cwd/PLOT3 $oname:r.pp3
if ( -e $cwd/GASPLT ) mv $cwd/GASPLT $oname:r.gsp
if ( -e $cwd/POLPLT ) mv $cwd/POLPLT $oname:r.nxp
if ( -e $cwd/PRGRSS ) mv $cwd/PRGRSS $oname:r.prg
exit

```


APPENDIX E
USE (MAKE) FILES FOR PROGRAM MAINTENANCE

```
$on control_Y then goto ctrl_exit
$on error then goto ctrl_exit
$write sys$output "Using PCGC2"
$ FOR/OBJ=bsb:PCGC2!O pccg:PCGC2! I
$ FOR/OBJ=bsb:AIM!O pccg:AIM! I
$ FOR/OBJ=bsb:BPROPS!O pccg:BPROPS! I
$ FOR/OBJ=bsb:CALACJ!O pccg:CALACJ! I
$ FOR/OBJ=bsb:CALAHJ!O pccg:CALAHJ! I
$ FOR/OBJ=bsb:CALCED!O pccg:CALCED! I
$ FOR/OBJ=bsb:CALCET!O pccg:CALCET! I
$ FOR/OBJ=bsb:CALCF!O pccg:CALCF! I
$ FOR/OBJ=bsb:CALCG!O pccg:CALCG! I
$ FOR/OBJ=bsb:CALCGE!O pccg:CALCGE! I
$ FOR/OBJ=bsb:CALCH!O pccg:CALCH! I
$ FOR/OBJ=bsb:CALCNJ!O pccg:CALCNJ! I
$ FOR/OBJ=bsb:CALCP!O pccg:CALCP! I
$ FOR/OBJ=bsb:CALCPP!O pccg:CALCPP! I
$ FOR/OBJ=bsb:CALCTE!O pccg:CALCTE! I
$ FOR/OBJ=bsb:CALCU!O pccg:CALCU! I
$ FOR/OBJ=bsb:CALCV!O pccg:CALCV! I
$ FOR/OBJ=bsb:CALCW!O pccg:CALCW! I
$ FOR/OBJ=bsb:CALCYFU!O pccg:CALCYFU! I
$ FOR/OBJ=bsb:COAL0!O pccg:COAL0! I
$ FOR/OBJ=bsb:COAL1!O pccg:COAL1! I
$ FOR/OBJ=bsb:COAL2!O pccg:COAL2! I
$ FOR/OBJ=bsb:CPUTIM!O pccg:CPUTIM! I
$ FOR/OBJ=bsb:CREE!O pccg:CREE! I
$ FOR/OBJ=bsb:DISORD!O pccg:DISORD! I
$ FOR/OBJ=bsb:EOLP!O pccg:EOLP! I
$ FOR/OBJ=bsb:ERF!O pccg:ERF! I
$ FOR/OBJ=bsb:FGTABL!O pccg:FGTABL! I
$ FOR/OBJ=bsb:FIND!O pccg:FIND! I
$ FOR/OBJ=bsb:FLINT!O pccg:FLINT! I
$ FOR/OBJ=bsb:FLUX!O pccg:FLUX! I
$ FOR/OBJ=bsb:FLUXR!O pccg:FLUXR! I
$ FOR/OBJ=bsb:FLUXT!O pccg:FLUXT! I
$ FOR/OBJ=bsb:FLUXX!O pccg:FLUXX! I
$ FOR/OBJ=bsb:FLUX0!O pccg:FLUX0! I
$ FOR/OBJ=bsb:GASE!O pccg:GASE! I
$ FOR/OBJ=bsb:GRDGRF!O pccg:GRDGRF! I
$ FOR/OBJ=bsb:GRID!O pccg:GRID! I
$ FOR/OBJ=bsb:INFLOW!O pccg:INFLOW! I
$ FOR/OBJ=bsb:INIT!O pccg:INIT! I
$ FOR/OBJ=bsb:LISOLV!O pccg:LISOLV! I
$ FOR/OBJ=bsb:PLTWRT!O pccg:PLTWRT! I
$ FOR/OBJ=bsb:PRINT!O pccg:PRINT! I
$ FOR/OBJ=bsb:PROFILE!O pccg:PROFILE! I
$ FOR/OBJ=bsb:PROG!O pccg:PROG! I
$ FOR/OBJ=bsb:PROMOD!O pccg:PROMOD! I
$ FOR/OBJ=bsb:PROPS!O pccg:PROPS! I
$ FOR/OBJ=bsb:PSICT!O pccg:PSICT! I
$ FOR/OBJ=bsb:PSICT0!O pccg:PSICT0! I
$ FOR/OBJ=bsb:PSOLVE!O pccg:PSOLVE! I
$ FOR/OBJ=bsb:RADCOF!O pccg:RADCOF! I
$ FOR/OBJ=bsb:RESTRT!O pccg:RESTRT! I
$ FOR/OBJ=bsb:SETUP!O pccg:SETUP! I
$ FOR/OBJ=bsb:SIGMAD!O pccg:SIGMAD! I
$ FOR/OBJ=bsb:SIGMAH!O pccg:SIGMAH! I
$ FOR/OBJ=bsb:STREAM!O pccg:STREAM! I
$ FOR/OBJ=bsb:TABLE!O pccg:TABLE! I
$ FOR/OBJ=bsb:CALHCN!O pccg:CALHCN! I
$ FOR/OBJ=bsb:CALCNO!O pccg:CALCNO! I
$ FOR/OBJ=bsb:NOXMN!O pccg:NOXMN! I
$ FOR/OBJ=bsb:RATE!O pccg:RATE! I
```

```

$ FOR/OBJ=bsb:RSTNOX!O pccg:RETNOX!I
$ FOR/OBJ=bsb:NCAR!O pccg:NCAR!I
$ COPY bsb:PCGC2.OBJ!I,-
bsb:AIM.OBJ!I,bsb:BPROPS.OBJ!I,-
bsb:CALCED.OBJ!I,bsb:CALCET.OBJ!I,-
bsb:CALCF.OBJ!I,bsb:CALCG.OBJ!I,-
bsb:CALCGE.OBJ!I,bsb:CALCH.OBJ!I,-
bsb:CALCNJ.OBJ!I,bsb:CALCP.OBJ!I,-
bsb:CALCPP.OBJ!I,bsb:CALCTE.OBJ!I,-
bsb:CALCU.OBJ!I,bsb:CALCV.OBJ!I,-
bsb:CALCW.OBJ!I,bsb:CALCYPH.OBJ!I -
bsb:SEG1.OBJ!O
$ COPY bsb:COAL0.OBJ!I,bsb:COAL1.OBJ!I,-
bsb:COAL2.OBJ!I bsb:SEG2.OBJ!O
$ COPY bsb:CPUTIM.OBJ!I,bsb:CFEE.OBJ!I,-
bsb:DISORD.OBJ!I,-
bsb:ERF.OBJ!I,bsb:FGTABL.OBJ!I,-
bsb:FIND.OBJ!I bsb:SEG3.OBJ!O
$ COPY bsb:FLUX.OBJ!I,bsb:FLUXR.OBJ!I,-
bsb:FLUXT.OBJ!I,bsb:FLUXX.OBJ!I,-
bsb:FLUXO.OBJ!I,bsb:GASE.OBJ!I,-
bsb:FLINT.OBJ!I bsb:SEG4.OBJ!O
$ COPY bsb:GRDGRF.OBJ!I,bsb:GRID.OBJ!I,bsb:ENFLOW.OBJ!I,-
bsb:INIT.OBJ!I,bsb:LISOLV.OBJ!I,bsb:PLTWRT.OBJ!I,-
bsb:PRINT.OBJ!I,bsb:PROFILE.OBJ!I,-
bsb:PROMOD.OBJ!I,bsb:PROPS.OBJ!I,-
bsb:PROC.OBJ!I bsb:SEG5.OBJ!O
$ COPY bsb:PSICT.OBJ!I,bsb:PSICT0.OBJ!I,-
bsb:PSOLVE.OBJ!I,bsb:EOLP.OBJ!I,-
bsb:CALACJ.OBJ!I,bsb:CAIANJ.OBJ!I -
bsb:SEG6.OBJ!O
$ COPY bsb:RADCOF.OBJ!I,bsb:RESTRT.OBJ!I,-
bsb:SETUP.OBJ!I,bsb:SIGMAD.OBJ!I,-
bsb:SIGMAM.OBJ!I,bsb:STREAM.OBJ!I,-
bsb:TABLE.OBJ!I bsb:SEG7.OBJ!O
$ COPY bsb:CALHCN.OBJ!I,bsb:CALCNO.OBJ!I,-
bsb:NOXMN.OBJ!I,bsb:RATE.OBJ!I,-
bsb:RSTNOX.OBJ!I bsb:SEG8.OBJ!O
$ LINK bsb:SEG1.OBJ!I,bsb:SEG2.OBJ!I,-
bsb:SEG3.OBJ!I,bsb:SEG4.OBJ!I,-
bsb:SEG5.OBJ!I,bsb:SEG6.OBJ!I,-
bsb:SEG7.OBJ!I,bsb:SEG8.OBJ!I,-
bsb:NCAR.OBJ!I -
/EXE=bsb:PCGC2!O
$exit
$ctrl_exit:
$exit 2

```

```
DEST      = /mnt/brewster/afr/pbug
EXTHDRS   =
HDRS      =
FFLAGS    = -O2
LDFLAGS   = -O2
LIBS      =
LINKER    = fc
MAKEFILE  = makefile
OBJS      = aim.o \
            b.o \
            bprops.o \
            calacj.o \
            calahj.o \
            calc.o \
            calced.o \
            calcet.o \
            calcf.o \
            calcg.o \
            calcge.o \
            calch.o \
            calcnj.o \
            calcno.o \
            calcp.o \
            calcpp.o \
            calcte.o \
            calcup.o \
            calcvp.o \
            calcw.o \
            calcyfu.o \
            calhcn.o \
            coal0.o \
            coal1.o \
            coal2.o \
            cputim.o \
            cree.o \
            cree0.o \
            dif.o \
            disord.o \
            eico2.o \
            eih2o.o \
            eolp.o \
            erf.o \
            fgtabl.o \
            find.o \
            flint.o \
            flux.o \
            flux0.o \
            fluxr.o \
```

```

fluxt.o \
fluxx.o \
frzfe.o \
frzfeh.o \
fstf.o \
fstfe.o \
fstfeh.o \
fstfh.o \
grdgrf.o \
grid.o \
grmap.o \
hcps.o \
inflow.o \
init.o \
intgrt.o \
lisolv.o \
mixfe.o \
noxmm.o \
oldrat.o \
pcgc2.o \
pej.o \
pltwrt.o \
print.o \
profil.o \
prog.o \
promod.o \
props.o \
prtar.o \
psict.o \
psict0.o \
psolve.o \
radcof.o \
rate.o \
ratrms.o \
restrt.o \
result.o \
rstnox.o \
rtarms2.o \
setup.o \
sigmad.o \
sigmam.o \
spece.o \
stream.o \
table.o \
tblf.o \
tblfe.o \
tblfeh.o \
tblfh.o \
tblrstfe.o \
tblrstfeh.o \
wall.o

```

PRINT = pr

PROGRAM = pcgc2

```
SRCS      = aim.f \
           b.f \
           bprops.f \
           calacj.f \
           calahj.f \
           calc.f \
           calced.f \
           calcet.f \
           calcf.f \
           calcg.f \
           calcge.f \
           calch.f \
           calcnj.f \
           calcno.f \
           calcp.f \
           calcpp.f \
           calcte.f \
           calcup.f \
           calcvp.f \
           calcw.f \
           calcyfu.f \
           calhcn.f \
           coal0.f \
           coal1.f \
           coal2.f \
           cputim.f \
           cree.f \
           cree0.f \
           dif.f \
           disord.f \
           eico2.f \
           eih2o.f \
           eolp.f \
           erf.f \
           fgtabl.f \
           find.f \
           flint.f \
           flux.f \
           flux0.f \
           fluxr.f \
           fluxt.f \
           fluxx.f \
           frzfe.f \
           frzfeh.f \
           fstf.f \
           fstfe.f \
           fstfeh.f \
           fstfh.f \
           grdgrf.f \
           grid.f \
           grmap.f \
           hcps.f \
           inflow.f \
           init.f \
           intgrt.f \
           lisolv.f \
```

```

mixfe.f \
noxmn.f \
oldrat.f \
pcgc2.f \
pej.f \
pltwrt.f \
print.f \
profil.f \
prog.f \
promod.f \
props.f \
prtar.f \
psict.f \
psict0.t \
psolve.f \
radcof.f \
rale.f \
ratrms.f \
restrt.f \
result.f \
rstnox.f \
rtrms2.f \
setup.f \
sigmad.f \
sigmam.f \
spece.f \
stream.f \
table.f \
tblf.f \
tblfe.f \
tblfeh.f \
tblfh.f \
tblrstfe.f \
tblrstfeh.f \
wall.f

all: $(PROGRAM)

$(PROGRAM): $(OBJS) $(LIBS)
echo -n "Loading $(PROGRAM) ... "
$(LINKER) $(LDFLAGS) $(OBJS) $(LIBS) -o $(PROGRAM)
echo "done"

clean:; rm -f $(OBJS)

depend:; mkmf -f $(MAKEFILE) PROGRAM=$(PROGRAM) DEST=$(DEST)

index:; tags -wx $(HDRS) $(SRCS)

install: $(PROGRAM)
echo Installing $(PROGRAM) in $(DEST)
install -s $(PROGRAM) $(DEST)

print:; $(PRINT) $(HDRS) $(SRCS)

program: $(PROGRAM)

```

```

tags:          $(HDRS) $(SRCS); ctags $(HDRS) $(SRCS)

update:        $(DEST); $(PROGRAM)

$(DEST)/$(PROGRAM): $(SRCS) $(LIBS) $(HDRS) $(EXTHDRS)
                  make -f $(MAKEFILE) DEST=$(DEST) install

###
aim.o: PARAMETER.INC COEF.INC FLUPR.INC
      fc -c -O1 aim.f
bprops.o: PARAMETER.INC ALL.INC CPARAM.INC CPART.INC CPEUL.INC FLUPR.INC \
      INTRUS.INC KASET1.INC SAVBP.INC VAR.INC VARR.INC
calacj.o: PARAMETER.INC INTRUS.INC ALL.INC CPART.INC CPSOU.INC VAR.INC \
      GEOM.INC FLUPR.INC COEF.INC TURB.INC PANDS.INC REACT.INC PARD.INC \
      TUBWAL.INC KASET1.INC CPEUL.INC SWPDIR.INC BOUND.INC CFLAG.INC \
      IPPAR.INC EULP.INC
calahj.o: PARAMETER.INC INTRUS.INC ALL.INC VAR.INC GEOM.INC FLUPR.INC \
      COEF.INC TURB.INC PARD.INC TUBWAL.INC KASET1.INC CPEUL.INC SWPDIR.INC \
      BOUND.INC CFLAG.INC IPPAR.INC EULP.INC CPART.INC CPSOU.INC PANDS.INC \
      REACT.INC
calc.o: PARAMETER.INC CCHEMI.INC CEQUIL.INC CINDEX.INC CMATRI.INC \
      CPARAM.INC CSPECE.INC PRIN.INC
calced.o: PARAMETER.INC ALL.INC TDIS.INC GEOM.INC FLUPR.INC COEF.INC \
      TURB.INC KASET1.INC CPSOU.INC INTRUS.INC SWPDIR.INC SUSP.INC VAR.INC
calcet.o: PARAMETER.INC ALL.INC CGASMF.INC VAR.INC GEOM.INC FLUPR.INC \
      COEF.INC TURB.INC MIXFR.INC KASET1.INC CPSEF.INC SWPDIR.INC CPSOU.INC \
      INTRUS.INC
calcf.o: PARAMETER.INC INTRUS.INC ALL.INC VAR.INC GEOM.INC FLUPR.INC \
      COEF.INC TURB.INC MIXFR.INC CPSOU.INC SWPDIR.INC KASET1.INC \
      TABRIT.INC CGASMF.INC CPSEF.INC
calcg.o: PARAMETER.INC ALL.INC VAR.INC GEOM.INC FLUPR.INC COEF.INC TURB.INC \
      FLUC.INC KASET1.INC CPSOU.INC SWPDIR.INC INTRUS.INC
calcge.o: PARAMETER.INC ALL.INC CGASMF.INC VAR.INC GEOM.INC FLUPR.INC \
      COEF.INC TURB.INC FLUC.INC KASET1.INC CPSOU.INC SWPDIR.INC INTRUS.INC
calch.o: PARAMETER.INC PRIN.INC INTRUS.INC ALL.INC ENTH.INC VAR.INC \
      GEOM.INC FLUPR.INC COEF.INC TURB.INC KASET1.INC CPSOU.INC SWPDIR.INC \
      RADCON.INC VARR.INC KRAD.INC
calcnj.o: PARAMETER.INC ALL.INC INTRUS.INC VAR.INC GEOM.INC FLUPR.INC \
      COEF.INC TURB.INC PARD.INC TUBWAL.INC KASET1.INC CPSOU.INC CPART.INC \
      CPEUL.INC SWPDIR.INC CFLAG.INC PANDS.INC REACT.INC IPPAR.INC EULP.INC
calcno.o: PARAMETER.INC ALL.INC INTRUS.INC VAR.INC GEOM.INC FLUPR.INC \
      COEF.INC TURB.INC FLUC.INC TUBWAL.INC KASET1.INC CPSOU.INC SWPDIR.INC \
      CALCYI.INC NSWPS.INC NOXRSD.INC
calcp.o: PARAMETER.INC PRIN.INC ALL.INC INTRUS.INC PCOR.INC VAR.INC \
      GEOM.INC COEF.INC CPSOU.INC SWPDIR.INC SIMPLE.INC FLUPR.INC \
      FLUPR2.INC
calcpp.o: PARAMETER.INC PRIN.INC ALL.INC INTRUS.INC PCOR.INC VAR.INC \
      GEOM.INC COEF.INC CPSOU.INC SWPDIR.INC SIMPLE.INC SWPALT.INC \
      FLUPR.INC FLUPR2.INC
calcte.o: PARAMETER.INC ALL.INC INTRUS.INC GRID.INC TEN.INC VAR.INC \
      GEOM.INC FLUPR.INC COEF.INC TURB.INC KASET1.INC SUSP.INC CPSOU.INC \
      SWPDIR.INC SWRL.INC
calcup.o: PARAMETER.INC AFR.INC ALL.INC INTRUS.INC UVEL.INC VAR.INC \
      GEOM.INC COEF.INC KASET1.INC CPSOU.INC SWPDIR.INC SIMPLE.INC \
      FLUPR.INC FLUPR2.INC PCOR.INC
calcvp.o: PARAMETER.INC ALL.INC INTRUS.INC VVEL.INC VAR.INC GEOM.INC \

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        COEF.INC KASET1.INC CPSOU.INC SWPDIR.INC SWRL.INC FLUPR.INC \
        FLUPR2.INC PCOR.INC
calcw.o: PARAMETER.INC ALL.INC INTRUS.INC WVEL.INC VAR.INC GEOM.INC \
        FLUPR.INC COEF.INC KASET1.INC CPSOU.INC SWPDIR.INC
calcyfu.o: PARAMETER.INC ALL.INC CGSMF.INC COEF.INC CPSEF.INC CPSOU.INC \
        FLUPR.INC GEOM.INC INTRUS.INC KASET1.INC MAGHJ.INC MIXFR.INC \
        SWPDIR.INC SSUM.INC TURB.INC VAR.INC
calhcn.o: PARAMETER.INC ALL.INC INTRUS.INC VAR.INC GEOM.INC FLUPR.INC \
        COEF.INC TURB.INC FLUC.INC CALCYI.INC NSWPS.INC KASET1.INC SWPDIR.INC \
        TUBWAL.INC CPSOU.INC NOXRSD.INC
coal0.o: PARAMETER.INC AFR.INC ALL.INC CFLAG.INC CPARAM.INC GPARAM.INC \
        CSPECE.INC CEQUIL.INC CWATER.INC CPSOU.INC CPART.INC CINDEX.INC \
        CHETRX.INC CTNBP.INC TRAJ.INC GEOM.INC VAR.INC FLUPR.INC KASET1.INC \
        PANDS.INC REACT.INC PRIN.INC CPLOT.INC CGSFLO.INC BUG.INC IPPAR.INC \
        HCAP.INC HREF.INC RCON.INC RCONT.INC RRAT.INC PFAC.INC CNDXCG.INC \
        UNDER.INC CPSEF.INC TABRIT.INC CCHEMI.INC PVAR.INC ICON.INC \
        TUBWAL.INC MRCK.INC
coal1.o: PARAMETER.INC PRIN.INC CSPECE.INC CEQUIL.INC CCHEMI.INC CINDEX.INC \
        CPARAM.INC DIFUS.INC RCON.INC RCONT.INC TRAJ.INC ICON.INC GPARAM.INC
coal2.o: PARAMETER.INC CPARAM.INC CCHEMI.INC CEQUIL.INC CINDEX.INC \
        CHETRX.INC CSPECE.INC CPART.INC RCON.INC IPPAR.INC HCAP.INC HREF.INC \
        RRAT.INC DIFEQN.INC VARR.INC RADCON.INC OMEGA.INC PECOR.INC PFAC.INC \
        PRIN.INC DIFUS.INC TRAJ.INC ICON.INC RCON.INC GPARAM.INC MRCK.INC
cree.o: PARAMETER.INC CCHEMI.INC CEQUIL.INC CINDEX.INC CPARAM.INC \
        CSPECE.INC PRIN.INC
cree0.o: PARAMETER.INC CCHEMI.INC CEQUIL.INC CINDEX.INC CMATRI.INC \
        CPARAM.INC CSPECE.INC PANDS.INC REACT.INC PRIN.INC CNDXCG.INC
disord.o: PARAMETER.INC KASET1.INC SHERX.INC RADCON.INC DISO.INC ALL.INC \
        GEOM.INC BCRAD.INC KRAD.INC INTRUS.INC FLUPR.INC VARR.INC GRID.INC \
        PRIN.INC PARD.INC
eolp.o: PARAMETER.INC PRIN.INC ALL.INC INTRUS.INC VAR.INC GEOM.INC \
        FLUPR.INC COEF.INC TURB.INC PARD.INC TUBWAL.INC KASET1.INC CPSOU.INC \
        CPART.INC CPEUL.INC SWPDIR.INC CFLAG.INC IPPAR.INC EULP.INC VARR.INC \
        CGSMF.INC CGSFLO.INC CPSEF.INC UNDER.INC TIMER.INC PANDS.INC \
        REACT.INC
fgtabl.o: CGAUSS.INC
flint.o: PARAMETER.INC ADFLO.INC ALL.INC CPART.INC CWATER.INC FLIN.INC \
        GRID.INC INTRUS.INC VAR.INC VVEL.INC GEOM.INC FLUPR.INC PANDS.INC \
        REACT.INC PVAR.INC KASET1.INC TUBWAL.INC STRFNC.INC CGSFLO.INC \
        NOXMN.INC PDIM.INC SHERX.INC GMAP.INC CGSMF.INC CPSEF.INC TURB.INC
flux.o: PARAMETER.INC ALL.INC INTRUS.INC PRIN.INC VARR.INC GEOM.INC \
        RADCON.INC CPART.INC KRAD.INC DISO.INC COEF.INC CSET.INC RADRES.INC
flux0.o: PARAMETER.INC KASET1.INC SHERX.INC ALL.INC CPART.INC CINDEX.INC \
        PRIN.INC GEOM.INC DISO.INC RADCON.INC BCRAD.INC
fluxr.o: PARAMETER.INC PRIN.INC BCRAD.INC COEF.INC GEOM.INC VARR.INC \
        KRAD.INC CPART.INC SWPDIR.INC CSET.INC RADRES.INC ALL.INC INTRUS.INC \
        RADCON.INC
fluxt.o: PARAMETER.INC ALL.INC INTRUS.INC COEF.INC GEOM.INC VARR.INC \
        KRAD.INC CPART.INC SWPDIR.INC CSET.INC RADRES.INC RADCON.INC
fluxx.o: PARAMETER.INC PRIN.INC ALL.INC BCRAD.INC INTRUS.INC COEF.INC \
        GEOM.INC VARR.INC KRAD.INC CPART.INC SWPDIR.INC CSET.INC RADRES.INC \
        KASET1.INC RADCON.INC
frzfe.o: PARAMETER.INC PRIN.INC CPARAM.INC UPNX.INC PVAR.INC DENS.INC \
        TABRIT.INC CTABLE.INC FLUPR.INC RTMTAB.INC
frzfeh.o: PARAMETER.INC PRIN.INC RTMTAB.INC CPARAM.INC CINDEX.INC UPNX.INC \
        PVAR.INC DENS.INC TABRIT.INC BUG.INC CCHEMI.INC CTABLE.INC FLUPR.INC \

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        CSPECE.INC
fstf.o: PARAMETER.INC PRIN.INC CPARAM.INC FLUPR.INC CTABLE.INC
fstfe.o: PARAMETER.INC PRIN.INC CPARAM.INC PVAR.INC BUG.INC CTABLE.INC \
        FLUPR.INC
fstfeh.o: PARAMETER.INC CPARAM.INC PVAR.INC PRIN.INC BUG.INC CTABLE.INC \
        FLUPR.INC
fstfh.o: PARAMETER.INC PRIN.INC CPARAM.INC FLUPR.INC CTABLE.INC
grid.o: PARAMETER.INC ALL.INC INTRUS.INC GRID.INC GEOM.INC KASET1.INC \
        TUBWAL.INC STRFNC.INC CGSFLO.INC NOXMN.INC PDIM.INC PRIN.INC
grmap.o: PARAMETER.INC ADFLO.INC ALL.INC INTRUS.INC GRID.INC GEOM.INC \
        TUBWAL.INC NOXMN.INC TIMER.INC PDIM.INC STRFNC.INC GMAP.INC \
        KASET1.INC PRIN.INC
hcps.o: PARAMETER.INC CCHEMI.INC CINDEX.INC CPARAM.INC CSPECE.INC
inflow.o: PARAMETER.INC PRIN.INC ADFLO.INC CGSFLO.INC CPSEF.INC FLIN.INC \
        KASET1.INC PANDS.INC REACT.INC PDIM.INC SWRL.INC
        fc -c -00 inflow.f
init.o: PARAMETER.INC ALL.INC INTRUS.INC WVEL.INC VVEL.INC ENTH.INC \
        MAGHJ.INC MIXFR.INC VAR.INC GEOM.INC FLUPR.INC CFLAG.INC KASET1.INC \
        COEF.INC CPSOU.INC CGASMF.INC STRFNC.INC KRAD.INC VARR.INC CGSFLO.INC \
        PANDS.INC REACT.INC CPSEF.INC UVEL.INC PCOR.INC SSUM.INC UNDER.INC
intgrt.o: PARAMETER.INC ALL.INC INTRUS.INC
lisolv.o: PARAMETER.INC COEF.INC SWPDIR.INC TIMER.INC SWPALT.INC
mixfe.o: PARAMETER.INC PRIN.INC CPARAM.INC PVAR.INC DENS.INC CCHEMI.INC \
        BUG.INC CGSFLO.INC PANDS.INC REACT.INC TABRIT.INC CTABLE.INC \
        FLUPR.INC
noxmn.o: PARAMETER.INC NSWPS.INC CALCYI.INC CPSEF.INC PANDS.INC REACT.INC \
        PVAR.INC CINDEX.INC SSUM.INC KASET1.INC GEOM.INC TUBWAL.INC NOXMN.INC \
        VAR.INC FLUPR.INC ALL.INC CPARAM.INC INTRUS.INC RATE.INC MOLWT.INC \
        RATPAR.INC INTRAT.INC MISC.INC NOXRTE.INC XRATE.INC NOXRSD.INC \
        PRIN.INC RATEST.INC CTABLE.INC
oldrat.o: PARAMETER.INC ALL.INC CPARAM.INC CPART.INC CPSOU.INC CINDEX.INC \
        CSPECE.INC INTRUS.INC PANDS.INC REACT.INC FLUPR.INC CTABLE.INC \
        DENS.INC VAR.INC GEOM.INC TURB.INC FLUC.INC CGASMF.INC PVAR.INC \
        MOLWT.INC BOUND.INC NOXRTE.INC RATE.INC RATPAR.INC CALCYI.INC \
        INTRAT.INC XRATE.INC CGAUSS.INC RATRMS.INC AREXP.INC PROPIN.INC
pcgc2.o: PARAMETER.INC AFR.INC ADFLO.INC ALL.INC CGASMF.INC CGSFLO.INC \
        CPARAM.INC CPART.INC CPSEF.INC CPSOU.INC CSPECE.INC CWATER.INC \
        ENTH.INC FLIN.INC FLUC.INC FLUPR.INC GRID.INC INTRUS.INC KASET1.INC \
        MAGHJ.INC MIXFR.INC OMEGA.INC PANDS.INC PARD.INC PCOR.INC PDIM.INC \
        PRIN.INC REACT.INC RRAT.INC SWRL.INC TDIS.INC TEN.INC UVEL.INC \
        VAR.INC VVEL.INC WVEL.INC GEOM.INC CTABLE.INC BUG.INC TURB.INC \
        SHEAR.INC COEF.INC TUBWAL.INC PROPIN.INC VARR.INC CPLOT.INC CPEUL.INC \
        STRFNC.INC SSUM.INC SWPDIR.INC UNDER.INC DENS.INC SIMPLE.INC \
        NOXMN.INC TABRIT.INC TIMER.INC PVAR.INC CFLAG.INC PLTVAR.INC \
        RESID.INC CCHEMI.INC SHERX.INC EULP.INC IPPAR.INC GMAP.INC
pej.o: PARAMETER.INC CINDEX.INC CSPECE.INC CTNBP.INC TRAJ.INC HCAP.INC \
        HREF.INC
pltwrt.o: PARAMETER.INC ALL.INC CPARAM.INC INTRUS.INC VAR.INC COEF.INC \
        GEOM.INC FLUPR.INC VARR.INC CPEUL.INC STRFNC.INC CGSFLO.INC \
        CGASMF.INC NOXMN.INC
profil.o: PARAMETER.INC ADFLO.INC ALL.INC VAR.INC GEOM.INC FLUPR.INC \
        KASET1.INC STRFNC.INC CGSFLO.INC TURB.INC NOXMN.INC TUBWAL.INC \
        PDIM.INC PANDS.INC REACT.INC SWRL.INC VVEL.INC
prog.o: PARAMETER.INC ALL.INC FLUC.INC VAR.INC CGASMF.INC FLUPR.INC \
        UVEL.INC VVEL.INC WVEL.INC PCOR.INC ENTH.INC TEN.INC TDIS.INC \
        MIXFR.INC PARD.INC

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promod.o: PARAMETER.INC ADFLO.INC INTRUS.INC ALL.INC MAGHJ.INC VVEL.INC \
    WVEL.INC PCOR.INC VAR.INC GEOM.INC FLUPR.INC SHERX.INC KASET1.INC \
    SUSP.INC COEF.INC TURB.INC MIXFR.INC SHEAR.INC TUBWAL.INC CGASMF.INC \
    SSUM.INC SWRL.INC TIMER.INC CPSEF.INC UVEL.INC
props.o: PARAMETER.INC ALL.INC INTRUS.INC PRIN.INC MAGHJ.INC CPARAM.INC \
    CPART.INC FLUPR.INC PANDS.INC REACT.INC CTABLE.INC CPEUL.INC
prtar.o: PARAMETER.INC ALL.INC CPART.INC INTRUS.INC CPEUL.INC PFAC.INC \
    AREXP.INC BOUND.INC GEOM.INC
psict.o: PARAMETER.INC AFR.INC OMEGA.INC ALL.INC CPARAM.INC CWATER.INC \
    CPART.INC CPSOU.INC INTRUS.INC GEOM.INC VAR.INC FLUPR.INC KASET1.INC \
    CGSFLO.INC CPLOT.INC CPEUL.INC SSUM.INC MOLWT.INC IPPAR.INC CFLAG.INC \
    RCONT.INC CGASMF.INC TUBWAL.INC RRAT.INC CPSEF.INC PRIN.INC TRAJ.INC \
    DIFEQN.INC PECOR.INC VARR.INC TURB.INC GPARAM.INC
psict0.o: PARAMETER.INC ALL.INC CFLAG.INC CGASMF.INC CGSFLO.INC CPART.INC \
    CPEUL.INC CPLOT.INC CPSEF.INC CPSOU.INC EULP.INC FLUPR.INC GEOM.INC \
    INTRUS.INC IPPAR.INC KASET1.INC PANDS.INC REACT.INC PRIN.INC \
    TUBWAL.INC VAR.INC
psolve.o: PARAMETER.INC ALL.INC CPARAM.INC CPART.INC CPSOU.INC TRAJ.INC \
    VAR.INC FLUPR.INC KASET1.INC CGSFLO.INC CPLOT.INC CPEUL.INC MOLWT.INC \
    IPPAR.INC CFLAG.INC RCONT.INC OMEGA.INC EULP.INC PRIN.INC VARR.INC \
    DIFEQN.INC PECOR.INC GEOM.INC
radcof.o: PARAMETER.INC ALL.INC CINDEX.INC CPEUL.INC CPART.INC DISO.INC \
    RADCON.INC KRAD.INC FLUPR.INC
rate.o: PARAMETER.INC ALL.INC CPARAM.INC CPART.INC CPSOU.INC CINDEX.INC \
    CSPECE.INC INTRUS.INC PANDS.INC REACT.INC FLUPR.INC CTABLE.INC \
    DENS.INC VAR.INC GEOM.INC TURB.INC FLUC.INC CGASMF.INC PVAR.INC \
    MOLWT.INC BOUND.INC NOXRTE.INC RATE.INC RATPAR.INC CALCYI.INC \
    INTRAT.INC XRATE.INC CGAUSS.INC RATRMS.INC AREXP.INC PROPIN.INC \
    PRIN.INC RATEST.INC RESID.INC
ratrms.o: PARAMETER.INC CPARAM.INC CINDEX.INC PVAR.INC FLUPR.INC RATRMS.INC \
    RATE.INC RATPAR.INC INTRAT.INC PANDS.INC REACT.INC CALCYI.INC \
    NOXRTE.INC MOLWT.INC CTABLE.INC
restrt.o: PARAMETER.INC ALL.INC VAR.INC FLUPR.INC MAGHJ.INC KASET1.INC \
    CGASMF.INC KRAD.INC VARR.INC TABRIT.INC FLUC.INC
result.o: PARAMETER.INC ALL.INC FLUPR.INC BCRAD.INC KRAD.INC GEOM.INC \
    DISO.INC VARR.INC PRIN.INC
rstnox.o: PARAMETER.INC ALL.INC KASET1.INC CGASMF.INC CALCYI.INC
rtrms2.o: PARAMETER.INC CPARAM.INC CINDEX.INC PVAR.INC FLUPR.INC RATRMS.INC \
    RATE.INC RATPAR.INC INTRAT.INC PANDS.INC REACT.INC CALCYI.INC \
    NOXRTE.INC MOLWT.INC CTABLE.INC
setup.o: PARAMETER.INC ALL.INC CPART.INC COEF.INC GEOM.INC KRAD.INC \
    CSET.INC VARR.INC RADCON.INC
spece.o: PARAMETER.INC CCHEMI.INC CEQUIL.INC CINDEX.INC CMATRI.INC \
    CPARAM.INC CSPECE.INC PRIN.INC
stream.o: PARAMETER.INC ALL.INC INTRUS.INC VAR.INC GEOM.INC FLUPR.INC \
    TUBWAL.INC STRFNC.INC CGSFLO.INC
table.o: PARAMETER.INC CPARAM.INC TABRIT.INC TIMER.INC CTABLE.INC
tblf.o: PARAMETER.INC PRIN.INC CPARAM.INC FLUPR.INC CCHEMI.INC TABRIT.INC \
    BUG.INC CGSFLO.INC PANDS.INC REACT.INC CTABLE.INC
tblfe.o: PARAMETER.INC PRIN.INC CPARAM.INC UPNX.INC PVAR.INC DENS.INC \
    TABRIT.INC CCHEMI.INC BUG.INC CGSFLO.INC PANDS.INC REACT.INC \
    CTABLE.INC FLUPR.INC RTMTAB.INC
tblfeh.o: PARAMETER.INC PRIN.INC CPARAM.INC RTMTAB.INC PVAR.INC DENS.INC \
    TABRIT.INC CCHEMI.INC BUG.INC CGSFLO.INC PANDS.INC REACT.INC UPNX.INC \
    CTABLE.INC FLUPR.INC
tblfh.o: PARAMETER.INC PRIN.INC CPARAM.INC FLUPR.INC CCHEMI.INC DENS.INC \

