

MIXING AND GASIFICATION OF COAL IN
ENTRAINED FLOW SYSTEMS.

Final Report, August 31, 1979

Volume 2.

USER'S MANUAL FOR
A COMPUTER PROGRAM FOR
1-DIMENSIONAL COAL COMBUSTION OR GASIFICATION (1-DICOG).

Philip J. Smith and L. Douglas Smoot

Combustion Laboratory
Department of Chemical Engineering
BRIGHAM YOUNG UNIVERSITY
Provo, Utah 84602

Prepared for
The United States Department of Energy

Under Contract No. EF-77-S-01-2666

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, 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 trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

FOREWORD

This document is the second volume of the final report, prepared for the Department of Energy (DOE). It is the User's Manual for a computer model for One-Dimensional Coal Combustion or Gasification. Work on this code was initiated under contract to EPRI and the U.S. Department of Energy in December of 1974.

Work during the past year has been supported by the Electric Power Research Institute, Palo Alto, California, under Contract No. RP-364-1-3 with Mr. John Dimmer as Contract Officer and by the U.S. Department of Energy, Washington, D.C. under Contract No. EF 77-S-01-2666 with Dr. Robert C. Wellek as Contract Officer. Financial cost sharing from the Research Division of Brigham Young University for development of this code is gratefully acknowledged. The assistance of Mr. Scott M. Woodfield with computer program development is also acknowledged.

CODE AVAILABILITY

This code can be obtained at a minimal cost from:

Dr. L. Douglas Smoot
270 CB
Brigham Young University
Provo, Utah 84602

Included in the materials to be provided are the User's Manual and the card deck. The cost of obtaining these materials provides for some assistance by telephone in implementing the code and interpreting the output.

ABSTRACT

A one-dimensional, steady-state model describing pulverized coal combustion and gasification is presented. While emphasis has been placed on the description of the coal reaction processes and gas-particle interactions, one-dimensional fluid mechanics and particle-particle, particle-wall radiation have been included. Moisture vaporization from the coal particles, multi-step coal pyrolysis, and heterogeneous char oxidation by multiple oxidizers are modeled for polydispersed coal particle sizes or types. Although the formulation is one-dimensional, mixing rates of primary and secondary streams and recirculation within the reactor have been accounted for as specified input. The resulting model predicts thermal, chemical and physical histories for both the gaseous and particle phases. Gas-particle interactions account for appropriate diffusion and kinetic rates. Gas phase reactions are assumed to be in local chemical equilibrium. The solution technique uses predictor-corrector methods for integration of the ordinary non-linear differential equations which are coupled with a number of auxiliary algebraic equations. An iterative approach is required for the radiant heat transfer calculations by the zone method. Stiffness in differential energy equations is overcome by a pseudo steady-state method when needed. The generalized nature of the model allows for calculation of both coal combustion and coal gasification characteristics. User information is presented, along with a sample computation and a listing of the program.

TABLE OF CONTENTS - VOLUME 2

FOREWORD	iii
CODE AVAILABILITY.	iii
ABSTRACT	iv
LIST OF FIGURES.	vi
LIST OF TABLES	vi
NOMENCLATURE	vii
 I. USER'S MANUAL FOR ONE-DIMENSIONAL COAL COMBUSTION OR GASIFICATION MODEL.	 1
A. Introduction.	1
 II. THEORETICAL MODEL DEVELOPMENT	 4
A. Model Basis	4
B. Differential Equations.	9
C. Enthalpy-Temperature Relationships.	12
D. Physical Properties	17
E. Radiative Heat Transfer	20
F. State and Mass Flow Continuity.	23
G. Convective and Conductive Heat Transfer	25
H. Particle Reactions.	27
I. Local Gas Phase Equilibrium	32
J. Specified Mixing Processes.	33
 III. SOLUTION TECHNIQUE.	 39
A. Differential Equation Solver.	39
B. Treatment for Radiation	41
C. Step Size Control	42
D. Numerical Stiffness	44
 IV. 1-DICOG CODE.	 46
A. General Description	46
B. Description of Subroutines.	48
C. Input	50
D. Output.	60
E. Code Operation.	60
 REFERENCES	 68
APPENDIX A - 1-DICOG SAMPLE CALCULATION.	A-1
APPENDIX B - 1-DICOG FORTRAN LISTING	B-1
APPENDIX C - SPECIES INPUT PARAMETERS FOR EQUILIBRIUM CALCULATIONS	C-1

LIST OF FIGURES

<u>Figure</u>	<u>Page</u>
1 Schematic diagram of volume element for 1-DICOG	5
2 Schematic of jth particle, illustrating constituents and reaction processes.	8
3 Schematic of energy partitioning during coal particle reaction.	15
4 Schematic representation of the secondary mixing process. .	34
5 Schematic representation of the recirculation process . . .	37
6 Information flow for 1-DICOG.	43
7 Initial guess at the jth particle type temperature profile.	62
8 Particle size distribution used for the three increment poly-dispersed combustion calculation of Appendix A	63

LIST OF TABLES

<u>Table</u>	<u>Page</u>
1 Summary of Key Assumptions and Conditions of Coal Reaction Model	6
2 Summary of Model Differential Equations	10
3 1-DICOG Constitutive Equations: Enthalpy-Temperature Relationships	13
4 1-DICOG Constitutive Equations: Physical Properties. . . .	18
5 1-DICOG Constitutive Equations: Radiative Heat Transfer. .	21
6 1-DICOG Constitutive Equations: State and Mass Flow Continuity.	24
7 1-DICOG Constitutive Equations: Convective and Conductive Heat Transfer	26
8 1-DICOG Constitutive Equations: Particle Reactions	28
9 Selected Kinetic Parameters for 1-DICOG	31
10 Input Data for 1-DICOG.	51
11 FORTRAN Variable Nomenclature	53
12 Coal Analysis for Sample Calculation of Appendix A.	66

NOMENCLATURE

<u>Symbol</u>	<u>Units</u>	<u>Definitions</u>
A_j	cm^2	Particle area
A	s^{-1}	Pre-exponential factor
A	cm^2	Corss sectional area
a	$\text{cal g}^{-1} \text{K}^{-(k)}$	Heat capacity coefficient (Eq. 33)
a	cm^{-1}	Radiative absorption coefficient
b	$\text{cal g}^{-1} \text{K}^{-(k)}$	Heat capacity coefficient (Eq. 59)
B	---	Blowing parameter
C	mol cm^{-3}	Molar concentration
C_p	$\text{cal g}^{-1} \text{K}^{-1}$	Heat capacity
D	$\text{cm}^2 \text{s}^{-1}$	Mass diffusivity
D_s	cm	Diameter of reactor chamber
d	cm	Particle diameter
E	cal mol^{-1}	Activation energy
E_λ	---	Absorption efficiency
h	$\text{cal s}^{-1} \text{cm}^{-2} \text{K}^{-1}$	Heat transfer coefficient
h	cal g^{-1}	Enthalpy
h	---	Step size
Δh	cal g^{-1}	Heat of reaction
I	$\text{cal cm}^{-2} \text{s}^{-1}$	Radiative intensity
J	---	Total number of particles
K	---	Total number of elements
k	$\text{s}^{-1}, \text{cm s}^{-1}$	Reaction rate coefficient
k	$\text{cal s}^{-1} \text{cm}^{-1} \text{K}^{-1}$	Thermal conductivity

k_c	cm s^{-1}	Mass transfer coefficient
k_g	$\text{cal s}^{-1} \text{cm}^{-1} \text{K}^{-1}$	Gas conductivity
k_x	$\text{moles cm}^{-2} \text{s}^{-1}$	Mass transfer coefficient
M	g mol^{-1}	Molecular weight
m	$\text{g cm}^{-1} \text{s}^{-1}$	Mass addition rate
Nu	---	Nusselt number
n	cm^{-3}	Particle number density
Pr	---	Prandtl number
p	atm	Pressure
Q	$\text{cal cm}^{-3} \text{s}^{-1}$	Particle-gas heat transfer rate
R	$\text{cal mol}^{-1} \text{K}^{-1}$	Gas constant
r	$\text{g cm}^{-3} \text{s}^{-1}$	Particle reaction rate
Re	---	Reynolds number
Sc	---	Schmidt number
T	K	Temperature
v	cm s^{-1}	Velocity
w	g s^{-1}	Mass flow rate
X	---	Mole fraction
x	cm	Axial space coordinate
y	---	Arbitrary independent variable
Y	---	Devolatilization coefficient
α	g	Coal component mass
δ	---	Stockmayer parameter
ϵ	---	Emmissivity
γ	---	Particle swelling parameter
ϕ	---	Interaction parameter
ϕ	---	Stoichiometric coefficient
σ	---	Particle internal area factor

μ	$\text{g cm}^{-1} \text{ s}^{-1}$	Viscosity
π	---	Pi, 3.14159
ρ	g cm^{-3}	Density
σ	$\text{\AA}$	Collision diameter
σ	$\text{cal s}^{-1} \text{ cm}^{-2} \text{ K}^{-4}$	Stefan-Boltzmann constant
ω	---	Mass fraction
Ω	---	Collision integral

Subscripts

a	ash
b	boundary
c	coal
c	convection
d	diffusion
e	equilibrium
f	flame
g	gas
h	char
i	gas species, summation index
j	particle type, surface of particle
k	kinetic, element, summation index
ℓ	char oxidation reaction
m	mean, mixture, devolatilization reaction, mass transfer
n	reaction order, total species, position
o	initial value, without blowing, oxidizer
p	radiation region, summation index
q	radiation region, summation index
r	radiation

s	secondary
v	volatiles
w	moisture
y	hydrocarbon
μ	viscosity
α	coal component
ρ	recirculation

I. USER'S MANUAL FOR ONE-DIMENSIONAL COAL COMBUSTION OR GASIFICATION MODEL

A. INTRODUCTION

1. Background

This manual presents the details of the one-dimensional computer code, referred to as 1-DICOG (1 - DIMensional Combustion Or Gasification), for describing pulverized coal combustion or gasification processes. A description of coal reaction processes, including devolatilization, char oxidation, gas-phase oxidation, and gas-particle interchange is emphasized. Coal and gas physical properties are also included. The resulting model, which describes the response of a coal particle to its thermal, chemical and physical environment, has been coupled with one-dimensional fluid mechanics and radiative heat transfer to form a working model to describe the performance of pulverized coal combustors and gasifiers. The formulation of the coal reaction processes can also be readily applied to other fluid mechanics models in order to extend investigations to multi-dimensional examples (1).

Development of an analytical treatment of pulverized coal-char behavior in reacting systems is based largely on experimental observations and kinetic parameters deduced from these observations. Since there are still unresolved questions regarding the kinetics of coal reaction, 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 ($<100 \mu\text{m}$) and heating rates are high (10^3 - 10^5 K s^{-1}). This treatment would not necessarily apply to fixed or fluidized bed processes without modification, but is intended for application to pulverized coal furnaces and entrained coal gasifiers.