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      BUG.INC CGSFLO.INC TABRIT.INC CTABLE.INC RTMTAB.INC
tblrstfe.o: PARAMETER.INC PRIN.INC CPARAM.INC UPNX.INC PVAR.INC DENS.INC \
      CCHEMI.INC BUG.INC TABRIT.INC CTABLE.INC FLUPR.INC RTMTAB.INC
tblrstfeh.o: PARAMETER.INC PRIN.INC CPARAM.INC UPNX.INC PVAR.INC DENS.INC \
      TABRIT.INC CCHEMI.INC BUG.INC CTABLE.INC FLUPR.INC RTMTAB.INC
wall.o: PARAMETER.INC ALL.INC INTRUS.INC COEF.INC
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APPENDIX F
METHANE COMBUSTION CASE

!NSAY..(SAY(I),I=1,NSAY) follows:

259

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F  2 F  2      !UPDAT,KOPUP,USDAT,KOPUS,...
F  0 F  0      !VPDAT,KOPVP,VSDAT,KOPVS,...
F  4 F  4      !WPDAT,KOPWP,WSDAT,KOPWS,...
F  1 F  1      !TIPDAT,KOPTIP,TISEAT,KOPTES,...
F  2 F  2      !EDPDAT,KOPEDP,EDSDAT,KOPEDS,...
0.00E+00, 0.00E-00,      !PLS,SLS,AISL...
1      8.50000E+00      !NSFORM,ALPHA0
1.25500E-02, 1.25500E-02, -5.50000E-02, !RP,RS1,RS2,
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AR	39.94800	0.0
C	12.01115	4.0
H	1.00797	1.0
O	15.9994	-2.0
N	14.0067	0.0

AR	1.5/66AR	1.00	0.00	0.00	0.0	300.000	5000.000
-0.25000000E	01	0.0	0.0	0.0	0.0	0.0	0.0
-0.74537500E	03	0.43660002E	01	0.25000000E	01	0.0	0.0
0.0	0.0	0.0	0.74537476E	03	0.43660002E	01	0.0
C02	J 9/65C	1.0	2.00	0.00	0.0	300.000	5000.000
0.44608040E	01	0.30981717E	02	0.12392566E	05	0.22741323E	09-0.15525948E-13
-0.48961438E	05	-0.98635978E	00	0.24007788E	01	0.87350905E	02-0.66070861E-05
0.20021860E	08	0.63274039E	15	-0.48377520E	05	0.96951447E	01
H20	J 3/61H	2.0	1.00	0.00	0.0	300.000	5000.000
0.27167616E	01	0.29451370E	02	-0.80224368E	06	0.10226681E	09-0.48472104E-14
-0.29905820E	05	0.66305666E	01	0.40701275E	01	-0.11084499E	02 0.41521180E-05
-0.29637404E	08	0.80762101E	12	-0.30279719E	05	-0.32270038E	00
M2	J 9/65N	2.0	0.0	0.0	0.0	300.000	5000.000
0.28963194E	01	0.15154863E	02	-0.57235275E	06	0.99807385E	10-0.65223536E-14
-0.90586182E	03	0.61615143E	01	0.36748257E	01	-0.12081496E	02 0.23240100E-05
-0.63217520E	09	-0.22577253E	12	-0.10611587E	04	0.23580418E	01
O2	J 9/65O	2.0	0.0	0.0	0.0	300.000	5000.000
0.36219521E	01	0.73618256E	03	-0.19652219E	06	0.36201556E	10-0.28945623E-14
-0.12019822E	04	0.36150942E	01	0.36255980E	01	-0.18782183E	02 0.70554543E-05
0.67635071E	08	0.21555977E	11	0.10475225E	04	0.43052769E	01
C0	J 9/65C	1.0	1.00	0.00	0.0	300.000	5000.000
0.29840689E	01	0.14891387E	02	0.57899678E	06	0.10364576E	09-0.69353499E-14
-0.14245227E	05	0.63479147E	01	0.37100916E	01	-0.16190964E	02 0.36923584E-05
0.20319673E	08	0.23953344E	12	0.14356309E	05	0.29555340E	01
H2	J 3/61H	2.0	0.0	0.0	0.0	300.000	5000.000
0.31901883E	01	0.51159458E	03	0.52644204E	07	-0.34909964E	10 0.36945341E-14
0.87738013E	03	0.19629412E	01	0.30574446E	01	0.26765198E	02-0.58099149E-05
0.55210343E	08	-0.18122726E	11	-0.98890430E	03	-0.22997046E	01
CN4	J 3/61C	1.0	4.00	0.00	0.0	300.000	5000.000
0.15027056E	01	0.10416795E	01	-0.39181514E	05	0.67777872E	09-0.44283706E-13
-0.99787031E	04	0.10707143E	02	0.38261929E	01	-0.39794557E	02 0.24558321E-04
0.22732920E	07	0.69626952E	11	-0.10144945E	05	0.86690062E	00
C(S)	J 3/61C	1.0	0.0	0.0	0.0	300.000	5000.000
0.13604937E	01	0.19132237E	02	-0.84040386E	06	0.16448705E	09-0.11672670E-13
-0.65713843E	03	-0.80070200E	01	-0.44778049E	00	0.53690970E	02-0.39775563E-06
-0.40459263E	08	0.21134925E	11	-0.94280670E	02	0.16840773E	01

3.418,124.,0.,
3.996,190.,0.,
2.641,809.1,1.0,
3.681,91.5,0.,
3.433,113.,0.,
3.59,110.,0.,
2.915,38.,0.,
3.822,137.,0.,
4.163,224.7,0.

C2H2	J 3/61C	2.0	2.00	0.00	0.0	300.000	5000.000
0.45751076E	01	0.51238351E	02	0.17452339E	05	0.28673064E	09-0.17951420E-13
0.25607426E	05	0.35737925E	01	0.14102755E	01	0.19057274E	01-0.24501380E-04
0.14390871E	07	0.41345443E	11	0.26188203E	05	0.11393826E	02
C2H4	J 9/65C	2.0	4.00	0.00	0.0	300.000	5000.000
0.34552135E	01	0.11491802E	01	0.43651744E	05	0.76155060E	09-0.50123195E-13
0.44773086E	04	0.26987944E	01	0.14256821E	01	0.11383139E	01 0.79890006E-05
0.16253676E	07	0.67491256E	11	0.53370703E	04	0.14621819E	02
C2H6	CR2178C	2H	60	00	00	300.000	5000.000
1.67107058E	00	1.88078150E	02	6.98943156E	06	1.16385735E	09 7.17707692E-14
1.14683543E	04	1.26347347E	01	1.92453270E	00	1.68224303E	02 2.24906498E-06

3.40875417E-09 1.49239675E-12 -1.14789269E+04 1.16292438E+01
H J 9/65H 1.00 0.00 0.00 0.0 300.000 5000.000
0.25000000E 01 0.0 0.0 0.0 0.0
0.25471625E 05 -0.46011758E 00 0.25000000E 01 0.0 0.0
0.0 0.0 0.25471625E 05 -0.46011758E 00
CN J 6/69C 1.N 1.0 0.0 0.0 300.000 5000.000
0.36036282E 01 0.33644354E-03 0.10028930E-06 -0.16318141E-10 -0.36286701E-15
0.51159828E 05 0.35454493E 01 0.37386303E 01 -0.19239220E-02 0.47035173E-05
0.31112999E-08 0.61675318E-12 0.51270926E 05 0.34490204E 01
CH J12/67C 1.H 1.0 0.0 0.0 300.000 5000.000
0.22673111E 01 0.22042997E-02 -0.62250189E-06 0.69689321E-10 -0.21274952E-14
0.70838000E 05 0.87889338E 01 0.35632744E 01 -0.20031372E-03 -0.46129811E-06
0.18226920E-08 -0.86768310E-12 0.70405500E 05 0.17628012E 01
C J 3/61C 1.00 0.00 0.00 0.0 300.000 5000.000
0.25810652E 01 -0.14696202E-03 0.74388026E-07 -0.79401066E-11 0.51900964E-16
0.85216250E 05 0.43128872E 01 0.25328703E 01 -0.15887640E-03 0.30682077E-06
-0.26770053E-09 0.87488827E-13 0.85240375E 05 0.46062365E 01
C(S) J 3/61C 1.0 0.0 0.0 0.0 300.000 5000.000
0.13604937E 01 0.19182237E-02 -0.84040386E-06 0.16448705E-09 -0.11672670E-13
-0.65713843E 03 -0.80070200E 01 -0.44778049E 00 0.5369070E-02 -0.39775563E-06
-0.40459263E-08 0.21134925E-11 -0.94280670E 02 0.16840773E 01
4.033,231.8,0.
4.163,224.7,0.

APPENDIX G
PULVERIZED COAL COMBUSTION CASE

```

5,          !NSAY..(SAY(I),I=1,NSAY) follows:
>>>>>>>> REACTING PARTICLES IN HOT FLOW <<<<<<<<<
          ASAY SUBBITUMINOUS COAL CASE
          also analyzed by HILL as case 5
          NEWEST CODE
          swirl no = 2.0
T      T      T      T      T      !INRST, INCALF, INCREK, INCALH, INCALG
T      T      F      T      T      !IPSICT, INPRST, INEACH, INCLET, INCLGE
T      F      F      F      F      !INCAIN, INCURF, LEULP, INTFRZ, INISMP
T      F      T      F      T      !INCNOX, POLLUT, INQRI, INCSWP, INCSWS
F      F      F      T      F      !INNOZZ, INFSOU, LTBUG, GRDOUT, INPROG
F      T      F      F      F      !INCFP, INRAD, INRDGE, INTRUS, MAGHJER
0.500,0.500,0.500,0.200,          !URFU, URFV, URFW, URFH
0.700,0.700,0.700,0.700,0.700,    !URFE, URFK, URFJ, URFV, URFVIS
0.500,0.700,0.700,1.000,0.700,    !URFDEN, URFETA, URFGET, URFHJ, URFPP, URFPP
2.22300E-02, 8.40000E-02, 0.20320 , !DIAP, DIAS, DIACH
7.6837 , 6.36000E-03,              !NDIA(real), THICK
1000, 1000, 50,                    !MAXIT, INDPRI, INDRST
10, 10, 30,                        !NJINP, NJINS, NIWQ
100.000, 1.100, 25, 1.100, 0.900,  !ALI, EPSX, NL, EPSI, EPSD
-410.0 , 10.0 , 0.0000E+00, !HRMIN, HRMAX, HLOSS
4, 35.000 , 4.00000E-02, !NIINO, QHA, QLX
1000.00, 1000.00, 1200.00, !TBN, TBW, TBE
1.79000E-05, 86000. ,          !VISCOS, PRES
0.01000000, 0.10000000,        !SORMAX, SORMIN
NLET 1          ! (Primary)
6.2276E-03, 1.000, 0.000, 0.150, !FLOW, FFLOW, SWIRLN, TINFLO
NLET 2          ! (Secondary)
1.9341E-02, 0.000, 2.000, 0.130, !FLOW, FFLOW, SWIRLN, TINFLO
!          (Blank line)
ELEMENTS
HERMO          !The react. sect. is formatted
EACTANTS 1
300.000        !TMP (unformatted)
2. 0. 0. 0. 02 0.21453 G
2. 0. 0. 0. 02 0.70027 G
R1. 0. 0. 0. 0. AR 0.06375 G
2. 0 1. 0. 0. H2O 0.02145 G
!          (Blank line)
EACTANTS 2
589.000        !TMP (unformatted)
2. 0. 0. 0. 02 0.23153 G
2. 0. 0. 0. 02 0.75560 G
R1. 0. 0. 0. 0. AR 0.01285 G
!          (Blank line)
10, 5,
0.45523,1340.000,
0.0000,0.0000,0.0000,0.0000,0.0000,
0.0000,0.0000,0.0000,0.0000,0.0000,
1.0000,1.0000,1.0000,1.0000,1.0000,
0.000, 0.000, 0.000, 0.000, 0.000,
0.000, 0.000, 0.000, 0.000, 0.000,
1.0000,1.0000,1.0000,1.0000,1.0000,
2.500E-05, 5.000E-05, 6.500E-05,
8.000E-05, 1.000E-04,
0.4000,0.2500,0.1500,0.1000,0.1000,
F      F      T      F      F
T      T      T      F
0.9500,0.0200,
15, 25, 3,
0.350,0.350,0.350,0.350,0.350,
!
! All Particles have the same Properties
T          !INCOAL

```

```

2 1 5 1 1 0
1.000E-02, 1.000E-06, 0.100 , 0.800 !NCRXN,NHRXN,NPROP,IEUCK,KEQ,NSHRNK
1.0000 !DELTPJ,DELRRJ,GAMMA,URFPM
1.0000 !XI(J)
5.61070E+05, 0.00000E+00, -1.50400E+07, !HCO(J),HHO(J),HAO(J)
-1.58800E+07, 373.15 , !HWO(J),TNBP
0.93110 , 0.00000E+00, 6.89000E-02, !OMEGAC(J),OMEGAH(J),OMEGAA(J)
0.00000E+00, !OMEGAW(J)
3.70000E+05, 7.36380E+07, 0.39000 , !AMJ(J,M),EMJ(J,M),YY(J,M)
0.00000E+00, !HGV(J,M)
1.46000E+13, 2.51040E+08, 0.80000 , !AMJ(J,M),EMJ(J,M),YY(J,M)
0.00000E+00, !HGV(J,M)
1.0051 , 8.53540E+07, 1.0000 , !AL(J,L),EL(J,L),EMM(J,L)
0.00000E+00, !HGH(J,L)
1225.2 , 0.00000E+00, 0.00000E+00, !CCP(J,N11,COMPONENT)
1225.2 , 0.00000E+00, 0.00000E+00, !CCP(J,N11,COMPONENT)
1225.2 , 0.00000E+00, 0.00000E+00, !CCP(J,N11,COMPONENT)
1.00000E-05, 0.71960 , 4.68000E-02, !(WIC(J,K) K = 1,3)
0.21640 , 1.16000E-02, !(WIC(J,K) K = 4,NLM)
H2O !SLRCNP
O2 !OXYD(L),L = 1,NHRXN
2.00, !PHIL(L) L = 1,NHRXN
T T T , 10 !LDISO,LGASE,LEMCR,MAXITR
0.9300,0.8600,0.8200,0.8200,0.8200, !(QAB,IPS),IPS = 1,NPS)
0.3300,0.3100,0.3000,0.3000,0.3000, !(QSC,IPS),IPS = 1,NPS)
0.8000, 0.00 !EMW,TOUT
1.0000,0.0000 !A0,AF
4, !NSAYNX..(SAYNX(I),I=1,NSAYNX) follows:
***** PCNOX *****
**** NOX POLLUTANT CALCULATION USING OUTPUT FROM PCGC-2 FOR THE ****
**** PHASE AND PARTICLE PROPERTIES THROUGHOUT THE FLOW FIELD ****
***** BASECASE *****
1.00000E+11, 3.00000E+12, 4.12510E-04, !A1,A2,A3
2.80500E+08, 2.51000E+08, 1.45240E+08, !EACT1,EACT2,EACT3
0.900,0.900, 0.050,0.800, 0.000,0.000, !PRNOX,PRHCN,FCTNO,FCTHCN,YHCNPR,YHCNS
100, 2, 100, !MXITNX,IYTNX,INDPNX
1.0000 1.0000 , 1.00000E-04, !XIANOX,ZEDA,MAXRES
T T T !IRSTNX,IPLTNX,INH1NX

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F 2 F 2          !UPDAT,KOPUP,USDAT,KOPUS,...
F 0 F 0          !VPDAT,KOPVP,VSDAT,KOPVS,...
F 4 F 4          !WPDAT,KOPWP,WSDAT,KOPWS,...
T 1 T 1          !TIPDAT,KOPTP,TISDAT,KOPTES,...
F 2 F 2          !EDPDAT,KOPEDP,EDSDAT,KOFEDS,...
0.00E+00, 0.00E+00,
1 8.50000E+00    !PLS,SLS,AIIS...
1.25500E-02, 1.25500E-02, 6.50000E-02, !NSFORM,ALPHA0.
30.150 , 0.00000E+00, 0.00000E+00, 8.00000E-02, 0.00000E+00, 0.00000E+00,
28.030 , 0.00000E+00, 0.00000E+00, 0.10000 , 0.00000E+00, 5.00000E-03,
25.350 , 0.00000E+00, 0.00000E+00, 0.16700 , 0.00000E+00, 1.00000E-02,
24.000 , 0.00000E+00, 0.00000E+00, 0.18000 , 0.00000E+00, 1.25000E-02,
27.000 , 0.00000E+00, 0.00000E+00, 0.18000 , 0.00000E+00, 1.26000E-02,
30.290 , 0.00000E+00, 0.00000E+00, 0.23000 , 0.00000E+00, 1.50000E-02,
32.770 , 0.00000E+00, 0.00000E+00, 0.22000 , 0.00000E+00, 2.00000E-02,
35.510 , 0.00000E+00, 0.00000E+00, 0.18000 , 0.00000E+00, 2.50000E-02,
36.700 , 0.00000E+00, 0.00000E+00, 0.17000 , 0.00000E+00, 3.00000E-02,
36.710 , 0.00000E+00, 0.00000E+00, 0.16000 , 0.00000E+00, 3.50000E-02,
37.040 , 0.00000E+00, 0.00000E+00, 0.17000 , 0.00000E+00, 4.00000E-02,
37.250 , 0.00000E+00, 0.00000E+00, 0.17000 , 0.00000E+00, 4.50000E-02,
37.290 , 0.00000E+00, 0.00000E+00, 0.16000 , 0.00000E+00, 5.00000E-02,
36.430 , 0.00000E+00, 0.00000E+00, 0.18000 , 0.00000E+00, 5.50000E-02,
31.070 , 0.00000E+00, 0.00000E+00, 0.24000 , 0.00000E+00, 6.00000E-02,
21.000 , 0.00000E+00, 0.00000E+00, 0.29000 , 0.00000E+00, 6.50000E-02,

```

ODE

34	29
5	15
6	7
4	5

22

X

XU

Y

YV

1	-5.0000E-03	0.0000E+00	-1.3000E-03	0.0000E+00
2	5.0000E-03	0.0000E+00	1.3000E-03	0.0000E+00
3	1.5000E-02	0.0000E+00	3.9005E-03	0.0000E+00
4	2.5000E-02	0.0000E+00	6.6544E-03	0.0000E+00
5	3.5000E-02	0.0000E+00	9.5708E-03	0.0000E+00
6	4.5000E-02	0.0000E+00	1.2659E-02	0.0000E+00
7	5.6046E-02	0.0000E+00	1.5748E-02	0.0000E+00
8	6.8246E-02	0.0000E+00	1.8836E-02	0.0000E+00
9	8.1723E-02	0.0000E+00	2.1925E-02	0.0000E+00
10	9.6608E-02	0.0000E+00	2.5013E-02	0.0000E+00
11	1.1305E-01	0.0000E+00	2.8102E-02	0.0000E+00
12	1.3121E-01	0.0000E+00	3.1190E-02	0.0000E+00
13	1.5127E-01	0.0000E+00	3.4279E-02	0.0000E+00
14	1.7343E-01	0.0000E+00	3.7367E-02	0.0000E+00
15	1.9790E-01	0.0000E+00	4.0456E-02	0.0000E+00
16	2.2494E-01	0.0000E+00	4.3544E-02	0.0000E+00
17	2.5480E-01	0.0000E+00	4.6942E-02	0.0000E+00
18	2.8778E-01	0.0000E+00	5.0679E-02	0.0000E+00
19	3.2421E-01	0.0000E+00	5.4789E-02	0.0000E+00
20	3.6445E-01	0.0000E+00	5.9311E-02	0.0000E+00
21	4.0890E-01	0.0000E+00	6.4285E-02	0.0000E+00
22	4.5800E-01	0.0000E+00	6.9757E-02	0.0000E+00
23	5.1223E-01	0.0000E+00	7.5775E-02	0.0000E+00
24	5.7213E-01	0.0000E+00	8.1794E-02	0.0000E+00
25	6.3829E-01	0.0000E+00	8.7211E-02	0.0000E+00
26	7.1137E-01	0.0000E+00	9.2086E-02	0.0000E+00
27	7.9210E-01	0.0000E+00	9.6474E-02	0.0000E+00
28	8.8126E-01	0.0000E+00	1.0042E-01	0.0000E+00
29	9.7975E-01	0.0000E+00	1.0278E-01	0.0000E+00
30	1.0825E+00	0.0000E+00	0.0000E+00	0.0000E+00
31	1.2087E+00	0.0000E+00	0.0000E+00	0.0000E+00
32	1.3414E+00	0.0000E+00	0.0000E+00	0.0000E+00
33	1.4880E+00	0.0000E+00	0.0000E+00	0.0000E+00
34	1.6346E+00	0.0000E+00	0.0000E+00	0.0000E+00
35	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
36	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
37	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
38	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
39	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
40	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

REACTOR BOUNDARIES AND FLOW DOMAIN

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34
29	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	
28	X	X	X	X	X	O	O	O	O	O	O	O	O	O	O	O	O	X	O	O	O	O	O	O	O	O	O	O	O	O	O	O	
27	X	X	X	X	X	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	
26	X	X	X	X	X	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	
25	X	X	X	X	X	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	
24	X	X	X	X	X	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	
23	X	X	X	X	X	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	
22	X	X	X	X	X	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	
21	X	X	X	X	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	
20	X	X	X	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	
19	X	X	X	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	
18	X	X	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	
17	X	X	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	
16	X	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	
15	S	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	
14	S	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	

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_DRBO: [ BREWSTER.PCGC.EXAMPLES]ASA?SUB.GRD;1
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17-DEC-1987 11:04

Page 2

13	S	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	C	O	O	O	O	O	O	O	O
12	S	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	G	D	O	C	O	O	O	O	O
11	S	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	C	O	O	O	O	O	O	O
10	S	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	G	D	O	C	O	O	O	O	O
9	S	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	G	D	O	C	O	O	O	O	O
8	S	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	G	D	O	C	O	O	O	O	O
7	X	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	C	B	O	O	O	O	O	O	O
6	X	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	C	B	O	O	O	O	O	O	O
5	P	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	C	B	O	O	O	O	O	O	O
4	P	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	C	B	O	O	O	O	O	O	O
3	P	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	C	B	O	O	O	O	O	O	O
2	P	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	C	B	O	O	O	O	O	O	O
1	P	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	O	C	B	O	O	O	O	O	O	O

NOTE: THE JPRIM,JSEC,NJINS,JQ:ART,AND IQ:ART
ARE SUPERCEDED BY THE X AND P AND S IN THE MAP WHEN
INTRUS=.TRUE.

\$ set noverify

%SET-W NOTSET, error modifying DRB0:
%CLI-E:INVALIDTYPE, invalid device type - specify a mailbox device
%DCL-I-SUPERSEDE, previous value of UTLTY has been superseded
%SYSTEM-W-NOTALLPRIV, not all requested privileges authorized
%SYSTEM-W-NOTALLPRIV, not all requested privileges authorized
26-SEP-1987 10:53:46

%DCL-I-SUPERSEDE, previous value of SYSSPRINT has been superseded
%COPY-S-COPIED, DRB0:[BREWSTER.WORK]ASAYSUB.RST;70 copied to DRB0:[BREWSTER.WORK]ASAYSUB.RST;71 (159 blocks)
%COPY-S-COPIED, DRB0:[BREWSTER.WORK]ASAYSUB.PSO;59 copied to DRB0:[BREWSTER.WORK]ASAYSUB.PSO;70 (289 blocks)
%COPY-S-COPIED, DRB0:[BREWSTER.WORK]ASAYSUB.RNX;73 copied to DRB0:[BREWSTER.WORK]ASAYSUB.RNX;74 (29 blocks)
%COPY-S-COPIED, DRB0:[BREWSTER.WORK]ASAYSUB.TBL;21 copied to DRB0:[BREWSTER.WORK]ASAYSUB.TBL;22 (270 blocks)

No explicit USE file named PCGC2.USE

Using default USE file

Using PCGC2

%DELETE-I-FILDEL, DRB0:[BREWSTER]PCGC2.USF;1 deleted (3 blocks)

Running PCGC2

%SET I-NEWLIMS, new working set: Limit = 500 Quota = 500 Extent = 2000

>>>>>>> REACTING PARTICLES IN HOT FLOW <<<<<<<<<
ASAY SUBMITUMINOUS COAL CASE
also analyzed by HILL as case 5
NEWEST CODE
swirl no = 2.0

29 34
I
I
I 5, 22
I
15 I
7 I
5 I
.....

NITER	SORCE	RESORU RESORP	RESORV RESORH	RESORW RESORF	RESORM RESOET	NCREE
There were 61 failures in the equilibrium algorithm						
1	5.305E+00	9.635E-01	1.522E-01	1.719E+00	1.685E+00	0
		0.000E+00	5.305E+00	1.576E+00	1.697E+00	
HRPMIN = -37.34556						
INT(HRPMIN/10)*10.0-10.0 = -40.00000						
HRMIN1 = -410.0000						
Changing HRMIN from -410. to -40.						
Generating new table...						
5	3.440E+01	3.440E+01	3.910E+00	1.594E+00	2.777E+00	148
		0.000E+00	3.132E+00	1.247E+00	1.144E+00	
HRPMIN = -230.4098						
HRMIN1 = -40.00000						
NCREE = 148						
NLIM = 100						
INT(HRPMIN/10)*10.0-10.0 = -240.0000						
Changing HRMIN from -40. to -240.						
Generating new table...						
There were 13 failures in the equilibrium algorithm						
10	1.792E+01	1.792E+01	1.620E+00	1.132E+00	1.954E+00	16
		0.000E+00	2.343E+00	9.913E-01	7.780E-01	
15	6.538E+00	6.538E+00	1.008E+00	1.439E+00	2.511E+00	20
		0.000E+00	2.360E+00	1.878E+00	1.374E+00	

20	1.552E+01	1.552E+01	9.035E-01	1.050E+00	7.944E-01	
		0.000E+00	1.862E+00	1.176E+00	9.444E-01	31
25	9.385E+00	9.385E+00	7.800E-01	6.767E-01	1.854E+00	
		0.000E+00	2.160E+00	7.221E-01	7.037E-01	39
30	6.756E+00	6.756E+00	4.289E-01	8.463E-01	9.424E-01	
		0.000E+00	2.439E+00	8.279E-01	7.686E-01	38
35	9.337E+00	9.337E+00	3.519E-01	9.632E-01	5.841E-01	
		0.000E+00	2.061E+00	8.936E-01	7.824E-01	36
40	2.395E+00	2.395E+00	2.712E-01	9.840E-01	5.108E-01	
		0.000E+00	1.535E+00	8.759E-01	7.942E-01	36
45	5.811E+00	5.811E+00	2.710E-01	7.332E-01	4.054E-01	
		0.000E+00	1.208E+00	6.305E-01	4.995E-01	37
50	3.564E+00	3.564E+00	2.576E-01	6.250E-01	7.634E-01	
		0.000E+00	1.266E+00	5.768E-01	5.185E-01	44
55	2.904E+00	2.904E+00	3.294E-01	6.563E-01	5.211E-01	
		0.000E+00	1.264E+00	5.734E-01	4.347E-01	45
60	3.985E+00	3.985E+00	2.409E-01	7.515E-01	2.692E-01	
		0.000E+00	1.263E+00	6.406E-01	5.129E-01	43
65	9.228E-01	7.711E-01	1.747E-01	7.485E-01	4.027E-01	
		0.000E+00	9.228E-01	6.070E-01	4.928E-01	43
70	2.525E+00	2.525E+00	1.150E-01	6.621E-01	1.301E-01	
		0.000E+00	7.553E-01	5.130E-01	4.018E-01	45
75	1.618E+00	1.618E+00	1.005E-01	6.273E-01	3.065E-01	
		0.000E+00	7.698E-01	4.819E-01	3.914E-01	47
80	1.219E+00	1.219E+00	1.089E-01	6.306E-01	2.535E-01	
		0.000E+00	7.311E-01	4.502E-01	3.426E-01	49
85	1.895E+00	1.895E+00	1.030E-01	6.480E-01	9.838E-02	
		0.000E+00	7.221E-01	4.351E-01	3.276E-01	49
90	6.467E-01	6.069E-01	8.297E-02	6.467E-01	1.928E-01	
		0.000E+00	5.845E-01	3.977E-01	3.017E-01	50
95	1.049E+00	1.049E+00	6.688E-02	6.193E-01	8.173E-02	
		0.000E+00	4.572E-01	3.490E-01	2.435E-01	49
100	8.922E-01	8.922E-01	5.223E-02	6.008E-01	1.274E-01	
		0.000E+00	4.492E-01	3.317E-01	2.386E-01	52
105	5.915E-01	4.383E-01	5.185E-02	5.915E-01	1.384E-01	
		0.000E+00	4.158E-01	3.135E-01	2.155E-01	55
110	9.282E-01	9.282E-01	5.208E-02	5.869E-01	4.554E-02	
		0.000E+00	3.909E-01	2.931E-01	1.965E-01	53
115	5.765E-01	4.849E-01	4.631E-02	5.765E-01	9.149E-02	
		0.000E+00	3.423E-01	2.708E-01	1.874E-01	53
120	5.577E-01	4.284E-01	3.789E-02	5.577E-01	6.184E-02	
		0.000E+00	2.704E-01	2.434E-01	1.573E-01	55
125	5.405E-01	4.958E-01	3.148E-02	5.405E-01	5.475E-02	
		0.000E+00	2.395E-01	2.285E-01	1.464E-01	56
130	5.251E-01	1.958E-01	3.143E-02	5.251E-01	7.765E-02	
		0.000E+00	2.152E-01	2.132E-01	1.374E-01	57
135	5.118E-01	4.424E-01	3.275E-02	5.118E-01	3.591E-02	
		0.000E+00	1.855E-01	1.968E-01	1.244E-01	58
140	4.973E-01	3.304E-01	3.106E-02	4.973E-01	4.779E-02	
		0.000E+00	1.726E-01	1.841E-01	1.188E-01	58
145	4.813E-01	2.001E-01	2.721E-02	4.813E-01	4.409E-02	
		0.000E+00	1.413E-01	1.683E-01	1.046E-01	58
150	4.654E-01	2.718E-01	2.422E-02	4.654E-01	2.720E-02	
		0.000E+00	1.255E-01	1.569E-01	9.600E-02	59
155	4.496E-01	1.581E-01	2.347E-02	4.496E-01	4.390E-02	
		0.000E+00	1.031E-01	1.469E-01	9.093E-02	60
160	4.347E-01	2.103E-01	2.406E-02	4.347E-01	3.022E-02	
		0.000E+00	7.915E-02	1.363E-01	8.277E-02	61
165	4.201E-01	2.073E-01	2.363E-02	4.201E-01	2.318E-02	
		0.000E+00	7.700E-02	1.277E-01	7.331E-02	61
170	4.055E-01	1.139E-01	2.236E-02	4.055E-01	3.118E-02	
		0.000E+00	7.044E-02	1.192E-01	7.379E-02	62
175	3.908E-01	1.494E-01	2.089E-02	3.908E-01	2.058E-02	
		0.000E+00	7.039E-02	1.124E-01	6.372E-02	63

180 3.761E-01 1.172E-01 1.956E-02 3.761E-01 2.614E-02 63
0.000E+00 6.599E-02 1.065E-01 6.608E-02
185 3.618E-01 1.040E-01 1.950E-02 3.618E-01 2.380E-02 63
0.000E+00 5.634E-02 1.004E-01 6.217E-02
190 3.481E-01 1.261E-01 1.939E-02 3.481E-01 1.867E-02 64
0.000E+00 5.541E-02 9.512E-02 5.986E-02
195 3.346E-01 8.359E-02 1.914E-02 3.346E-01 2.238E-02 64
0.000E+00 5.881E-02 9.056E-02 5.827E-02
200 3.211E-01 8.702E-02 1.829E-02 3.211E-01 1.833E-02 64
0.000E+00 6.484E-02 8.676E-02 5.574E-02
205 3.079E-01 8.298E-02 1.731E-02 3.079E-01 1.761E-02 64
0.000E+00 6.988E-02 8.346E-02 5.425E-02
210 2.948E-01 6.414E-02 1.686E-02 2.948E-01 1.839E-02 64
0.000E+00 6.899E-02 8.012E-02 5.240E-02
215 2.822E-01 7.709E-02 1.662E-02 2.822E-01 1.507E-02 63
0.000E+00 6.770E-02 7.707E-02 5.070E-02
220 2.700E-01 6.539E-02 1.653E-02 2.700E-01 1.637E-02 62
0.000E+00 6.882E-02 7.440E-02 4.992E-02
225 2.579E-01 5.859E-02 1.600E-02 2.579E-01 1.548E-02 63
0.000E+00 7.096E-02 7.194E-02 4.845E-02
230 2.461E-01 5.975E-02 1.541E-02 2.461E-01 1.357E-02 63
0.000E+00 7.307E-02 6.966E-02 4.712E-02
235 2.346E-01 5.102E-02 1.471E-02 2.346E-01 1.429E-02 63
0.000E+00 7.199E-02 6.722E-02 4.573E-02
240 2.234E-01 5.037E-02 1.428E-02 2.234E-01 1.306E-02 62
0.000E+00 6.885E-02 6.480E-02 4.416E-02
245 2.127E-01 4.944E-02 1.409E-02 2.127E-01 1.250E-02 62
0.000E+00 6.650E-02 6.254E-02 4.306E-02
250 2.022E-01 4.397E-02 1.372E-02 2.022E-01 1.250E-02 62
0.000E+00 6.514E-02 6.033E-02 4.172E-02
255 1.920E-01 4.416E-02 1.327E-02 1.920E-01 1.132E-02 62
0.000E+00 6.444E-02 5.818E-02 4.025E-02
260 1.821E-01 4.109E-02 1.263E-02 1.821E-01 1.104E-02 61
0.000E+00 6.273E-02 5.598E-02 3.878E-02
265 1.726E-01 3.739E-02 1.205E-02 1.726E-01 1.068E-02 60
0.000E+00 5.948E-02 5.368E-02 3.719E-02
270 1.635E-01 3.713E-02 1.172E-02 1.635E-01 9.901E-03 60
0.000E+00 5.597E-02 5.145E-02 3.581E-02
275 1.547E-01 3.470E-02 1.142E-02 1.547E-01 9.805E-03 60
0.000E+00 5.304E-02 4.924E-02 3.440E-02
280 1.462E-01 3.371E-02 1.102E-02 1.462E-01 9.248E-03 59
0.000E+00 5.073E-02 4.706E-02 3.286E-02
285 1.380E-01 3.263E-02 1.049E-02 1.380E-01 8.609E-03 59
0.000E+00 4.836E-02 4.489E-02 3.131E-02
290 1.302E-01 3.023E-02 9.904E-03 1.302E-01 8.349E-03 59
0.000E+00 4.535E-02 4.266E-02 2.972E-02
295 1.227E-01 2.895E-02 9.477E-03 1.227E-01 7.907E-03 59
0.000E+00 4.191E-02 4.044E-02 2.818E-02
300 1.156E-01 2.796E-02 9.153E-03 1.156E-01 7.882E-03 59
0.000E+00 3.866E-02 3.825E-02 2.671E-02
305 1.087E-01 2.700E-02 8.862E-03 1.087E-01 8.981E-03 59
0.000E+00 3.588E-02 3.609E-02 2.519E-02
310 1.152E-01 2.660E-02 1.500E-02 1.021E-01 1.152E-01 59
0.000E+00 3.356E-02 3.396E-02 2.366E-02
315 9.578E-02 2.519E-02 8.030E-03 9.578E-02 8.102E-03 58
0.000E+00 3.078E-02 3.184E-02 2.214E-02
320 8.978E-02 2.403E-02 7.563E-03 8.978E-02 6.578E-03 58
0.000E+00 2.806E-02 2.976E-02 2.064E-02
325 8.407E-02 2.330E-02 7.193E-03 8.407E-02 5.734E-03 58
0.000E+00 2.537E-02 2.771E-02 1.922E-02
330 7.864E-02 2.262E-02 6.851E-03 7.864E-02 5.299E-03 59
0.000E+00 2.291E-02 2.572E-02 1.782E-02
335 7.349E-02 2.207E-02 6.502E-03 7.349E-02 4.876E-03 59
0.000E+00 2.076E-02 2.379E-02 1.643E-02

340	6.860E-02	2.142E-02	6.140E-03	6.860E-02	4.480E-03	
		0.000E+00	1.879E-02	2.192E-02	1.510E-02	59
345	6.398E-02	2.059E-02	5.769E-03	6.398E-02	4.177E-03	
		0.000E+00	1.688E-02	2.011E-02	1.381E-02	59
350	5.964E-02	1.990E-02	5.427E-03	5.964E-02	3.883E-03	
		0.000E+00	1.500E-02	1.839E-02	1.260E-02	59
355	5.556E-02	1.934E-02	5.116E-03	5.556E-02	3.651E-03	
		0.000E+00	1.333E-02	1.675E-02	1.145E-02	59
360	5.174E-02	1.881E-02	4.815E-03	5.174E-02	3.421E-03	
		0.000E+00	1.187E-02	1.519E-02	1.036E-02	59
365	4.815E-02	1.829E-02	4.512E-03	4.815E-02	3.166E-03	
		0.000E+00	1.059E-02	1.374E-02	9.343E-03	59
370	4.480E-02	1.767E-02	4.208E-03	4.480E-02	2.949E-03	
		0.000E+00	9.452E-03	1.239E-02	8.392E-03	59
375	4.169E-02	1.702E-02	3.920E-03	4.169E-02	2.759E-03	
		0.000E+00	8.410E-03	1.113E-02	7.518E-03	59
380	3.879E-02	1.645E-02	3.661E-03	3.879E-02	2.592E-03	
		0.000E+00	7.455E-03	9.973E-03	6.724E-03	59
385	3.611E-02	1.591E-02	3.419E-03	3.611E-02	2.445E-03	
		0.000E+00	6.648E-03	8.912E-03	6.001E-03	59
390	3.362E-02	1.539E-02	3.189E-03	3.362E-02	2.291E-03	
		0.000E+00	5.986E-03	7.952E-03	5.345E-03	59
395	3.132E-02	1.484E-02	2.967E-03	3.132E-02	2.139E-03	
		0.000E+00	5.422E-03	7.089E-03	4.753E-03	59
400	2.919E-02	1.425E-02	2.756E-03	2.919E-02	2.009E-03	
		0.000E+00	4.933E-03	6.308E-03	4.227E-03	59
405	2.723E-02	1.368E-02	2.564E-03	2.723E-02	1.888E-03	
		0.000E+00	4.497E-03	5.617E-03	3.764E-03	59
410	2.541E-02	1.314E-02	2.391E-03	2.541E-02	1.783E-03	
		0.000E+00	4.124E-03	4.997E-03	3.356E-03	59
415	2.373E-02	1.262E-02	2.231E-03	2.373E-02	1.681E-03	
		0.000E+00	3.816E-03	4.455E-03	3.001E-03	59
420	2.219E-02	1.210E-02	2.082E-03	2.219E-02	1.587E-03	
		0.000E+00	3.567E-03	3.981E-03	2.683E-03	59
425	2.075E-02	1.157E-02	1.939E-03	2.075E-02	1.487E-03	
		0.000E+00	3.349E-03	3.566E-03	2.410E-03	59
430	1.943E-02	1.105E-02	1.808E-03	1.943E-02	1.403E-03	
		0.000E+00	3.154E-03	3.198E-03	2.171E-03	59
435	1.821E-02	1.054E-02	1.692E-03	1.821E-02	1.330E-03	
		0.000E+00	2.974E-03	2.882E-03	1.963E-03	59
440	1.707E-02	1.007E-02	1.584E-03	1.707E-02	1.259E-03	
		0.000E+00	2.819E-03	2.605E-03	1.785E-03	59
445	1.602E-02	9.610E-03	1.484E-03	1.602E-02	1.189E-03	
		0.000E+00	2.685E-03	2.364E-03	1.629E-03	59
450	1.504E-02	9.157E-03	1.392E-03	1.504E-02	1.119E-03	
		0.000E+00	2.564E-03	2.156E-03	1.492E-03	59
455	1.414E-02	8.710E-03	1.303E-03	1.414E-02	1.054E-03	
		0.000E+00	2.450E-03	1.976E-03	1.373E-03	59
460	1.329E-02	8.282E-03	1.223E-03	1.329E-02	9.971E-04	
		0.000E+00	2.339E-03	1.819E-03	1.273E-03	59
465	1.250E-02	7.878E-03	1.150E-03	1.250E-02	9.482E-04	
		0.000E+00	2.234E-03	1.683E-03	1.183E-03	59
470	1.177E-02	7.493E-03	1.084E-03	1.177E-02	8.927E-04	
		0.000E+00	2.137E-03	1.565E-03	1.105E-03	59
475	1.108E-02	7.123E-03	1.018E-03	1.108E-02	8.421E-04	
		0.000E+00	2.046E-03	1.460E-03	1.034E-03	59
480	1.044E-02	6.763E-03	9.589E-04	1.044E-02	7.992E-04	
		0.000E+00	1.959E-03	1.371E-03	9.727E-04	59

NJITER		SORCE		RESNJ'S	
SCATTER	ITER: 0	ITERATION:	1	FRAC CHANGE IN TOT NET WALL FLUX:	1.000E+00
SCATTER	ITER: 0	ITERATION:	2	FRAC CHANGE IN TOT NET WALL FLUX:	5.418E-01
SCATTER	ITER: 0	ITERATION:	3	FRAC CHANGE IN TOT NET WALL FLUX:	2.016E-01
SCATTER	ITER: 0	ITERATION:	4	FRAC CHANGE IN TOT NET WALL FLUX:	7.955E-02

SCATTER ITER: 0 ITERATION: 5 FRAC CHANGE IN TOT NET WALL FLUX: 3.063E-02
 SCATTER ITER: 0 ITERATION: 6 FRAC CHANGE IN TOT NET WALL FLUX: 1.133E-02
 SCATTER ITER: 0 ITERATION: 7 FRAC CHANGE IN TOT NET WALL FLUX: 4.149E-03
 SCATTER ITER: 1 ITERATION: 1 FRAC CHANGE IN TOT NET WALL FLUX: 3.215E-02
 SCATTER ITER: 1 ITERATION: 2 FRAC CHANGE IN TOT NET WALL FLUX: 1.025E-02
 SCATTER ITER: 1 ITERATION: 3 FRAC CHANGE IN TOT NET WALL FLUX: 1.614E-03
 SCATTER ITER: 0 ITERATION: 1 FRAC CHANGE IN TOT NET WALL FLUX: 1.000E+00
 SCATTER ITER: 0 ITERATION: 2 FRAC CHANGE IN TOT NET WALL FLUX: 5.418E-01
 SCATTER ITER: 0 ITERATION: 3 FRAC CHANGE IN TOT NET WALL FLUX: 2.016E-01
 SCATTER ITER: 0 ITERATION: 4 FRAC CHANGE IN TOT NET WALL FLUX: 7.955E-02
 SCATTER ITER: 0 ITERATION: 5 FRAC CHANGE IN TOT NET WALL FLUX: 3.063E-02
 SCATTER ITER: 0 ITERATION: 6 FRAC CHANGE IN TOT NET WALL FLUX: 1.133E-02
 SCATTER ITER: 0 ITERATION: 7 FRAC CHANGE IN TOT NET WALL FLUX: 4.149E-03
 SCATTER ITER: 1 ITERATION: 1 FRAC CHANGE IN TOT NET WALL FLUX: 3.215E-02
 SCATTER ITER: 1 ITERATION: 2 FRAC CHANGE IN TOT NET WALL FLUX: 1.025E-02
 SCATTER ITER: 1 ITERATION: 3 FRAC CHANGE IN TOT NET WALL FLUX: 1.614E-03

IF IT HITS THE WALLS IT STICKS

ISL= 1, IPS= 1, TERMINATED AT: IV=34, JU= 2 TIME= 2.429E-01 NPOINT= 476
 ISL= 1, IPS= 2, TERMINATED AT: IV=34, JU= 2 TIME= 2.381E-01 NPOINT= 519
 ISL= 1, IPS= 3, TERMINATED AT: IV=34, JU= 2 TIME= 2.384E-01 NPOINT= 481
 ISL= 1, IPS= 4, TERMINATED AT: IV=34, JU= 2 TIME= 2.306E-01 NPOINT= 643
 ISL= 1, IPS= 5, TERMINATED AT: IV=34, JU= 2 TIME= 2.196E-01 NPOINT= 534
 ISL= 2, IPS= 1, TERMINATED AT: IV=34, JU= 6 TIME= 2.444E-01 NPOINT= 375
 ISL= 2, IPS= 2, TERMINATED AT: IV=34, JU= 5 TIME= 2.428E-01 NPOINT= 510
 ISL= 2, IPS= 3, TERMINATED AT: IV=34, JU= 5 TIME= 2.389E-01 NPOINT= 472
 ISL= 2, IPS= 4, TERMINATED AT: IV=34, JU= 5 TIME= 2.274E-01 NPOINT= 447
 ISL= 2, IPS= 5, TERMINATED AT: IV=34, JU= 4 TIME= 2.186E-01 NPOINT= 527
 ISL= 3, IPS= 1, TERMINATED AT: IV=34, JU=12 TIME= 2.429E-01 NPOINT= 587
 ISL= 3, IPS= 2, TERMINATED AT: IV=34, JU= 9 TIME= 2.363E-01 NPOINT= 361
 ISL= 3, IPS= 3, TERMINATED AT: IV=34, JU= 8 TIME= 2.365E-01 NPOINT= 427
 ISL= 3, IPS= 4, TERMINATED AT: IV=34, JU= 7 TIME= 2.271E-01 NPOINT= 485
 ISL= 3, IPS= 5, TERMINATED AT: IV=34, JU= 7 TIME= 2.215E-01 NPOINT= 512
 ISL= 4, IPS= 1, TERMINATED AT: IV=34, JU=17 TIME= 2.398E-01 NPOINT= 463
 ISL= 4, IPS= 2, TERMINATED AT: IV=34, JU=13 TIME= 2.359E-01 NPOINT= 343
 ISL= 4, IPS= 3, TERMINATED AT: IV=34, JU=12 TIME= 2.365E-01 NPOINT= 561
 ISL= 4, IPS= 4, TERMINATED AT: IV=34, JU=11 TIME= 2.327E-01 NPOINT= 439
 ISL= 4, IPS= 5, TERMINATED AT: IV=34, JU= 9 TIME= 2.247E-01 NPOINT= 585
 ISL= 5, IPS= 1, TERMINATED AT: IV=34, JU=19 TIME= 2.394E-01 NPOINT= 400
 ISL= 5, IPS= 2, TERMINATED AT: IV=34, JU=17 TIME= 2.378E-01 NPOINT= 275
 ISL= 5, IPS= 3, TERMINATED AT: IV=34, JU=14 TIME= 2.345E-01 NPOINT= 392
 ISL= 5, IPS= 4, TERMINATED AT: IV=34, JU=13 TIME= 2.304E-01 NPOINT= 431
 ISL= 5, IPS= 5, TERMINATED AT: IV=34, JU=11 TIME= 2.246E-01 NPOINT= 567
 ISL= 6, IPS= 1, TERMINATED AT: IV=34, JU=21 TIME= 2.486E-01 NPOINT= 503
 ISL= 6, IPS= 2, TERMINATED AT: IV=34, JU=20 TIME= 2.347E-01 NPOINT= 276
 ISL= 6, IPS= 3, TERMINATED AT: IV=34, JU=18 TIME= 2.339E-01 NPOINT= 331
 ISL= 6, IPS= 4, TERMINATED AT: IV=34, JU=17 TIME= 2.283E-01 NPOINT= 464
 ISL= 6, IPS= 5, TERMINATED AT: IV=34, JU=15 TIME= 2.233E-01 NPOINT= 588
 ISL= 7, IPS= 1, TERMINATED AT: IV=34, JU=22 TIME= 2.648E-01 NPOINT= 567
 ISL= 7, IPS= 2, TERMINATED AT: IV=34, JU=21 TIME= 2.329E-01 NPOINT= 310
 ISL= 7, IPS= 3, TERMINATED AT: IV=34, JU=20 TIME= 2.344E-01 NPOINT= 366
 ISL= 7, IPS= 4, TERMINATED AT: IV=34, JU=18 TIME= 2.282E-01 NPOINT= 459
 ISL= 7, IPS= 5, TERMINATED AT: IV=34, JU=16 TIME= 2.227E-01 NPOINT= 615
 TRAJECTORY ISL= 8, IPS= 1 RECIRCULATES
 ISL= 8, IPS= 1, TERMINATED AT: IV=34, JU=24 TIME= 2.591E-01 NPOINT= 493
 ISL= 8, IPS= 2, TERMINATED AT: IV=34, JU=23 TIME= 2.413E-01 NPOINT= 430
 ISL= 8, IPS= 3, TERMINATED AT: IV=34, JU=22 TIME= 2.330E-01 NPOINT= 320
 ISL= 8, IPS= 4, TERMINATED AT: IV=34, JU=21 TIME= 2.283E-01 NPOINT= 357
 ISL= 8, IPS= 5, TERMINATED AT: IV=34, JU=20 TIME= 2.253E-01 NPOINT= 605
 TRAJECTORY ISL= 9, IPS= 1 RECIRCULATES
 ISL= 9, IPS= 1, TERMINATED AT: IV=34, JU=25 TIME= 2.460E-01 NPOINT= 582
 ISL= 9, IPS= 2, TERMINATED AT: IV=34, JU=23 TIME= 2.530E-01 NPOINT= 377
 ISL= 9, IPS= 3, TERMINATED AT: IV=34, JU=23 TIME= 2.396E-01 NPOINT= 376
 ISL= 9, IPS= 4, TERMINATED AT: IV=34, JU=22 TIME= 2.340E-01 NPOINT= 375
 ISL= 9, IPS= 5, TERMINATED AT: IV=34, JU=21 TIME= 2.248E-01 NPOINT= 615

TRAJECTORY ISL=10, IPS= 1 RECIRCULATES
 ISL=10, IPS= 1, TERMINATED AT: IV=34, JU=27 TIME= 2.391E-01 NPOINT= 444
 TRAJECTORY ISL=10, IPS= 2 RECIRCULATES
 ISL=10, IPS= 2, TERMINATED AT: IV=34, JU=24 TIME= 3.249E-01 NPOINT= 544
 ISL=10, IPS= 3, TERMINATED AT: IV=34, JU=24 TIME= 2.498E-01 NPOINT= 327
 ISL=10, IPS= 4, TERMINATED AT: IV=34, JU=23 TIME= 2.349E-01 NPOINT= 434
 ISL=10, IPS= 5, TERMINATED AT: IV=34, JU=22 TIME= 2.289E-01 NPOINT= 593

SUM OF SOLID PHASE COUPLING

SSPE = 3.226E-04
 SSPF = 0.000E+00
 SSPM = 3.226E-04
 SSPU = 8.218E-03
 SSPV = -5.514E-06
 SSPH = 0.000E+00

AT X = 1.49 , COAL BURNOUT = 0.7679

>>>>FOLP COMPLETE, END OF PARTICLE ITERATION # 1

NITER	SORCE	RESORU RESORP	FESORV FESORH	RESORW RESORF	RESORM RESOET	NCREE
1	1.271E+00	1.841E-01	3.757E-02	4.141E-02	1.455E-01	
	1.270870	0.000E+00	1.141E-01	2.143E-01	1.271E+00	59
5	1.398E+00	1.398E+00	6.889E-01	2.321E-01	3.04CE-01	
		0.000E+00	2.894E-01	3.513E-01	5.898E-01	58
10	1.278E+00	1.278E+00	3.365E-01	3.478E-01	2.219E-01	
		0.000E+00	4.126E-01	4.139E-01	1.067E+00	55
15	1.232E+00	1.232E+00	3.218E-01	2.835E-01	2.327E-01	
		0.000E+00	4.337E-01	3.791E-01	8.958E-01	51
20	8.923E-01	8.923E-01	2.504E-01	2.271E-01	2.261E-01	
		0.000E+00	4.194E-01	3.186E-01	7.355E-01	45
25	6.369E-01	6.369E-01	2.372E-01	2.100E-01	1.618E-01	
		0.000E+00	5.072E-01	2.905E-01	6.369E-01	40
30	6.021E-01	6.021E-01	1.332E-01	1.763E-01	1.067E-01	
		0.000E+00	5.583E-01	2.430E-01	6.021E-01	37
35	5.444E-01	5.444E-01	8.997E-02	1.437E-01	8.631E-02	
		0.000E+00	5.139E-01	1.975E-01	5.444E-01	30
40	5.757E-01	5.757E-01	7.555E-02	1.275E-01	7.543E-02	
		0.000E+00	4.316E-01	1.828E-01	4.905E-01	29
45	4.437E-01	4.437E-01	5.755E-02	1.226E-01	9.752E-02	
		0.000E+00	3.561E-01	1.827E-01	4.437E-01	24
50	4.048E-01	4.048E-01	4.385E-02	1.130E-01	6.947E-02	
		0.000E+00	3.027E-01	1.690E-01	4.048E-01	23
55	3.801E-01	3.801E-01	3.812E-02	1.042E-01	3.676E-02	
		0.000E+00	2.838E-01	1.585E-01	3.801E-01	21
60	3.550E-01	3.550E-01	3.284E-02	9.855E-02	4.527E-02	
		0.000E+00	2.509E-01	1.574E-01	3.550E-01	18
65	3.233E-01	3.233E-01	2.742E-02	9.614E-02	3.010E-02	
		0.000E+00	2.068E-01	1.584E-01	3.233E-01	18
70	2.992E-01	2.992E-01	2.076E-02	9.204E-02	2.978E-02	
		0.000E+00	1.675E-01	1.566E-01	2.992E-01	17
75	2.747E-01	2.747E-01	1.699E-02	8.546E-02	3.155E-02	
		0.000E+00	1.328E-01	1.543E-01	2.747E-01	16
80	2.567E-01	2.567E-01	1.405E-02	7.758E-02	1.936E-02	
		0.000E+00	1.126E-01	1.527E-01	2.567E-01	16
85	2.403E-01	2.403E-01	1.019E-02	7.122E-02	2.944E-02	
		0.000E+00	1.013E-01	1.515E-01	2.403E-01	15
90	2.227E-01	2.227E-01	7.134E-02	6.653E-02	2.899E-02	
		0.000E+00	8.755E-02	1.498E-01	2.227E-01	15
95	2.064E-01	2.064E-01	5.012E-02	6.232E-02	1.829E-02	

275

100	1.897E-01	0.000E+00	7.432E-02	1.461E-01	2.064E-01	15
		5.930E-02	1.358E-02	5.761E-02	2.191E-02	
		0.000E+00	6.427E-02	1.423E-01	1.897E-01	15
105	1.791E-01	4.660E-02	1.312E-02	5.242E-02	1.915E-02	
		0.000E+00	5.651E-02	1.385E-01	1.791E-01	15
110	1.694E-01	5.691E-02	1.274E-02	4.772E-02	1.541E-02	
		0.000E+00	5.481E-02	1.348E-01	1.694E-01	15
115	1.613E-01	2.559E-02	1.178E-02	4.367E-02	1.732E-02	
		0.000E+00	5.286E-02	1.302E-01	1.613E-01	15
120	1.506E-01	5.492E-02	1.007E-02	3.979E-02	1.242E-02	
		0.000E+00	4.841E-02	1.254E-01	1.506E-01	15
125	1.417E-01	5.831E-02	8.092E-03	3.601E-02	1.150E-02	
		0.000E+00	4.302E-02	1.190E-01	1.417E-01	15
130	1.329E-01	2.778E-02	7.271E-03	3.245E-02	1.291E-02	
		0.000E+00	3.878E-02	1.140E-01	1.329E-01	15
135	1.273E-01	3.165E-02	6.825E-03	2.920E-02	9.181E-03	
		0.000E+00	3.771E-02	1.082E-01	1.273E-01	15
140	1.211E-01	3.089E-02	6.514E-03	2.615E-02	8.112E-03	
		0.000E+00	3.729E-02	1.035E-01	1.211E-01	15
145	1.142E-01	3.005E-02	5.892E-03	2.324E-02	8.129E-03	
		0.000E+00	3.478E-02	9.799E-02	1.142E-01	15
150	1.066E-01	4.556E-02	4.891E-03	2.055E-02	6.610E-03	
		0.000E+00	3.052E-02	9.255E-02	1.066E-01	15
155	9.902E-02	3.780E-02	4.029E-03	1.827E-02	8.370E-03	
		0.000E+00	2.623E-02	8.695E-02	9.902E-02	14
160	9.271E-02	2.799E-02	3.882E-03	1.621E-02	7.937E-03	
		0.000E+00	2.283E-02	8.142E-02	9.271E-02	14
165	8.723E-02	3.109E-02	3.629E-03	1.431E-02	5.561E-03	
		0.000E+00	2.086E-02	7.654E-02	8.723E-02	14
170	8.225E-02	2.715E-02	3.472E-03	1.268E-02	5.660E-03	
		0.000E+00	1.880E-02	7.165E-02	8.225E-02	14
175	7.710E-02	2.827E-02	3.041E-03	1.143E-02	4.822E-03	
		0.000E+00	1.591E-02	6.714E-02	7.710E-02	14
180	7.210E-02	3.036E-02	2.429E-03	1.045E-02	4.078E-03	
		0.000E+00	1.298E-02	6.287E-02	7.210E-02	14
185	6.709E-02	2.348E-02	2.110E-03	9.555E-03	4.459E-03	
		0.000E+00	1.044E-02	5.888E-02	6.709E-02	14
190	6.185E-02	2.294E-02	1.935E-03	8.638E-03	3.339E-03	
		0.000E+00	8.654E-03	5.546E-02	6.185E-02	14
195	5.675E-02	2.216E-02	1.732E-03	7.812E-03	2.413E-03	
		0.000E+00	7.566E-03	5.226E-02	5.675E-02	14
200	5.164E-02	1.805E-02	1.532E-03	7.192E-03	2.439E-03	
		0.000E+00	6.344E-03	4.927E-02	5.164E-02	14
205	4.650E-02	1.902E-02	1.282E-03	6.750E-03	1.767E-03	
		0.000E+00	4.974E-03	4.633E-02	4.650E-02	13
210	4.325E-02	1.731E-02	1.054E-03	6.367E-03	1.785E-03	
		0.000E+00	3.857E-03	4.325E-02	4.163E-02	12
215	4.011E-02	1.446E-02	9.976E-04	5.951E-03	1.723E-03	
		0.000E+00	2.907E-03	4.011E-02	3.685E-02	12
220	3.693E-02	1.486E-02	9.082E-04	5.509E-03	1.131E-03	
		0.000E+00	2.405E-03	3.693E-02	3.234E-02	12
225	3.380E-02	1.312E-02	8.435E-04	5.122E-03	1.175E-03	
		0.000E+00	2.108E-03	3.380E-02	2.828E-02	12
230	3.070E-02	1.101E-02	7.790E-04	4.849E-03	1.127E-03	
		0.000E+00	1.723E-03	3.070E-02	2.444E-02	12
235	2.767E-02	1.107E-02	7.043E-04	4.644E-03	8.174E-04	
		0.000E+00	1.385E-03	2.767E-02	2.106E-02	12
240	2.479E-02	9.521E-03	6.701E-04	4.431E-03	9.602E-04	
		0.000E+00	1.125E-03	2.479E-02	1.803E-02	12
245	2.204E-02	8.924E-03	6.557E-04	4.193E-03	8.854E-04	
		0.000E+00	9.160E-04	2.204E-02	1.525E-02	12
250	1.948E-02	8.667E-03	6.064E-04	3.959E-03	7.689E-04	
		0.000E+00	8.763E-04	1.948E-02	1.288E-02	12
255	1.709E-02	7.269E-03	5.654E-04	3.783E-03	9.075E-04	

		0.000E+00	8.522E-04	1.709E-02	1.078E-02	13
260	1.488E-02	6.578E-03	5.220E-04	3.671E-03	7.922E-04	
		0.000E+00	7.828E-04	1.488E-02	8.962E-03	13
265	1.288E-02	6.243E-03	4.794E-04	3.575E-03	7.076E-04	
		0.000E+00	7.550E-04	1.288E-02	7.515E-03	13
270	1.107E-02	5.440E-03	4.753E-04	3.470E-03	7.421E-04	
		0.000E+00	7.041E-04	1.107E-02	6.262E-03	13

NJITER SOURCE RESNJ'S

SCATTER ITER: 0	ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX:	1.000E+00
SCATTER ITER: 0	ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX:	5.296E-01
SCATTER ITER: 0	ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX:	1.822E-01
SCATTER ITER: 0	ITERATION: 4	FRAC CHANGE IN TOT NET WALL FLUX:	7.618E-02
SCATTER ITER: 0	ITERATION: 5	FRAC CHANGE IN TOT NET WALL FLUX:	2.731E-02
SCATTER ITER: 0	ITERATION: 6	FRAC CHANGE IN TOT NET WALL FLUX:	1.039E-02
SCATTER ITER: 0	ITERATION: 7	FRAC CHANGE IN TOT NET WALL FLUX:	3.653E-03
SCATTER ITER: 1	ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX:	2.909E-02
SCATTER ITER: 1	ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX:	1.237E-02
SCATTER ITER: 1	ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX:	2.101E-03
SCATTER ITER: 0	ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX:	1.000E+00
SCATTER ITER: 0	ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX:	5.296E-01
SCATTER ITER: 0	ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX:	1.822E-01
SCATTER ITER: 0	ITERATION: 4	FRAC CHANGE IN TOT NET WALL FLUX:	7.618E-02
SCATTER ITER: 0	ITERATION: 5	FRAC CHANGE IN TOT NET WALL FLUX:	2.731E-02
SCATTER ITER: 0	ITERATION: 6	FRAC CHANGE IN TOT NET WALL FLUX:	1.039E-02
SCATTER ITER: 0	ITERATION: 7	FRAC CHANGE IN TOT NET WALL FLUX:	3.653E-03
SCATTER ITER: 1	ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX:	2.909E-02
SCATTER ITER: 1	ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX:	1.237E-02
SCATTER ITER: 1	ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX:	2.101E-03

IF IT HITS THE WALLS IT STICKS

ISL= 1, IPS= 1, TERMINATED AT: IV=34, JU= 2	TIME= 2.351E-01	NPOINT= 350
ISL= 1, IPS= 2, TERMINATED AT: IV=34, JU= 2	TIME= 2.297E-01	NPOINT= 439
ISL= 1, IPS= 3, TERMINATED AT: IV=34, JU= 2	TIME= 2.277E-01	NPOINT= 485
ISL= 1, IPS= 4, TERMINATED AT: IV=34, JU= 2	TIME= 2.240E-01	NPOINT= 417
ISL= 1, IPS= 5, TERMINATED AT: IV=34, JU= 2	TIME= 2.177E-01	NPOINT= 425
ISL= 2, IPS= 1, TERMINATED AT: IV=34, JU= 7	TIME= 2.375E-01	NPOINT= 338
ISL= 2, IPS= 2, TERMINATED AT: IV=34, JU= 5	TIME= 2.291E-01	NPOINT= 439
ISL= 2, IPS= 3, TERMINATED AT: IV=34, JU= 4	TIME= 2.267E-01	NPOINT= 463
ISL= 2, IPS= 4, TERMINATED AT: IV=34, JU= 4	TIME= 2.243E-01	NPOINT= 443
ISL= 2, IPS= 5, TERMINATED AT: IV=34, JU= 3	TIME= 2.223E-01	NPOINT= 457
ISL= 3, IPS= 1, TERMINATED AT: IV=34, JU=11	TIME= 2.426E-01	NPOINT= 510
ISL= 3, IPS= 2, TERMINATED AT: IV=34, JU= 8	TIME= 2.317E-01	NPOINT= 422
ISL= 3, IPS= 3, TERMINATED AT: IV=34, JU= 6	TIME= 2.284E-01	NPOINT= 488
ISL= 3, IPS= 4, TERMINATED AT: IV=34, JU= 5	TIME= 2.298E-01	NPOINT= 482
ISL= 3, IPS= 5, TERMINATED AT: IV=34, JU= 5	TIME= 2.209E-01	NPOINT= 463
ISL= 4, IPS= 1, TERMINATED AT: IV=34, JU=15	TIME= 2.493E-01	NPOINT= 480
ISL= 4, IPS= 2, TERMINATED AT: IV=34, JU=11	TIME= 2.361E-01	NPOINT= 427
ISL= 4, IPS= 3, TERMINATED AT: IV=34, JU= 9	TIME= 2.338E-01	NPOINT= 503
ISL= 4, IPS= 4, TERMINATED AT: IV=34, JU= 7	TIME= 2.310E-01	NPOINT= 491
ISL= 4, IPS= 5, TERMINATED AT: IV=34, JU= 6	TIME= 2.253E-01	NPOINT= 477
ISL= 5, IPS= 1, TERMINATED AT: IV=34, JU=18	TIME= 2.549E-01	NPOINT= 406
ISL= 5, IPS= 2, TERMINATED AT: IV=34, JU=13	TIME= 2.457E-01	NPOINT= 465
ISL= 5, IPS= 3, TERMINATED AT: IV=34, JU=10	TIME= 2.398E-01	NPOINT= 546
ISL= 5, IPS= 4, TERMINATED AT: IV=34, JU= 9	TIME= 2.344E-01	NPOINT= 479
ISL= 5, IPS= 5, TERMINATED AT: IV=34, JU= 8	TIME= 2.246E-01	NPOINT= 438
ISL= 6, IPS= 1, TERMINATED AT: IV=34, JU=20	TIME= 2.709E-01	NPOINT= 419
ISL= 6, IPS= 2, TERMINATED AT: IV=34, JU=15	TIME= 2.533E-01	NPOINT= 367
ISL= 6, IPS= 3, TERMINATED AT: IV=34, JU=13	TIME= 2.411E-01	NPOINT= 532
ISL= 6, IPS= 4, TERMINATED AT: IV=34, JU=11	TIME= 2.354E-01	NPOINT= 480
ISL= 6, IPS= 5, TERMINATED AT: IV=34, JU=10	TIME= 2.282E-01	NPOINT= 457
ISL= 7, IPS= 1, TERMINATED AT: IV=34, JU=22	TIME= 2.866E-01	NPOINT= 518
ISL= 7, IPS= 2, TERMINATED AT: IV=34, JU=18	TIME= 2.562E-01	NPOINT= 425
ISL= 7, IPS= 3, TERMINATED AT: IV=34, JU=15	TIME= 2.489E-01	NPOINT= 531
ISL= 7, IPS= 4, TERMINATED AT: IV=34, JU=13	TIME= 2.415E-01	NPOINT= 535