The fluid mechanics model is time-steady in one space dimension and requires input specification of the rates of jet mixing and recirculation. The potential uses and advantages of this model include: 1) low computer costs for investigating effects of operating and configurational variables on coal reaction processes; 2) a method for evaluating various descriptions of coal kinetics together with model parameters; 3) a basis for development of multi-dimensional codes of coal reaction processes; 4) interpretation of experimental data; 5) a single model for describing both combustion and gasification processes for pulverized coal systems; and 6) potential use as a component in systems analysis codes that describe processes with a combustion or gasification step. This one-dimensional model is not well-suited for comparison with local measurements in two or more dimensions inside combustors or gasifiers. Further, it would not be applicable to the detailed design or optimization of such systems.

In this volume of the final report, review of other pulverized coal combustion and gasification models is presented. The basis for the model is then explained including a description of all model equations and required assumptions. The numerical solution technique is discussed and methods used for improved computational efficiency are disclosed. User information regarding the 1-DICOG code is then presented. The appendices contain a sample calculation, the program listing and helpful equilibrium parameters.

2. Literature Review

Several models have been developed for combustion of pulverized coal systems, but relatively few have been applied to gasification. The complex fluid mechanics involved in both must be coupled with the local heterogeneous and homogeneous gas and particle-phase reactions. Overcoming these types of complexities has forced most modeling efforts to look at a more macroscopic level of approximation, where larger areas of the reactor are characterized by simplifying assumptions, rather than defining the detailed mechanisms throughout the reactor. A notable exception to this is the multi-dimensional work originating at Imperial College (2), where modeling in gaseous-fired furnaces is being extended to coal-fired systems. It is to this type of modeling effort that the present formulation of coal reaction processes may make the largest contribution.

Models for pulverized coal combustion include those of Vulis (3), Hedley and Jackson (4), Horn et al. (5) and Field et al. (6). These models may be considered to be plug-flow in nature, where some have been modified to include the effects of recirculation. Beer and Lee (7) have developed a model which incorporates a combination of perfectly-stirred reactors and plug-flow reactors. Lewellen et al. (8) have recently developed a model for a swirling-coal combustor, wherein they identified the dominant physical processes in four regions of interest. Some initial efforts have been expended to incorporate coal combustion with complex two-dimensional turbulent fluid mechanics by Richter and Quack (9); and Gibson and Morgan (10). In all such cases very simple coal reaction models were used in order to accommodate the more detailed mixing.

Entrained flow gasification models are only recently being developed. Batchelder et al. (11) presented some of the earliest work in this area. Mehta (12) has developed a model combining perfectly-stirred reactors and plug-flow reactors to describe a three-stage, entrained gasifier. Two models of gasification are being developed by George et al. (13), one being a combination of perfectly-stirred reactors and plug-flow reactors, the other based on a characteristic-time approach. Lewis et al. (14) are preparing a gasification model consisting of two parts, one part containing the single particle chemistry, etc., the other part containing the fluid mechanics and homogeneous chemistry. Blake (15) has initiated development of a generalized, multidimensional, gasification model and some work has been done to include coal combustion in two dimensional models similar to that described in Section 4 of Volume 1 of this report, and by Gibson and by Morgan (10); and Richter and Quack (11).

The formulation incorporated in 1-DICOG contains physical and chemical descriptions which extend beyond any that have been included in previous mathematical models for pulverized coal entrained flow reactors, whether for combustion or gasification. Currently, researchers engaged in developing coal conversion models on this level include Sprouse (16), Blake (15) and Stickler (18). Sprouse is formulating a one-dimensional model much like 1-DICOG. Blake, as already mentioned, is developing a multi-dimensional approach. Also, a two-dimensional, axi-symmetric, combustion and gasification model incorporating the concepts of 1-DICOG is being developed by the BYU Combustion Laboratory as reported by Smoot and Hedman (1); and Smoot and Pratt (17). Stickler et al. (18) have developed a one-dimensional coal combustion model designed to simulate MHD power generators. Although radiation has been ignored in their model, the approach is very similar to 1-DICOG.

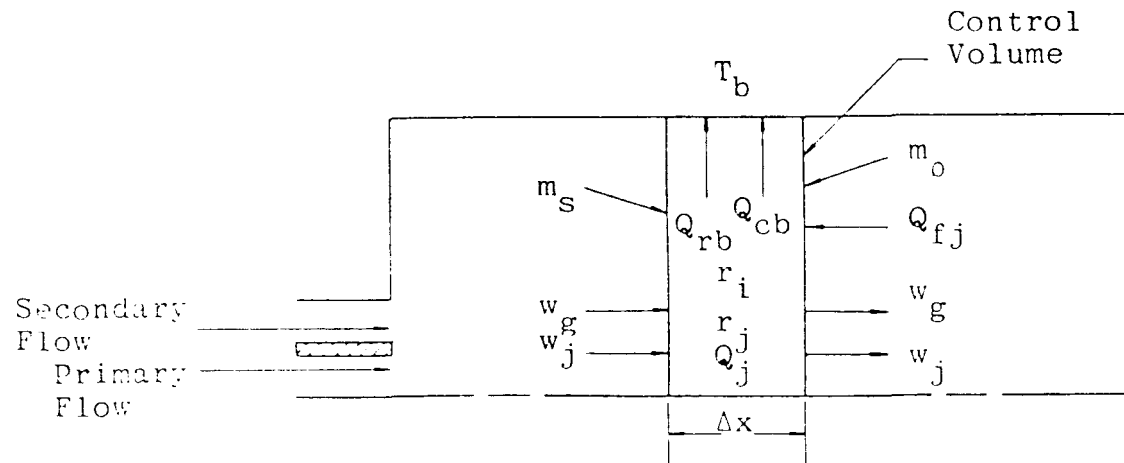
II. THEORETICAL MODEL DEVELOPMENT

A. MODEL BASIS

1-DICOG, by its one-dimensional formulation, assumes no gradients normal to the direction of flow. The differential formulation is based on a volume element inside a gasifier or furnace as depicted in the schematic shown in Figure 1. As depicted by this schematic, the following aspects of pulverized coal combustion and gasification have been included in the model: 1) mixing of primary and secondary streams (specified as input); 2) recirculation of reacted products (specified as input); 3) devolatilization and swelling of the coal; 4) reaction of the char by oxygen, steam carbon dioxide, hydrogen or any arbitrary oxidizer; 5) conductive heat transfer between the coal or char particles and the gases; 6) convective losses to the reactor wall; 7) variations in composition of inlet gases and solids; 8) variation in coal or char particle sizes; 9) oxidation of the coal devolatilization products; 10) radiative interchange among particles and with the reactor walls; and 11) inclusion of multiple sizes or types of coal particles, each with their own individual properties, composition, reaction rates, etc.

The following are considered to be the major limitations of the one-dimensional model (1-DICOG). 1) The model does not predict local mean or fluctuating properties within the pulverized coal reactor as a function of both radial and axial position. 2) The model does not predict rates of jet mixing or recirculation; rather, these values are required input. 3) The detailed behavior of coal reactions is not yet well understood, which leads to uncertainty in the kinetic description and parameters for the pulverized coal systems. 4) Some details of the pulverized coal gasification and combustion processes have been neglected to reduce model complexity and computation time. These include particle velocity lag effects, micromixing processes, gas-phase rate-limiting reactions and gas-phase radiation. A complete summary of key model assumptions and conditions is given in Table 1.

1-DICOG has been developed for an arbitrary number of chemical elements (K in total number). All equations are derived for elemental balances as opposed to species balances. This simplification is rendered tractable by the local gas phase chemical equilibrium approximation. Local equilibrium signifies that the gas phase species are in chemical equilibrium at each point within the reactor, which is equivalent to assuming infinite gas-phase reaction rates. It does not imply that neighboring elements are in equilibrium with each other. The elemental balances simplify the approach in two ways. First, the number of differential equations involved in elemental balances is usually much smaller than those required for species balances. Secondly, this greatly simplifies the required link with the coal reaction model. Volatiles, for example, need not be specified by species composition, which are difficult to identify, but only by elemental composition which is easier to define from an ultimate analysis of the char. From the element balances and the calculated energy level, the Gibb's free energy is minimized and



m_s = rate of flow of secondary stream into control volume	r_j = rate of pyrolysis and oxidation of coal/char
w_g = rate of gas flow into control volume	r_i = rate of reaction of gas species
w_j = rate of particle flow into control volume	Q_{cb} = rate of heat loss by convection
m_p = rate of recirculated product flow into control volume	Q_{rb} = rate of heat loss by radiation
Q_j = heat transferred by conduction between gas and particles.	Q_{fj} = rate of radiative heat transfer in reactor
	T_b = wall temperature

Figure 1. Schematic diagram of volume element for 1-DICOG (1).

TABLE 1

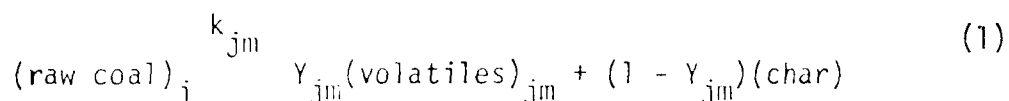
SUMMARY OF KEY ASSUMPTIONS AND CONDITIONS OF
COAL REACTION MODEL (1-DICOG)
(Modified from Smoot and Pratt (1))

1. Steady-state, compressible gas, with specified uniform pressure or specified pressure variation, and specified reactor area variation.
2. Particles and gases in dynamic equilibrium.
3. Specified secondary gas and recirculated product input along reactor with instantaneous mixing at each interval of reactor area.
4. Multiple particle sizes or types.
5. Each particle size and type and gas are distinct phases.
6. Negligible gas conduction, molecular diffusion, thermal diffusion, gravity effects, particle interactions, wall friction, viscous dissipation, work on surroundings, gas phase radiation, particle-phase convective losses, kinetic energy, particle volume.
7. Coal reactions take place by competing processes of devolatilization and char oxidation.
8. Rate-limiting steps include upstream radiative transport, rate of gross oxidizer/fuel mixing, rate of product recirculation, rate of coal particle devolatilization, rate of char reaction (with O_2 , CO_2 , H_2 and H_2O), rate of molecular diffusion to/from particle surface, and rate of heat transfer by conduction to/from particle surface.
9. Gas phase in local equilibrium.
10. Particles are composed of raw coal, char, ash and moisture.
11. Ash is inert and remains with the particle. Any volatile mineral matter is considered part of volatiles or char content.
12. Coal devolatilization is by an arbitrary sequence of irreversible, parallel, activated processes with specified activation energies.
13. Coal particle swelling is proportional to extent of devolatilization.
14. Spherical particles of uniform local particle temperature with arbitrary change in char particle diameter during reaction and with internal and external surface reactions according to specified burn area per particle.
15. Char contains specified proportions of other elements which enter the gas phase at a rate proportional to the carbon reaction.
16. Coal moisture loss controlled by vapor diffusion and heat transfer.
17. Devolatilization produces a fuel-rich product whose gases block diffusion and conduction by surface transpiration.

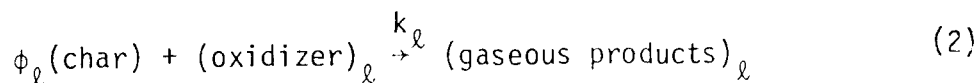
complete species composition, gas temperature, and other properties are computed from the assumption of local equilibrium.