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ISL= 7, IPS= 5, TERMINATED AT: IV=34, JU=11 TIME= 2.319E-01 NPOINT= 416
ISL= 8, IPS= 1, TERMINATED AT: IV=34, JU=23 TIME= 3.551E-01 NPOINT= 377
ISL= 8, IPS= 2, TERMINATED AT: IV=34, JU=20 TIME= 2.691E-01 NPOINT= 309
ISL= 8, IPS= 3, TERMINATED AT: IV=34, JU=18 TIME= 2.573E-01 NPOINT= 508
ISL= 8, IPS= 4, TERMINATED AT: IV=34, JU=16 TIME= 2.498E-01 NPOINT= 520
ISL= 8, IPS= 5, TERMINATED AT: IV=34, JU=14 TIME= 2.411E-01 NPOINT= 440
TRAJECTORY ISL= 9, IPS= 1 RECIRCULATES
ISL= 9, IPS= 1, TERMINATED AT: IV=34, JU=27 TIME= 3.193E-01 NPOINT= 434
ISL= 9, IPS= 2, TERMINATED AT: IV=34, JU=21 TIME= 2.854E-01 NPOINT= 406
ISL= 9, IPS= 3, TERMINATED AT: IV=34, JU=19 TIME= 2.680E-01 NPOINT= 499
ISL= 9, IPS= 4, TERMINATED AT: IV=34, JU=18 TIME= 2.542E-01 NPOINT= 486
ISL= 9, IPS= 5, TERMINATED AT: IV=34, JU=16 TIME= 2.433E-01 NPOINT= 444
TRAJECTORY ISL=10, IPS= 1 RECIRCULATES
ISL=10, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 3.435E-01 NPOINT= 420
ISL=10, IPS= 2, TERMINATED AT: IV=34, JU=22 TIME= 3.261E-01 NPOINT= 351
ISL=10, IPS= 3, TERMINATED AT: IV=34, JU=21 TIME= 2.813E-01 NPOINT= 445
ISL=10, IPS= 4, TERMINATED AT: IV=34, JU=19 TIME= 2.668E-01 NPOINT= 458
ISL=10, IPS= 5, TERMINATED AT: IV=34, JU=18 TIME= 2.483E-01 NPOINT= 431