1-DICOG is also derived for an arbitrary number of particle types (J in total number). This is an important feature of the model since George et al. (13) have indicated that approximating a pulverized coal system with a mono-dispersed particle size might lead to significant error. The code allows for the formal examination of different sizes or types in the same reactor. This will be evidenced in the equation set by noting that all particle equations will be written with a subscript j denoting the equation for the jth particle classification. The most common application of this option would be to examine the effect of a particle size distribution, but this is not the only possibility. The description is such that each particle type may have its own properties such as composition, rate of devolatilization, rate of oxidation, and rate of swelling. This option could be used to study the effects of feeding a mixture of different coal types, or perhaps recycling some char along with makeup coal.

The process by which each particle reacts is schematically presented in Figure 2. The reacting particle is composed of specified amounts of raw coal, char, ash, and moisture. 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 oxidizer (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:



The ash is defined as that portion of the particle which remains inert throughout the entire combustion or gasification process. Moisture loss is controlled by heat transfer to the particle surface and water vapor diffusion away. During devolatilization, the particle swells at a rate proportional to the extent of devolatilization. After completion of devolatilization, the particle may continue heterogeneous char oxidation as either a constant diameter, changing-density particle, or a constant density, shrinking-diameter particle. The details of this coal submodel are presented in the following sections and also in Smoot and Pratt (17).

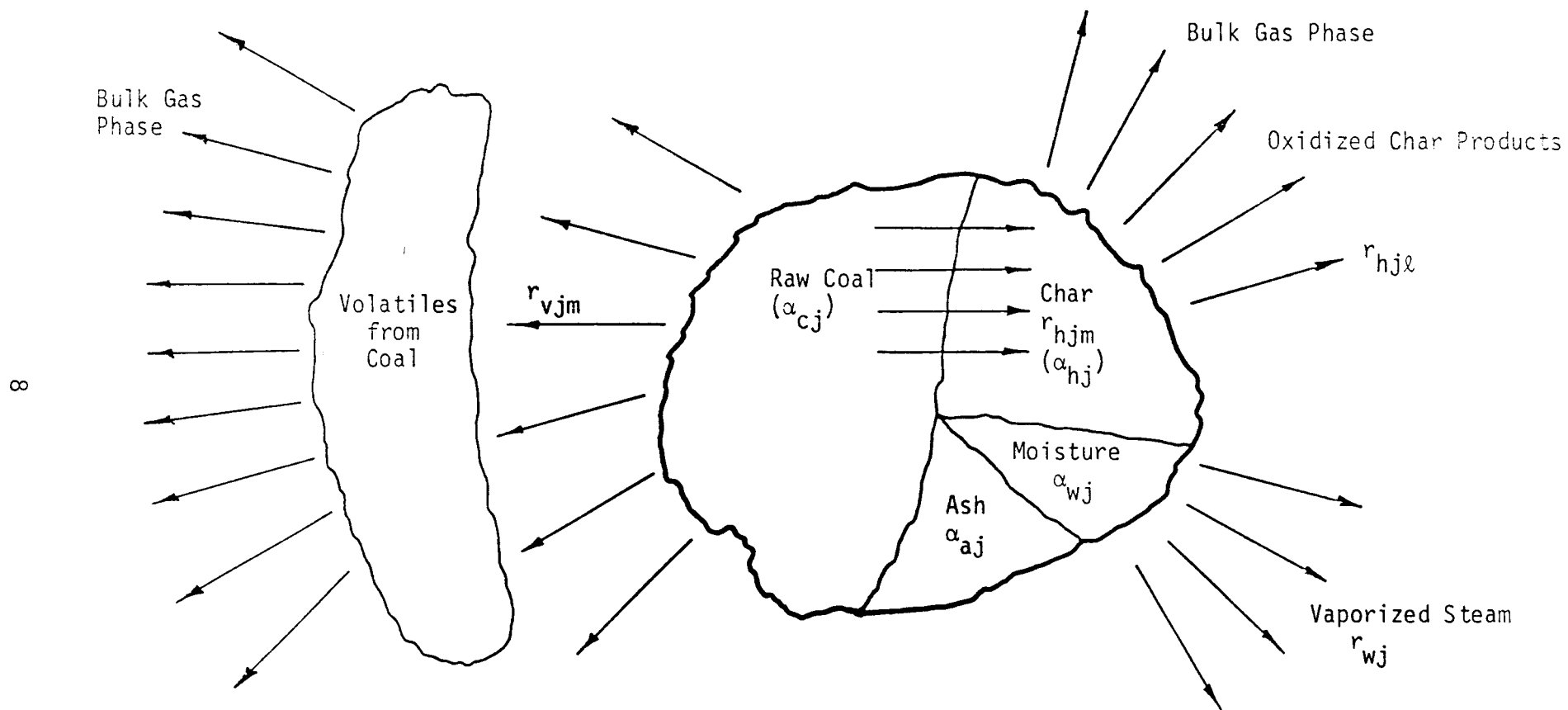


Figure 2. Schematic of j th particle, illustrating constituents and reaction processes (1).

The required set of differential equations will be discussed next. In addition, a number of auxiliary or constitutive algebraic equations are required as component model parts. These equations describe the following aspects of the coal reaction process: (1) enthalpy-temperature relationships; (2) physical properties including heat capacity, thermal conductivity, diffusivity, and viscosity; (3) radiative interchange inside the gasifier; (4) equations of state and mass flow continuity; (5) convective and conductive heat interchange among the gases, particles and walls; and (6) rates of devolatilization and oxidation of coal and char. Each of these aspects of the model will then be discussed in turn. Finally, the local gas phase equilibrium calculations will be described.

B. DIFFERENTIAL EQUATIONS

The differential equation set which is solved by 1-DICOG is summarized in Table 2. This set of non-linear, highly coupled, ordinary differential equations is derived for a volume element as depicted in Figure 1 (see for example, Bird et al. 19). A general derivation of equations governing pulverized coal systems is given by Smoot and Pratt (17). The set is reduced to ordinary differential equations where derivatives are taken with respect to the one space dimension by considering the system to be at steady-state and only one-dimensional.

Equation 3 (Table 2) depicts the mass rate of change of each element. There is one of these equations solved for each of the K total elements considered. The sources or sinks of elemental mass addition or depletion for the gas phase are only three in number. Mass addition or depletion may take place through reaction with any of the J particle classifications. This is shown in the first term on the right hand side of Eq. 3. The summation is required since each of the particle phases represents a potential contributor. The final two terms represent sources or sinks due to secondary mixing and recirculation. As mentioned previously, these last two terms must be specified by the user, since they represent two-dimensional effects that might be important in the early regions of the reactor. Modeling of these terms is discussed in the sub-section entitled "Specified Mixing Processes".

Equation 4 represents the mass rate of change of each particle phase. There is one of these equations for each particle phase classification. As with the gas phase elemental balances of Eq. 3 the only sources and sinks are the overall particle reaction, secondary mixing and recirculation. No summation is required since the equation is written for each individual particle classification. Note particularly the sign on the reaction rate term in Eqs. 3 and 4. Reaction rates are written as the rate of mass addition to the gas phase per unit gas volume per unit time; thus, a positive reaction rate signifies a source of mass for the gas phase and a sink for the particle phase.

Equation 5 is the gas phase energy balance. Again, the first two terms on the right hand side depict the energy exchange due to secondary mixing and recirculation respectively. The final terms enclosed between parentheses represent all other gas phase heat transfer mechanisms. Q_j accounts for the conductive heat transfer from the j th particle type

TABLE 2
SUMMARY OF MODEL DIFFERENTIAL EQUATIONS

NO.	TYPE	EQUATION	NO. OF EQNS.
3	Gas Element Continuity (k^{th})	$d(w_g \omega_k)/dx = A \sum_j r_{jk} + m_{sgk} + m_{pgk}$	K
4	j^{th} Particle Phase Continuity	$dw_j/dx = -Ar_j + m_{sj} + m_{pj}$	J
5	Gas Energy	$d(w_g h_g)/dx = h_{sg} m_{sg} + h_{pg} m_{pg} + A(\sum_j Q_j - Q_{cb} + \sum_j r_j h_{jg})$	1
6	Particle Energy	$d(w_j h_j)/dx = m_{sj} h_{sj} + m_{pj} h_{pj} + A(Q_{fj} - Q_{rbj} - Q_j - r_j h_j)$	J
7	Particle Number	$d(vn_j A)/dx = (m_{pj}/\alpha_j) + (m_{sj}/\alpha_j)$	J
8	Total Gas Continuity	$d(w_g)/dx = A \sum_j r_j + m_{sg} + m_{pg}$	1
9	Coal Mass	$d(\alpha_{cj})/dx = (r_{cj}/n_j v)$	J
10	Char Mass	$d(\alpha_{hj})/dx = (r_{hj}/n_j v)$	J
11	Moisture Mass	$d(\alpha_{wj})/dx = -(r_{wj}/n_j v)$	J

to the gas. Q_{cb} is the convective heat transfer from the gas to the boundary or reactor walls. The last term is the energy carried to the gas by the mass addition from the particle phase. The summation over each of the particle terms accounts for all particle classifications.

Equation 6 is the analogous particle phase energy equation. Energy exchange due to secondary mixing or recirculation of j th particle phase is accounted for in the first two terms. The particle energy is similar to the gas phase energy equation with the exception of two radiation terms and no convective wall term. The radiation terms include particle phase radiation but with the assumption of no gas phase radiation. Q_{fj} accounts for particle-particle radiation within the reactor. Q_{rbi} is the radiative heat transfer rate from the particle cloud to the reactor boundaries. There is a separate particle energy equation for each particle phase. The Q_i term arising in both the particle and gas energy equations results in the tightest coupling of any of the differential equations. Numerical techniques which are used to avoid problems with this tight coupling are discussed in the Solution Technique section.

Equation 7 represents the linear rate of change of the particle number for each of the j particle types. The only source or sink terms in this case are recirculation or secondary mixing of the j th particle class. In other words, if there is no recirculation or secondary addition of the coal particles in the j th classification, then the number of particles passing any point in the reactor per unit time ($v_n A$) is constant. This observation emphasizes another approximation in the coal reaction model. The particles are not allowed to break or fragment during the history of the reaction process. Some studies, such as Padia et al. (20), have counted many more particles (up to 3-5 per coal particle) evolving from the combustion process than were input; however, the fragmentation is thought to occur during the final burnout phases of char combustion when the fine ash structure is not mechanically strong enough to remain integral. This being the case, the assumption of no fragmentation may not introduce significant error in the estimate of particle burnout times. It should be realized that this approximation is at least a conservative one, since smaller fragments should react even faster than the larger particles.

Equation 8 represents the rate of change of the gas phase mass flow rate and is exactly analogous to Eq. 4. It is also the sum of the gas element balances (Eq. 3) over all of the elements. Equation 3 and 8 are independent equations. It is possible to write continuity equations for each element mass fraction (ω_k), the sum of the mass fractions ($\sum \omega_k = 1$), and an overall gas phase mass continuity (w_g). Thus, there are $K + 2$ equations, of which any $K + 1$ are independent. 1-DICOG makes use of the equations in ω_k and w_g . The sum of the mass fractions is not used. The solution of Eq. 8 gives the history of the gas phase mass flow rate. With this information and the solution to Eq. 1 for each element, the history of the gas phase elemental composition is known.