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SUM OF SOLID PHASE COUPLING

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SSPE = 3.397E-04
SSPF = 0.000E+00
SSPN = 3.397E-04
SSPU = 6.871E-03
SSPV = -3.343E-06
SSPH = 0.000E+00

```

AT X = 1.49 , COAL BURNOUT = 0.8086

>>>>EOLP COMPLETE, END OF PARTICLE ITERATION # 2

274

277

NITER	SORCE	RESORU RESORP	RESCRV RESCRH	RESORW RESORF	RESORM RESOET	NCREE
1	5.423E-01	8.710E-02 0.000E+00	2.653E-02 3.438E-02	1.664E-02 6.961E-02	5.664E-02 5.423E-01	13
HRPMIN = -480.6645 HRMINI = -240.0000 NCREE = 13 NLIM = 0 INT(HRPMIN/10)*10.0-10.0 = -490.0000 Changing HRMIN from -240. to -490. Generating new table... There were 75 failures in the equilibrium algorithm 5 3.914E-01 3.914E-01 1.986E-01 5.846E-02 1.050E-01 0.000E+00 1.217E-01 9.617E-02 2.846E-01 1						
Changing HRMAX from 10. to 20. Generating new table... There were 69 failures in the equilibrium algorithm 10 3.379E-01 3.379E-01 9.918E-02 7.904E-02 6.920E-02 0.000E+00 9.248E-02 9.382E-02 2.594E-01 0						
HRPMIN = -386.4065 INT(HRPMIN/10)*10.0-10.0 = -390.0000 HRMINI = -490.0000 Changing HRMIN from -490. to -390. Generating new table... There were 57 failures in the equilibrium algorithm 15 2.560E-01 2.560E-01 1.045E-01 6.993E-02 5.996E-02 0.000E+00 8.816E-02 9.211E-02 2.141E-01 0						
20 1.796E-01 1.540E-01 6.601E-02 6.748E-02 4.950E-02 0.000E+00 9.355E-02 1.008E-01 1.796E-01 0						
25 1.590E-01 1.357E-01 6.162E-02 6.174E-02 4.212E-02						

		0.000E+00	1.021E-01	9.345E-02	1.550E-01	0
30	1.472E-01	1.059E-01	5.005E-02	5.882E-02	3.243E-02	
		0.000E+00	1.064E-01	8.162E-02	1.472E-01	0
35	1.306E-01	1.083E-01	3.569E-02	5.380E-02	2.510E-02	
		0.000E+00	1.011E-01	6.518E-02	1.306E-01	0
40	1.401E-01	1.401E-01	2.597E-02	4.987E-02	2.076E-02	
		0.000E+00	8.932E-02	5.767E-02	1.116E-01	0
45	1.016E-01	1.016E-01	2.031E-02	4.635E-02	2.429E-02	
		0.000E+00	7.553E-02	5.162E-02	9.778E-02	0

HRPMIN = -377.6133

INT(HRPMIN/10)*10.0-10.0 = -380.0000

HRMIN1 = -390.0000

Changing HRMIN from -390. to -380.

Generating new table...

There were 49 failures in the equilibrium algorithm

50	8.987E-02	4.777E-02	1.696E-02	4.314E-02	2.154E-02	
		0.000E+00	6.650E-02	4.649E-02	8.987E-02	0
55	8.309E-02	5.097E-02	1.484E-02	4.004E-02	1.131E-02	
		0.000E+00	6.003E-02	4.048E-02	8.309E-02	0
60	7.752E-02	3.759E-02	1.253E-02	3.764E-02	1.115E-02	
		0.000E+00	5.392E-02	3.677E-02	7.752E-02	0

HRPMIN = -367.6340

INT(HRPMIN/10)*10.0-10.0 = -370.0000

HRMIN1 = -380.0000

Changing HRMIN from -380. to -370.

Generating new table...

There were 43 failures in the equilibrium algorithm

65	7.180E-02	5.728E-02	1.106E-02	3.438E-02	9.210E-03	
		0.000E+00	4.549E-02	3.367E-02	7.180E-02	0
70	6.686E-02	6.686E-02	9.403E-03	3.121E-02	7.989E-03	
		0.000E+00	3.667E-02	3.144E-02	6.616E-02	0
75	6.261E-02	4.000E-02	7.841E-03	2.839E-02	9.931E-03	
		0.000E+00	3.046E-02	2.956E-02	6.261E-02	0
80	6.090E-02	2.840E-02	6.569E-03	2.616E-02	6.789E-03	
		0.000E+00	2.794E-02	2.819E-02	6.090E-02	0
85	6.039E-02	2.663E-02	5.298E-03	2.395E-02	5.289E-03	
		0.000E+00	2.745E-02	2.740E-02	6.039E-02	0

HRPMIN = -359.8350

INT(HRPMIN/10)*10.0-10.0 = -360.0000

HRMIN1 = -370.0000

Changing HRMIN from -370. to -360.

Generating new table...

There were 45 failures in the equilibrium algorithm

90	5.924E-02	3.001E-02	5.867E-03	2.262E-02	6.353E-03	
		0.000E+00	2.664E-02	2.708E-02	5.924E-02	0
95	5.751E-02	4.513E-02	4.562E-03	2.103E-02	4.660E-03	
		0.000E+00	2.425E-02	2.610E-02	5.751E-02	0
100	5.548E-02	4.269E-02	4.208E-03	1.975E-02	5.287E-03	
		0.000E+00	2.171E-02	2.510E-02	5.548E-02	0
105	5.394E-02	3.008E-02	3.798E-03	1.838E-02	5.554E-03	
		0.000E+00	2.005E-02	2.416E-02	5.394E-02	0
110	5.260E-02	2.663E-02	3.445E-03	1.720E-02	3.927E-03	
		0.000E+00	1.937E-02	2.371E-02	5.260E-02	0
115	5.114E-02	2.610E-02	3.017E-03	1.608E-02	4.048E-03	
		0.000E+00	1.853E-02	2.324E-02	5.114E-02	0
120	4.881E-02	2.976E-02	2.854E-03	1.524E-02	4.060E-03	
		0.000E+00	1.676E-02	2.261E-02	4.881E-02	0
125	4.634E-02	3.276E-02	2.883E-03	1.457E-02	3.418E-03	
		0.000E+00	1.435E-02	2.165E-02	4.634E-02	0
130	4.370E-02	2.686E-02	2.886E-03	1.388E-02	3.755E-03	
		0.000E+00	1.215E-02	2.090E-02	4.370E-02	0

HRPMIN = -349.2851

INT(HRPMIN/10)*10.0-10.0 = -350.0000

HRMIN1 = -360.0000

Changing HRMIN from -360. to -350.

Generating new table...

There were 42 failures in the equilibrium algorithm

135	4.169E-02	2.256E-02	4.333E-03	1.361E-02	3.781E-03	
		0.000E+00	1.068E-02	2.053E-02	4.169E-02	0
140	3.906E-02	2.099E-02	2.707E-03	1.292E-02	3.243E-03	
		0.000E+00	9.473E-03	1.987E-02	3.906E-02	0
145	3.614E-02	1.752E-02	2.213E-03	1.219E-02	3.605E-03	
		0.000E+00	8.131E-03	1.887E-02	3.614E-02	0
150	3.269E-02	1.855E-02	2.129E-03	1.145E-02	3.232E-03	
		0.000E+00	6.470E-03	1.763E-02	3.269E-02	0
155	2.987E-02	1.707E-02	2.185E-03	1.095E-02	2.807E-03	
		0.000E+00	4.973E-03	1.657E-02	2.987E-02	0
160	2.699E-02	1.260E-02	2.100E-03	1.050E-02	2.782E-03	
		0.000E+00	3.876E-03	1.553E-02	2.699E-02	0
165	2.453E-02	1.203E-02	1.907E-03	1.006E-02	2.654E-03	
		0.000E+00	3.154E-03	1.447E-02	2.453E-02	0
170	2.188E-02	1.043E-02	1.701E-03	9.637E-03	2.994E-03	
		0.000E+00	2.629E-03	1.332E-02	2.188E-02	0
175	1.968E-02	8.261E-03	1.615E-03	9.288E-03	3.138E-03	
		0.000E+00	2.079E-03	1.232E-02	1.968E-02	0
180	1.769E-02	8.505E-03	1.642E-03	8.981E-03	2.790E-03	
		0.000E+00	1.622E-03	1.124E-02	1.769E-02	0

HRPMIN = -339.9317

INT(HRPMIN/10)*10.0-10.0 = -340.0000

HRMINI = -350.0000

Changing HRMIN from -350. to -340.

Generating new table...

There were 43 failures in the equilibrium algorithm

185	1.651E-02	8.070E-03	3.314E-03	9.111E-03	3.155E-03	
		0.000E+00	1.570E-03	1.093E-02	1.651E-02	0
190	1.503E-02	7.364E-03	2.085E-03	8.794E-03	2.704E-03	
		0.000E+00	1.363E-03	1.008E-02	1.503E-02	0
195	1.366E-02	6.483E-03	1.619E-03	8.365E-03	2.671E-03	
		0.000E+00	1.300E-03	9.291E-03	1.366E-02	0
200	1.249E-02	4.622E-03	1.507E-03	7.831E-03	2.703E-03	
		0.000E+00	1.143E-03	8.335E-03	1.249E-02	0
205	1.148E-02	4.791E-03	1.449E-03	7.425E-03	2.360E-03	
		0.000E+00	9.600E-04	7.495E-03	1.148E-02	0
210	1.087E-02	4.179E-03	1.389E-03	7.067E-03	2.092E-03	
		0.000E+00	8.373E-04	6.825E-03	1.087E-02	1

HRPMIN = -340.0816

HRMINI = -340.0000

NCRE = 1

NLIN = 0

INT(HRPMIN/10)*10.0-10.0 = -350.0000

Changing HRMIN from -340. to -350.

Generating new table...

There were 42 failures in the equilibrium algorithm

215	1.046E-02	4.559E-03	2.805E-03	6.933E-03	2.274E-03	
		0.000E+00	9.353E-04	6.483E-03	1.046E-02	0
220	1.002E-02	3.627E-03	1.983E-03	6.543E-03	1.995E-03	
		0.000E+00	9.254E-04	6.055E-03	1.002E-02	0

NUMBER SOURCE

RESNJ'S

SCATTER ITER: 0	ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX:	1.000E+00
SCATTER ITER: 0	ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX:	5.124E-01
SCATTER ITER: 0	ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX:	1.604E-01
SCATTER ITER: 0	ITERATION: 4	FRAC CHANGE IN TOT NET WALL FLUX:	6.695E-02
SCATTER ITER: 0	ITERATION: 5	FRAC CHANGE IN TOT NET WALL FLUX:	2.197E-02
SCATTER ITER: 0	ITERATION: 6	FRAC CHANGE IN TOT NET WALL FLUX:	8.299E-03
SCATTER ITER: 1	ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX:	2.822E-02
SCATTER ITER: 1	ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX:	1.238E-02
SCATTER ITER: 1	ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX:	2.125E-03

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SCATTER ITER: 0 ITERATION: 1 FRAC CHANGE IN TOT NET WALL FLUX: 1.000E+00
SCATTER ITER: 0 ITERATION: 2 FRAC CHANGE IN TOT NET WALL FLUX: 5.124E-01
SCATTER ITER: 0 ITERATION: 3 FRAC CHANGE IN TOT NET WALL FLUX: 1.604E-01
SCATTER ITER: 0 ITERATION: 4 FRAC CHANGE IN TOT NET WALL FLUX: 6.695E-02
SCATTER ITER: 0 ITERATION: 5 FRAC CHANGE IN TOT NET WALL FLUX: 2.197E-02
SCATTER ITER: 0 ITERATION: 6 FRAC CHANGE IN TOT NET WALL FLUX: 8.299E-03
SCATTER ITER: 1 ITERATION: 1 FRAC CHANGE IN TOT NET WALL FLUX: 2.822E-02
SCATTER ITER: 1 ITERATION: 2 FRAC CHANGE IN TOT NET WALL FLUX: 1.238E-02
SCATTER ITER: 1 ITERATION: 3 FRAC CHANGE IN TOT NET WALL FLUX: 2.125E-03

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IF IT HITS THE WALLS IT STICKS

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ISL= 1, IPS= 1, TERMINATED AT: IV=34, JU= 2 TIME= 2.411E-01 NPOINT= 446
ISL= 1, IPS= 2, TERMINATED AT: IV=34, JU= 2 TIME= 2.381E-01 NPOINT= 421
ISL= 1, IPS= 3, TERMINATED AT: IV=34, JU= 2 TIME= 2.351E-01 NPOINT= 474
ISL= 1, IPS= 4, TERMINATED AT: IV=34, JU= 2 TIME= 2.362E-01 NPOINT= 494
ISL= 1, IPS= 5, TERMINATED AT: IV=34, JU= 2 TIME= 2.305E-01 NPOINT= 458
ISL= 2, IPS= 1, TERMINATED AT: IV=34, JU= 7 TIME= 2.413E-01 NPOINT= 350
ISL= 2, IPS= 2, TERMINATED AT: IV=34, JU= 5 TIME= 2.386E-01 NPOINT= 455
ISL= 2, IPS= 3, TERMINATED AT: IV=34, JU= 4 TIME= 2.349E-01 NPOINT= 460
ISL= 2, IPS= 4, TERMINATED AT: IV=34, JU= 4 TIME= 2.369E-01 NPOINT= 508
ISL= 2, IPS= 5, TERMINATED AT: IV=34, JU= 3 TIME= 2.305E-01 NPOINT= 459
ISL= 3, IPS= 1, TERMINATED AT: IV=34, JU=10 TIME= 2.471E-01 NPOINT= 373
ISL= 3, IPS= 2, TERMINATED AT: IV=34, JU= 8 TIME= 2.414E-01 NPOINT= 461
ISL= 3, IPS= 3, TERMINATED AT: IV=34, JU= 6 TIME= 2.365E-01 NPOINT= 495
ISL= 3, IPS= 4, TERMINATED AT: IV=34, JU= 6 TIME= 2.365E-01 NPOINT= 463
ISL= 3, IPS= 5, TERMINATED AT: IV=34, JU= 5 TIME= 2.271E-01 NPOINT= 439
ISL= 4, IPS= 1, TERMINATED AT: IV=34, JU=14 TIME= 2.584E-01 NPOINT= 428
ISL= 4, IPS= 2, TERMINATED AT: IV=34, JU=10 TIME= 2.501E-01 NPOINT= 477
ISL= 4, IPS= 3, TERMINATED AT: IV=34, JU= 9 TIME= 2.398E-01 NPOINT= 545
ISL= 4, IPS= 4, TERMINATED AT: IV=34, JU= 8 TIME= 2.394E-01 NPOINT= 484
ISL= 4, IPS= 5, TERMINATED AT: IV=34, JU= 6 TIME= 2.337E-01 NPOINT= 452
ISL= 5, IPS= 1, TERMINATED AT: IV=34, JU=17 TIME= 2.705E-01 NPOINT= 394
ISL= 5, IPS= 2, TERMINATED AT: IV=34, JU=13 TIME= 2.561E-01 NPOINT= 493
ISL= 5, IPS= 3, TERMINATED AT: IV=34, JU=11 TIME= 2.451E-01 NPOINT= 573
ISL= 5, IPS= 4, TERMINATED AT: IV=34, JU=10 TIME= 2.437E-01 NPOINT= 517
ISL= 5, IPS= 5, TERMINATED AT: IV=34, JU= 8 TIME= 2.320E-01 NPOINT= 479
ISL= 6, IPS= 1, TERMINATED AT: IV=34, JU=20 TIME= 2.833E-01 NPOINT= 421
ISL= 6, IPS= 2, TERMINATED AT: IV=34, JU=16 TIME= 2.612E-01 NPOINT= 525
ISL= 6, IPS= 3, TERMINATED AT: IV=34, JU=14 TIME= 2.555E-01 NPOINT= 541
ISL= 6, IPS= 4, TERMINATED AT: IV=34, JU=12 TIME= 2.491E-01 NPOINT= 497
ISL= 6, IPS= 5, TERMINATED AT: IV=34, JU=10 TIME= 2.403E-01 NPOINT= 445
ISL= 7, IPS= 1, TERMINATED AT: IV=34, JU=22 TIME= 3.221E-01 NPOINT= 487
ISL= 7, IPS= 2, TERMINATED AT: IV=34, JU=18 TIME= 2.771E-01 NPOINT= 520
ISL= 7, IPS= 3, TERMINATED AT: IV=34, JU=16 TIME= 2.607E-01 NPOINT= 443
ISL= 7, IPS= 4, TERMINATED AT: IV=34, JU=14 TIME= 2.531E-01 NPOINT= 473
ISL= 7, IPS= 5, TERMINATED AT: IV=34, JU=12 TIME= 2.439E-01 NPOINT= 418
TRAJECTORY ISL= 8, IPS= 1 RECIRCULATES
ISL= 8, IPS= 1, TERMINATED AT: IV=34, JU=25 TIME= 3.477E-01 NPOINT= 439
ISL= 8, IPS= 2, TERMINATED AT: IV=34, JU=20 TIME= 2.965E-01 NPOINT= 491
ISL= 8, IPS= 3, TERMINATED AT: IV=34, JU=18 TIME= 2.751E-01 NPOINT= 446
ISL= 8, IPS= 4, TERMINATED AT: IV=34, JU=16 TIME= 2.647E-01 NPOINT= 477
ISL= 8, IPS= 5, TERMINATED AT: IV=34, JU=14 TIME= 2.488E-01 NPOINT= 441
TRAJECTORY ISL= 9, IPS= 1 RECIRCULATES
ISL= 9, IPS= 1, TERMINATED AT: IV=34, JU=27 TIME= 3.249E-01 NPOINT= 438
ISL= 9, IPS= 2, TERMINATED AT: IV=34, JU=21 TIME= 3.201E-01 NPOINT= 531
ISL= 9, IPS= 3, TERMINATED AT: IV=34, JU=19 TIME= 2.864E-01 NPOINT= 381
ISL= 9, IPS= 4, TERMINATED AT: IV=34, JU=18 TIME= 2.676E-01 NPOINT= 422
ISL= 9, IPS= 5, TERMINATED AT: IV=34, JU=15 TIME= 2.504E-01 NPOINT= 431
TRAJECTORY ISL=10, IPS= 1 RECIRCULATES
ISL=10, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 3.665E-01 NPOINT= 503
TRAJECTORY ISL=10, IPS= 2 RECIRCULATES
ISL=10, IPS= 2, TERMINATED AT: IV=34, JU=24 TIME= 3.509E-01 NPOINT= 497
ISL=10, IPS= 3, TERMINATED AT: IV=34, JU=20 TIME= 3.065E-01 NPOINT= 474
ISL=10, IPS= 4, TERMINATED AT: IV=34, JU=19 TIME= 2.837E-01 NPOINT= 459
ISL=10, IPS= 5, TERMINATED AT: IV=34, JU=18 TIME= 2.634E-01 NPOINT= 423

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SUM OF SOLID PHASE COUPLING

SSPE = 3.420E-04
 SSPF = 0.000E+00
 SSPM = 3.420E-04
 SSPU = 6.524E-03
 SSPV = -3.458E-06
 SSPH = 0.000E+00

AT X = 1.49 , COAL BURNOUT = 0.8141

>>>>EOLP COMPLETE, END OF PARTICLE ITERATION # 3

221

NITER	SOURCE	RESORU RESORP	RESORV RESORH	RESORW RESORF	RESORM RESORT	NCREE
1	4.175E-01	8.180E-02	2.686E-02	1.107E-02	4.167E-02	
	0.4174700	0.000E+00	4.009E-02	5.259E-02	4.175E-01	0
5	1.663E-01	1.663E-01	1.316E-01	4.282E-02	4.581E-02	
		0.000E+00	4.882E-02	8.492E-02	1.477E-01	0
10	1.019E-01	1.019E-01	5.989E-02	4.738E-02	3.104E-02	
		0.000E+00	4.717E-02	8.233E-02	9.585E-02	0
15	7.611E-02	5.068E-02	3.461E-02	3.605E-02	1.609E-02	
		0.000E+00	3.990E-02	5.809E-02	7.611E-02	0
20	6.447E-02	6.447E-02	2.204E-02	2.311E-02	1.260E-02	
		0.000E+00	3.391E-02	3.858E-02	6.245E-02	0
25	5.588E-02	4.214E-02	1.539E-02	2.008E-02	1.249E-02	
		0.000E+00	3.395E-02	3.483E-02	5.588E-02	0
30	5.183E-02	4.228E-02	1.177E-02	1.783E-02	7.227E-03	
		0.000E+00	3.146E-02	2.801E-02	5.183E-02	0
35	4.779E-02	3.380E-02	1.079E-02	1.634E-02	5.728E-03	
		0.000E+00	2.808E-02	2.379E-02	4.779E-02	0
40	4.340E-02	2.630E-02	7.331E-03	1.520E-02	4.587E-03	
		0.000E+00	2.381E-02	2.142E-02	4.340E-02	0
45	3.926E-02	2.148E-02	5.976E-03	1.531E-02	3.461E-03	
		0.000E+00	1.988E-02	2.047E-02	3.926E-02	0
50	3.664E-02	1.981E-02	4.914E-03	1.550E-02	2.502E-03	
		0.000E+00	1.673E-02	1.914E-02	3.664E-02	0
55	3.529E-02	1.666E-02	4.015E-03	1.526E-02	2.186E-03	
		0.000E+00	1.437E-02	1.730E-02	3.529E-02	0
60	3.464E-02	1.546E-02	3.590E-03	1.468E-02	1.837E-03	
		0.000E+00	1.250E-02	1.543E-02	3.464E-02	0
65	3.466E-02	1.467E-02	3.343E-03	1.421E-02	2.119E-03	
		0.000E+00	1.095E-02	1.386E-02	3.466E-02	0
70	3.475E-02	1.211E-02	3.159E-03	1.381E-02	2.407E-03	
		0.000E+00	9.451E-03	1.287E-02	3.475E-02	0
75	3.488E-02	1.157E-02	2.766E-03	1.334E-02	2.304E-03	
		0.000E+00	8.556E-03	1.221E-02	3.488E-02	0
80	3.477E-02	1.091E-02	2.466E-03	1.283E-02	2.435E-03	
		0.000E+00	8.397E-03	1.152E-02	3.477E-02	0
85	3.458E-02	1.294E-02	2.338E-03	1.223E-02	2.683E-03	
		0.000E+00	8.381E-03	1.109E-02	3.458E-02	0
90	3.431E-02	1.470E-02	2.368E-03	1.171E-02	2.874E-03	
		0.000E+00	8.305E-03	1.083E-02	3.431E-02	0
95	3.397E-02	1.423E-02	2.340E-03	1.117E-02	3.075E-03	
		0.000E+00	8.204E-03	1.057E-02	3.397E-02	0
100	3.362E-02	1.308E-02	2.240E-03	1.063E-02	3.060E-03	
		0.000E+00	8.139E-03	1.038E-02	3.362E-02	0
105	3.305E-02	1.278E-02	2.101E-03	1.012E-02	2.942E-03	
		0.000E+00	8.062E-03	1.015E-02	3.305E-02	0
110	3.241E-02	1.305E-02	2.003E-03	9.594E-03	2.892E-03	

115 3.146E-02 0.000E+00 7.778E-03 9.980E-03 3.241E-02 0
 1.342E-02 1.920E-03 9.133E-03 2.784E-03
 0.000E+00 7.236E-03 9.817E-03 3.146E-02 0
 120 3.041E-02 1.293E-02 1.846E-03 8.700E-03 2.637E-03 0
 0.000E+00 6.558E-03 9.708E-03 3.041E-02 0
 HRPMIN = -339.2996
 INT(HRPMIN/10)*10.0-10.0 = -340.0000
 HRMIN1 = -350.0000
 Changing HRMIN from -350. to -340.
 Generating new table...
 There were 43 failures in the equilibrium algorithm
 125 2.940E-02 1.248E-02 3.355E-03 8.665E-03 2.872E-03 0
 0.000E+00 6.050E-03 1.003E-02 2.940E-02
 130 2.804E-02 1.149E-02 2.137E-03 8.386E-03 2.443E-03 0
 0.000E+00 5.452E-03 1.006E-02 2.804E-02
 135 2.637E-02 9.870E-03 1.723E-03 8.036E-03 2.330E-03 0
 0.000E+00 4.848E-03 9.938E-03 2.637E-02
 140 2.453E-02 9.236E-03 1.550E-03 7.556E-03 2.172E-03 0
 0.000E+00 4.040E-03 9.439E-03 2.453E-02
 145 2.257E-02 8.374E-03 1.445E-03 7.130E-03 1.929E-03 0
 0.000E+00 3.289E-03 8.925E-03 2.257E-02
 150 2.090E-02 7.103E-03 1.342E-03 6.800E-03 1.771E-03 0
 0.000E+00 2.706E-03 8.642E-03 2.090E-02
 155 1.902E-02 6.398E-03 1.217E-03 6.489E-03 1.664E-03 0
 0.000E+00 2.275E-03 8.235E-03 1.902E-02
 160 1.750E-02 5.863E-03 1.099E-03 6.131E-03 1.645E-03 0
 0.000E+00 1.950E-03 7.916E-03 1.750E-02
 165 1.584E-02 4.749E-03 1.014E-03 5.810E-03 1.653E-03 0
 0.000E+00 1.669E-03 7.520E-03 1.584E-02
 170 1.459E-02 4.246E-03 9.700E-04 5.509E-03 1.559E-03 0
 0.000E+00 1.444E-03 7.211E-03 1.459E-02
 175 1.334E-02 3.775E-03 9.410E-04 5.208E-03 1.484E-03 0
 0.000E+00 1.285E-03 6.876E-03 1.334E-02
 180 1.238E-02 3.333E-03 8.976E-04 4.915E-03 1.445E-03 0
 0.000E+00 1.190E-03 6.566E-03 1.238E-02
 185 1.143E-02 3.078E-03 8.441E-04 4.624E-03 1.405E-03 0
 0.000E+00 1.097E-03 6.259E-03 1.143E-02
 190 1.068E-02 2.682E-03 7.983E-04 4.335E-03 1.391E-03 0
 0.000E+00 9.886E-04 5.942E-03 1.068E-02
 195 1.002E-02 2.352E-03 7.643E-04 4.071E-03 1.329E-03 0
 0.000E+00 8.718E-04 5.681E-03 1.002E-02 0
 NJITER SOURCE FESNJ'S
 SCATTER ITER: 0 ITERATION: 1 FRAC CHANGE IN TOT NET WALL FLUX: 1.000E+00
 SCATTER ITER: 0 ITERATION: 2 FRAC CHANGE IN TOT NET WALL FLUX: 5.114E-01
 SCATTER ITER: 0 ITERATION: 3 FRAC CHANGE IN TOT NET WALL FLUX: 1.578E-01
 SCATTER ITER: 0 ITERATION: 4 FRAC CHANGE IN TOT NET WALL FLUX: 6.573E-02
 SCATTER ITER: 0 ITERATION: 5 FRAC CHANGE IN TOT NET WALL FLUX: 2.133E-02
 SCATTER ITER: 0 ITERATION: 6 FRAC CHANGE IN TOT NET WALL FLUX: 8.014E-03
 SCATTER ITER: 1 ITERATION: 1 FRAC CHANGE IN TOT NET WALL FLUX: 2.855E-02
 SCATTER ITER: 1 ITERATION: 2 FRAC CHANGE IN TOT NET WALL FLUX: 1.257E-02
 SCATTER ITER: 1 ITERATION: 3 FRAC CHANGE IN TOT NET WALL FLUX: 2.159E-03
 SCATTER ITER: 0 ITERATION: 1 FRAC CHANGE IN TOT NET WALL FLUX: 1.000E+00
 SCATTER ITER: 0 ITERATION: 2 FRAC CHANGE IN TOT NET WALL FLUX: 5.114E-01
 SCATTER ITER: 0 ITERATION: 3 FRAC CHANGE IN TOT NET WALL FLUX: 1.578E-01
 SCATTER ITER: 0 ITERATION: 4 FRAC CHANGE IN TOT NET WALL FLUX: 6.573E-02
 SCATTER ITER: 0 ITERATION: 5 FRAC CHANGE IN TOT NET WALL FLUX: 2.133E-02
 SCATTER ITER: 0 ITERATION: 6 FRAC CHANGE IN TOT NET WALL FLUX: 8.014E-03
 SCATTER ITER: 1 ITERATION: 1 FRAC CHANGE IN TOT NET WALL FLUX: 2.855E-02
 SCATTER ITER: 1 ITERATION: 2 FRAC CHANGE IN TOT NET WALL FLUX: 1.257E-02
 SCATTER ITER: 1 ITERATION: 3 FRAC CHANGE IN TOT NET WALL FLUX: 2.159E-03
 IF IT HITS THE WALLS IT STICKS
 ISL= 1, IPS= 1, TERMINATED AT: IV=34, JU= 2 TIME= 2.471E-01 NPCINT= 467
 ISL= 1, IPS= 2, TERMINATED AT: IV=34, JU= 2 TIME= 2.425E-01 NPCINT= 454

ISL= 1, IPS= 3, TERMINATED AT: IV=34, JU= 2 TIME= 2.442E-01 NPOINT= 499
 ISL= 1, IPS= 4, TERMINATED AT: IV=34, JU= 2 TIME= 2.391E-01 NPOINT= 498
 ISL= 1, IPS= 5, TERMINATED AT: IV=34, JU= 2 TIME= 2.338E-01 NPOINT= 447
 ISL= 2, IPS= 1, TERMINATED AT: IV=34, JU= 6 TIME= 2.495E-01 NPOINT= 479
 ISL= 2, IPS= 2, TERMINATED AT: IV=34, JU= 5 TIME= 2.436E-01 NPOINT= 384
 ISL= 2, IPS= 3, TERMINATED AT: IV=34, JU= 4 TIME= 2.438E-01 NPOINT= 479
 ISL= 2, IPS= 4, TERMINATED AT: IV=34, JU= 4 TIME= 2.419E-01 NPOINT= 518
 ISL= 2, IPS= 5, TERMINATED AT: IV=34, JU= 3 TIME= 2.343E-01 NPOINT= 447
 ISL= 3, IPS= 1, TERMINATED AT: IV=34, JU=10 TIME= 2.551E-01 NPOINT= 401
 ISL= 3, IPS= 2, TERMINATED AT: IV=34, JU= 8 TIME= 2.512E-01 NPOINT= 445
 ISL= 3, IPS= 3, TERMINATED AT: IV=34, JU= 6 TIME= 2.464E-01 NPOINT= 490
 ISL= 3, IPS= 4, TERMINATED AT: IV=34, JU= 6 TIME= 2.405E-01 NPOINT= 538
 ISL= 3, IPS= 5, TERMINATED AT: IV=34, JU= 5 TIME= 2.378E-01 NPOINT= 468
 ISL= 4, IPS= 1, TERMINATED AT: IV=34, JU=14 TIME= 2.612E-01 NPOINT= 373
 ISL= 4, IPS= 2, TERMINATED AT: IV=34, JU=10 TIME= 2.499E-01 NPOINT= 411
 ISL= 4, IPS= 3, TERMINATED AT: IV=34, JU= 9 TIME= 2.475E-01 NPOINT= 469
 ISL= 4, IPS= 4, TERMINATED AT: IV=34, JU= 8 TIME= 2.462E-01 NPOINT= 560
 ISL= 4, IPS= 5, TERMINATED AT: IV=34, JU= 6 TIME= 2.373E-01 NPOINT= 458
 ISL= 5, IPS= 1, TERMINATED AT: IV=34, JU=17 TIME= 2.727E-01 NPOINT= 415
 ISL= 5, IPS= 2, TERMINATED AT: IV=34, JU=13 TIME= 2.621E-01 NPOINT= 381
 ISL= 5, IPS= 3, TERMINATED AT: IV=34, JU=11 TIME= 2.496E-01 NPOINT= 535
 ISL= 5, IPS= 4, TERMINATED AT: IV=34, JU= 9 TIME= 2.491E-01 NPOINT= 558
 ISL= 5, IPS= 5, TERMINATED AT: IV=34, JU= 8 TIME= 2.388E-01 NPOINT= 498
 ISL= 5, IPS= 1, TERMINATED AT: IV=34, JU=20 TIME= 2.890E-01 NPOINT= 465
 ISL= 5, IPS= 2, TERMINATED AT: IV=34, JU=16 TIME= 2.697E-01 NPOINT= 376
 ISL= 5, IPS= 3, TERMINATED AT: IV=34, JU=13 TIME= 2.610E-01 NPOINT= 446
 ISL= 6, IPS= 4, TERMINATED AT: IV=34, JU=11 TIME= 2.531E-01 NPOINT= 510
 ISL= 6, IPS= 5, TERMINATED AT: IV=34, JU=10 TIME= 2.450E-01 NPOINT= 456
 ISL= 7, IPS= 1, TERMINATED AT: IV=34, JU=21 TIME= 3.220E-01 NPOINT= 467
 ISL= 7, IPS= 2, TERMINATED AT: IV=34, JU=18 TIME= 2.807E-01 NPOINT= 405
 ISL= 7, IPS= 3, TERMINATED AT: IV=34, JU=15 TIME= 2.637E-01 NPOINT= 441
 ISL= 7, IPS= 4, TERMINATED AT: IV=34, JU=13 TIME= 2.573E-01 NPOINT= 520
 ISL= 7, IPS= 5, TERMINATED AT: IV=34, JU=11 TIME= 2.475E-01 NPOINT= 475
 TRAJECTORY ISL= 8, IPS= 1 RECIRCULATES
 ISL= 8, IPS= 1, TERMINATED AT: IV=34, JU=24 TIME= 3.531E-01 NPOINT= 422
 ISL= 8, IPS= 2, TERMINATED AT: IV=34, JU=19 TIME= 2.942E-01 NPOINT= 362
 ISL= 8, IPS= 3, TERMINATED AT: IV=34, JU=17 TIME= 2.768E-01 NPOINT= 462
 ISL= 8, IPS= 4, TERMINATED AT: IV=34, JU=16 TIME= 2.646E-01 NPOINT= 483
 ISL= 8, IPS= 5, TERMINATED AT: IV=34, JU=13 TIME= 2.538E-01 NPOINT= 486
 TRAJECTORY ISL= 9, IPS= 1 RECIRCULATES
 ISL= 9, IPS= 1, TERMINATED AT: IV=34, JU=27 TIME= 3.274E-01 NPOINT= 521
 ISL= 9, IPS= 2, TERMINATED AT: IV=34, JU=21 TIME= 3.185E-01 NPOINT= 386
 ISL= 9, IPS= 3, TERMINATED AT: IV=34, JU=19 TIME= 2.855E-01 NPOINT= 438
 ISL= 9, IPS= 4, TERMINATED AT: IV=34, JU=17 TIME= 2.706E-01 NPOINT= 496
 ISL= 9, IPS= 5, TERMINATED AT: IV=34, JU=16 TIME= 2.607E-01 NPOINT= 467
 TRAJECTORY ISL=10, IPS= 1 RECIRCULATES
 ISL=10, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 3.740E-01 NPOINT= 445
 TRAJECTORY ISL=10, IPS= 2 RECIRCULATES
 ISL=10, IPS= 2, TERMINATED AT: IV=34, JU=24 TIME= 3.697E-01 NPOINT= 541
 ISL=10, IPS= 3, TERMINATED AT: IV=34, JU=20 TIME= 3.043E-01 NPOINT= 492
 ISL=10, IPS= 4, TERMINATED AT: IV=34, JU=19 TIME= 2.838E-01 NPOINT= 464
 ISL=10, IPS= 5, TERMINATED AT: IV=34, JU=17 TIME= 2.673E-01 NPOINT= 438

SUM OF SOLID PHASE COUPLING

SSPE = 3.434E-04
 SSPF = 0.000E+00
 SSPM = 3.434E-04
 SSPU = 6.502E-03
 SSPV = -3.137E-06
 SSPH = 0.000E+00

AT X = 1.49 , COAL BURNOUT = 0.8173

>>>>FOLD COMPLETE, END OF PARTICLE ITERATION # 4

196

NITER	SORCE	RESORU RESORP	RESORV RESORH	RESORW RESORF	RESORM RESOET	NCREE
1	3.551E-01	4.608E-02	2.139E-02	9.025E-03	4.088E-02	0
0.3550613		0.000E+00	3.917E-02	5.456E-02	3.551E-01	
5	1.410E-01	1.410E-01	1.226E-01	4.051E-02	3.766E-02	0
		0.000E+00	4.156E-02	9.343E-02	1.136E-01	
10	9.389E-02	8.241E-02	6.216E-02	4.754E-02	2.325E-02	0
		0.000E+00	4.030E-02	9.389E-02	8.466E-02	
15	7.894E-02	5.834E-02	4.366E-02	4.207E-02	1.498E-02	0
		0.000E+00	3.390E-02	7.894E-02	7.428E-02	
20	6.298E-02	5.758E-02	2.916E-02	2.913E-02	5.601E-03	0
		0.000E+00	2.646E-02	5.530E-02	6.298E-02	
25	5.392E-02	3.679E-02	2.148E-02	2.398E-02	5.821E-03	0
		0.000E+00	2.278E-02	4.652E-02	5.392E-02	
30	4.851E-02	2.853E-02	1.397E-02	1.979E-02	6.444E-03	0
		0.000E+00	1.838E-02	3.947E-02	4.851E-02	
35	4.570E-02	2.190E-02	1.020E-02	1.630E-02	4.302E-03	0
		0.000E+00	1.599E-02	3.488E-02	4.570E-02	
40	4.350E-02	1.667E-02	7.744E-03	1.390E-02	3.055E-03	0
		0.000E+00	1.409E-02	3.187E-02	4.350E-02	
45	4.144E-02	1.686E-02	6.238E-03	1.208E-02	3.192E-03	0
		0.000E+00	1.241E-02	2.958E-02	4.144E-02	
50	3.948E-02	1.459E-02	5.345E-03	1.072E-02	3.776E-03	0
		0.000E+00	1.118E-02	2.782E-02	3.948E-02	
55	3.716E-02	1.415E-02	4.915E-03	9.595E-03	3.389E-03	0
		0.000E+00	1.002E-02	2.628E-02	3.716E-02	
60	3.486E-02	1.380E-02	4.375E-03	8.729E-03	2.756E-03	0
		0.000E+00	9.005E-03	2.472E-02	3.486E-02	
65	3.274E-02	1.140E-02	3.566E-03	7.813E-03	2.523E-03	0
		0.000E+00	8.184E-03	2.315E-02	3.274E-02	
70	3.076E-02	9.567E-03	2.979E-03	7.109E-03	2.132E-03	0
		0.000E+00	7.425E-03	2.156E-02	3.076E-02	
75	2.892E-02	8.819E-03	2.456E-03	6.339E-03	1.922E-03	0
		0.000E+00	6.589E-03	2.021E-02	2.892E-02	
80	2.764E-02	7.819E-03	2.008E-03	5.681E-03	1.718E-03	0
		0.000E+00	5.687E-03	1.905E-02	2.764E-02	
85	2.621E-02	7.403E-03	1.636E-03	5.006E-03	1.366E-03	0
		0.000E+00	5.056E-03	1.819E-02	2.621E-02	
90	2.539E-02	6.680E-03	1.342E-03	4.472E-03	1.233E-03	0
		0.000E+00	4.821E-03	1.752E-02	2.539E-02	
95	2.446E-02	6.358E-03	1.134E-03	3.979E-03	1.134E-03	0
		0.000E+00	4.619E-03	1.699E-02	2.446E-02	
100	2.343E-02	6.315E-03	1.015E-03	3.620E-03	1.038E-03	0
		0.000E+00	4.221E-03	1.647E-02	2.343E-02	
105	2.264E-02	5.863E-03	9.012E-04	3.300E-03	1.076E-03	0
		0.000E+00	3.761E-03	1.596E-02	2.264E-02	
110	2.142E-02	5.577E-03	8.094E-04	3.098E-03	1.002E-03	0
		0.000E+00	3.325E-03	1.550E-02	2.142E-02	
115	2.048E-02	5.276E-03	7.110E-04	2.909E-03	8.879E-04	0
		0.000E+00	2.882E-03	1.496E-02	2.048E-02	
120	1.926E-02	4.621E-03	6.202E-04	2.795E-03	8.518E-04	0
		0.000E+00	2.439E-03	1.440E-02	1.926E-02	
125	1.813E-02	4.072E-03	5.426E-04	2.667E-03	7.803E-04	0
		0.000E+00	2.109E-03	1.367E-02	1.813E-02	
130	1.693E-02	3.663E-03	4.746E-04	2.574E-03	7.426E-04	0
		0.000E+00	1.915E-03	1.301E-02	1.693E-02	
135	1.570E-02	3.366E-03	4.161E-04	2.468E-03	7.130E-04	0
		0.000E+00	1.822E-03	1.218E-02	1.570E-02	
140	1.452E-02	3.418E-03	3.778E-04	2.363E-03	6.340E-04	

145	1.332E-02	0.000E+00 1.796E-03 1.147E-02 1.452E-02	0
		3.141E-03 3.592E-04 2.242E-03 5.855E-04	
		0.000E+00 1.804E-03 1.061E-02 1.332E-02	0
150	1.225E-02	2.612E-03 3.361E-04 2.115E-03 5.575E-04	
		0.000E+00 1.824E-03 9.872E-03 1.225E-02	0
155	1.122E-02	2.340E-03 3.129E-04 1.976E-03 5.022E-04	
		0.000E+00 1.821E-03 9.020E-03 1.122E-02	0
160	1.028E-02	2.233E-03 2.864E-04 1.824E-03 4.987E-04	
		0.000E+00 1.766E-03 8.280E-03 1.028E-02	0

NJITER	SORCE	RESNJ'S
SCATTER ITER: 0	ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX: 1.000E+00
SCATTER ITER: 0	ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX: 5.134E-01
SCATTER ITER: 0	ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX: 1.617E-01
SCATTER ITER: 0	ITERATION: 4	FRAC CHANGE IN TOT NET WALL FLUX: 6.764E-02
SCATTER ITER: 0	ITERATION: 5	FRAC CHANGE IN TOT NET WALL FLUX: 2.235E-02
SCATTER ITER: 0	ITERATION: 6	FRAC CHANGE IN TOT NET WALL FLUX: 8.464E-03
SCATTER ITER: 1	ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX: 2.881E-02
SCATTER ITER: 1	ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX: 1.274E-02
SCATTER ITER: 1	ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX: 2.182E-03
SCATTER ITER: 0	ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX: 1.000E+00
SCATTER ITER: 0	ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX: 5.134E-01
SCATTER ITER: 0	ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX: 1.617E-01
SCATTER ITER: 0	ITERATION: 4	FRAC CHANGE IN TOT NET WALL FLUX: 6.764E-02
SCATTER ITER: 0	ITERATION: 5	FRAC CHANGE IN TOT NET WALL FLUX: 2.235E-02
SCATTER ITER: 0	ITERATION: 6	FRAC CHANGE IN TOT NET WALL FLUX: 8.464E-03
SCATTER ITER: 1	ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX: 2.881E-02
SCATTER ITER: 1	ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX: 1.274E-02
SCATTER ITER: 1	ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX: 2.182E-03

IF IT HITS THE WALLS IT STICKS

ISL= 1, IPS= 1, TERMINATED AT: IV=34, JU= 2	TIME= 2.461E-01	NPOINT= 436
ISL= 1, IPS= 2, TERMINATED AT: IV=34, JU= 2	TIME= 2.432E-01	NPOINT= 401
ISL= 1, IPS= 3, TERMINATED AT: IV=34, JU= 2	TIME= 2.382E-01	NPOINT= 542
ISL= 1, IPS= 4, TERMINATED AT: IV=34, JU= 2	TIME= 2.403E-01	NPOINT= 497
ISL= 1, IPS= 5, TERMINATED AT: IV=34, JU= 2	TIME= 2.320E-01	NPOINT= 462
ISL= 2, IPS= 1, TERMINATED AT: IV=34, JU= 6	TIME= 2.483E-01	NPOINT= 450
ISL= 2, IPS= 2, TERMINATED AT: IV=34, JU= 5	TIME= 2.411E-01	NPOINT= 394
ISL= 2, IPS= 3, TERMINATED AT: IV=34, JU= 4	TIME= 2.385E-01	NPOINT= 509
ISL= 2, IPS= 4, TERMINATED AT: IV=34, JU= 4	TIME= 2.408E-01	NPOINT= 490
ISL= 2, IPS= 5, TERMINATED AT: IV=34, JU= 3	TIME= 2.351E-01	NPOINT= 465
ISL= 3, IPS= 1, TERMINATED AT: IV=34, JU=10	TIME= 2.502E-01	NPOINT= 480
ISL= 3, IPS= 2, TERMINATED AT: IV=34, JU= 8	TIME= 2.459E-01	NPOINT= 419
ISL= 3, IPS= 3, TERMINATED AT: IV=34, JU= 7	TIME= 2.428E-01	NPOINT= 528
ISL= 3, IPS= 4, TERMINATED AT: IV=34, JU= 5	TIME= 2.417E-01	NPOINT= 513
ISL= 3, IPS= 5, TERMINATED AT: IV=34, JU= 5	TIME= 2.327E-01	NPOINT= 463
ISL= 4, IPS= 1, TERMINATED AT: IV=34, JU=14	TIME= 2.586E-01	NPOINT= 499
ISL= 4, IPS= 2, TERMINATED AT: IV=34, JU=10	TIME= 2.536E-01	NPOINT= 435
ISL= 4, IPS= 3, TERMINATED AT: IV=34, JU= 9	TIME= 2.444E-01	NPOINT= 534
ISL= 4, IPS= 4, TERMINATED AT: IV=34, JU= 7	TIME= 2.436E-01	NPOINT= 535
ISL= 4, IPS= 5, TERMINATED AT: IV=34, JU= 6	TIME= 2.372E-01	NPOINT= 478
ISL= 5, IPS= 1, TERMINATED AT: IV=34, JU=17	TIME= 2.744E-01	NPOINT= 506
ISL= 5, IPS= 2, TERMINATED AT: IV=34, JU=13	TIME= 2.559E-01	NPOINT= 424
ISL= 5, IPS= 3, TERMINATED AT: IV=34, JU=11	TIME= 2.489E-01	NPOINT= 547
ISL= 5, IPS= 4, TERMINATED AT: IV=34, JU= 9	TIME= 2.464E-01	NPOINT= 517
ISL= 5, IPS= 5, TERMINATED AT: IV=34, JU= 8	TIME= 2.398E-01	NPOINT= 464
ISL= 6, IPS= 1, TERMINATED AT: IV=34, JU=20	TIME= 2.885E-01	NPOINT= 444
ISL= 6, IPS= 2, TERMINATED AT: IV=34, JU=16	TIME= 2.692E-01	NPOINT= 388
ISL= 6, IPS= 3, TERMINATED AT: IV=34, JU=13	TIME= 2.602E-01	NPOINT= 472
ISL= 6, IPS= 4, TERMINATED AT: IV=34, JU=12	TIME= 2.523E-01	NPOINT= 510
ISL= 6, IPS= 5, TERMINATED AT: IV=34, JU= 9	TIME= 2.380E-01	NPOINT= 438
ISL= 7, IPS= 1, TERMINATED AT: IV=34, JU=22	TIME= 3.229E-01	NPOINT= 465
ISL= 7, IPS= 2, TERMINATED AT: IV=34, JU=18	TIME= 2.771E-01	NPOINT= 382
ISL= 7, IPS= 3, TERMINATED AT: IV=34, JU=16	TIME= 2.641E-01	NPOINT= 467
ISL= 7, IPS= 4, TERMINATED AT: IV=34, JU=14	TIME= 2.548E-01	NPOINT= 479


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ISL= 7, IPS= 5, TERMINATED AT: IV=34, JU=11 TIME= 2.432E-01 NPOINT= 475
TRAJECTORY ISL= 8, IPS= 1 RECIRCULATES
ISL= 8, IPS= 1, TERMINATED AT: IV=34, JU=25 TIME= 3.507E-01 NPOINT= 425
ISL= 8, IPS= 2, TERMINATED AT: IV=34, JU=20 TIME= 3.014E-01 NPOINT= 348
ISL= 8, IPS= 3, TERMINATED AT: IV=34, JU=18 TIME= 2.827E-01 NPOINT= 487
ISL= 8, IPS= 4, TERMINATED AT: IV=34, JU=16 TIME= 2.671E-01 NPOINT= 497
ISL= 8, IPS= 5, TERMINATED AT: IV=34, JU=14 TIME= 2.546E-01 NPOINT= 474
TRAJECTORY ISL= 9, IPS= 1 RECIRCULATES
ISL= 9, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 3.263E-01 NPOINT= 471
ISL= 9, IPS= 2, TERMINATED AT: IV=34, JU=21 TIME= 3.239E-01 NPOINT= 424
ISL= 9, IPS= 3, TERMINATED AT: IV=34, JU=19 TIME= 2.943E-01 NPOINT= 476
ISL= 9, IPS= 4, TERMINATED AT: IV=34, JU=18 TIME= 2.748E-01 NPOINT= 476
ISL= 9, IPS= 5, TERMINATED AT: IV=34, JU=16 TIME= 2.586E-01 NPOINT= 474
TRAJECTORY ISL=10, IPS= 1 RECIRCULATES
ISL=10, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 3.934E-01 NPOINT= 498
TRAJECTORY ISL=10, IPS= 2 RECIRCULATES
ISL=10, IPS= 2, TERMINATED AT: IV=34, JU=24 TIME= 3.552E-01 NPOINT= 518
ISL=10, IPS= 3, TERMINATED AT: IV=34, JU=21 TIME= 3.165E-01 NPOINT= 453
ISL=10, IPS= 4, TERMINATED AT: IV=34, JU=19 TIME= 2.856E-01 NPOINT= 495
ISL=10, IPS= 5, TERMINATED AT: IV=34, JU=18 TIME= 2.671E-01 NPOINT= 449

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SUM OF SOLID PHASE COUPLING

SSPE = 3.421E-C4

SSPF = 0.000E+C0

SSPM = 3.421E-C4

SSPU = 6.485E-C3

SSPV = -2.995E-C6

SSPII = 0.000E+C0

AT X = 1.49 , COAL BURNOUT = 0.8151

>>>>EOLP COMPLETE; END OF PARTICLE ITERATION # 5

162

NITER	SORCE	RESORU RESORP	RESORV RESORH	RESORW RESORF	RESORM RESOET	NCREC
1	2.689E-01	4.910E-02	2.014E-02	4.609E-03	2.848E-02	
	0.2688537	0.000E+00	2.802E-02	3.849E-02	2.689E-01	0
5	1.141E-01	1.141E-01	1.088E-01	2.616E-02	3.075E-02	
		0.000E+00	2.723E-02	6.829E-02	8.457E-02	0
10	7.133E-02	5.183E-02	4.548E-02	2.999E-02	1.733E-02	
		0.000E+00	2.400E-02	7.133E-02	5.861E-02	0
15	5.627E-02	3.734E-02	2.641E-02	2.743E-02	9.706E-03	
		0.000E+00	1.802E-02	5.627E-02	4.198E-02	0
20	4.434E-02	3.620E-02	1.760E-02	2.001E-02	6.355E-03	
		0.000E+00	1.357E-02	4.434E-02	3.112E-02	0
25	3.761E-02	2.311E-02	9.415E-03	1.498E-02	5.377E-03	
		0.000E+00	1.169E-02	3.761E-02	2.673E-02	0
30	3.279E-02	1.630E-02	5.538E-03	1.122E-02	3.798E-03	
		0.000E+00	1.046E-02	3.279E-02	2.279E-02	0
35	2.790E-02	1.181E-02	4.064E-03	9.214E-03	2.568E-03	
		0.000E+00	9.938E-03	2.790E-02	1.968E-02	0
40	2.425E-02	9.170E-03	3.426E-03	7.185E-03	2.266E-03	
		0.000E+00	1.024E-02	2.425E-02	1.740E-02	0
45	2.167E-02	8.149E-03	2.932E-03	6.263E-03	2.095E-03	
		0.000E+00	1.066E-02	2.167E-02	1.630E-02	0
50	1.955E-02	7.512E-03	2.368E-03	5.598E-03	1.999E-03	
		0.000E+00	1.070E-02	1.955E-02	1.535E-02	0
55	1.779E-02	6.581E-03	1.902E-03	4.876E-03	1.717E-03	
		0.000E+00	1.047E-02	1.779E-02	1.414E-02	0
60	1.624E-02	5.794E-03	1.598E-03	4.178E-03	1.515E-03	

65	1.485E-02	0.000E+00	9.962E-03	1.624E-02	1.276E-02	0
		4.944E-03	1.358E-03	3.633E-03	1.409E-03	
		0.000E+00	9.284E-03	1.485E-02	1.151E-02	0
70	1.356E-02	4.500E-03	1.188E-03	3.256E-03	1.235E-03	
		0.000E+00	8.429E-03	1.356E-02	1.041E-02	0
75	1.240E-02	4.135E-03	1.070E-03	2.938E-03	1.126E-03	
		0.000E+00	7.424E-03	1.240E-02	9.347E-03	0
80	1.132E-02	3.685E-03	9.712E-04	2.647E-03	1.025E-03	
		0.000E+00	6.384E-03	1.132E-02	8.327E-03	0
85	1.044E-02	3.312E-03	8.632E-04	2.382E-03	9.403E-04	
		0.000E+00	5.401E-03	1.044E-02	7.356E-03	0

NUMBER SOURCE RESNJS

SCATTER	ITER: 0	ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX:	1.000E+00
SCATTER	ITER: 0	ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX:	5.138E-01
SCATTER	ITER: 0	ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX:	1.591E-01
SCATTER	ITER: 0	ITERATION: 4	FRAC CHANGE IN TOT NET WALL FLUX:	6.664E-02
SCATTER	ITER: 0	ITERATION: 5	FRAC CHANGE IN TOT NET WALL FLUX:	2.176E-02
SCATTER	ITER: 0	ITERATION: 6	FRAC CHANGE IN TOT NET WALL FLUX:	8.236E-03
SCATTER	ITER: 1	ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX:	2.871E-02
SCATTER	ITER: 1	ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX:	1.268E-02
SCATTER	ITER: 1	ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX:	2.172E-03
SCATTER	ITER: 0	ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX:	1.000E+00
SCATTER	ITER: 0	ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX:	5.138E-01
SCATTER	ITER: 0	ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX:	1.591E-01
SCATTER	ITER: 0	ITERATION: 4	FRAC CHANGE IN TOT NET WALL FLUX:	6.664E-02
SCATTER	ITER: 0	ITERATION: 5	FRAC CHANGE IN TOT NET WALL FLUX:	2.176E-02
SCATTER	ITER: 0	ITERATION: 6	FRAC CHANGE IN TOT NET WALL FLUX:	8.236E-03
SCATTER	ITER: 1	ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX:	2.871E-02
SCATTER	ITER: 1	ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX:	1.268E-02
SCATTER	ITER: 1	ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX:	2.172E-03

IF IT HITS THE WALLS IT STICKS

ISL= 1, IPS= 1, TERMINATED AT: IV=34, JU= 2	TIME= 2.455E-01	NPOINT= 457
ISL= 1, IPS= 2, TERMINATED AT: IV=34, JU= 2	TIME= 2.411E-01	NPOINT= 444
ISL= 1, IPS= 3, TERMINATED AT: IV=34, JU= 2	TIME= 2.402E-01	NPOINT= 453
ISL= 1, IPS= 4, TERMINATED AT: IV=34, JU= 2	TIME= 2.396E-01	NPOINT= 518
ISL= 1, IPS= 5, TERMINATED AT: IV=34, JU= 2	TIME= 2.328E-01	NPOINT= 457
ISL= 2, IPS= 1, TERMINATED AT: IV=34, JU= 6	TIME= 2.491E-01	NPOINT= 499
ISL= 2, IPS= 2, TERMINATED AT: IV=34, JU= 5	TIME= 2.464E-01	NPOINT= 426
ISL= 2, IPS= 3, TERMINATED AT: IV=34, JU= 4	TIME= 2.448E-01	NPOINT= 428
ISL= 2, IPS= 4, TERMINATED AT: IV=34, JU= 4	TIME= 2.412E-01	NPOINT= 563
ISL= 2, IPS= 5, TERMINATED AT: IV=34, JU= 4	TIME= 2.358E-01	NPOINT= 486
ISL= 3, IPS= 1, TERMINATED AT: IV=34, JU=10	TIME= 2.535E-01	NPOINT= 490
ISL= 3, IPS= 2, TERMINATED AT: IV=34, JU= 8	TIME= 2.500E-01	NPOINT= 391
ISL= 3, IPS= 3, TERMINATED AT: IV=34, JU= 7	TIME= 2.419E-01	NPOINT= 484
ISL= 3, IPS= 4, TERMINATED AT: IV=34, JU= 6	TIME= 2.424E-01	NPOINT= 532
ISL= 3, IPS= 5, TERMINATED AT: IV=34, JU= 5	TIME= 2.322E-01	NPOINT= 464
ISL= 4, IPS= 1, TERMINATED AT: IV=34, JU=14	TIME= 2.610E-01	NPOINT= 480
ISL= 4, IPS= 2, TERMINATED AT: IV=34, JU=11	TIME= 2.551E-01	NPOINT= 437
ISL= 4, IPS= 3, TERMINATED AT: IV=34, JU= 9	TIME= 2.491E-01	NPOINT= 410
ISL= 4, IPS= 4, TERMINATED AT: IV=34, JU= 8	TIME= 2.453E-01	NPOINT= 529
ISL= 4, IPS= 5, TERMINATED AT: IV=34, JU= 7	TIME= 2.340E-01	NPOINT= 489
ISL= 5, IPS= 1, TERMINATED AT: IV=34, JU=17	TIME= 2.715E-01	NPOINT= 461
ISL= 5, IPS= 2, TERMINATED AT: IV=34, JU=13	TIME= 2.613E-01	NPOINT= 410
ISL= 5, IPS= 3, TERMINATED AT: IV=34, JU=11	TIME= 2.491E-01	NPOINT= 479
ISL= 5, IPS= 4, TERMINATED AT: IV=34, JU=10	TIME= 2.477E-01	NPOINT= 508
ISL= 5, IPS= 5, TERMINATED AT: IV=34, JU= 8	TIME= 2.357E-01	NPOINT= 484
ISL= 6, IPS= 1, TERMINATED AT: IV=34, JU=20	TIME= 2.915E-01	NPOINT= 575
ISL= 6, IPS= 2, TERMINATED AT: IV=34, JU=16	TIME= 2.677E-01	NPOINT= 403
ISL= 6, IPS= 3, TERMINATED AT: IV=34, JU=13	TIME= 2.590E-01	NPOINT= 493
ISL= 6, IPS= 4, TERMINATED AT: IV=34, JU=12	TIME= 2.501E-01	NPOINT= 542
ISL= 6, IPS= 5, TERMINATED AT: IV=34, JU=10	TIME= 2.424E-01	NPOINT= 481
ISL= 7, IPS= 1, TERMINATED AT: IV=34, JU=22	TIME= 3.241E-01	NPOINT= 445
ISL= 7, IPS= 2, TERMINATED AT: IV=34, JU=18	TIME= 2.779E-01	NPOINT= 418

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ISL= 7, IPS= 3, TERMINATED AT: IV=34, JU=15 TIME= 2.619E-01 NPOINT= 481
ISL= 7, IPS= 4, TERMINATED AT: IV=34, JU=13 TIME= 2.515E-01 NPOINT= 533
ISL= 7, IPS= 5, TERMINATED AT: IV=34, JU=12 TIME= 2.431E-01 NPOINT= 489
TRAJECTORY ISL= 8, IPS= 1 RECIRCULATES
ISL= 8, IPS= 1, TERMINATED AT: IV=34, JU=25 TIME= 3.449E-01 NPOINT= 498
ISL= 8, IPS= 2, TERMINATED AT: IV=34, JU=20 TIME= 2.926E-01 NPOINT= 411
ISL= 8, IPS= 3, TERMINATED AT: IV=34, JU=18 TIME= 2.798E-01 NPOINT= 473
ISL= 8, IPS= 4, TERMINATED AT: IV=34, JU=16 TIME= 2.624E-01 NPOINT= 463
ISL= 8, IPS= 5, TERMINATED AT: IV=34, JU=14 TIME= 2.550E-01 NPOINT= 424
TRAJECTORY ISL= 9, IPS= 1 RECIRCULATES
ISL= 9, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 3.346E-01 NPOINT= 474
ISL= 9, IPS= 2, TERMINATED AT: IV=34, JU=21 TIME= 3.140E-01 NPOINT= 537
ISL= 9, IPS= 3, TERMINATED AT: IV=34, JU=19 TIME= 2.953E-01 NPOINT= 448
ISL= 9, IPS= 4, TERMINATED AT: IV=34, JU=18 TIME= 2.770E-01 NPOINT= 451
ISL= 9, IPS= 5, TERMINATED AT: IV=34, JU=15 TIME= 2.548E-01 NPOINT= 438
TRAJECTORY ISL=10, IPS= 1 RECIRCULATES
ISL=10, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 4.041E-01 NPOINT= 516
TRAJECTORY ISL=10, IPS= 2 RECIRCULATES
ISL=10, IPS= 2, TERMINATED AT: IV=34, JU=24 TIME= 3.572E-01 NPOINT= 499
ISL=10, IPS= 3, TERMINATED AT: IV=34, JU=21 TIME= 3.145E-01 NPOINT= 434
ISL=10, IPS= 4, TERMINATED AT: IV=34, JU=19 TIME= 2.899E-01 NPOINT= 466
ISL=10, IPS= 5, TERMINATED AT: IV=34, JU=17 TIME= 2.632E-01 NPOINT= 434

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SUM OF SOLID PHASE COUPLING

```

SSPE = 3.431E-04
SSPF = 0.000E+00
SSPM = 3.431E-04
SSPU = 6.492E-03
SSPV = -3.056E-06
SSPH = 0.000E+00

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AT X = 1.49 , COAL BURNOUT = 0.8168

>>>>EOLP COMPLETE, END OF PARTICLE ITERATION # 6

88

NITER	SORCE	RESORU RESORP	RESORV RESORH	FESORW RESORF	RESORM RESOET	NCREE
1	2.716E-01	4.456E-02	1.779E-02	5.419E-03	2.749E-02	0
0.2716434		0.000E+00	2.557E-02	4.275E-02	2.716E-01	
5	8.639E-02	8.370E-02	7.798E-02	2.168E-02	2.275E-02	0
		0.000E-00	2.664E-02	5.905E-02	8.535E-02	
10	5.546E-02	4.008E-02	4.136E-02	2.387E-02	1.637E-02	0
		0.000E+00	2.442E-02	5.539E-02	5.546E-02	
15	4.602E-02	3.903E-02	2.893E-02	2.421E-02	1.007E-02	0
		0.000E+00	2.176E-02	4.632E-02	4.375E-02	
20	3.402E-02	3.306E-02	1.725E-02	1.892E-02	7.373E-03	1
		0.000E+00	1.720E-02	3.212E-02	3.402E-02	

HRPMIN = -340.1540
 HRMIN1 = -340.0000
 NCREE = 1
 NLIM = 0
 ENT(HRPMIN/10)*10.0-10.0 = -350.0000
 Changing HRMIN from -340. to -350.
 Generating new table...
 There were 42 failures in the equilibrium algorithm

25	2.753E-02	2.348E-02	1.140E-02	1.365E-02	6.449E-03	0
		0.000E+00	1.358E-02	2.363E-02	2.753E-02	
30	2.368E-02	2.023E-02	7.565E-03	9.650E-03	4.626E-03	0
		0.000E+00	1.127E-02	1.904E-02	2.368E-02	

HRPMIN = -339.9836

INT(HRPMIN/10)*10.0-10.0 = -340.0000

HRMIN1 = -350.0000

Changing HRMIN from -350. to -340.

Generating new table...