Equations 9 through 11 show the rate of change of each of the constituents of each of the particle classifications considered. Initially, the reacting particles are represented as being composed of specified

amounts of raw coal (α_{cjo}), char (α_{hjo}), moisture (α_{wjo}), and ash (α_{ajo}). The only sink terms for any of these constituents is their respective reaction rate terms. Ash is defined in this code as that portion of the initial particle which is inert to any reaction. The ash content is thus constant, and no differential equation is required. The sign on the reaction rate term for the moisture mass is different from the others simply due to the definition of the reaction rates of the raw coal and char which, by convention, are taken to be the rate of disappearance of each of these constituents per unit volume of reacting, particle-gas mixture. All other reaction rates use the opposite convention.

The solution strategy for this set of $6J + K + 2$ differential equations is given in the section entitled "Solution Technique". The solution of these equations determines the history of ω_k , w_j , h_g , h_j , n_j , w_g , α_{cj} , α_{hj} and α_{wj} .

C. ENTHALPY-TEMPERATURE RELATIONSHIPS

The temperature of the gas and particle phases are determined by tracking the enthalpy of each phase by means of the differential energy equations represented in Eqs. 5 and 6 of Table 2. Auxiliary enthalpy-temperature relationships are required to solve these energy equations and to obtain the temperature history for each particle classification and for the gas phase. These relationships are indicated in Table 3 and are now discussed in more detail.

The particle enthalpy is obtained directly from the particle differential energy equation. No additional enthalpy terms appear on the right hand side of Eq. 6 in Table 2 other than the dependent variable (h_j) itself. The temperature of the individual particle phase is determined directly from Eq. 12 of Table 3 once the enthalpy (h_j) has been found from the differential equation set. The finite difference approximation used is completely acceptable, since each element used for the differential equation solution technique must be small enough for only mild temperature changes to occur across it (see Solution Technique section). The heat capacity (C_{pj}) is treated as a quadratic equation in temperature. Since the particle temperature must be known to calculate the heat capacity and vice versa, the solution of Eq. 12 must be accomplished by iteration, but convergence is rapid and straightforward.

The gas temperature is calculated in the gas phase chemical equilibrium sub-routine but requires the pressure, the local enthalpy level and elemental composition of the gas phase as input. The gas enthalpy comes from the differential energy equation which requires the term h_{jg} which appears on the right hand side of Eq. 6 in Table 2. The remainder of this section will deal with this term.

Equation 13 shows the constitutive equation used to calculate h_{jg} . This term represents the net enthalpy given to the gas phase due to products evolving from the j th particle phase. There are three sources of gaseous products in this coal particle model: devolatilization, heterogeneous char oxidation, and moisture vaporization. The corresponding terms appear on the right hand side of Eq. 13. The reaction rate fraction (i.e., r_{wj}/r_j) tells what fraction of each unit mass added to the gas

TABLE 3

T-DICOG CONSTITUTIVE EQUATIONS: ENTHALPY-TEMPERATURE RELATIONSHIPS

NO.	TYPE	EQUATION
12	Particle temperature	$\Delta T_j = \Delta h_j / C_{pj}$
13	Net particle product (gas) enthalpy	$h_{jg} = (\sum_m r_{vjm} h_{vjm} + h_{hj} \sum_{\ell} r_{hj\ell} + r_{wj} h_{wj}) / r_j$
14	Volatiles enthalpy	$h_{vjm} = \int C_{pvjm} dT_j + h_{vjm}^{\circ}$
15	Char enthalpy	$h_{hj} = \int C_{phj} dT_j + h_{hj}^{\circ}$
16	Mositure enthalpy	$h_{wj} = \int C_{pwj} dT_j + h_{wj}^{\circ}$

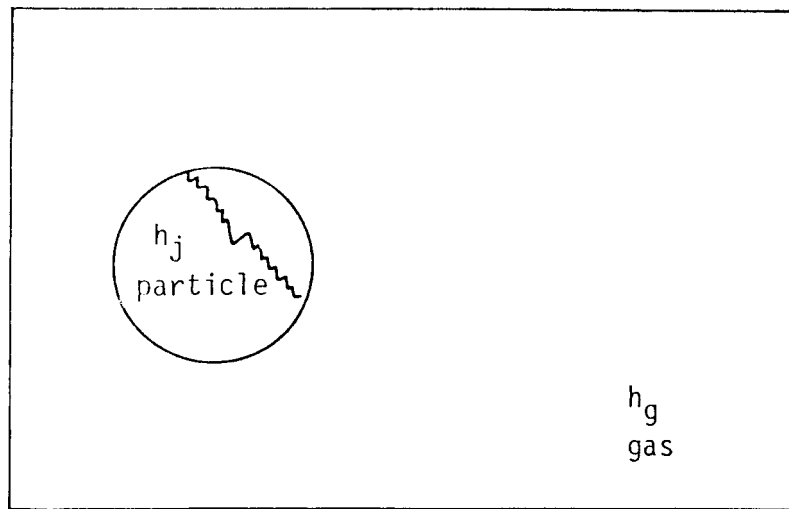
phase corresponds to the respective source. The denominator, r_i , being the total particle reaction rate (see Eq. 65, Table 8) and the terms in the numerator are the net rates for reaction of each source. The three enthalpy terms (h_{vi} , h_{hj} , h_{wj}) represent the net energy level of each source. These enthalpies are calculated in the last three equations of Table 3.

At this point another modeling assumption is required. Since the three reactions which are responsible for exchanging matter and energy between the particle and gas phases are two-phase reactions, it is not immediately obvious to which phase to credit the heat of reaction. This credit (or debit for endothermic reaction) could be given to either the particle or the gas phase or both. Experimental evidence indicating which should be the proper choice is hard to obtain. Ayling, et al. (21) have reported measurements of both particle and gas temperatures in a reacting system. Their particle measurements seem to be 200-300 K higher than the gas temperatures indicating that the particle receives some of the heat of reaction. Since physical arguments could be made for all three cases and since this author feels that the experimental evidence is inconclusive, the choice is made, somewhat arbitrarily, to give all heats of reaction to the gas phase. This is the way the model was developed and coded. The methodology for the other two assumptions is given at the end of this section. It should be realized that whichever assumption is chosen it is not crucial to the overall prediction. 1-DICOG allows for energy exchange between the particle and gas phases by conduction, which gives rise to a certain amount of self-adjusting between the two phases.

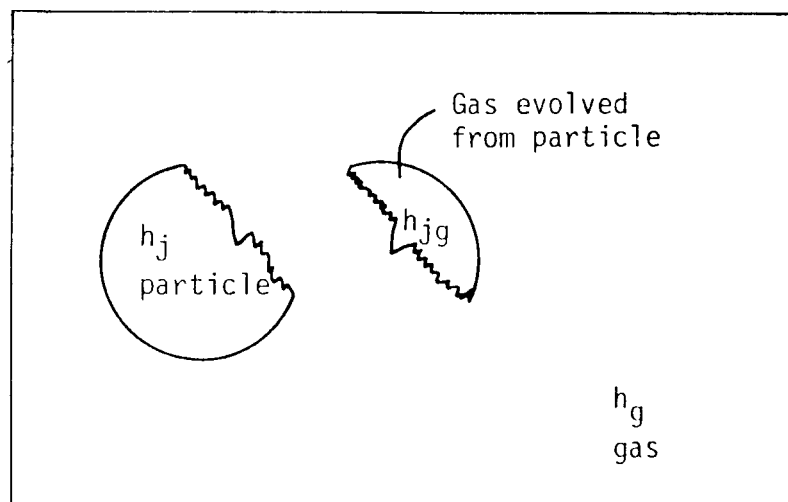
Equations 14, 15 and 16 are all analogous. The enthalpy level of each constituent is composed of the integrated heat capacity and the standard heat of formation; however, this formulation requires some subtle observations. Since the heat of reaction of each is given to the gas phase, the heat of reaction does not even appear in the equations. All three terms (h_{vi} , h_{hj} , h_{wj}) are based on the particle-phase constituents, not on the respective gas-phase constituents. The adiabatic reaction process may be considered to take place completely in the gas phase; therefore, the energy added is only that energy carried by the corresponding particle (solid) phase material being added to the gas. Figure 3 may help in visualizing this process. With the added assumption that the evolving gases from the particle are leaving at or near the particle temperature, the formulation is complete. With a quadratic equation in temperature for each of the heat capacities, the integration can be formally performed from 298 K to the particle temperature. The respective heats of formation (h_{vi}° , h_{hj}° , h_{wj}°) are for each constituent in the particle phase. For example, the moisture may be considered to be bound in a liquid state thus:

$$h_{wj}^{\circ} = -3792 \text{ cal g}^{-1} \quad (17)$$

If the char is considered to be mostly solid carbon:



(a) Before reaction



(b) After reaction

Figure 3. Schematic of energy partitioning during coal particle reaction.

$$h_{hj}^{\circ} = 0.0 \text{ cal g}^{-1} \quad (18)$$

An approximate heat of formation for the solid volatiles matter may be obtained from an ultimate analysis and heating value data of the coal. From Eq. 1 it can be seen that:

$$h_{(\text{raw coal})}^{\circ} = Y h_{(\text{vol.})}^{\circ} + (1 - Y) h_{(\text{char})}^{\circ} \quad (19)$$

$$h_{(\text{vol.})}^{\circ} = h_{(\text{raw coal})}^{\circ} / Y$$

The raw coal is the dry, ash-free portion of the coal analysis; thus:

$$h_{vj}^{\circ} = h_{(\text{vol})}^{\circ} = h^{\circ}(\text{DAF coal}) / Y$$

$$= [h_{(\text{total combustion products})}^{\circ} + (\text{heating value of DAF coal})] / Y \quad (20)$$

Finally, how does the formulation change if it is assumed that the heat liberated during particle reaction is assigned to the particle phase instead of the gas phase or if the heats of reaction were partitioned between the two phases? The approach is straightforward. When all heats of reaction are given to the solid phase, Eqs. 14, 15 and 16 of Table 3 must be charged for these heats of reaction; therefore,

$$h_{vjm} = \int C_{pvjm} dT_j + h_{vjm}^{\circ} - \Delta h_{vjm} \quad (21)$$

$$h_{hj} = \int C_{phj} dT_j + h_{hj}^{\circ} - \Delta h_{hj} \quad (22)$$

$$h_{wj} = \int C_{pwj} dT_j + h_{wj}^{\circ} - \Delta h_{wj} \quad (23)$$

where the h terms represent the respective heats of reaction in question. In addition, these heats of reaction must be given to the solid phase and Eq. 6 of Table 2 must have the following term added to the right hand side:

TABLE 4

1-DICOG CONSTITUTIVE EQUATIONS: PHYSICAL PROPERTIES

NO.	TYPE	EQUATION
25	Particle heat capacity	$C_{pj} = \omega_{hj}C_{phj} + \omega_{cj}C_{pcj} + \omega_{wj}C_{pwj} + \omega_{aj}C_{paj}$
26	Gas species conductivity	$k_i = [C_{pi} + (5R/4M_i)]\mu_i$
27	Gas mixture conductivity	$k_g = \sum_i [X_i k_i / \sum_k X_k \phi_{ik}]$
28	Gas species viscosity	$\mu_i = 2.67 \times 10^{-5} (M_i T_g)^{1/2} / \sigma_i^2 \Omega_\mu$
29	Interaction parameter	$\phi_{ik} = (1/8)^{1/2} [1 + M_i/M_k]^{-1/2} [1 + (\mu_i/\mu_k)^{1/2} (M_k/M_i)^{1/4}]^2$
30	Gas mixture viscosity	$\mu_g = \sum_i [X_i \mu_i / \sum_k X_k \phi_{ik}]$
31	Species diffusivity	$D_{ik} = 1.84 \times 10^{-3} T_g^{3/2} [(1/M_k) + (1/M_i)]^{1/2} / p \sigma_{ik}^2 \Omega_d$
32	Mixture diffusivity	$D_{im} = (1 - X_i) / \sum_{k \neq i} (X_k / D_{ik})$
33	Particle diameter	$d_j = d_{jo} [1 + \gamma(\alpha_{cjo} - \alpha_{cj}) / \alpha_{cjo}]$
34	Particle surface area	$A_j = \pi d_j^2$

$$+ A(\sum_m r_{vm} \Delta h_{vm} + \Delta h_{hj} \sum_\ell r_{hj\ell} + r_{wj} \Delta h_{wj}) \quad (24)$$

If partitioning of the heats of reaction between the particle and gas phase is desired, all the respective heats of reaction need only be weighted by that proportion which is to be given to the particle phase.

D. PHYSICAL PROPERTIES

A number of physical properties of the gas and particle phases are required. Table 4 shows how each of these are calculated. Equation 25 simply shows how to calculate the weighted heat capacity for the j th particle type. This comes from the coal model depicted in Figure 2 which shows the four constituents of the modeled particle. As in the previous section, all heat capacities are given as quadratic equations in temperature. The constituent particle mass fractions are calculated directly from the local constituent mass as obtained from the differential equation set (Eqs. 9, 10, 11 of Table 2). For example:

$$\omega_{hj} = \alpha_{hj} / \alpha_j \quad (35)$$

where

$$\alpha_j = \alpha_{cj} + \alpha_{hj} + \alpha_{wj} + \alpha_{aj} \quad (36)$$

The overall particle heat capacity (C_{pj}) is needed to determine particle temperature in Eq. 12 of Table 3.

Equations 26 and 27 comprise the computations for the gaseous thermal conductivity which will be needed in the convective and conductive heat transfer calculations. These equations are based on a semi-empirical method of handling energy exchange in polyatomic gases Bird et al. (19). Equation 26 shows Eucken's formula for a single gaseous species i and Eq. 27 shows the equation used to estimate the conductivity of a gaseous mixture (22). This procedure requires the individual species viscosity (μ_i) and the coefficient ϕ_{ik} defined in Eq. 29.

The gaseous viscosity is calculated by means of Eqs. 28, 29 and 30. Equation 28 for a single gaseous species is based on a derivation for pure monatomic gases. The Stockmayer collision diameter σ and collision integral Ω_u , which is a slowly varying function of the dimensionless temperature (kT/ϵ) and the polar parameter ($\delta = (\text{dipole moment})^2 / 2\epsilon\sigma^3$), may be obtained from tabulated values (23). As with the thermal conductivity, the semi-empirical formula of Wilke (19) is used for the viscosity of the multicomponent gas mixture at low densities through Eq. 30.

The mass diffusivity for a single gaseous species i through the gas mixture m is determined with Eqs. 31, 32. This diffusivity is needed in both the devolatilization and oxidation equations and in the heat

transfer equations. For ordinary binary diffusion, the Chapman-Enskog formula for gaseous diffusivity at low density and for an ideal gas is given in Eq. 31 (19). The collision integral for diffusion Ω_d is a dimensionless function of the temperature and of the intermolecular potential field for one molecule of i and one of k . This function can be conveniently approximated by a Lennard-Jones function, (19, 23). This requires a suitable estimate of the Lennard-Jones parameters σ_{ik} and ϵ_{ik} from the individual species parameters σ_i and ϵ_i by

$$\sigma_{ik} = 1/2(\sigma_i + \sigma_k) \quad (37)$$

$$\epsilon_{ik} = \sqrt{\epsilon_i \epsilon_k} \quad (38)$$

The effective binary diffusivity of species i in the multicomponent mixture (D_{im}) is calculated as shown in Eq. 32. This formulation assumes that each species in the mixture moves with the same velocity (19).

Finally, the physical characteristics of the j th particle type are calculated with Eqs. 33 and 34. The particle is allowed to swell linearly with the extent of devolatilization as shown in Eq. 33. The swelling coefficient y must be specified a priori. This swelling during devolatilization is an experimentally observed phenomenon (24). This average particle diameter increase is often in the order of 10% (25). Experimental quantification of particle diameter change after devolatilization and during heterogeneous char oxidation do not seem to be available. Two possible options regarding the diameter of the char residue have been proposed and incorporated in the model. 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. This situation seems to be substantiated by visual observation of scanning electron micrographs of coal particle samples taken from combustors (24, 1, 26). Alternatively, the particle may be perceived to react mostly on the surface and thus burn out at a near constant density but as a shrinking particle. In this case

$$d_j = [6\alpha_j / (\pi\rho_{\sigma j})]^{1/3} \quad (39)$$

where ρ_j is the solid density of the j th particle type after complete devolatilization (ie. when $\alpha_j=0$). Both options have been coded in 1-DICOG. External particle surface area is shown in Eq. 34.

The calculations of gaseous properties such as thermal conductivity, coefficient of viscosity, and mass diffusivity require a large number of algebraic computations for each individual species as well as summations over all species. To minimize computational time, these iterative calculations for physical properties have been modularized in the computer code. This permits these calculations to be performed only when required due to significant property variations, rather than at every element. This strategy for computational efficiency is discussed further in the Solution Technique section.

E. RADIATIVE HEAT TRANSFER

The processes involved in coal conversion systems are known to be strongly influenced by radiative heat transfer within the reactor (27). Table 5 summarizes the equations required to solve the radiative interchange within a one-dimensional, particle-laden reacting system. The additional assumptions are made of a radiatively transparent gas phase and radiatively gray, non-scattering particles. The only radiative energy transfer is thus between the particles within the reactor and between the particle cloud and the reactor walls.

Radiative transfer involves an integral analysis arising from integration over all of the individual surface areas which are emitting and absorbing energy throughout the entire system. The zone method (27) is a rigorous technique for determining radiative transport, given the temperature and number density distributions. Its weakness lies in obtaining these distributions and in uncertainty of radiative properties of the solids. The resulting problem is solved by assuming an initial distribution for all T_j and n_j , calculating the resulting radiative fluxes by the zone method and then solving all the differential and constitutive equations with the given radiative transfer as input. The assumed profiles are then updated and the procedure is repeated. This iterative technique for the zone method is discussed further in the Solution Technique section.

The one-dimensional nature of this model simplifies the radiation solution technique. The entire length of the reactor is divided into a number of zones (usually about 250), each assumed uniform in ϵ_j and T_j and thin enough so that it may be assumed that no particle is hidden from view by any other particle within the zone. It is emphasized that in the formulation of 1-DICOG, these radiation regions or zones do not usually correspond with the elements used for numerically solving the differential equation set.

Equation 40 shows the net rate of radiative heat transfer per unit reactor volume to the j th particle classification from all other particles within the reactor. The first term on the right hand side depicts the absorbed portion of the total radiative energy arriving at that particle type surface per unit volume from all other particle surfaces within the reactor. The absorptivity is assumed equal to the

TABLE 5

1-DICOG CONSTITUTIVE EQUATIONS: RADIATIVE HEAT TRANSFER

NO.	TYPE	EQUATION
40	Radiative heat transfer in reactor	$Q_{fj} = (\pi/4) I_{qt} n_j d_j^2 \epsilon_j - I_{qoj} / \Delta x_p$
41	Local radiative intensity	$I_{qt} = \sum_p I_{pq}$
42	Radiative emission	$I_{poj} = (a_j T_j^4)_p \sigma \Delta x_p$
43	Radiative intensity	$I_{pq} = \left(\sum_j I_{poj} \right) \exp \left[- \sum_{p \neq q} \left(\sum_j a_j \right)_p \Delta x_p \right]$
44	Radiative adsorption coefficient	$a_j = (\pi/4) \epsilon_j n_j d_j^2$
45	Radiative heat exchange	$Q_{rbj} = (4\sigma \epsilon_b / D_s) (T_j^4 - T_b^4) \{ 1 - \exp[-E_\lambda (\pi/4) (D_s/2) d_j^2 n_j] \}$

emissivity ϵ_j . I_{gt} is the total intensity of the radiative energy reaching the zone q where the local n_j and d_j are assumed known. The second term depicts the energy emitted from the j th particle type originating in the q th zone.

Equation 41 shows how the total radiative intensity arriving at each zone q must be summed over all zones in the reactor. Eq. 42 represents the energy intensity emitted from the j th particle type at each of the p zones. Equation 43 is simply the Bouger-Lambert Law (27) for the attenuation of the one-dimensional beam due to its passage through the absorbing, non-scattering, particle cloud. The exponent term is the transmittance of the beam and $(\sum_j I_{p0j})$ is the intensity entering the p zone of thickness Δx_p . The radiative absorption coefficient for each particle type in each zone is given the local properties by means of Eq. 44. If both absorption and scattering were to be considered, this coefficient should be the total extinction coefficient, which would be the sum of the given absorption coefficients and scattering coefficients.

The above scheme is formal and correct with the given assumptions; however, it gives rise to some significant numerical problems in some applications. As mentioned previously, the zones must be selected so that each particle is optically visible; in other words, no significant attenuation must take place across the chosen radiative zone. Some gasification systems at high pressure and heavy particle loading do not readily satisfy the criterion. The BI-GAS gasification system is a case in point (28). In this case the optical depth is so small that the zone technique requires unrealistically small zones. In such cases improved computational efficiency and accuracy is achieved by treating the radiative transfer as a diffusion process for such systems.

For optically dense systems, Eq. 15 may be replaced by the diffusion equation as shown by Hottel and Sarofim (27).

$$Q_{fj} = \frac{-16\sigma T_j^3}{3\Delta x_p (\sum_j a_j)} \frac{dT_j}{dx} \quad (46)$$

The derivative of the j th particle temperature may be expressed in terms of the differential equation variables of Table 2 as follows:

$$\frac{dT_j}{dx} = \left[\frac{d(w_j h_j)}{dx} - h_j \frac{dw_j}{dx} \right] (1/w_j C_{pj}) \quad (47)$$

When Eq. 47 is substituted into Eq. 46 and subsequently into Eq. 6 of Table 2 and rearranged, the particle energy equation becomes:

$$\frac{d(w_j h_j)}{dx} = \left(\frac{1}{1 - A C_{rj}} \right) [m_{sj} h_{sj} + m_{pj} h_{pj} - A(C_{rj} h_j \frac{dw_j}{dx} + Q_{rbj} + Q_j + r_j h_j)] \quad (48)$$

where:

$$C_{rj} = (-16\sigma T_j^3) / (3\Delta x_p (\sum_j a_j) w_j C_{pj}) \quad (49)$$

This approach greatly simplifies the solution strategy for optically thick systems, since the radiation treatment no longer needs an iterative technique but can be solved directly with the differential equations. In this case, Δx_p becomes the volume element width. The reason for this simplification is that the diffusion approximation transforms the integral equations for radiation into differential equations of a form similar to the other differential equations of the model. 1-DICOG is coded to permit calculation by either the zone method or the diffusional approximation method described above.