There were 43 failures in the equilibrium algorithm

35	2.161E-02	1.248E-02	5.676E-03	7.945E-03	4.178E-03	0
		0.000E+00	1.003E-02	1.697E-02	2.161E-02	
40	1.937E-02	1.042E-02	4.673E-03	5.993E-03	2.348E-03	0
		0.000E+00	8.480E-03	1.436E-02	1.937E-02	
45	1.851E-02	8.498E-03	3.241E-03	4.860E-03	1.798E-03	0
		0.000E+00	7.744E-03	1.295E-02	1.851E-02	
50	1.764E-02	9.220E-03	2.713E-03	4.116E-03	1.726E-03	0
		0.000E+00	7.000E-03	1.197E-02	1.764E-02	
55	1.650E-02	1.048E-02	2.293E-03	3.765E-03	1.263E-03	0
		0.000E+00	6.016E-03	1.114E-02	1.650E-02	
60	1.545E-02	8.130E-03	1.871E-03	3.425E-03	1.456E-03	0
		0.000E+00	5.187E-03	1.055E-02	1.545E-02	
65	1.439E-02	6.224E-03	1.560E-03	3.161E-03	1.233E-03	0
		0.000E+00	4.543E-03	1.002E-02	1.439E-02	
70	1.359E-02	6.981E-03	1.355E-03	2.913E-03	7.536E-04	0
		0.000E+00	4.000E-03	9.557E-03	1.359E-02	
75	1.260E-02	5.459E-03	1.159E-03	2.682E-03	8.981E-04	0
		0.000E+00	3.428E-03	9.140E-03	1.260E-02	
80	1.180E-02	4.783E-03	9.680E-04	2.505E-03	7.270E-04	0
		0.000E+00	2.859E-03	8.880E-03	1.180E-02	
85	1.106E-02	4.253E-03	8.277E-04	2.312E-03	6.094E-04	0
		0.000E+00	2.444E-03	8.621E-03	1.106E-02	
90	1.028E-02	3.600E-03	7.150E-04	2.166E-03	7.023E-04	0
		0.000E+00	2.197E-03	8.389E-03	1.028E-02	

209

NOITER	SORCE	RESNJ'S
SCATTER	ITER: 0	ITERATION: 1
SCATTER	ITER: 0	ITERATION: 2
SCATTER	ITER: 0	ITERATION: 3
SCATTER	ITER: 0	ITERATION: 4
SCATTER	ITER: 0	ITERATION: 5
SCATTER	ITER: 0	ITERATION: 6
SCATTER	ITER: 1	ITERATION: 1
SCATTER	ITER: 1	ITERATION: 2
SCATTER	ITER: 1	ITERATION: 3
SCATTER	ITER: 0	ITERATION: 1
SCATTER	ITER: 0	ITERATION: 2
SCATTER	ITER: 0	ITERATION: 3
SCATTER	ITER: 0	ITERATION: 4
SCATTER	ITER: 0	ITERATION: 5
SCATTER	ITER: 0	ITERATION: 6
SCATTER	ITER: 1	ITERATION: 1
SCATTER	ITER: 1	ITERATION: 2
SCATTER	ITER: 1	ITERATION: 3

IF IT HITS THE WALLS IT STICKS

ISL= 1, IPS= 1, TERMINATED AT: IV=34, JU= 2	TIME= 2.455E-01	NPOINT= 455
ISL= 1, IPS= 2, TERMINATED AT: IV=34, JU= 2	TIME= 2.413E-01	NPOINT= 430
ISL= 1, IPS= 3, TERMINATED AT: IV=34, JU= 2	TIME= 2.445E-01	NPOINT= 459
ISL= 1, IPS= 4, TERMINATED AT: IV=34, JU= 2	TIME= 2.381E-01	NPOINT= 524
ISL= 1, IPS= 5, TERMINATED AT: IV=34, JU= 2	TIME= 2.305E-01	NPOINT= 494
ISL= 2, IPS= 1, TERMINATED AT: IV=34, JU= 6	TIME= 2.475E-01	NPOINT= 463
ISL= 2, IPS= 2, TERMINATED AT: IV=34, JU= 5	TIME= 2.431E-01	NPOINT= 431
ISL= 2, IPS= 3, TERMINATED AT: IV=34, JU= 5	TIME= 2.450E-01	NPOINT= 463
ISL= 2, IPS= 4, TERMINATED AT: IV=34, JU= 4	TIME= 2.358E-01	NPOINT= 532
ISL= 2, IPS= 5, TERMINATED AT: IV=34, JU= 4	TIME= 2.329E-01	NPOINT= 462
ISL= 3, IPS= 1, TERMINATED AT: IV=34, JU=10	TIME= 2.530E-01	NPOINT= 483
ISL= 3, IPS= 2, TERMINATED AT: IV=34, JU= 8	TIME= 2.498E-01	NPOINT= 382
ISL= 3, IPS= 3, TERMINATED AT: IV=34, JU= 7	TIME= 2.477E-01	NPOINT= 489
ISL= 3, IPS= 4, TERMINATED AT: IV=34, JU= 6	TIME= 2.436E-01	NPOINT= 538

ISL= 3, IPS= 5, TERMINATED AT: IV=34, JU= 6 TIME= 2.367E-01 NPOINT= 492
 ISL= 4, IPS= 1, TERMINATED AT: IV=34, JU=14 TIME= 2.601E-01 NPOINT= 447
 ISL= 4, IPS= 2, TERMINATED AT: IV=34, JU=11 TIME= 2.510E-01 NPOINT= 396
 ISL= 4, IPS= 3, TERMINATED AT: IV=34, JU=10 TIME= 2.504E-01 NPOINT= 495
 ISL= 4, IPS= 4, TERMINATED AT: IV=34, JU= 8 TIME= 2.452E-01 NPOINT= 544
 ISL= 4, IPS= 5, TERMINATED AT: IV=34, JU= 7 TIME= 2.387E-01 NPOINT= 488
 ISL= 5, IPS= 1, TERMINATED AT: IV=34, JU=17 TIME= 2.716E-01 NPOINT= 560
 ISL= 5, IPS= 2, TERMINATED AT: IV=34, JU=14 TIME= 2.611E-01 NPOINT= 376
 ISL= 5, IPS= 3, TERMINATED AT: IV=34, JU=12 TIME= 2.562E-01 NPOINT= 485
 ISL= 5, IPS= 4, TERMINATED AT: IV=34, JU=10 TIME= 2.479E-01 NPOINT= 523
 ISL= 5, IPS= 5, TERMINATED AT: IV=34, JU= 9 TIME= 2.360E-01 NPOINT= 482
 ISL= 6, IPS= 1, TERMINATED AT: IV=34, JU=20 TIME= 2.929E-01 NPOINT= 410
 ISL= 6, IPS= 2, TERMINATED AT: IV=34, JU=16 TIME= 2.681E-01 NPOINT= 412
 ISL= 6, IPS= 3, TERMINATED AT: IV=34, JU=14 TIME= 2.618E-01 NPOINT= 456
 ISL= 6, IPS= 4, TERMINATED AT: IV=34, JU=12 TIME= 2.511E-01 NPOINT= 528
 ISL= 6, IPS= 5, TERMINATED AT: IV=34, JU=11 TIME= 2.435E-01 NPOINT= 517
 ISL= 7, IPS= 1, TERMINATED AT: IV=34, JU=22 TIME= 3.245E-01 NPOINT= 488
 ISL= 7, IPS= 2, TERMINATED AT: IV=34, JU=18 TIME= 2.818E-01 NPOINT= 353
 ISL= 7, IPS= 3, TERMINATED AT: IV=34, JU=16 TIME= 2.645E-01 NPOINT= 429
 ISL= 7, IPS= 4, TERMINATED AT: IV=34, JU=14 TIME= 2.584E-01 NPOINT= 512
 ISL= 7, IPS= 5, TERMINATED AT: IV=34, JU=13 TIME= 2.464E-01 NPOINT= 509
 TRAJECTORY ISL= 8, IPS= 1 RECIRCULATES
 ISL= 8, IPS= 1, TERMINATED AT: IV=34, JU=25 TIME= 3.417E-01 NPOINT= 428
 ISL= 8, IPS= 2, TERMINATED AT: IV=34, JU=20 TIME= 2.950E-01 NPOINT= 406
 ISL= 8, IPS= 3, TERMINATED AT: IV=34, JU=18 TIME= 2.789E-01 NPOINT= 449
 ISL= 8, IPS= 4, TERMINATED AT: IV=34, JU=16 TIME= 2.654E-01 NPOINT= 482
 ISL= 8, IPS= 5, TERMINATED AT: IV=34, JU=15 TIME= 2.556E-01 NPOINT= 485
 TRAJECTORY ISL= 9, IPS= 1 RECIRCULATES
 ISL= 9, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 3.419E-01 NPOINT= 519
 ISL= 9, IPS= 2, TERMINATED AT: IV=34, JU=21 TIME= 3.175E-01 NPOINT= 422
 ISL= 9, IPS= 3, TERMINATED AT: IV=34, JU=19 TIME= 2.911E-01 NPOINT= 455
 ISL= 9, IPS= 4, TERMINATED AT: IV=34, JU=18 TIME= 2.780E-01 NPOINT= 484
 ISL= 9, IPS= 5, TERMINATED AT: IV=34, JU=16 TIME= 2.566E-01 NPOINT= 459
 TRAJECTORY ISL=10, IPS= 1 RECIRCULATES
 ISL=10, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 4.060E-01 NPOINT= 619
 TRAJECTORY ISL=10, IPS= 2 RECIRCULATES
 ISL=10, IPS= 2, TERMINATED AT: IV=34, JU=24 TIME= 3.571E-01 NPOINT= 522
 ISL=10, IPS= 3, TERMINATED AT: IV=34, JU=21 TIME= 3.121E-01 NPOINT= 444
 ISL=10, IPS= 4, TERMINATED AT: IV=34, JU=19 TIME= 2.902E-01 NPOINT= 460
 ISL=10, IPS= 5, TERMINATED AT: IV=34, JU=18 TIME= 2.671E-01 NPOINT= 435

SUM OF SOLID PHASE COUPLING

SSPE = 3.441E-04
 SSPF = 0.000E+00
 SSPM = 3.441E-04
 SSPU = 6.498E-03
 SSPV = -3.067E-06
 SSPH = 0.000E+00

AT X = 1.49 , COAL BURNOUT = 0.8190

>>>FOLP COMPLETE, END OF PARTICLE ITERATION # 7

93

NITER	SORCE	RESORU RESORP	RESORV RESORH	RESORW RESORF	RESORM RESOET	NCREE
1	1.977E-01	2.974E-02	1.514E-02	3.948E-03	2.235E-02	0
0.1977319		0.000E+00	1.398E-02	2.805E-02	1.977E-01	
5	5.564E-02	4.773E-02	4.214E-02	1.247E-02	1.491E-02	0
		0.000E+00	1.332E-02	3.328E-02	5.564E-02	
10	3.898E-02	2.571E-02	2.132E-02	1.416E-02	9.321E-03	

		0.000E+00	1.378E-02	3.108E-02	3.898E-02	0
15	3.183E-02	2.402E-02	1.475E-02	1.453E-02	5.639E-03	0
		0.000E+00	1.246E-02	2.767E-02	3.183E-02	0
20	2.588E-02	2.140E-02	9.767E-03	1.237E-02	4.569E-03	0
		0.000E+00	9.568E-03	2.086E-02	2.588E-02	0
25	2.203E-02	1.473E-02	6.781E-03	9.644E-03	3.813E-03	0
		0.000E+00	7.389E-03	1.637E-02	2.203E-02	0
30	1.937E-02	1.205E-02	4.500E-03	7.506E-03	2.672E-03	0
		0.000E+00	6.447E-03	1.407E-02	1.937E-02	0
35	1.750E-02	8.296E-03	3.360E-03	6.276E-03	2.017E-03	0
		0.000E+00	5.859E-03	1.269E-02	1.750E-02	0
40	1.594E-02	7.385E-03	2.701E-03	5.109E-03	1.135E-03	0
		0.000E+00	5.310E-03	1.139E-02	1.594E-02	0
45	1.467E-02	5.904E-03	2.140E-03	4.214E-03	1.026E-03	0
		0.000E+00	4.792E-03	1.025E-02	1.467E-02	0
50	1.343E-02	5.290E-03	1.722E-03	3.513E-03	8.696E-04	0
		0.000E+00	4.281E-03	9.324E-03	1.343E-02	0
55	1.234E-02	5.222E-03	1.457E-03	3.076E-03	6.428E-04	0
		0.000E+00	3.731E-03	8.430E-03	1.234E-02	0
60	1.132E-02	4.048E-03	1.229E-03	2.715E-03	6.262E-04	0
		0.000E+00	3.294E-03	7.670E-03	1.132E-02	0
65	1.044E-02	3.466E-03	1.041E-03	2.452E-03	5.540E-04	0
		0.000E+00	2.990E-03	6.944E-03	1.044E-02	0

NUMBER	SOURCE	RESN1'S
SCATTER	ITER: 0 ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX: 1.000E+00
SCATTER	ITER: 0 ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX: 5.157E-01
SCATTER	ITER: 0 ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX: 1.588E-01
SCATTER	ITER: 0 ITERATION: 4	FRAC CHANGE IN TOT NET WALL FLUX: 6.671E-02
SCATTER	ITER: 0 ITERATION: 5	FRAC CHANGE IN TOT NET WALL FLUX: 2.171E-02
SCATTER	ITER: 0 ITERATION: 6	FRAC CHANGE IN TOT NET WALL FLUX: 8.241E-03
SCATTER	ITER: 1 ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX: 2.887E-02
SCATTER	ITER: 1 ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX: 1.278E-02
SCATTER	ITER: 1 ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX: 2.191E-03
SCATTER	ITER: 0 ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX: 1.000E+00
SCATTER	ITER: 0 ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX: 5.157E-01
SCATTER	ITER: 0 ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX: 1.588E-01
SCATTER	ITER: 0 ITERATION: 4	FRAC CHANGE IN TOT NET WALL FLUX: 6.671E-02
SCATTER	ITER: 0 ITERATION: 5	FRAC CHANGE IN TOT NET WALL FLUX: 2.171E-02
SCATTER	ITER: 0 ITERATION: 6	FRAC CHANGE IN TOT NET WALL FLUX: 8.241E-03
SCATTER	ITER: 1 ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX: 2.887E-02
SCATTER	ITER: 1 ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX: 1.278E-02
SCATTER	ITER: 1 ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX: 2.191E-03

IF IT HITS THE WALLS IT STICKS

ISL= 1, IPS= 1, TERMINATED AT: IV=34, JU= 2	TIME= 2.451E-01	NPOINT= 363
ISL= 1, IPS= 2, TERMINATED AT: IV=34, JU= 2	TIME= 2.436E-01	NPOINT= 451
ISL= 1, IPS= 3, TERMINATED AT: IV=34, JU= 2	TIME= 2.413E-01	NPOINT= 521
ISL= 1, IPS= 4, TERMINATED AT: IV=34, JU= 2	TIME= 2.410E-01	NPOINT= 563
ISL= 1, IPS= 5, TERMINATED AT: IV=34, JU= 2	TIME= 2.327E-01	NPOINT= 488
ISL= 2, IPS= 1, TERMINATED AT: IV=34, JU= 7	TIME= 2.478E-01	NPOINT= 463
ISL= 2, IPS= 2, TERMINATED AT: IV=34, JU= 5	TIME= 2.445E-01	NPOINT= 431
ISL= 2, IPS= 3, TERMINATED AT: IV=34, JU= 4	TIME= 2.450E-01	NPOINT= 533
ISL= 2, IPS= 4, TERMINATED AT: IV=34, JU= 4	TIME= 2.409E-01	NPOINT= 510
ISL= 2, IPS= 5, TERMINATED AT: IV=34, JU= 4	TIME= 2.354E-01	NPOINT= 484
ISL= 3, IPS= 1, TERMINATED AT: IV=34, JU=10	TIME= 2.548E-01	NPOINT= 397
ISL= 3, IPS= 2, TERMINATED AT: IV=34, JU= 8	TIME= 2.496E-01	NPOINT= 456
ISL= 3, IPS= 3, TERMINATED AT: IV=34, JU= 7	TIME= 2.437E-01	NPOINT= 535
ISL= 3, IPS= 4, TERMINATED AT: IV=34, JU= 6	TIME= 2.377E-01	NPOINT= 518
ISL= 3, IPS= 5, TERMINATED AT: IV=34, JU= 5	TIME= 2.359E-01	NPOINT= 490
ISL= 4, IPS= 1, TERMINATED AT: IV=34, JU=14	TIME= 2.598E-01	NPOINT= 463
ISL= 4, IPS= 2, TERMINATED AT: IV=34, JU=10	TIME= 2.487E-01	NPOINT= 470
ISL= 4, IPS= 3, TERMINATED AT: IV=34, JU= 9	TIME= 2.460E-01	NPOINT= 529
ISL= 4, IPS= 4, TERMINATED AT: IV=34, JU= 8	TIME= 2.396E-01	NPOINT= 524
ISL= 4, IPS= 5, TERMINATED AT: IV=34, JU= 7	TIME= 2.383E-01	NPOINT= 498

ISL= 5, IPS= 1, TERMINATED AT: IV=34, JU=17 TIME= 2.712E-01 NPOINT= 468
 ISL= 5, IPS= 2, TERMINATED AT: IV=34, JU=13 TIME= 2.554E-01 NPOINT= 418
 ISL= 5, IPS= 3, TERMINATED AT: IV=34, JU=11 TIME= 2.488E-01 NPOINT= 536
 ISL= 5, IPS= 4, TERMINATED AT: IV=34, JU=10 TIME= 2.454E-01 NPOINT= 558
 ISL= 5, IPS= 5, TERMINATED AT: IV=34, JU= 9 TIME= 2.416E-01 NPOINT= 455
 ISL= 6, IPS= 1, TERMINATED AT: IV=34, JU=20 TIME= 2.929E-01 NPOINT= 451
 ISL= 6, IPS= 2, TERMINATED AT: IV=34, JU=16 TIME= 2.652E-01 NPOINT= 327
 ISL= 6, IPS= 3, TERMINATED AT: IV=34, JU=14 TIME= 2.601E-01 NPOINT= 503
 ISL= 6, IPS= 4, TERMINATED AT: IV=34, JU=12 TIME= 2.506E-01 NPOINT= 538
 ISL= 6, IPS= 5, TERMINATED AT: IV=34, JU=11 TIME= 2.444E-01 NPOINT= 454
 ISL= 7, IPS= 1, TERMINATED AT: IV=34, JU=22 TIME= 3.252E-01 NPOINT= 396
 ISL= 7, IPS= 2, TERMINATED AT: IV=34, JU=18 TIME= 2.784E-01 NPOINT= 357
 ISL= 7, IPS= 3, TERMINATED AT: IV=34, JU=16 TIME= 2.676E-01 NPOINT= 463
 ISL= 7, IPS= 4, TERMINATED AT: IV=34, JU=14 TIME= 2.530E-01 NPOINT= 502
 ISL= 7, IPS= 5, TERMINATED AT: IV=34, JU=12 TIME= 2.479E-01 NPOINT= 491
 TRAJECTORY ISL= 8, IPS= 1 RECIRCULATES
 ISL= 8, IPS= 1, TERMINATED AT: IV=34, JU=25 TIME= 3.356E-01 NPOINT= 452
 ISL= 8, IPS= 2, TERMINATED AT: IV=34, JU=20 TIME= 2.945E-01 NPOINT= 409
 ISL= 8, IPS= 3, TERMINATED AT: IV=34, JU=18 TIME= 2.797E-01 NPOINT= 413
 ISL= 8, IPS= 4, TERMINATED AT: IV=34, JU=16 TIME= 2.640E-01 NPOINT= 500
 ISL= 8, IPS= 5, TERMINATED AT: IV=34, JU=15 TIME= 2.526E-01 NPOINT= 479
 TRAJECTORY ISL= 9, IPS= 1 RECIRCULATES
 ISL= 9, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 3.442E-01 NPOINT= 501
 ISL= 9, IPS= 2, TERMINATED AT: IV=34, JU=21 TIME= 3.154E-01 NPOINT= 412
 ISL= 9, IPS= 3, TERMINATED AT: IV=34, JU=19 TIME= 2.911E-01 NPOINT= 458
 ISL= 9, IPS= 4, TERMINATED AT: IV=34, JU=18 TIME= 2.745E-01 NPOINT= 534
 ISL= 9, IPS= 5, TERMINATED AT: IV=34, JU=16 TIME= 2.590E-01 NPOINT= 443
 TRAJECTORY ISL=10, IPS= 1 RECIRCULATES
 ISL=10, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 4.023E-01 NPOINT= 662
 TRAJECTORY ISL=10, IPS= 2 RECIRCULATES
 ISL=10, IPS= 2, TERMINATED AT: IV=34, JU=24 TIME= 3.600E-01 NPOINT= 520
 ISL=10, IPS= 3, TERMINATED AT: IV=34, JU=21 TIME= 3.126E-01 NPOINT= 457
 ISL=10, IPS= 4, TERMINATED AT: IV=34, JU=19 TIME= 2.890E-01 NPOINT= 504
 ISL=10, IPS= 5, TERMINATED AT: IV=34, JU=18 TIME= 2.670E-01 NPOINT= 436

SUM OF SOLID PHASE COUPLING

SSPE = 3.426E-04
 SSPF = 0.000E+00
 SSPM = 3.426E-04
 SSPU = 6.488E-03
 SSPV = -3.102E-06
 SSPH = 0.000E+00

AT X = 1.49 , COAL BURNOUT = 0.8154

>>>>HOLP COMPLETE, END OF PARTICLE ITERATION # 8

66

NITER	SORCE	RESORU RESORP	RESORV RESORH	RESORW RESORF	RESORM RESOET	NCREE
1	1.734E-01	2.239E-02	8.904E-03	3.874E-03	1.709E-02	
		0.000E+00	1.423E-02	2.420E-02	1.734E-01	0
0.1733967						
5	4.746E-02	4.369E-02	4.113E-02	1.022E-02	1.190E-02	
		0.000E+00	1.190E-02	3.175E-02	4.746E-02	0
10	3.523E-02	2.153E-02	2.076E-02	1.211E-02	7.173E-03	
		0.000E+00	1.040E-02	3.081E-02	3.523E-02	0
15	2.975E-02	1.638E-02	1.165E-02	1.149E-02	4.879E-03	
		0.000E+00	7.494E-03	2.258E-02	2.975E-02	0
20	2.482E-02	1.683E-02	9.186E-03	9.239E-03	3.842E-03	
		0.000E+00	5.436E-03	1.494E-02	2.482E-02	0
25	2.130E-02	9.522E-03	5.527E-03	6.780E-03	3.351E-03	

30	1.869E-02	0.000E+00	4.071E-03	1.053E-02	2.130E-02	0
		8.363E-03	3.161E-03	5.306E-03	2.062E-03	
35	1.685E-02	0.000E+00	3.373E-03	8.521E-03	1.869E-02	0
		6.874E-03	2.326E-03	4.390E-03	1.367E-03	
40	1.554E-02	0.000E+00	2.698E-03	6.937E-03	1.685E-02	0
		4.780E-03	1.763E-03	3.703E-03	1.065E-03	
45	1.459E-02	0.000E+00	2.215E-03	5.706E-03	1.554E-02	0
		4.399E-03	1.461E-03	3.216E-03	8.618E-04	
50	1.380E-02	0.000E+00	1.825E-03	4.989E-03	1.459E-02	0
		3.692E-03	1.229E-03	2.888E-03	9.651E-04	
55	1.314E-02	0.000E+00	1.552E-03	4.624E-03	1.380E-02	0
		3.131E-03	1.009E-03	2.611E-03	9.175E-04	
60	1.256E-02	0.000E+00	1.495E-03	4.459E-03	1.314E-02	0
		3.581E-03	8.779E-04	2.327E-03	7.787E-04	
65	1.199E-02	0.000E+00	1.546E-03	4.296E-03	1.256E-02	0
		3.116E-03	7.532E-04	2.119E-03	7.987E-04	
70	1.151E-02	0.000E+00	1.562E-03	4.174E-03	1.199E-02	0
		2.507E-03	6.482E-04	1.968E-03	7.656E-04	
75	1.099E-02	0.000E+00	1.442E-03	4.054E-03	1.151E-02	0
		2.427E-03	5.751E-04	1.838E-03	7.133E-04	
80	1.043E-02	0.000E+00	1.237E-03	3.890E-03	1.099E-02	0
		2.395E-03	5.085E-04	1.739E-03	7.504E-04	
85	9.868E-03	0.000E+00	1.086E-03	3.769E-03	1.043E-02	0
		2.918E-03	4.627E-04	1.636E-03	6.905E-04	
		0.000E+00	9.964E-04	3.617E-03	9.868E-03	0

NJITER SOURCE RESNJ'S
 SCATTER ITER: 0 ITERATION: 1 FRAC CHANGE IN TOT NET WALL FLUX: 1.000E+00
 SCATTER ITER: 0 ITERATION: 2 FRAC CHANGE IN TOT NET WALL FLUX: 5.154E-01
 SCATTER ITER: 0 ITERATION: 3 FRAC CHANGE IN TOT NET WALL FLUX: 1.587E-01
 SCATTER ITER: 0 ITERATION: 4 FRAC CHANGE IN TOT NET WALL FLUX: 6.654E-02
 SCATTER ITER: 0 ITERATION: 5 FRAC CHANGE IN TOT NET WALL FLUX: 2.167E-02
 SCATTER ITER: 0 ITERATION: 6 FRAC CHANGE IN TOT NET WALL FLUX: 8.212E-03
 SCATTER ITER: 1 ITERATION: 1 FRAC CHANGE IN TOT NET WALL FLUX: 2.900E-02
 SCATTER ITER: 1 ITERATION: 2 FRAC CHANGE IN TOT NET WALL FLUX: 1.282E-02
 SCATTER ITER: 1 ITERATION: 3 FRAC CHANGE IN TOT NET WALL FLUX: 2.201E-03
 SCATTER ITER: 0 ITERATION: 1 FRAC CHANGE IN TOT NET WALL FLUX: 1.000E+00
 SCATTER ITER: 0 ITERATION: 2 FRAC CHANGE IN TOT NET WALL FLUX: 5.154E-01
 SCATTER ITER: 0 ITERATION: 3 FRAC CHANGE IN TOT NET WALL FLUX: 1.587E-01
 SCATTER ITER: 0 ITERATION: 4 FRAC CHANGE IN TOT NET WALL FLUX: 6.654E-02
 SCATTER ITER: 0 ITERATION: 5 FRAC CHANGE IN TOT NET WALL FLUX: 2.167E-02
 SCATTER ITER: 0 ITERATION: 6 FRAC CHANGE IN TOT NET WALL FLUX: 8.212E-03
 SCATTER ITER: 1 ITERATION: 1 FRAC CHANGE IN TOT NET WALL FLUX: 2.900E-02
 SCATTER ITER: 1 ITERATION: 2 FRAC CHANGE IN TOT NET WALL FLUX: 1.282E-02
 SCATTER ITER: 1 ITERATION: 3 FRAC CHANGE IN TOT NET WALL FLUX: 2.201E-03

IF IT HITS THE WALLS IT STICKS

ISL= 1, IPS= 1, TERMINATED AT: IV=34, JU= 2 TIME= 2.455E-01 NPOINT= 437
 ISL= 1, IPS= 2, TERMINATED AT: IV=34, JU= 2 TIME= 2.440E-01 NPOINT= 365
 ISL= 1, IPS= 3, TERMINATED AT: IV=34, JU= 2 TIME= 2.382E-01 NPOINT= 515
 ISL= 1, IPS= 4, TERMINATED AT: IV=34, JU= 2 TIME= 2.411E-01 NPOINT= 518
 ISL= 1, IPS= 5, TERMINATED AT: IV=34, JU= 2 TIME= 2.323E-01 NPOINT= 508
 ISL= 2, IPS= 1, TERMINATED AT: IV=34, JU= 6 TIME= 2.486E-01 NPOINT= 476
 ISL= 2, IPS= 2, TERMINATED AT: IV=34, JU= 5 TIME= 2.460E-01 NPOINT= 411
 ISL= 2, IPS= 3, TERMINATED AT: IV=34, JU= 4 TIME= 2.390E-01 NPOINT= 528
 ISL= 2, IPS= 4, TERMINATED AT: IV=34, JU= 4 TIME= 2.401E-01 NPOINT= 489
 ISL= 2, IPS= 5, TERMINATED AT: IV=34, JU= 3 TIME= 2.347E-01 NPOINT= 480
 ISL= 3, IPS= 1, TERMINATED AT: IV=34, JU=10 TIME= 2.544E-01 NPOINT= 431
 ISL= 3, IPS= 2, TERMINATED AT: IV=34, JU= 8 TIME= 2.493E-01 NPOINT= 427
 ISL= 3, IPS= 3, TERMINATED AT: IV=34, JU= 6 TIME= 2.407E-01 NPOINT= 530
 ISL= 3, IPS= 4, TERMINATED AT: IV=34, JU= 6 TIME= 2.415E-01 NPOINT= 503
 ISL= 3, IPS= 5, TERMINATED AT: IV=34, JU= 5 TIME= 2.321E-01 NPOINT= 484
 ISL= 4, IPS= 1, TERMINATED AT: IV=34, JU=14 TIME= 2.637E-01 NPOINT= 471
 ISL= 4, IPS= 2, TERMINATED AT: IV=34, JU=10 TIME= 2.505E-01 NPOINT= 502
 ISL= 4, IPS= 3, TERMINATED AT: IV=34, JU= 9 TIME= 2.446E-01 NPOINT= 494

ISL= 4, IPS= 4, TERMINATED AT: IV=34, JU= 8 TIME= 2.448E-01 NPOINT= 533
 ISL= 4, IPS= 5, TERMINATED AT: IV=34, JU= 6 TIME= 2.384E-01 NPOINT= 485
 ISL= 5, IPS= 1, TERMINATED AT: IV=34, JU=17 TIME= 2.712E-01 NPOINT= 529
 ISL= 5, IPS= 2, TERMINATED AT: IV=34, JU=13 TIME= 2.551E-01 NPOINT= 447
 ISL= 5, IPS= 3, TERMINATED AT: IV=34, JU=11 TIME= 2.485E-01 NPOINT= 514
 ISL= 5, IPS= 4, TERMINATED AT: IV=34, JU=10 TIME= 2.484E-01 NPOINT= 503
 ISL= 5, IPS= 5, TERMINATED AT: IV=34, JU= 8 TIME= 2.383E-01 NPOINT= 539
 ISL= 6, IPS= 1, TERMINATED AT: IV=34, JU=20 TIME= 2.888E-01 NPOINT= 420
 ISL= 6, IPS= 2, TERMINATED AT: IV=34, JU=16 TIME= 2.686E-01 NPOINT= 351
 ISL= 6, IPS= 3, TERMINATED AT: IV=34, JU=13 TIME= 2.600E-01 NPOINT= 470
 ISL= 6, IPS= 4, TERMINATED AT: IV=34, JU=12 TIME= 2.526E-01 NPOINT= 497
 ISL= 6, IPS= 5, TERMINATED AT: IV=34, JU=10 TIME= 2.441E-01 NPOINT= 544
 ISL= 7, IPS= 1, TERMINATED AT: IV=34, JU=22 TIME= 3.280E-01 NPOINT= 403
 ISL= 7, IPS= 2, TERMINATED AT: IV=34, JU=18 TIME= 2.749E-01 NPOINT= 384
 ISL= 7, IPS= 3, TERMINATED AT: IV=34, JU=16 TIME= 2.669E-01 NPOINT= 465
 ISL= 7, IPS= 4, TERMINATED AT: IV=34, JU=14 TIME= 2.583E-01 NPOINT= 496
 ISL= 7, IPS= 5, TERMINATED AT: IV=34, JU=12 TIME= 2.479E-01 NPOINT= 488
 TRAJECTORY ISL= 8, IPS= 1 RECIRCULATES
 ISL= 8, IPS= 1, TERMINATED AT: IV=34, JU=25 TIME= 3.350E-01 NPOINT= 448
 ISL= 8, IPS= 2, TERMINATED AT: IV=34, JU=20 TIME= 2.934E-01 NPOINT= 451
 ISL= 8, IPS= 3, TERMINATED AT: IV=34, JU=18 TIME= 2.770E-01 NPOINT= 453
 ISL= 8, IPS= 4, TERMINATED AT: IV=34, JU=16 TIME= 2.673E-01 NPOINT= 490
 ISL= 8, IPS= 5, TERMINATED AT: IV=34, JU=14 TIME= 2.563E-01 NPOINT= 512
 TRAJECTORY ISL= 9, IPS= 1 RECIRCULATES
 ISL= 9, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 3.464E-01 NPOINT= 522
 ISL= 9, IPS= 2, TERMINATED AT: IV=34, JU=21 TIME= 3.184E-01 NPOINT= 399
 ISL= 9, IPS= 3, TERMINATED AT: IV=34, JU=19 TIME= 2.910E-01 NPOINT= 428
 ISL= 9, IPS= 4, TERMINATED AT: IV=34, JU=18 TIME= 2.743E-01 NPOINT= 509
 ISL= 9, IPS= 5, TERMINATED AT: IV=34, JU=16 TIME= 2.565E-01 NPOINT= 494
 TRAJECTORY ISL=10, IPS= 1 RECIRCULATES
 ISL=10, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 4.030E-01 NPOINT= 648
 TRAJECTORY ISL=10, IPS= 2 RECIRCULATES
 ISL=10, IPS= 2, TERMINATED AT: IV=34, JU=24 TIME= 3.587E-01 NPOINT= 534
 ISL=10, IPS= 3, TERMINATED AT: IV=34, JU=21 TIME= 3.130E-01 NPOINT= 424
 ISL=10, IPS= 4, TERMINATED AT: IV=34, JU=19 TIME= 2.889E-01 NPOINT= 496
 ISL=10, IPS= 5, TERMINATED AT: IV=34, JU=18 TIME= 2.668E-01 NPOINT= 427

SUM OF SOLID PHASE COUPLING

SSPE = 3.424E-04
 SSPF = 0.000E+00
 SSPM = 3.424E-04
 SSPU = 6.485E-03
 SSPV = -2.940E-06
 SSPH = 0.000E+00

AT X = 1.49 , COAL BURNOUT = 0.8150

>>>>EOLP COMPLETE, END OF PARTICLE ITERATION # 9

85

NITER	SORCE	RESORU RESORP	RESORV RESORH	RESORW RESORF	RESORM RESOET	NCREE
1	1.605E-01	2.419E-02	8.001E-03	3.145E-03	1.625E-02	
0.1605134		0.000E+00	1.132E-02	2.052E-02	1.605E-01	0
5	4.928E-02	4.613E-02	4.332E-02	1.067E-02	1.225E-02	
		0.000E+00	1.239E-02	3.202E-02	4.928E-02	0
10	3.648E-02	2.234E-02	2.223E-02	1.234E-02	7.761E-03	
		0.000E+00	1.098E-02	3.051E-02	3.648E-02	0
15	3.009E-02	1.738E-02	1.188E-02	1.124E-02	4.977E-03	
		0.000E+00	8.484E-03	2.300E-02	3.009E-02	0
20	2.506E-02	1.512E-02	9.089E-03	8.870E-03	3.923E-03	