Equation 45 presents the radiative heat transfer rate per unit reactor volume for energy exchange between the reactor walls and the cloud of the j th particles. This approximation assumes a gray, bounding surface with equal emissivity and absorptivity ϵ_b . The particle cloud is also assumed to have equal emissivity and absorptivity, approximated by the terms enclosed within the braces. This expression allows for reduction of either of the primary beams, (i.e. cloud to surface or surface to cloud). Secondary reflections are ignored. If the wall is considered black, there are no secondary reflections. The exponent within the brackets assumes spherical particles and a characteristic dimension taken to be the radius of the vessel ($D_s/2$). The other terms in the exponent between the brackets represent the projected area of randomly oriented particles with no negative curvature. E_s is an absorption efficiency and usually taken as unity. In order for Q_{rbj} to have the proper units, the area to volume ratio of the reactor must be identified. The term $(4/D_s)$, contained within the first set of parenthesis on the right hand side of Eq. 45 represents the cylindrical geometry chosen for 1-DICOG.

F. STATE AND MASS FLOW CONTINUITY

This set of constitutive equations shown in Table 6 is straightforward and requires little explanation. Eq. 50 shows the ideal gas equation of state chosen for this formulation for its simplicity and accuracy for high-temperature systems. Equations 52 through 57 show how the total particle mass is composed of each of its constitutive

TABLE 6

1-DICOG CONSTITUTIVE EQUATIONS: STATE AND MASS FLOW CONTINUITY

NO.	TYPE	EQUATION
50	Molar gas concentration	$C_g = p/RT_g$
51	Gas velocity	$v = w_g/\rho_g A$
52	Particle density	$\rho_j = \rho_{cj} + \rho_{hj} + \rho_{aj} + \rho_{wj}$
53	Coal density	$\rho_{cj} = \alpha_{cj} n_j$
54	Moisture density	$\rho_{wj} = \alpha_{wj} n_j$
55	Char density	$\rho_{hj} = \alpha_{hj} n_j$
56	Ash density	$\rho_{aj} = \alpha_{aj} n_j$
57	Particle mass	$\alpha_j = \alpha_{hj} + \alpha_{cj} + \alpha_{aj} + \alpha_{wj}$

parts, raw coal, char, ash and moisture. The density of each constituent (constitutive particle mass per unit reactor volume) is obtained from the constituent mass and the particle number density, each of which is obtained from the differential equation set.

Equation 51 deserves some discussion. In the formulation of 1-DICOG, the assumption is made of no velocity lag between the particle and gas phases; thus, the velocity of the gas is also the velocity of each particle. In addition, the particles may be assumed to occupy a negligible volume as compared to the gas phase volume. Under these conditions, the velocity is calculated directly from the equation of continuity for the gas phase as shown in Eq. 51. This approach alleviates the need to solve a momentum differential equation. Since the completion of 1-DICOG, there has been some motivation to incorporate the effects of particle drag. It is thought that the most significant effect would be to alter the particle-gas heat transfer rates due to increased convection. Stickler et al. (18) have incorporated particle lag by tracking the velocity difference between each particle classification and the gas phase. By assuming that the time scale for particle acceleration is small compared to that for mass loss, explicit integration of a conveniently chosen drag law reduces the formulation to a simple algebraic equation. This approach is feasible with 1-DICOG but is not included in the present version.

G. CONVECTIVE AND CONDUCTIVE HEAT TRANSFER

All heat transfer within the reactor comes from either radiation or conduction. Conduction may also be modified or augmented by convective flow. The previous Radiative Heat Transfer section, discussed the assumptions and equations for radiative heat transfer in 1-DICOG. This section concludes the discussion and heat transfer phenomena. An important aspect of the conductive/convective heat transfer is the effect of simultaneous mass transfer. The mass transfer aspects of the problem are discussed in more detail under the Particle Reactions section; thus, the next two sections are closely related.

Equation 58 of Table 7 represents the heat transfer rate per unit reactor volume between the j th particle classification and the gas phase. This equation reflects the assumptions of spherical particles and no slip between the gas and particle phases. The leading number 2 represents the mean conductive Nusselt Number for heat transfer from spheres without the presence of particle blowing. The term enclosed between brackets is the correction on the heat transfer rate for the presence of mass transfer or particle blowing. Smith (29) discusses the derivation of this term based on classical film theory as well as introducing other approximate corrections from other considerations. The blowing parameter or transpiration parameter for heat transfer is given in Eq. 60. The relationship of this parameter to that for mass transfer is also discussed in Smith (29). A transformed form of this parameter is sometimes called the Spalding Number (see Smith 29). The resulting Q_j is required for both the particle and gas differential energy equations.

TABLE 7

1-DICOG CONSTITUTIVE EQUATIONS: CONVECTIVE AND CONDUCTIVE HEAT TRANSFER

NO.	TYPE	EQUATION
58	Particle-gas heat transfer	$Q_j = 2\pi[B_j/(\exp B_j - 1)]k_g(T_j - T_g)d_jn_j$
59	Convective heat exchange with surroundings	$Q_{cb} = 4h_m(T_g - T_b)/D_s$
60	Transpiration parameter	$B_j = r_j C_{pg}/2\pi d_j k_g n_j$
61	Heat transfer coefficient-wall losses	$(h_m D_s/k_g) = 0.023 (Re_g)^{0.8} (Pr_g)^{1/3}$
62	Reynolds No.	$Re_g = D_s w_g/(\mu_g A_s)$
63	Prandtl No.	$Pr_g = (C_{pg} \mu_g/k_g)$

The sub-section entitled State and Mass Flow Continuity introduced a method of incorporating particle drag. Correspondingly, Eq. 58 would require modification. The mean Nusselt Number without mass transfer would change from 2.0 to

$$Nu_{jg} = 2.0 + 0.65 (Re_{jg})^{1/2} (Pr_g)^{1/3} \quad (64)$$

or some similar expression to account for the enhanced convective flow (see for example Kreith, (30)). Here Re_{jg} is the local relative Reynolds Number between the j th particle group and the gas.

The energy balance also accounts for convective heat exchange of the gas phase with the reactor walls. Equation 59 shows the expression for calculating Q_{cb} as a function of a mean heat transfer coefficient (h_m). This heat transfer coefficient can be obtained through empirical correlations for the Nusselt Number such as shown in Eqs. 61 to 63 (30).

H. 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 effect of oxidizer diffusion and high rates of mass transfer or particle blowing are incorporated. As presented schematically in Figure 2, the three overall mass loss processes for each particle are moisture vaporization, devolatilization and heterogeneous char oxidation. The corresponding equations are shown in Table 8. The model allows one moisture vaporization rate expression per particle, M devolatilization reactions per particle type of the form shown in Eq. 1, and L char oxidation reactions per particle type of the form shown in Eq. 2. Each of these reaction sets will be discussed in turn. The total reaction rate of the j th particle classification per unit reactor volume is then the sum of each of these reactions, $(L+M+1)$ in total number, as shown in Eq. 65.

The moisture vaporization rate is computed from the rate of diffusion of the moisture from the particle surface to the bulk gas phase. At the particle surface, the moisture mole fraction is assumed to be in equilibrium with the particle and is therefore be calculated from the equilibrium vapor pressure by use of Raoult's Law, as shown in Eq. 77. The vapor pressure is calculated from the particle temperature by either an Antoine Eq. 7 or an empirically fitted, five-term, power series in particle temperature. 1-DICOG was coded for either option. The resulting moisture vaporization rate, corrected for the presence of high mass transfer rates, is shown in Eq. 76. The derivation of this type of expression is discussed in Smith (29).

The devolatilization reaction Eq. 1 for the j th particle has been proposed by Ubayakar et al. (31). The kinetic rate of production of volatiles from the m th reaction is given in Eq. 72, where the reaction rate constant is given in Eq. 75 and the mass density of the raw coal

TABLE 8

1-DICOG CONSTITUTIVE EQUATIONS: PARTICLE REACTIONS

NO.	TYPE	EQUATION
65	Particle reaction rate to gas phase	$r_j = \sum_{\ell} r_{hj\ell} + \sum_m r_{vjm} + r_{wj}$
66	Net char reaction rate	$r_{hj} = \sum_m r_{hjm} - \sum_{\ell} r_{hj\ell}$
67	Oxidizer-char reaction rate	$r_{hj\ell} = (A_j n_j)^2 M_{hj} M_g \phi_{\ell} k_{cj\ell} k_{j\ell} \zeta_j C_{o\ell} C_g / [M_g A_j n_j C_g (\zeta_j k_{j\ell} + k_{cj\ell}) + r_j]$
68	Kinetic char rate	$k_{j\ell} = A_{j\ell} T_j^m \exp(-E_{j\ell}/RT_j)$
69	Transpiration parameter for mass transfer	$B_{mj} = r_j / (2\pi D_{om} \rho_g d_j n_j)$
70	Char mass transfer coefficient	$k_{cj\ell} = 2D_{om} B_{mj} / [d_j (\exp B_{mj} - 1)]$
71	Total coal reaction rate	$r_{cj} = \sum_m r_{cjm} = -[\sum_m (r_{hjm} + r_{vjm})]$
72	Volatiles reaction rate	$r_{vjm} = k_{mj} Y_{mj} \rho_{cj}$

TABLE 8 (Cont.)

NO.	TYPE	EQUATION
73	Char production rate	$r_{hjm} = r_{vjm}(1 - Y_{mj})/Y_{mj}$
74	Gas element production	$r_{jk} = \phi_{wjk}r_{wj} + \sum_{\ell} \phi_{h k \ell} r_{h j \ell} + \sum_m \phi_{v j k m} r_{v j m}$
75	Coal kinetic rate	$k_{mj} = A_{mj} \exp(-E_{mj}/RT_j)$
76	Moisture vaporization rate	$r_{jw} = [2\pi B_{mj}/(\exp B_{mj} - 1)] C_g M_w (X_{wj} - X_{wg}) d_j n_j D_{wg}$ $+ x_{wj} r_j$
77	Moisture equilibrium mole fraction	$X_{wj} = p_{ej}/p$

per unit reactor volume ($\rho_{c,j}$) was previously explained in Eq. 53 of Table 6. It is possible that volatile products could accumulate at the particle surface and in the particle pores. In this case, the rate of volatiles depletion would be affected by diffusion or convection from particle blow holes and from the immediate surface into the bulk gas phase while competing with condensation or repolymerization processes. If this were true, diffusion would affect the reaction rate and an expression similar to the moisture vaporization rate could be included (also see Smith (29)). It is important to realize that diffusional effects only become important when the volatiles can repolymerize or condense prior to diffusion into the gas phase. Because of uncertainties in the repolymerization rate coefficients, the nature of the volatiles diffusion process, and because the techniques and models used to correlate existing pyrolysis data most often have utilized forms like Eq. 72, 1-DICOG has been formulated with the pyrolysis model based on Eq. 72.