25	2.190E-02	0.000E+00	6.809E-03	1.654E-02	2.506E-02	0
		1.198E-02	5.103E-03	6.315E-03	2.965E-03	
30	1.941E-02	0.000E+00	5.631E-03	1.301E-02	2.190E-02	0
		9.011E-03	2.802E-03	4.789E-03	2.017E-03	
35	1.768E-02	0.000E+00	4.988E-03	1.197E-02	1.941E-02	0
		6.947E-03	2.004E-03	3.779E-03	1.301E-03	
40	1.627E-02	0.000E+00	4.484E-03	1.097E-02	1.768E-02	0
		5.609E-03	1.790E-03	3.081E-03	1.148E-03	
45	1.521E-02	0.000E+00	4.006E-03	1.008E-02	1.627E-02	0
		4.568E-03	1.428E-03	2.627E-03	9.469E-04	
50	1.415E-02	0.000E+00	3.501E-03	9.260E-03	1.521E-02	0
		3.852E-03	1.125E-03	2.375E-03	8.625E-04	
55	1.315E-02	0.000E+00	3.048E-03	8.526E-03	1.415E-02	0
		3.722E-03	8.863E-04	2.172E-03	6.906E-04	
60	1.220E-02	0.000E+00	2.690E-03	7.843E-03	1.315E-02	0
		3.360E-03	7.759E-04	1.972E-03	5.683E-04	
65	1.137E-02	0.000E+00	2.447E-03	7.270E-03	1.220E-02	0
		2.710E-03	6.700E-04	1.809E-03	5.653E-04	
70	1.061E-02	0.000E+00	2.259E-03	6.792E-03	1.137E-02	0
		2.604E-03	5.891E-04	1.695E-03	4.900E-04	
		0.000E+00	2.080E-03	6.378E-03	1.061E-02	0

NJITER SOURCE RESNJ'S
 SCATTER ITER: 0 ITERATION: 1 FRAC CHANGE IN TOT NET WALL FLUX: 1.000E+00
 SCATTER ITER: 0 ITERATION: 2 FRAC CHANGE IN TOT NET WALL FLUX: 5.153E-01
 SCATTER ITER: 0 ITERATION: 3 FRAC CHANGE IN TOT NET WALL FLUX: 1.583E-01
 SCATTER ITER: 0 ITERATION: 4 FRAC CHANGE IN TOT NET WALL FLUX: 6.636E-02
 SCATTER ITER: 0 ITERATION: 5 FRAC CHANGE IN TOT NET WALL FLUX: 2.160E-02
 SCATTER ITER: 0 ITERATION: 6 FRAC CHANGE IN TOT NET WALL FLUX: 8.181E-03
 SCATTER ITER: 1 ITERATION: 1 FRAC CHANGE IN TOT NET WALL FLUX: 2.899E-02
 SCATTER ITER: 1 ITERATION: 2 FRAC CHANGE IN TOT NET WALL FLUX: 1.281E-02
 SCATTER ITER: 1 ITERATION: 3 FRAC CHANGE IN TOT NET WALL FLUX: 2.199E-03
 SCATTER ITER: 0 ITERATION: 1 FRAC CHANGE IN TOT NET WALL FLUX: 1.000E+00
 SCATTER ITER: 0 ITERATION: 2 FRAC CHANGE IN TOT NET WALL FLUX: 5.153E-01
 SCATTER ITER: 0 ITERATION: 3 FRAC CHANGE IN TOT NET WALL FLUX: 1.583E-01
 SCATTER ITER: 0 ITERATION: 4 FRAC CHANGE IN TOT NET WALL FLUX: 6.636E-02
 SCATTER ITER: 0 ITERATION: 5 FRAC CHANGE IN TOT NET WALL FLUX: 2.160E-02
 SCATTER ITER: 0 ITERATION: 6 FRAC CHANGE IN TOT NET WALL FLUX: 8.181E-03
 SCATTER ITER: 1 ITERATION: 1 FRAC CHANGE IN TOT NET WALL FLUX: 2.899E-02
 SCATTER ITER: 1 ITERATION: 2 FRAC CHANGE IN TOT NET WALL FLUX: 1.281E-02
 SCATTER ITER: 1 ITERATION: 3 FRAC CHANGE IN TOT NET WALL FLUX: 2.199E-03

IF IT HITS THE WALLS IT STICKS

ISL= 1, IPS= 1, TERMINATED AT: IV=34, JU= 2 TIME= 2.424E-01 NPOINT= 511
 ISL= 1, IPS= 2, TERMINATED AT: IV=34, JU= 2 TIME= 2.459E-01 NPOINT= 393
 ISL= 1, IPS= 3, TERMINATED AT: IV=34, JU= 2 TIME= 2.381E-01 NPOINT= 494
 ISL= 1, IPS= 4, TERMINATED AT: IV=34, JU= 2 TIME= 2.405E-01 NPOINT= 554
 ISL= 1, IPS= 5, TERMINATED AT: IV=34, JU= 2 TIME= 2.294E-01 NPOINT= 478
 ISL= 2, IPS= 1, TERMINATED AT: IV=34, JU= 7 TIME= 2.450E-01 NPOINT= 511
 ISL= 2, IPS= 2, TERMINATED AT: IV=34, JU= 5 TIME= 2.442E-01 NPOINT= 431
 ISL= 2, IPS= 3, TERMINATED AT: IV=34, JU= 5 TIME= 2.439E-01 NPOINT= 513
 ISL= 2, IPS= 4, TERMINATED AT: IV=34, JU= 4 TIME= 2.407E-01 NPOINT= 518
 ISL= 2, IPS= 5, TERMINATED AT: IV=34, JU= 4 TIME= 2.324E-01 NPOINT= 473
 ISL= 3, IPS= 1, TERMINATED AT: IV=34, JU=11 TIME= 2.542E-01 NPOINT= 578
 ISL= 3, IPS= 2, TERMINATED AT: IV=34, JU= 8 TIME= 2.441E-01 NPOINT= 435
 ISL= 3, IPS= 3, TERMINATED AT: IV=34, JU= 7 TIME= 2.434E-01 NPOINT= 378
 ISL= 3, IPS= 4, TERMINATED AT: IV=34, JU= 6 TIME= 2.414E-01 NPOINT= 549
 ISL= 3, IPS= 5, TERMINATED AT: IV=34, JU= 5 TIME= 2.370E-01 NPOINT= 514
 ISL= 4, IPS= 1, TERMINATED AT: IV=34, JU=14 TIME= 2.624E-01 NPOINT= 517
 ISL= 4, IPS= 2, TERMINATED AT: IV=34, JU=10 TIME= 2.495E-01 NPOINT= 456
 ISL= 4, IPS= 3, TERMINATED AT: IV=34, JU= 9 TIME= 2.486E-01 NPOINT= 516
 ISL= 4, IPS= 4, TERMINATED AT: IV=34, JU= 8 TIME= 2.450E-01 NPOINT= 527
 ISL= 4, IPS= 5, TERMINATED AT: IV=34, JU= 7 TIME= 2.391E-01 NPOINT= 558
 ISL= 5, IPS= 1, TERMINATED AT: IV=34, JU=17 TIME= 2.710E-01 NPOINT= 439
 ISL= 5, IPS= 2, TERMINATED AT: IV=34, JU=13 TIME= 2.552E-01 NPOINT= 429

ISL= 5, IPS= 3, TERMINATED AT: IV=34, JU=11 TIME= 2.493E-01 NPOINT= 506
 ISL= 5, IPS= 4, TERMINATED AT: IV=34, JU=10 TIME= 2.472E-01 NPOINT= 553
 ISL= 5, IPS= 5, TERMINATED AT: IV=34, JU= 9 TIME= 2.387E-01 NPOINT= 538
 ISL= 6, IPS= 1, TERMINATED AT: IV=34, JU=20 TIME= 2.920E-01 NPOINT= 508
 ISL= 6, IPS= 2, TERMINATED AT: IV=34, JU=16 TIME= 2.684E-01 NPOINT= 427
 ISL= 6, IPS= 3, TERMINATED AT: IV=34, JU=13 TIME= 2.591E-01 NPOINT= 404
 ISL= 6, IPS= 4, TERMINATED AT: IV=34, JU=12 TIME= 2.519E-01 NPOINT= 525
 ISL= 6, IPS= 5, TERMINATED AT: IV=34, JU=10 TIME= 2.441E-01 NPOINT= 543
 ISL= 7, IPS= 1, TERMINATED AT: IV=34, JU=22 TIME= 3.353E-01 NPOINT= 405
 ISL= 7, IPS= 2, TERMINATED AT: IV=34, JU=18 TIME= 2.743E-01 NPOINT= 404
 ISL= 7, IPS= 3, TERMINATED AT: IV=34, JU=16 TIME= 2.676E-01 NPOINT= 412
 ISL= 7, IPS= 4, TERMINATED AT: IV=34, JU=14 TIME= 2.528E-01 NPOINT= 496
 ISL= 7, IPS= 5, TERMINATED AT: IV=34, JU=12 TIME= 2.464E-01 NPOINT= 533
 TRAJECTORY ISL= 8, IPS= 1 RECIRCULATES
 ISL= 8, IPS= 1, TERMINATED AT: IV=34, JU=25 TIME= 3.351E-01 NPOINT= 477
 ISL= 8, IPS= 2, TERMINATED AT: IV=34, JU=20 TIME= 2.903E-01 NPOINT= 407
 ISL= 8, IPS= 3, TERMINATED AT: IV=34, JU=18 TIME= 2.797E-01 NPOINT= 434
 ISL= 8, IPS= 4, TERMINATED AT: IV=34, JU=16 TIME= 2.641E-01 NPOINT= 414
 ISL= 8, IPS= 5, TERMINATED AT: IV=34, JU=14 TIME= 2.566E-01 NPOINT= 516
 TRAJECTORY ISL= 9, IPS= 1 RECIRCULATES
 ISL= 9, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 3.183E-01 NPOINT= 403
 ISL= 9, IPS= 2, TERMINATED AT: IV=34, JU=21 TIME= 3.141E-01 NPOINT= 354
 ISL= 9, IPS= 3, TERMINATED AT: IV=34, JU=19 TIME= 2.365E-01 NPOINT= 422
 ISL= 9, IPS= 4, TERMINATED AT: IV=34, JU=18 TIME= 2.761E-01 NPOINT= 505
 ISL= 9, IPS= 5, TERMINATED AT: IV=34, JU=16 TIME= 2.596E-01 NPOINT= 495
 TRAJECTORY ISL=10, IPS= 1 RECIRCULATES
 ISL=10, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 4.041E-01 NPOINT= 668
 TRAJECTORY ISL=10, IPS= 2 RECIRCULATES
 ISL=10, IPS= 2, TERMINATED AT: IV=34, JU=24 TIME= 3.578E-01 NPOINT= 514
 ISL=10, IPS= 3, TERMINATED AT: IV=34, JU=21 TIME= 3.52E-01 NPOINT= 392
 ISL=10, IPS= 4, TERMINATED AT: IV=34, JU=19 TIME= 2.901E-01 NPOINT= 477
 ISL=10, IPS= 5, TERMINATED AT: IV=34, JU=18 TIME= 2.665E-01 NPOINT= 429

SUM OF SOLID PHASE COUPLING

SSPE = 3.431E-04
 SSPF = 0.000E+00
 SSPM = 3.431E-04
 SSPU = 6.491E-03
 SSPV = -2.957E-06
 SSPH = 0.000E+00

AT X = 1.49 , COAL BURNOUT = 0.8167

>>>>EOLP COMPLETE, END OF PARTICLE ITERATION # 10

74

NITER	SORCE	RESORU RESORP	RESORV RESORH	RESORW RESORF	RESOFM RESOET	NCRSE
1	1.189E-01	2.304E-02	7.906E-03	2.405E-03	1.331E-02	
		0.000E+00	8.312E-03	1.718E-02	1.189E-01	0
0.1189421						
5	3.147E-02	2.881E-02	2.626E-02	7.158E-03	3.559E-03	
		0.000E+00	8.801E-03	2.189E-02	3.147E-02	0
10	2.264E-02	1.389E-02	1.327E-02	7.583E-03	5.164E-03	
		0.000E+00	7.655E-03	1.951E-02	2.264E-02	0
15	1.806E-02	1.072E-02	7.212E-03	7.059E-03	2.920E-03	
		0.000E+00	6.206E-03	1.526E-02	1.806E-02	0
20	1.491E-02	1.067E-02	5.275E-03	5.755E-03	2.420E-03	
		0.000E+00	4.721E-03	1.180E-02	1.491E-02	0
25	1.320E-02	7.024E-03	3.172E-03	4.400E-03	1.654E-03	
		0.000E+00	3.807E-03	1.012E-02	1.320E-02	0
30	1.192E-02	5.285E-03	2.066E-03	3.591E-03	1.085E-03	

35	1.084E-02	0.000E+00 3.280E-03 9.295E-03 1.192E-02	0
		4.108E-03 1.588E-03 3.064E-03 6.976E-04	
		0.000E+00 2.949E-03 8.456E-03 1.084E-02	0
40	1.003E-02	3.506E-03 1.396E-03 2.747E-03 5.943E-04	
		0.000E+00 2.654E-03 7.615E-03 1.003E-02	0

ITER	SOURCE	RESNLS
SCATTER ITER: 0	ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX: 1.000E+00
SCATTER ITER: 0	ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX: 5.156E-01
SCATTER ITER: 0	ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX: 1.583E-01
SCATTER ITER: 0	ITERATION: 4	FRAC CHANGE IN TOT NET WALL FLUX: 6.637E-02
SCATTER ITER: 0	ITERATION: 5	FRAC CHANGE IN TOT NET WALL FLUX: 2.160E-02
SCATTER ITER: 0	ITERATION: 6	FRAC CHANGE IN TOT NET WALL FLUX: 8.184E-03
SCATTER ITER: 1	ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX: 2.899E-02
SCATTER ITER: 1	ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX: 1.282E-02
SCATTER ITER: 1	ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX: 2.199E-03
SCATTER ITER: 0	ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX: 1.000E+00
SCATTER ITER: 0	ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX: 5.156E-01
SCATTER ITER: 0	ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX: 1.583E-01
SCATTER ITER: 0	ITERATION: 4	FRAC CHANGE IN TOT NET WALL FLUX: 6.637E-02
SCATTER ITER: 0	ITERATION: 5	FRAC CHANGE IN TOT NET WALL FLUX: 2.160E-02
SCATTER ITER: 0	ITERATION: 6	FRAC CHANGE IN TOT NET WALL FLUX: 8.184E-03
SCATTER ITER: 1	ITERATION: 1	FRAC CHANGE IN TOT NET WALL FLUX: 2.899E-02
SCATTER ITER: 1	ITERATION: 2	FRAC CHANGE IN TOT NET WALL FLUX: 1.282E-02
SCATTER ITER: 1	ITERATION: 3	FRAC CHANGE IN TOT NET WALL FLUX: 2.199E-03

IF IT HITS THE WALLS IT STICKS

ISL= 1, IPS= 1, TERMINATED AT: IV=34, JU= 2 TIME= 2.450E-01 NPOINT= 531
ISL= 1, IPS= 2, TERMINATED AT: IV=34, JU= 2 TIME= 2.420E-01 NPOINT= 414
ISL= 1, IPS= 3, TERMINATED AT: IV=34, JU= 2 TIME= 2.408E-01 NPOINT= 504
ISL= 1, IPS= 4, TERMINATED AT: IV=34, JU= 2 TIME= 2.397E-01 NPOINT= 528
ISL= 1, IPS= 5, TERMINATED AT: IV=34, JU= 2 TIME= 2.322E-01 NPOINT= 493
ISL= 2, IPS= 1, TERMINATED AT: IV=34, JU= 7 TIME= 2.483E-01 NPOINT= 566
ISL= 2, IPS= 2, TERMINATED AT: IV=34, JU= 5 TIME= 2.433E-01 NPOINT= 365
ISL= 2, IPS= 3, TERMINATED AT: IV=34, JU= 5 TIME= 2.389E-01 NPOINT= 483
ISL= 2, IPS= 4, TERMINATED AT: IV=34, JU= 4 TIME= 2.404E-01 NPOINT= 525
ISL= 2, IPS= 5, TERMINATED AT: IV=34, JU= 4 TIME= 2.351E-01 NPOINT= 515
ISL= 3, IPS= 1, TERMINATED AT: IV=34, JU=10 TIME= 2.537E-01 NPOINT= 457
ISL= 3, IPS= 2, TERMINATED AT: IV=34, JU= 8 TIME= 2.459E-01 NPOINT= 439
ISL= 3, IPS= 3, TERMINATED AT: IV=34, JU= 7 TIME= 2.407E-01 NPOINT= 499
ISL= 3, IPS= 4, TERMINATED AT: IV=34, JU= 6 TIME= 2.397E-01 NPOINT= 523
ISL= 3, IPS= 5, TERMINATED AT: IV=34, JU= 5 TIME= 2.312E-01 NPOINT= 524
ISL= 4, IPS= 1, TERMINATED AT: IV=34, JU=14 TIME= 2.626E-01 NPOINT= 473
ISL= 4, IPS= 2, TERMINATED AT: IV=34, JU=11 TIME= 2.491E-01 NPOINT= 458
ISL= 4, IPS= 3, TERMINATED AT: IV=34, JU= 9 TIME= 2.495E-01 NPOINT= 513
ISL= 4, IPS= 4, TERMINATED AT: IV=34, JU= 8 TIME= 2.404E-01 NPOINT= 533
ISL= 4, IPS= 5, TERMINATED AT: IV=34, JU= 7 TIME= 2.341E-01 NPOINT= 559
ISL= 5, IPS= 1, TERMINATED AT: IV=34, JU=17 TIME= 2.712E-01 NPOINT= 442
ISL= 5, IPS= 2, TERMINATED AT: IV=34, JU=13 TIME= 2.548E-01 NPOINT= 429
ISL= 5, IPS= 3, TERMINATED AT: IV=34, JU=11 TIME= 2.514E-01 NPOINT= 443
ISL= 5, IPS= 4, TERMINATED AT: IV=34, JU=10 TIME= 2.486E-01 NPOINT= 495
ISL= 5, IPS= 5, TERMINATED AT: IV=34, JU= 9 TIME= 2.358E-01 NPOINT= 539
ISL= 6, IPS= 1, TERMINATED AT: IV=34, JU=20 TIME= 2.891E-01 NPOINT= 393
ISL= 6, IPS= 2, TERMINATED AT: IV=34, JU=16 TIME= 2.665E-01 NPOINT= 377
ISL= 6, IPS= 3, TERMINATED AT: IV=34, JU=14 TIME= 2.593E-01 NPOINT= 446
ISL= 6, IPS= 4, TERMINATED AT: IV=34, JU=12 TIME= 2.523E-01 NPOINT= 506
ISL= 6, IPS= 5, TERMINATED AT: IV=34, JU=11 TIME= 2.439E-01 NPOINT= 551
ISL= 7, IPS= 1, TERMINATED AT: IV=34, JU=22 TIME= 3.398E-01 NPOINT= 411
ISL= 7, IPS= 2, TERMINATED AT: IV=34, JU=18 TIME= 2.756E-01 NPOINT= 356
ISL= 7, IPS= 3, TERMINATED AT: IV=34, JU=16 TIME= 2.633E-01 NPOINT= 411
ISL= 7, IPS= 4, TERMINATED AT: IV=34, JU=14 TIME= 2.519E-01 NPOINT= 507
ISL= 7, IPS= 5, TERMINATED AT: IV=34, JU=12 TIME= 2.480E-01 NPOINT= 537
TRAJECTORY ISL= 8, IPS= 1 RECIRCULATES
ISL= 8, IPS= 1, TERMINATED AT: IV=34, JU=26 TIME= 3.335E-01 NPOINT= 438
ISL= 8, IPS= 2, TERMINATED AT: IV=34, JU=19 TIME= 2.899E-01 NPOINT= 434

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ISL= 8, IPS= 3, TERMINATED AT: IV=34, JU=18 TIME= 2.770E-01 NPOINT= 443
ISL= 8, IPS= 4, TERMINATED AT: IV=34, JU=16 TIME= 2.621E-01 NPOINT= 461
ISL= 8, IPS= 5, TERMINATED AT: IV=34, JU=14 TIME= 2.504E-01 NPOINT= 503
TRAJECTORY ISL= 9, IPS= 1 RECIRCULATES
ISL= 9, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 3.540E-01 NPOINT= 537
ISL= 9, IPS= 2, TERMINATED AT: IV=34, JU=21 TIME= 3.153E-01 NPOINT= 401
ISL= 9, IPS= 3, TERMINATED AT: IV=34, JU=19 TIME= 2.865E-01 NPOINT= 385
ISL= 9, IPS= 4, TERMINATED AT: IV=34, JU=18 TIME= 2.745E-01 NPOINT= 416
ISL= 9, IPS= 5, TERMINATED AT: IV=34, JU=16 TIME= 2.609E-01 NPOINT= 509
TRAJECTORY ISL=10, IPS= 1 RECIRCULATES
ISL=10, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 4.051E-01 NPOINT= 669
TRAJECTORY ISL=10, IPS= 2 RECIRCULATES
ISL=10, IPS= 2, TERMINATED AT: IV=34, JU=24 TIME= 3.573E-01 NPOINT= 460
ISL=10, IPS= 3, TERMINATED AT: IV=34, JU=21 TIME= 3.134E-01 NPOINT= 406
ISL=10, IPS= 4, TERMINATED AT: IV=34, JU=19 TIME= 2.886E-01 NPOINT= 418
ISL=10, IPS= 5, TERMINATED AT: IV=34, JU=18 TIME= 2.671E-01 NPOINT= 472

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SUM OF SOLID PHASE COUPLING

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SSPE = 3.432E-04
SSPF = 0.000E+00
SSPM = 3.432E-04
SSPI = 6.491E-03
SSPV = -3.013E-06
SSPH = 0.000E+00

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AT X = 1.49 , COAL BURNOUT = 0.8169

>>>>FOLD COMPLETE, END OF PARTICLE ITERATION # 11

41

ITER	SORCE	RESORU RESORP	RESORV RESORH	RESORW RESORF	RESOR+4 RESORFT	NCREER
1	9.191E-02	1.564E-02	6.134E-03	2.629E-03	1.102E-02	0
CONVERGED BY SORMIN CRITERION						
5	1.976E-02	1.126E-02	7.577E-03	3.128E-03	3.739E-03	0
10	1.334E-02	5.969E-03	4.269E-03	3.464E-03	1.967E-03	0
15	1.042E-02	5.377E-03	2.376E-03	3.531E-03	1.237E-03	0

NIITER	SORCE	RESNJ'S
SCATTER ITER: 0	ITERATION: 1	FFAC CHANGE IN TOT NET WALL FLUX: 1.000E+00
SCATTER ITER: 0	ITERATION: 2	FFAC CHANGE IN TOT NET WALL FLUX: 5.158E-01
SCATTER ITER: 0	ITERATION: 3	FFAC CHANGE IN TOT NET WALL FLUX: 1.583E-01
SCATTER ITER: 0	ITERATION: 4	FFAC CHANGE IN TOT NET WALL FLUX: 6.636E-02
SCATTER ITER: 0	ITERATION: 5	FFAC CHANGE IN TOT NET WALL FLUX: 2.160E-02
SCATTER ITER: 0	ITERATION: 6	FFAC CHANGE IN TOT NET WALL FLUX: 8.183E-03
SCATTER ITER: 1	ITERATION: 1	FFAC CHANGE IN TOT NET WALL FLUX: 2.900E-02
SCATTER ITER: 1	ITERATION: 2	FFAC CHANGE IN TOT NET WALL FLUX: 1.282E-02
SCATTER ITER: 1	ITERATION: 3	FFAC CHANGE IN TOT NET WALL FLUX: 2.200E-03
SCATTER ITER: 0	ITERATION: 1	FFAC CHANGE IN TOT NET WALL FLUX: 1.000E+00
SCATTER ITER: 0	ITERATION: 2	FFAC CHANGE IN TOT NET WALL FLUX: 5.158E-01
SCATTER ITER: 0	ITERATION: 3	FFAC CHANGE IN TOT NET WALL FLUX: 1.583E-01
SCATTER ITER: 0	ITERATION: 4	FFAC CHANGE IN TOT NET WALL FLUX: 6.636E-02
SCATTER ITER: 0	ITERATION: 5	FFAC CHANGE IN TOT NET WALL FLUX: 2.160E-02
SCATTER ITER: 0	ITERATION: 6	FFAC CHANGE IN TOT NET WALL FLUX: 8.183E-03
SCATTER ITER: 1	ITERATION: 1	FFAC CHANGE IN TOT NET WALL FLUX: 2.900E-02
SCATTER ITER: 1	ITERATION: 2	FFAC CHANGE IN TOT NET WALL FLUX: 1.282E-02
SCATTER ITER: 1	ITERATION: 3	FFAC CHANGE IN TOT NET WALL FLUX: 2.200E-03

IF IT HITS THE WALLS IT STICKS

ISL= 1, IPS= 1, TERMINATED AT: IV=34, JU= 2 TIME= 2.450E-01 NPOINT= 561
 ISL= 1, IPS= 2, TERMINATED AT: IV=34, JU= 2 TIME= 2.409E-01 NPOINT= 433
 ISL= 1, IPS= 3, TERMINATED AT: IV=34, JU= 2 TIME= 2.384E-01 NPOINT= 509
 ISL= 1, IPS= 4, TERMINATED AT: IV=34, JU= 2 TIME= 2.404E-01 NPOINT= 559
 ISL= 1, IPS= 5, TERMINATED AT: IV=34, JU= 2 TIME= 2.297E-01 NPOINT= 483
 ISL= 2, IPS= 1, TERMINATED AT: IV=34, JU= 7 TIME= 2.472E-01 NPOINT= 541
 ISL= 2, IPS= 2, TERMINATED AT: IV=34, JU= 5 TIME= 2.422E-01 NPOINT= 383
 ISL= 2, IPS= 3, TERMINATED AT: IV=34, JU= 5 TIME= 2.443E-01 NPOINT= 507
 ISL= 2, IPS= 4, TERMINATED AT: IV=34, JU= 4 TIME= 2.383E-01 NPOINT= 519
 ISL= 2, IPS= 5, TERMINATED AT: IV=34, JU= 4 TIME= 2.352E-01 NPOINT= 509
 ISL= 3, IPS= 1, TERMINATED AT: IV=34, JU=10 TIME= 2.535E-01 NPOINT= 459
 ISL= 3, IPS= 2, TERMINATED AT: IV=34, JU= 8 TIME= 2.494E-01 NPOINT= 395
 ISL= 3, IPS= 3, TERMINATED AT: IV=34, JU= 7 TIME= 2.467E-01 NPOINT= 505
 ISL= 3, IPS= 4, TERMINATED AT: IV=34, JU= 6 TIME= 2.398E-01 NPOINT= 568
 ISL= 3, IPS= 5, TERMINATED AT: IV=34, JU= 6 TIME= 2.319E-01 NPOINT= 519
 ISL= 4, IPS= 1, TERMINATED AT: IV=34, JU=14 TIME= 2.615E-01 NPOINT= 427
 ISL= 4, IPS= 2, TERMINATED AT: IV=34, JU=11 TIME= 2.498E-01 NPOINT= 446
 ISL= 4, IPS= 3, TERMINATED AT: IV=34, JU= 9 TIME= 2.491E-01 NPOINT= 506
 ISL= 4, IPS= 4, TERMINATED AT: IV=34, JU= 8 TIME= 2.445E-01 NPOINT= 522
 ISL= 4, IPS= 5, TERMINATED AT: IV=34, JU= 7 TIME= 2.383E-01 NPOINT= 565
 ISL= 5, IPS= 1, TERMINATED AT: IV=34, JU=17 TIME= 2.712E-01 NPOINT= 448
 ISL= 5, IPS= 2, TERMINATED AT: IV=34, JU=13 TIME= 2.553E-01 NPOINT= 469
 ISL= 5, IPS= 3, TERMINATED AT: IV=34, JU=11 TIME= 2.488E-01 NPOINT= 464
 ISL= 5, IPS= 4, TERMINATED AT: IV=34, JU=10 TIME= 2.474E-01 NPOINT= 505
 ISL= 5, IPS= 5, TERMINATED AT: IV=34, JU= 9 TIME= 2.404E-01 NPOINT= 546
 ISL= 6, IPS= 1, TERMINATED AT: IV=34, JU=20 TIME= 2.893E-01 NPOINT= 406
 ISL= 6, IPS= 2, TERMINATED AT: IV=34, JU=16 TIME= 2.641E-01 NPOINT= 358
 ISL= 6, IPS= 3, TERMINATED AT: IV=34, JU=14 TIME= 2.545E-01 NPOINT= 440
 ISL= 6, IPS= 4, TERMINATED AT: IV=34, JU=12 TIME= 2.527E-01 NPOINT= 497
 ISL= 6, IPS= 5, TERMINATED AT: IV=34, JU=11 TIME= 2.438E-01 NPOINT= 555
 ISL= 7, IPS= 1, TERMINATED AT: IV=34, JU=22 TIME= 3.441E-01 NPOINT= 479
 ISL= 7, IPS= 2, TERMINATED AT: IV=34, JU=18 TIME= 2.754E-01 NPOINT= 355
 ISL= 7, IPS= 3, TERMINATED AT: IV=34, JU=16 TIME= 2.654E-01 NPOINT= 397
 ISL= 7, IPS= 4, TERMINATED AT: IV=34, JU=14 TIME= 2.520E-01 NPOINT= 496
 ISL= 7, IPS= 5, TERMINATED AT: IV=34, JU=12 TIME= 2.453E-01 NPOINT= 533
 TRAJECTORY ISL= 8, IPS= 1 RECIRCULATES
 ISL= 8, IPS= 1, TERMINATED AT: IV=34, JU=25 TIME= 3.320E-01 NPOINT= 506
 ISL= 8, IPS= 2, TERMINATED AT: IV=34, JU=20 TIME= 2.944E-01 NPOINT= 400
 ISL= 8, IPS= 3, TERMINATED AT: IV=34, JU=18 TIME= 2.735E-01 NPOINT= 447
 ISL= 8, IPS= 4, TERMINATED AT: IV=34, JU=16 TIME= 2.621E-01 NPOINT= 471
 ISL= 8, IPS= 5, TERMINATED AT: IV=34, JU=14 TIME= 2.541E-01 NPOINT= 500
 TRAJECTORY ISL= 9, IPS= 1 RECIRCULATES
 ISL= 9, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 3.501E-01 NPOINT= 529
 ISL= 9, IPS= 2, TERMINATED AT: IV=34, JU=21 TIME= 3.152E-01 NPOINT= 353
 ISL= 9, IPS= 3, TERMINATED AT: IV=34, JU=19 TIME= 2.855E-01 NPOINT= 442
 ISL= 9, IPS= 4, TERMINATED AT: IV=34, JU=18 TIME= 2.716E-01 NPOINT= 403
 ISL= 9, IPS= 5, TERMINATED AT: IV=34, JU=16 TIME= 2.576E-01 NPOINT= 480
 TRAJECTORY ISL=10, IPS= 1 RECIRCULATES
 ISL=10, IPS= 1, TERMINATED AT: IV=34, JU=28 TIME= 4.051E-01 NPOINT= 679
 TRAJECTORY ISL=10, IPS= 2 RECIRCULATES
 ISL=10, IPS= 2, TERMINATED AT: IV=34, JU=24 TIME= 3.556E-01 NPOINT= 526
 ISL=10, IPS= 3, TERMINATED AT: IV=34, JU=21 TIME= 3.149E-01 NPOINT= 398
 ISL=10, IPS= 4, TERMINATED AT: IV=34, JU=19 TIME= 2.890E-01 NPOINT= 420
 ISL=10, IPS= 5, TERMINATED AT: IV=34, JU=18 TIME= 2.673E-01 NPOINT= 484

SUM OF SOLID PHASE COUPLING

SSPE = 3.433E-04
 SSPE = 0.000E+00
 SSPM = 3.433E-04
 SSPU = 6.491E-03
 SSPV = 3.039E-06
 SSPH = 0.000E+00

AT X = 1.49 , COAL BURNOUT = 0.8170

>>>EQLP COMPLETE, END OF PARTICLE ITERATION # 12

CONVERGED BY MINITP CRITERION

17

NOX POLLUTANT CALCULATIONS CALLED FOLLOWING CONVERGENCE OF PGCC2

NITNOX	MAXSOR	RESNOX	RESNOX	NCREE
2	2.685E-02	2.685E-02	1.220E-02	0
4	4.453E-03	1.453E-03	2.045E-03	0
6	8.484E-04	3.484E-04	3.445E-04	0
8	1.492E-04	1.492E-04	5.764E-05	0

AT X = 1.48803 NOXAVG = 347.05 PPM HCN AVG = 0.08 PPM

FRACTION OF NODE ITERATIONS WITH INSTANTANEOUS OXYGEN CONCENTRATIONS
BETWEEN 2500 AND 18000 PPM = 0.6828

THIS IS A CONVERGED CASE

TOTAL CPU TIME: 34 hours, 47 minutes, 14.961 seconds!

TTOT= 125234.96
TPROPS= 93105.91
TEQLP= 11027.65
TTABLE= 218.52
TGRID = 1.12
TPRINT= 56.46
TCLCUP= 6701.42
TCALC= 10745.35
TRST= 164.38
TPIOTS= 5.86

FORTTRAN STOP

BREWSTER job terminated at 28-SEP-1987 00:36:30.53

Accounting information:

Buffered I/O count:	1652	Peak working set size:	2000
Direct I/O count:	6759	Peak page file size:	5117
Page faults:	7852	Mounted volumes:	0
Charged CPU time:	1 10:47:49.69	Elapsed time:	1 13:43:03.70

APPENDIX H
HIGH-PRESSURE COAL GASIFICATION CASE


```

7,      !NSAY..(SAY(1),I=1,NSAY) follows:
PGCG-2 %%%% BRIGHAM YOUNG UNIVERSITY GASIFIER %%%% HOT FLOW
>>>>>>> PE-MIXED CASE <<<<<<<<
>>>>>>> FOR UTA-I COAL AT 60 PSIA <<<<<<<<
NOX CALCULATIONS INCLUDED
Comment: Experimental work was performed by
        Azuhata and Nichols
*****
T      T      T      F      T      !INRST, INCALF, INCREF, INCALH, INCALG
T      T      F      F      T      !IPSTCT, INPRST, INEACH, INCLFF, INCLGE
T      F      F      F      T      !INCALN, INCORF, LEOLP, INFERZ, INISMP
F      F      T      F      F      !INCNOX, POLIUT, INCRIL, INCSWP, INCSWS
F      F      F      T      F      !INNOZ, INFSOU, LTHIG, GIBOUT, IMPROG
T      T      F      F      F      !INCFP, INRAD, INRCD, INTRUS, MAGIJER
0.500, 0.500, 0.500, 0.900,      !URFU, URFV, URFW, URFH
0.700, 0.700, 0.700, 0.700, 0.700, !URFE, URFK, URFI, URFJ, URFYIS
0.500, 0.800, 0.800, 1.000, 1.000, 1.000, !URFDEN, URFETA, URFGE, URFNJ, URFPP, URF
1.31000E-02, 2.87000E-02, 0.20000, !DIAP, DIAS, DIACH
8.6500, 3.17500E-03,      !NDIA(real), THICK
1000, 1000, 50,      !MAXIT, INDPRI, INIRST
4, 5, 32,      !NJINP, NJINS, NIWOQ
2.200, 1.200, 40, 1.088, 0.916,      !ALI, EPSX, NI, EPSI, EPSD
100.0, 200.0, 0.00000, !IRMIN, IIRMAX, ILOSS
8, 36.300, 5.92000E-02, !INIIO, OHA, QLX
1000.00, 1100.00, 1000.00, !THN, TBW, TBE
1.79000E-05, 4.13685E-05, !VISCOS, PRES
0.01000000, 0.10000000, !SORMAX, SORMIN
NLET 1      ! (Primary)
1.0753E-02, 1.000, 0.000, 0.100, !FLOW, PFLOW, SWIRLN, TINFLO
NLET 2      ! (Secondary)
4.1700E-03, 0.000, 0.000, 0.100, !FLOW, PFLOW, SWIRLN, TINFLO
!      (Blank line)
LEMENTS
HERMO
EACTANTS 1
367.000      !TMP (unformatted)
2. 0. 0. 0. 0. 02 0.78017 G
R1. 0. 0. 0. 0. AR 0.16663 G
2. 0 1. 0. 0. 0. H2O 0.05321 G
!      (Blank line)
EACTANTS 2
367.000      !TMP (unformatted)
2. 0. 0. 0. 0. N2 1.00000 G
!      (Blank line)
10, 5,      !NSL, NPS
0.83804, 1340.000,      !PLOADP, PDEN
0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,      !YPS(ISL), ISL = 1,5
0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,      !YPS(ISL), ISL = 6, NSL
1.0000, 1.0000, 1.0000, 1.0000, 1.0000, 1.0000,      !UPLAG(IPS), IPS = 1, NPS
0.000, 0.000, 0.000, 0.000, 0.000, 0.000,      !SPRANG(ISL), ISL = 1,5
0.000, 0.000, 0.000, 0.000, 0.000, 0.000,      !SPRANG(ISL), ISL = 6, NSL
0.9500, 0.9500, 0.9500, 0.9500, 0.9500, 0.9500,      !TLAG(IPS), IPS = 1, NPS
1.076E-05, 1.842E-05, 2.614E-05,      !PD(IPS), IPS = 1,3
3.721E-05, 6.937E-05,      !PD(IPS), IPS = 4, NPS
0.2000, 0.2000, 0.2000, 0.2000, 0.2000, 0.2000,      !PMF(IPS), IPS = 1, NPS
F      F      T      F      F      !LDEBUG, LYPS, LPARTP, LPARTS, LPIOTH
T      T      T      F      !LSPM, LSPU, LSPV, LSPH
0.9900, 0.0100,      !YPSH, YPSL
15, 25, 3,      !MAXITP, MINITP, IGASV
0.350, 0.350, 0.350, 0.350, 0.350,      !PRK(IPS), IPS = 1, NPS
1      !NCARD...COMMENT(1), I=1, NCARD) follows:
All Particles Have the same Properties
T      !INCOAL,
2 3 5 1 2 0      !NCRXN, NIIRXN, NPROP, IEUCK, KE2, ESHRNK

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1.000E-02, 1.000E-03, 0.100, 0.300 !DELTPJ,DELRRJ,GAMMA,URFPM
1.000C !X1(J)
1.5040CE+06, 0.00000E+00, -1.41600E+07, !HCO(J),HHO(J),HAO(J)
1.5880CE+07, 373.15, !HWO(J),TNBP
0.8389E, 0.00000E+00, 0.16101, !OMEGAC(J),OMEGAH(J),OMEGAA(J)
0.0000CE+00, !OMEGAW(J)
3.7000CE+05, -7.36380E+07, 0.38500, !AMJ(J,M),EMJ(J,M),YY(J,M)
0.0000CE+00, !HGV(J,M)
1.4600CE+13, 2.51040E+08, 0.80000, !AMJ(J,M),EMJ(J,M),YY(J,M)
0.0000CE+00, !HGV(J,M)
1.0257, 7.48500E+07, 1.0000, !AL(J,L).EL(J,L),EMM(J,L)
0.0000CE+00, !HGH(J,L)
1158.4, 2.58700E+07, 1.0000, !AL(J,L).EL(J,L),EMM(J,L)
-0.0000CE+00, !HGH(J,L)
207.56, 2.40000E+08, 1.0000, !AL(J,L).EL(J,L),EMM(J,L)
0.0000CE+00, !HGH(J,L)
1225.2, 0.00000E+00, 0.00000E+00, !CCP(J,N11,COMPONENT)
1225.2, 0.00000E+00, 0.00000E+00, !CCP(J,N11,COMPONENT)
1225.2, 0.00000E+00, 0.00000E+00, !CCP(J,N11,COMPONENT)
1.00000E-05, 0.79700, 6.25300E-02, ! (WIC(J,X) K = 1,3)
0.11766, 1.69500E-02, 5.84700E-03, ! (WIC(J,X) K = 4,NLM)
H2O !SLRCMP
O2 CO2 H2O !OXYD(L),L = 1,NHRRN
2.00, 1.00, 1.00, !PHIL(L) L = 1,NHRRN
T T F 10 !LDISO,LGASE,LEMCOR,MAXITR
0.9300,0.8600,0.8200,0.8200,0.8200, ! (QAB(IPS),IPS = 1,NPS)
1.3600,1.3400,1.3300,1.3200,1.3000, ! (QSC(IPS),IPS = 1,NPS)
0.8000,1500.00 !EMW,TOUT
1.0000,0.0000 !AO,AF
4, !NSAYNX..(SAYNX(I),I=1,NSAYNX) follows:
***** PCNOX *****
**** NOX POLLUTANT CALCULATION USING OUTPUT FROM PCGC-2 FOR THE ****
**** PHASE AND PARTICLE PROPERTIES THROUGHOUT THE FLOW FIELD ****
*****
1.00000E+11, 3.00000E+12, 4.12510E-04, !A1,A2,A3
2.80500E+08, 2.51200E+08, 1.45240E+08, !EACT1,EACT2,EACT3
0.900,0.900, 0.050,0.800, 0.000,0.000, !PRNOX,PRHCN,FCTNO,FCTHCN,YHCNPR,YHCNS
50, 2, 50, !MXITNX,ITYNX,INDPNX
1.0000, 1.0000, 1.00000E-05, !XIANOX,ZEDA,MAXRES
F T T !IRSTNX,IPLTNX,INITNX

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F	1	F	1	!UPDAT,KOPUP,USDAT,KOFUS,...
F	1	F	1	!VPPDAT,KOPVP,VSDAT,KOFVS,...
F	4	F	4	!WPPDAT,KOPWP,WSDAT,KOFWS,...
F	2	F	2	!TIPDAT,KOPTED,TESDAT,KOPTES,...
F	2	F	2	!EDPDAT,KOPEDP,EDEDAT,KOPEDS,...
1.30E-02, 2.30E-02,				!PLS.SLS,ATLS...
1	5.00000E+00			!NSFORM,ALPHA0
1.25500E-02, 1.25500E-02, 6.50000E-02,				!RP,RS1,RS2,

AR 39.94800 0.0
C 12.01115 4.0
H 1.00797 1.0
O 15.9994 -2.0
N 14.0067 0.0
S 32.06 4.0

AR L 5/86AR 1.00 0.00 0.00 0.0 300.000 5000.000
0.25000000E 01 0.0 0.0 0.0 0.0
-0.74537500E 03 0.43660002E 01 0.25000000E 01 0.0 0.0
0.0 0.0 -0.74537476E 03 0.43660002E 01
CO2 J 9/65C 1.0 2.00 0.00 0.0 300.000 5000.000
0.44638040E 01 0.30981717E-02-0.12392566E-05 0.22741323E-09-0.15525948E-13
-0.48951438E 05-0.98635978E 00 0.24007788E 01 0.87350905E-02-0.66070861E-05
0.20021860E-08 0.63274039E-15-0.48377520E 05 0.96951447E 01
H2O J 3/61H 2.0 1.00 0.00 0.0 300.000 5000.000
0.27157616E 01 0.29451370E-02-0.80224368E-06 0.10226681E-09-0.48472104E-14
-0.29905820E 05 0.66305666E 01 0.40701275E 01-0.11084499E-02 0.41521180E-05
-0.29637404E-08 0.80702101E-12-0.30279719E 05-0.32270038E 00
N2 J 9/65N 2.0 0.0 0.0 0.0 300.000 5000.000
0.28963194E 01 0.15154863E-02-0.57235275E-06 0.99807385E-10-0.65223536E-14
-0.90586182E 03 0.61615143E 01 0.36748257E 01-0.12081496E-02 0.23240100E-05
-0.63217520E-09-0.22577253E-12-0.10611587E 04 0.23580418E 01
O2 J 9/65O 2.0 0.0 0.0 0.0 300.000 5000.000
0.36219521E 01 0.73618256E-03-0.19652219E-06 0.36201556E-10-0.28945623E-14
0.12019822E 04 0.36150942E 01 0.36255980E 01-0.18782183E 02 0.70554543E-05
-0.67635071E-08 0.21555977E 11-0.10475225E 04 0.43052769E 01
CO J 9/65C 1.0 1.00 0.00 0.0 300.000 5000.000
0.29840689E 01 0.14891387E-02-0.57899678E-06 0.10364576E-09-0.69353499E-14
0.14245227E 05 0.63479147E 01 0.37100916E 01-0.16190964E-02 0.36923584E-05
0.20319673E 08 0.23953344E 12-0.14356309E 05 0.29555340E 01
H2 J 3/61H 2.0 0.0 0.0 0.0 300.000 5000.000
0.31001883E 01 0.51119458E-03 0.52644204E-07-0.34909964E-10 0.36945341E-14
-0.87738013E 03-0.19629412E 01 0.30574446E 01 0.26765198E-02-0.58099149E-05
0.55210343E-08-0.18122726E-11-0.98890430E 03-0.22997046E 01
CH4 J 3/61C 1.0 4.00 0.00 0.0 300.000 5000.000
0.15027056E 01 0.10416795E-01-0.39181514E-05 0.67777872E-09-0.44283706E-13
-0.99787031E 04 0.10707143E 02 0.38261929E 01-0.39794557E-02 0.24558321E-04
0.22712920E-07 0.69626952E-11-0.10144945E 05 0.86690062E 00
SO2 J 6/61S 1.0 2.00 0.00 0.0 300.000 5000.000
0.52411363E 01 0.19704204E-02-0.80375759E-06 0.15149969E-09-0.10557998E-13
-0.37558227E 05-0.10873518E 01 0.32665329E 01 0.53237863E-02 0.68437544E-06
-0.52809987E-08 0.25590450E-11-0.36908145E 05 0.96513473E 01
SO3 J 9/65S 1.0 3.00 0.00 0.0 300.000 5000.000
0.70757370E 01 0.31763383E-02-0.13535755E-05 0.25630875E-09-0.17936038E-13
0.50211375E 05 0.11200791E 02 0.25780373E 01 0.14556330E-01-0.91764159E-05
-0.79203022E-09 0.19709460E-11-0.48931750E 05 0.12251863E 02
COS J 3/61C 1.0 1.5 1.00 0.0 300.000 5000.000
0.52391987E 01 0.24100584E-02-0.96064377E-06 0.17778347E-09-0.12235703E-13
-0.18480449E 05-0.30910501E 01 0.24625311E 01 0.11947986E-01-0.13794370E-04
0.80707672E-08-0.18327640E-11-0.17803980E 05 0.10792556E 02
H2S J12/65H 2.5 1.00 0.00 0.0 300.000 5000.000
0.28479090E 01 0.38415990E-02-0.14099360E-05 0.24278735E-09-0.15783280E-13
-0.34469788E 04 0.74781399E 01 0.38811293E 01-0.13211856E-03 0.36517713E-05
-0.21820441E-08 0.28783779E-12-0.36350916E 04 0.25161505E 01
SO J12/65S 1.0 1.00 0.00 0.0 300.000 5000.000
0.38280144E 01 0.75593102E-03-0.30791631E-06 0.57880131E-10-0.40204419E-14
0.43632666E 03 0.44528189E 01 0.31224213E 01 0.13797339E-02 0.20611933E-05
0.38700776E 08 0.16366249E-11 0.17847565E 03 0.84176922E 01
C(S) J 3/61C 1.0 0.0 0.0 0.0 300.000 5000.000
0.13604937E 01 0.19182237E-02 0.84040386E-06 0.16448705E-09-0.11672670E-13
0.65713843E 03-0.80070200E 01-0.44778049E 00 0.53690970E-02-0.39775563E-06
-0.40459263E-08 0.21134925E-11-0.94280670E 02 0.16840773E 01

3.418,124.,0.,
 3.996,190.,0.,
 2.641,809.1,1.0,
 3.681,91.5,0.,
 3.433,113.,0.,
 3.59,110.,0.,
 2.915,38.,0.,
 3.758,148.6,0.0
 4.290,252.,.42,
 4.290,200.,.25
 4.130,336.0.,.25
 3.623,301.1,.15
 2.950,150.,.1
 3.822,137.,0.

C2H2 J 3/61C 2.H 2.00 0.00 0.0 300.000 5000.000
 0.45751076E 01 0.51238351E-02-0.17452339E-05 0.28673054E-03-0.17951420E-13
 0.25607426E 05-0.35737925E 01 0.14102755E 01 0.19057274E-01-0.24501380E-04
 0.16390871E-07-0.41345443E-11 0.26188203E 05 0.11393826E 02
 C2H4 J 9/65C 2.H 4.00 0.00 0.0 300.000 5000.000
 0.34552135E 01 0.11491802E-01-0.43651744E-05 0.76155050E-09 0.50123195E 13
 0.44773086E 04 0.26987944E 01 0.14256821E 01 0.11383139E-01 0.79890006E-05
 -0.16253676E-07 0.67491256E-11 0.53370703E 04 0.14621819E 02
 C2H6 CR2178C 2H 60 00 00 300.000 5000.000
 1.67107058E+00 1.88078150E-02-6.98943156E-06 1.16385735E-09-7.17707692E-14
 -1.14663543E+04 1.26317347E+01 0.92453270E+00 1.68224303E-02-2.24906498E-06
 -3.40875417E-09 1.49239675E-12-1.14789269E+04 1.16292438E+01
 H J 9/65H 1 00 0.00 0.00 0.0 300.000 5000.000
 0.25000000E 01 0.0 0.0 0.0 0.0
 0.25471625E 05-0.46011758E 00 0.25000000E 01 0.0 0.0
 0.0 0.0 0.25471625E 05-0.46011758E 00
 CN J 6/69C 1.N 1.0 0.0 0.0 300.000 5000.000
 0.36036282E 01 0.33644354E-03 0.10028930E-06-0.16318141E-10-0.36286701E-15
 0.51159828E 05 0.35454493E 01 0.37386303E 01-0.19239220E-02 0.47635173E-05
 -0.31112999E-08 0.61675318E-12 0.51270926E 05 0.34490204E 01
 CH J12/67C 1.H 1.0 0.0 0.0 300.000 5000.000
 0.22673111E 01 0.22042997E-02-1.62250189E-06 0.69689921E-10-0.21274952E-14
 0.70838000E 05 0.87889338E 01 0.35632744E 01-0.20031372E-03-0.40129811E-06
 0.18226920E-08-0.86768310E-12 0.70405500E 05 0.17628012E 01
 C J 3/61C 1.00 0.00 0.00 0.0 300.000 5000.000
 0.25810652E 01-0.14696202E-03 0.74388026E-07-0.79481066E-11 0.58500964E-16
 0.85216250E 05 0.43128872E 01 0.25328703E 01-0.15887640E-03 0.30682077E-06
 -0.26770053E-09 0.87488827E-13 0.85240375E 05 0.46062365E 01

APPENDIX I
COAL-WATER MIXTURE COMBUSTION CASE

10, INSAY..(SAY(1),I=1,NSAY) follows:
DOE-8 LIGNITE SLURRY COMBUSTION CASE-DAEM devolatilization model.

DATA COLLECTED 4/86 - 6/86

TEST CONDITIONS: LABORATORY NOZZLE

SR = 1.1

A/S = 0.7

SN = 1.5

OPERATORS: DOUG RAWLINS

CRAIG EATOUGH

ROB JONES

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F      T      T      F      T      ! INRST, INCAIF, INCRK, INCALH, INCALG
T      F      F      T      T      ! IPSICT, IMPHST, INRACH, INCIET, INCIJE
T      F      F      F      T      ! INCAIN, INCRF, IEQUIP, INTERZ, INISMP
F      F      T      F      T      ! INCNOX, POLIOP, INCEL, INCSWP, INCSWS
T      T      F      T      F      ! INNOZ, INESOL, ITHIG, GRIOUT, INPROG
T      T      T      T      F      ! INCEP, INEAF, INRIGD, INTRUS, MAGHIER
0.900,0.900,0.900,0.900,0.900,    ! URFU, URFV, URFW, URTU
0.900,0.900,0.900,0.900,0.900,    ! URFE, URFF, URFG, URTG, URFVIS
0.750,0.900,0.900,1.000,1.000,1.000,    ! URFDEN, URFETA, URFGET, URFNJ, URFPP, URFPP
3.20000E-03, 0.14500, 0.35000,    ! DIAP, DIAS, CIACH
8.5714, 4.20500E-02,    ! INDIA( coal ), THICK
1999, 2000, 50,    ! MAXIT, INIPRI, INIRST
1, 5, 29,    ! NJINP, NJINS, NIWOC
3.050, 1.100, 39, 1.120, 0.900,    ! ALI, EPSX, NL, EPSI, EPSD
1200.0, 1200.0, 0.00000E+00,    ! HRMIN, HRMAX, HRLOSS
10, 35.000, 0.13910,    ! INTINO, QHF, CLX
1100.00, 1100.00, 1100.00,    ! TBN, TBW, TBF
5.00000E-05, 85460,    ! VISCOS, PFES
0.00700000, 0.07000000,    ! SCORMAX, SCORMIN
INLET 1    ! (Primary)
4.8680E-03, 0.000, 0.020, 0.200,    ! FLOW, FFLCW, SWIRLN, TINFLO
INLET 2    ! (Secondary)
3.1190E-02, 0.000, 1.520, 0.200,    ! FLOW, FFLCW, SWIRLN, TINFLO
!    (Blank line)

ELEMENTS
THERMO    ! The react. sect. is formatted
REACTANTS 1
295.200    ! TMP (unformatted)
H 2. 0 1. 0. 0. HEQ(L) 1.000C0 L    !
!    (Blank line)

REACTANTS 2
688.400    ! TMP (unformatted)
G 2. 0. 0. 0. 0. O2 0.22750 G
N 2. 0. 0. 0. 0. N2 0.74150 G
AR1. 0. 0. 0. 0. AR 0.02750 G
HE1. 0. 0. 0. 0. HE 0.00250 G
!    (Blank line)

10, 5,    ! NSI, NPS
1.43000,1214.300,1.0,    ! PLOADP, PCEN, UPDOWN
0.0000,0.0000,0.0000,0.0000,0.0000,    ! YPS(1SL), 1SL = 1,5
0.0000,0.0000,0.0000,0.0000,0.0000,    ! YPS(1SL), 1SL = 6,NSI
1.0000,1.0000,0.7000,0.5000,0.3000,    ! UPLAG(IPS), IPS = 1,NPS
0.500, 1.500, 3.000, 4.000, 5.000,    ! SPRANG(1SL), 1SL = 1,5
6.000, 7.000, 9.000,12.000,15.000,    ! SPRANG(1SL), 1SL = 6,NSI
0.4360,0.4360,0.4360,0.4360,0.4360,    ! TLAG(IPS), IPS = 1,NPS
1.700E-05, 2.600E-05, 3.600E-05,    ! PD(IPS), IPS = 1,3
5.100E-05, 1.000E-04,    ! PD(IPS), IPS = 4,NPS
0.2000,0.2000,0.2000,0.2000,0.2000,    ! PMF(IPS), IPS = 1,NPS
F      F      T      F      F      ! LDEBUG, LAPS, LPARTI, LPARTS, LPBOTH
T      T      T      F      F      ! LSPM, LSPU, LSPV, LSPH
0.9500,0.0200,    ! YPSH, YPSI
30, 40, 3,    ! MAXITP, MINITP, IGASV
0.340,0.340,0.340,0.340,0.340,    ! PRK(IPS), IPS = 1,NPS

```

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1
      All Particles have the same Properties
!NCARD...COMENT(1),I=1,NCARD follows:
!INCOAL
!NCRXN,NHRXN,NPROP,IEUCK,KEQ,NSHRNK
!DELTPJ,DELTRJ,GAMMA,UREPM
!X1(J)
2.68205E+06, 0.00000E+00,-1.50400E+07,
!HCO(J),HHO(J),HAO(J)
-1.58800E+07, 373.15,
!HWO(J),TNBP
0.47960, 0.00000E+00, 8.04000E-02,
!OMEGAC(J),OMEGAH(J),OMEGAA(J)
0.44000,
!OMEGAW(J)
1.67000E+13, 2.36000E+08, 0.41000,
!AMJ(J,M),EMJ(J,M),YY(J,M)
0.00000E+00, 0.00000E+00,
!HGV(J,M),SIGDEV(J,M)
1.0051, 8.53540E+07, 1.0000,
!AL(J,L),EL(J,L),EMM(J,L)
0.00000E+00,
!HGH(J,L)
1225.2, 0.00000E+00, 0.00000E+00,
!CCP(J,N11,COMPONENT)
1225.2, 0.00000E+00, 0.00000E+00,
!CCP(J,N11,COMPONENT)
1225.2, 0.00000E+00, 0.00000E+00,
!CCP(J,N11,COMPONENT)
1.00000E-09, 0.75260, 4.73000E-02,
!(WIC(J,K) K = 1,3)
0.00000E+00, 0.17280, 1.47000E-02,
!(WIC(J,K) K = 4,6)
1.26000E-02,
!WIC(J,7)
H2O
!SLRCMP
O2
!OXYD(L),L = 1,NHRXN
2.00,
!PH11(L) L = 1,NHRXN
T T T 10
!LDISO,LGASE,LEMCOR,MAXITR
0.8700,0.8300,0.8200,0.8200,0.8200,
!(QAB(IPS),IPS = 1,NPS)
1.3600,1.3200,1.3000,1.3000,1.3000,
!(QSC(IPS),IPS = 1,NPS)
0.8000, 0.00
!EMW,TOUT
1.0000,0.0000
!A0,AF

```



```

F 2 F 2          !UPDAT,KOPUP,USDAT,KOPUS,...
T 2 F 2          !VPDAT,KOPVP,VSDAT,KOPVS,...
F 2 F 2          !WPDAT,KOPWP,WSDAT,KOPWS,...
F 1 F 1          !TIPDAT,KOPTEP,TISDAT,KOPTES,...
F 1 F 1          !EDPDAT,KOPEDP,EDSDAT,KOPEDS,...
2.0 , 8.5
2 8.00000E+00    !PLS,SLS,A11S...
2.92240E-03, 1.25000E-02, 6.50000E-02, !NSFORM,ALPHA0
0.00000E+00, 0.00000E+00, 0.00000E+00, !RP,RS1,RS2,
0.00000E+00, 30.000 , 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 31.000 , 0.00000E+00, 0.00000E+00, 0.00000E+00, 1.00000E-03,
0.00000E+00, 32.000 , 0.00000E+00, 0.00000E+00, 0.00000E+00, 1.50000E-03,
0.00000E+00, 33.000 , 0.00000E+00, 0.00000E+00, 0.00000E+00, 2.00000E-03,
0.00000E+00, 28.000 , 0.00000E+00, 0.00000E+00, 0.00000E+00, 2.50000E-03,
0.00000E+00, 29.000 , 0.00000E+00, 0.00000E+00, 0.00000E+00, 5.24163E-03,
0.00000E+00, 30.000 , 0.00000E+00, 0.00000E+00, 0.00000E+00, 9.88014E-03,
0.00000E+00, 31.000 , 0.00000E+00, 0.00000E+00, 0.00000E+00, 1.45187E-02,
0.00000E+00, 32.000 , 0.00000E+00, 0.00000E+00, 0.00000E+00, 1.91572E-02,
24.000 , 33.000 , 0.00000E+00, 4.3200 , 0.00000E+00, 1.25000E-02,
36.310 , 0.00000E+00, 21.210 , 7.3700 , 0.00000E+00, 1.50000E-02,
36.980 , 0.00000E+00, 26.380 , 7.1600 , 0.00000E+00, 2.00000E-02,
37.620 , 0.00000E+00, 28.650 , 7.0500 , 0.00000E+00, 2.50000E-02,
37.170 , 0.00000E+00, 29.020 , 7.3000 , 0.00000E+00, 3.00000E-02,
37.430 , 0.00000E+00, 29.480 , 7.0100 , 0.00000E+00, 3.50000E-02,
36.890 , 0.00000E+00, 29.170 , 7.0500 , 0.00000E+00, 4.00000E-02,
36.130 , 0.00000E+00, 27.790 , 6.9000 , 0.00000E+00, 4.50000E-02,
35.750 , 0.00000E+00, 26.230 , 6.8000 , 0.00000E+00, 5.00000E-02,
35.450 , 0.00000E+00, 24.760 , 6.6600 , 0.00000E+00, 5.50000E-02,
34.910 , 0.00000E+00, 21.580 , 6.3300 , 0.00000E+00, 6.00000E-02,
34.010 , 0.00000E+00, 18.270 , 6.1200 , 0.00000E+00, 6.50000E-02,

```

AR 39.9480 0.0
C 12.01115 4.0
H 1.00797 1.0
HE 4.00260 0.0
O 15.9994 -2.0
N 14.0067 0.0
S 32.06 4.0

AR 1.5/66AR 1.00 0.00 0.00 0.0 300.000 5000.000
0.25000000E 01 0.0 0.0 0.0 0.0
0.74537500E 03 0.43660002E 01 0.25000000E 01 0.0 0.0
0.0 0.0 -0.74537476E 03 0.43660002E 01
CH4 J 3/61C 1.0 4.00 0.00 0.0 300.000 5000.000
0.15027056E 01 0.10416795E 01 0.39181514E -05 0.67777872E -09 0.44283706E -13
-0.99787031E 04 0.10707143E 02 0.38261929E 01 -0.39794557E -02 0.24558321E -04
-0.22732920E -07 0.69626952E -11 0.10144945E 05 0.86690062E 00
CO J 9/65C 1.0 1.00 0.00 0.0 300.000 5000.000
0.29840689E 01 0.14891387E -02 -0.57899678E -06 0.10364576E -09 -0.69353499E -14
-0.14245227E 05 0.63479147E 01 0.37100916E 01 -0.16190964E -02 0.36923584E -05
-0.20319673E -08 0.23953344E -12 -0.14356309E 05 0.29555340E 01
CS2 J 9/65C 1.0 2.00 0.00 0.0 300.000 5000.000
0.44608040E 01 0.30981717E -02 -0.12392566E -05 0.22741323E -09 0.15525948E -13
-0.48961438E 05 -0.98635978E 00 0.24007788E 01 0.87350905E -02 -0.66070861E -05
-0.20021860E -08 0.63274039E -15 -0.48377520E 05 0.96951447E 01
COS J 3/61C 1.0 1.5 1.00 0.0 300.000 5000.000
0.52391987E 01 0.24100584E -02 -0.96064377E -06 0.17778347E -09 0.12235703E -13
0.18480449E 05 0.30910501E 01 0.24625311E 01 0.11947986E 01 0.13794370E 04
0.80707672E -08 -0.18327640E -11 -0.17803980E 05 0.10792556E 02
CS2 J 6/61C 1.5 2.0 0.0 0.0 300.000 5000.000
0.59867716E 01 0.16394432E -02 0.68384838E -06 0.12836890E -09 0.89167396E -14
0.12043848E 05 0.63998213E 01 0.32144232E 01 0.10443844E -01 -0.11062989E -04
0.52967657E -08 0.83022695E 12 0.12745867E 05 0.76185751E 01
H2 J 3/61H 2.0 0.0 0.0 0.0 300.000 5000.000
0.31001883E 01 0.51119458E -03 0.52644204E -07 -0.34909964E -10 0.36945341E -14
0.87738013E 03 -0.19629412E 01 0.30574446E 01 0.26765198E -02 0.58099149E -05
0.55210343E -08 -0.18122726E -11 0.98890430E 03 -0.22997046E 01
HK L 5/66HE 1.00 0.00 0.00 0.0 300.000 5000.000
0.25000000E 01 0.0 0.0 0.0 0.0
-0.74537476E 03 0.91534883E 00 0.25000000E 01 0.0 0.0
0.0 0.0 0.74537476E 03 0.91534883E 00
H2O J 3/61H 2.0 1.00 0.00 0.0 300.000 5000.000
0.27167616E 01 0.29451370E -02 0.80224368E -06 0.10226681E -09 0.48472104E -14
0.29905820E 05 0.66305666E 01 0.40701275E 01 -0.11084499E 02 0.41521180E 05
0.29637404E -08 0.80702101E -12 0.30279719E 05 -0.32270038E 00
H2S J 12/65H 2.5 1.00 0.00 0.0 300.000 5000.000
0.28479090E 01 0.38415990E 02 0.14099360E 05 0.24278735E -09 0.15783280E -13
0.34469788E 04 0.74781399E 01 0.38811293E 01 -0.13211856E -03 0.36517713E -05
-0.21820441E -08 0.28783779E -12 -0.36350916E 04 0.25161505E 01
N2 J 9/65N 2.0 0.0 0.0 0.0 300.000 5000.000
0.28963194E 01 0.15154863E -02 -0.57235275E -06 0.99807385E -10 -0.65223536E -14
-0.90586182E 03 0.61615143E 01 0.36748257E 01 -0.12081496E -02 0.23240100E -05
-0.63217520E -09 -0.22577253E -12 0.10611587E 04 0.23580418E 01
O2 J 9/65O 2.0 0.0 0.0 0.0 300.000 5000.000
0.36219521E 01 0.73618256E -03 -0.19652219E -06 0.36201556E -10 -0.28945623E -14
-0.12019822E 04 0.36150942E 01 0.36255980E 01 -0.18782183E -02 0.70554543E -05
0.67635071E 08 0.21555977E -11 -0.10475225E 04 0.43052769E 01
SO J 12/65S 1.0 1.00 0.00 0.0 300.000 5000.000
0.38280144E 01 0.75593102E -03 -0.30791631E -06 0.57880131E -10 -0.40204419E -14
-0.43632666E 03 0.44528189E 01 0.31224213E 01 0.13797339E -02 0.20611933E -05
0.38700776E -08 0.16366249E -11 -0.17847565E 03 0.84176922E 01
SO2 J 6/61S 1.0 2.00 0.00 0.0 300.000 5000.000
0.52451363E 01 0.19704204E -02 -0.80375759E -06 0.15149969E -09 0.10557998E -13
0.17558227E 05 -0.10873518E 01 0.32665329E 01 0.53237863E -02 0.68437544E -06
0.52809987E -08 0.25590450E -11 -0.36908145E 05 0.96513472E 01

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H2O(L)      1.11/65H  2.0  1.00 0.00 0.4  273.150  373.150
-1.00000000E 04 0.00000000E 00 0.0      0.0      0.0
 3.69780000E 06 5.92300000E 04 0.12712782E 02-0.17662790E-01-0.22556633E-04
 0.20820897E-06-0.24078606E-09-0.37483195E 05-0.59115326E 02
C(S)        J 3/61C  1.0  0.0  0.0  0.5  300.000  5000.000
 0.13604937E-01 0.19182237E-02-0.84040386E-06 0.16448705E-09 0.11672670E-13
-0.65713843E 03-0.80070200E 01-0.44778049E 00 0.53690970E-02-0.39775563E-06
-0.40459263E-08 0.21134925E-11-0.94280670E 02 0.16840773E 01

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3.418,124.,0.,      AR  ! ALL DATA FROM RP&S EXCEPT AS NOTED.
3.758,148.6,0.0,    CH4
3.59,110.,0.,      CO
3.996,190.,0.,      CO2
4.13,335.0,0.15     COS !STOCKMEYER POTENTIAL GUESSED, BS&L OTHERWISE
4.438,488.6,0.0     CS2 !DITTO
2.915,38.,0.,      H2
2.576,10.2,0.0     HE  !BS&L
2.641,809.1,1.0,    H2O
3.49,343.0,0.21     H2S
3.681,91.5,0.,      N2
1.434,113.,0.,      O2
4.0,240.,0.0        SO  !BLIND GUESS
4.04,347.0,0.42     SO2
2.641,809.1,1.0,    H2O(L)
3.822,137.,0.,      C(S)

```