The recommended rate constants for devolatilization are shown in Table 9. The chosen two-step mechanism of Ubhayakar et al. (31) seemed to be a reasonable compromise between the simple one-step mechanism of Badzioch et al. (12), which would not account for the effect of particle history on volatiles yield, and a more complex, multistep mechanism of (i.e., Reidelbach and Summerfield (33)) which could increase computational time.

In accordance with Eq. 1 the devolatilization of the raw coal also produces char. A simple mass balance results in the rate of formation of char from the j th particle type per unit reactor volume from the m th reaction as shown in Eq. 73. Finally, the net rate of disappearance of the raw coal in the j th particle class may be obtained by summing over all of the m reactions. The rate of raw coal disappearance is the negative of the sum of the rate of char and volatiles formation according to Eq. 1 and as shown in Eq. 71.

Char is assumed to react heterogeneously by a gaseous oxidizer that diffuses to the particle surface, adsorbs, reacts with char, desorbs and diffuses back into 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. 67. The derivation of this equation is shown in Smith (29). 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. 68. Following the recommendations of Smoot and Pratt (17), values of the experimental constants are shown in Table 9. The mass transfer coefficient, which is also required must be corrected for particle blowing or high rates of mass transfer according to one of the theories discussed in Smith (29). The mass transfer coefficient without blowing may be calculated from an empirical correlation for the Sherwood Number such as (19):

TABLE 9

SELECTED KINETIC PARAMETERS FOR 1-DICOG

PROCESS	REFERENCE	REACTION	RATE CONSTANT	PARAMETERS
Devolatilization	Ubayakar et al. (17)	$\text{raw coal} \xrightarrow{k_1} Y_1(\text{volatiles})_1 + (1-Y_1)(\text{char})$	$k_1 = A_1 \exp(-E_1/RT_j)$	$Y_1 = 0.39$
		simultaneously with reaction 2		$A_1 = 3.7 \times 10^5 \text{ s}^{-1}$
				$E_1 = 17.6 \text{ kcal mol}^{-1}$
		$\text{raw coal} \xrightarrow{k_2} Y_2(\text{volatiles})_2 + (1-Y_2)(\text{char})$	$k_2 = A_2 \exp(-E_2/RT_j)$	$Y_2 = 0.8$
		simultaneously with reaction 1		$A_2 = 1.46 \times 10^{13} \text{ s}^{-1}$
				$E_2 = 60.0 \text{ kcal mol}^{-1}$
Char Oxidation with O_2	Field (20)	$2C + O_2 \xrightarrow{k} CO$	$k = T_j(A + BT_j)$	$A = -1.68 \times 10^{-2} \text{ ms}^{-1}K^{-1}$
				$B = 1.32 \times 10^{-5} \text{ ms}^{-1}K^{-2}$
Char Oxidation with CO_2	Mayers (21)	$C + CO_2 \xrightarrow{k} 2CO$	$k = AT_j^n \exp(-E/RT_j)$	$n = 1.0$
				$A = 4.40 \text{ ms}^{-1}K^{-1}$
				$E = 38.7 \text{ kcal mol}^{-1}$
Char Oxidation with H_2O	Mayers (22)	$C + H_2O \xrightarrow{k} CO + H_2$	$k = AT_j^n \exp(-E/RT_j)$	$n = 1.0$
				$A = 1.33 \text{ ms}^{-1}K^{-1}$
				$E = 35.1 \text{ kcal mol}^{-1}$

$$Sh = (k_{co} d_j) / (D_{im}) = 2.0 + 0.65 (Re_{jg})^{1/2} (Sc)^{1/3} \quad (78)$$

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 the gas phases. When there is no particle lag, as is assumed in this version of 1-DICOG, this expression reduces to the theoretical value of 2.0 for molecular diffusion and the resulting expression for k_{co} , corrected for particle blowing, is given in Eq. 70. In this case, the blowing parameter is that for mass transfer as described in Smith (29) and shown in Eq. 69.

Since char is being formed by each of the m devolatilization reactions and also being depleted by each of the ℓ oxidation reactions, the net rate of char reaction is given in Eq. 66. Since the heterogeneous reaction is zero order with respect to the char concentration, heterogeneous ignition is permitted. Thus ignition phenomenon of the coal is not limited to devolatilization. Heterogeneous surface ignition is possible even if devolatilization has not been initiated.

Finally, each of the particle reactions act as a source for gas-phase material. In keeping with the local gas phase equilibrium assumption discussed in the next section, only element balances need be tracked. The total rate of production per unit reactor volume of the k th element from the j th particle is shown in Eq. 74. It is simply the sum of the stoichiometric coefficient times the reaction rate for each of the particle reactions. All of the r_{jk} values are needed for Eq. 1 of the differential equation set as shown in Table 2.

I. LOCAL GAS PHASE EQUILIBRIUM

By use of the gas phase continuity equation (Eq. 3, Table 2), the mass fraction of the elements in the gas phase may be followed. The energy balance for the gas phase (Eq. 5, Table 2) gives the history of the energy level throughout the reactor. This information, together with the specified reactor pressure, is sufficient to permit gaseous equilibrium calculations which produce the gaseous species composition and the local gas temperature. This local gas phase equilibrium assumption is justified if it can be assumed that the heterogeneous and particle reactions are much slower than gas phase kinetics. In addition, the one-dimensional assumption requires instantaneous radial mixing and ignores turbulent fluctuations. The equilibrium assumption is at least consistent with other levels of approximation in 1-DICOG.

Calculating the complex equilibrium states and temperature at prescribed pressure and enthalpy is not a simple task. Three schemes could be considered, namely: equating of forward and reverse rates, equilibrium constant formulation, and Gibbs function minimization. The first, dynamic equilibrium scheme, encounters all the difficulties of a full kinetic scheme. Even if all the reactions could be identified, there still remains the task of finding accurate experimental rate constants, to say nothing of the numerical scheme to solve the set of equations. The second scheme, the equilibrium constant approach, is perhaps the most familiar and conceptually the easiest to formulate; however,

it is known to be equivalent to the Gibbs function minimization principle for a mixture at specified energy level and pressure, but is highly inefficient for complex chemical systems. The third scheme which determines the mixture composition corresponding to the minimum total Gibbs free energy of the reacting mixture was first described by White et al. (37). This approach has been proven to be vastly superior in its computational efficiency to the other schemes. Algorithms for calculating chemical equilibrium based on this principle have been developed. Among the more well known of these are the NASA-Lewis program (38) and the Edwards Air Force Base program (39). Both were developed for the aerospace industry.

1-DICOG was coded with a thermochemical equilibrium subroutine based on the Edwards program (39). The existing code was stripped of all statements not pertaining directly to the equilibrium calculations and then implemented straightforwardly. The efficiency of this subroutine is crucial since its complex equilibrium calculation may be performed as many as 30,000 times during the course of a computer computation for a typical coal reactor.

J. SPECIFIED MIXING PROCESSES

Since entrainment of the secondary air into the primary jet is a multidimensional process, it cannot be predicted by a one-dimensional calculation. Likewise, the recirculation process within the reactor is not predictable without multidimensional computations. These two processes are accounted for in 1-DICOG by the a priori specification of these respective rates of entrainment and recirculation (m_s , m_p). This section discusses ways of modeling these terms. It should be noted that 1-DICOG does not require either of these processes to be included. For example, if a plug flow approximation is valid throughout the computational domain, then m_s and m_p are set to zero.

1. Secondary Mixing

When incorporating the effects of secondary mixing, the one-dimensional scheme of 1-DICOG may be thought of as following the progress of the primary jet. As shown in Figure 4, the jet is assumed to expand into the reaction chamber at a growth angle θ . This jet expansion is observed to be nearly linear and appropriate values for the growth angle θ may be obtained from Abramovich (40). The flow within the jet is assumed to have a uniform velocity profile at all axial positions in accordance with the one-dimensional nature of the computation. The secondary stream is allowed to entrain into the primary jet at a mass addition rate m_s (mass of secondary per unit time per unit axial length). Several of these parameters must be identified to completely specify the problem, each of which is needed for the differential equation set of Table 2. These are:

m_{sg} : total mass-addition rate of the gas from the secondary stream ($\text{g cm}^{-1} \text{s}^{-1}$)

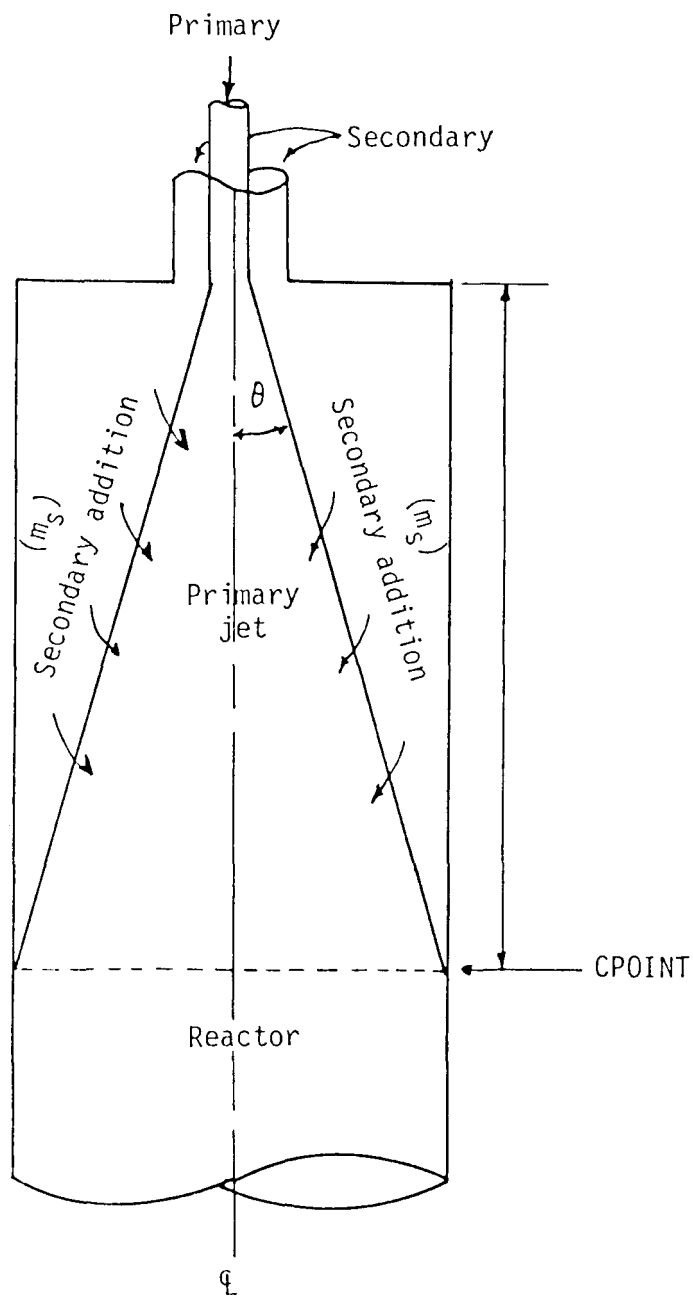


Figure 4. Schematic representation of the secondary mixing process.

m_{sj} : total mass addition rate of the j th particle classification from the secondary stream ($\text{g cm}^{-1} \text{s}^{-1}$)

m_{sgk} : total mass addition rate of the k th gas phase element from the secondary stream ($\text{g cm}^{-1} \text{s}^{-1}$)

h_{sg} : enthalpy of the gas phase portion of the secondary stream ($\text{g cm}^{-1} \text{s}^{-1}$)

h_{sj} : enthalpy of the j th particle classification in the secondary stream (cal g^{-1})

Often, there are no particles in the secondary stream in which case $m_{sj} = 0$. The elemental mass addition rate (m_{sgk}) is readily obtained from the elemental composition of the secondary stream together with the secondary gaseous addition rate m_{sg} . The enthalpy levels of the secondary components (h_{sg} , h_{sj}) required by 1-DICOG from the reference state of 298 K, are evaluated at the secondary temperature. For example:

$$h_{sg} = h_{sg}^o + \int_{298}^{T_s} C_{psg} dT \quad (79)$$

This value is taken as constant throughout the mixing process.

The final value to be specified (m_{sg}), must be defined as an appropriate function of the axial coordinate x . In reference to Figure 4 the value of m_{sg} must be finite and positive for $0 < x < \text{CPOINT}$ and must have a zero value for all $x = \text{CPOINT}$. Within the code the FORTRAN variable CPOINT identifies the end of the mixing region. This value is obtained directly from the given growth angle r and the reactor dimensions. Any reasonable function for m_{sg} is permissible. An additional requirement is the conservation of mass such that:

$$w_{gs} = \int_0^{\text{CPOINT}} m_{gs} dx \quad (80)$$

Stickler et al. (18) have used an exponential form for m_{sg} . The present version of 1-DICOG is coded to handle any power series in x up to a quadratic. This could be easily altered to take any arbitrary function of x by changing only a few FORTRAN statements.

2. Recirculation

The recirculation process downstream of a sudden dump region fed by two coaxial jets with particles is extremely complex. If this process is to be specified in a one-dimensional framework, the description can only be expected to be qualitative at best.

The same parameters for recirculation must be prescribed for use in the differential equation set of Table 2 as were needed for secondary mixing; namely m_{pg} , m_{pj} , m_{pgk} , h_{pg} and h_{pj} . Figure 5 schematically represents the recirculation process. In this case, there is a region of detrainment as well as one of entrainment with respect to the primary jet.

Determining the amount and distribution of recirculation of gases and particles is a difficult task. Thring and Newby (41) have proposed a simple theoretical treatment for recirculation based on empirical laws of entrainment for a free jet. More refined theories for confined jets have been put forward by Craya and Curtet (42), Barchilon and Curtet (42) and Hill (44). These empirical theories have been reviewed by Field et al. (6) and Beer and Chigier (45). None of these approaches were meant for two coaxial jets with a sudden-dump configuration, so they could not be expected to apply directly; however, they are able to give guidance for order-of-magnitude estimates of the amount of recirculating material.

To construct general functions in x for each of the gaseous recirculation parameters is difficult. An overall mass balance requires that:

$$\int_0^{\text{CPOINT}} (m_{pg} + \sum_j m_{pj}) dx = 0 \quad (81)$$

In addition an overall energy balance requires that:

$$\int_0^{\text{CPOINT}} (h_{pg} m_{pg} + \sum_j h_{pj} m_{pj}) dx = 0 \quad (82)$$

These two statements require that no net change in mass or energy is permitted through the recirculation process.

1-DICOG has been formulated and coded to allow the user to incorporate any function he deems realistic with a minimum of statement changes. The difficulty in formulating an approach lies in the fact that in the recirculation zone itself, the particles can continue to react. The extent of reaction is very much dependent on the point of exit from the primary jet, the length of time in the recirculation zone, and the

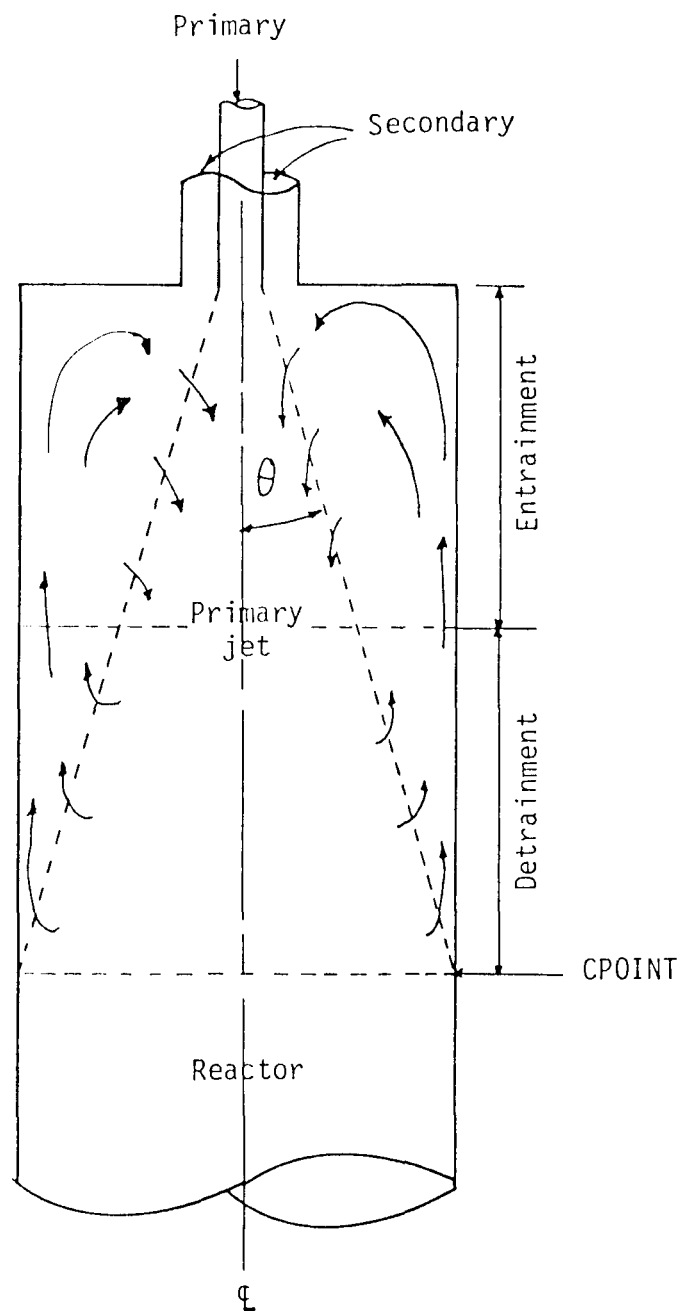


Figure 5. Schematic representation of the recirculation process.

point of reentry. The composition of the gas is also changing due to particle reaction in the recirculation zone. In addition, there will be a different history involved with the particles that are recirculated and those that are not. Without a full, multi-dimensional calculation, the exact influence of these parameters can not be stated. The approach which is outlined next is only meant to be an example of how this might be handled.

First, it has been observed experimentally (26) that, in some reactors, the particle dispersion is very much slower than gas mixing. In this limiting case, there are comparatively few particles that are recirculated. By making the assumption of no particle recirculation, the problem is already greatly simplified, since none of the particle recirculation parameters are required. The constraints are now reduced to:

$$\int_0^{CPOINT} m_{pg} dx = 0 \quad (83)$$

$$\int_0^{CPOINT} m_{pgk} dx = \int_0^{CPOINT} \omega_{pgk} m_{pg} dx = 0 \quad (84)$$

$$\int_0^{CPOINT} h_{pg} m_{pg} dx = 0 \quad (85)$$

Next, the midpoint of the recirculation zone is defined as the dividing point between detrainment and entrainment (see Figure 5). Since there are no particles in the recirculation zone, no reaction is allowed to take place in this region. The properties (ω_{pgk} , h_{pg}) of this recirculating gas are chosen to be constant and equal to the properties of the gas stream at some average location in the detrainment stage of the process (for example where $x = 3CPOINT/4$). This means that ω_{pgk} and h_{pg} can be factored from Eqs. 84 and 85 and all three constraints reduce to Eq. 83. The solution technique is iterative due to the radiation treatment. It is consequently, a straightforward matter to initially guess values for ω_{pgk} and h_{pg} and find the correct values iteratively. Finally, m_{pg} is defined as a function of x to meet the constraint of Eq. 83. A reasonable approach would be to choose any function symmetric about $CPOINT/2$ and the x axis. A simple but reasonable function is a straight line with x -intercept at $CPOINT/2$. The total mass flow rate of recirculated gas is determined by one of the integrals below

$$\int_0^{CPOINT/2} m_{pg} dx = \int_{CPOINT/2}^{CPOINT} -m_{pg} dx = w_{pg} \quad (86)$$

By choosing an appropriate ω_{pg} the problem is completely defined.

III. SOLUTION TECHNIQUE

The set of $6J + K + 2$ first order, non-linear, ordinary differential equations of Table 2, and the associated constitutive algebraic equations must be solved simultaneously in a numerical scheme. The zone method for radiation and the recirculation treatment both require an iterative solution technique. The tight coupling between differential equations through particle-gas interaction terms causes numerical stiffness. The overall procedure for overcoming these obstacles and obtaining an economic and efficient solution procedure is discussed in this section.

A. DIFFERENTIAL EQUATION SOLVER

There are many numerical techniques available for solving ordinary differential equations. The solution strategy chosen for 1-DICOG was an Adams-Moulton Predictor-Corrector method. Several recent, efficient implicit algorithms were also examined (46, 47). These methods require Jacobian information which cannot be obtained explicitly with the differential equations of Table 2. The Jacobian could be determined through a numerical differentiation scheme but this was not thought to be an efficient approach. This particular equation set requires a large amount of computation for an evaluation of a derivative. As can be studying Table 2, each time a derivative is to be determined all of the constitutive equations must be solved, including the complex thermochemical equilibrium algorithm. The attractive advantage of the predictor-corrector methods is that they require a minimal number of derivative evaluations to be computed at each step (as compared with four evaluations for the Runge-Kutta method, for example).

The method incorporated in 1-DICOG calls for an Adams-Bashforth Predictor, namely:

$$y_{n+1} = y_n + \frac{h}{24} (55y'_n - 59y'_{n-1} + 37y'_{n-2} - 9y'_{n-3}) \quad (87)$$

In this equation, y represents the independent variable and y' is the derivative with respect to the dependent variable, n is the particular step in question and h is the step size. The predicted function value is thus based on the last function value and the derivatives at four back points. The error term associated with this predictor (48) is:

$$\left(\frac{251}{6}\right) \frac{h^5 y^{(5)}}{5!} \quad (88)$$

After predicting the value of each function at $(n+1)$ from Eq. 87 the predicted values of y_{n+1} are used in the differential equation

set and in the constitutive equations to determine a predicted value for each derivative at (n+1). After this evaluation, the predicted value of the function is then corrected with an Adams-Moulton corrector

$$y_{n+1}^{(c)} = y_n + \frac{h}{24}(9y_{n+1}'^{(p)} + 19y_n' - 5y_{n-1}' + y_{n-2}') \quad (89)$$

In this equation, y_{n+1} is the corrected functional value at (n+1) and y_{n+1}' is the predicted derivative at the (n+1) step. The accuracy is thus greatly enhanced. With the new corrected value of each function at (n+1), the derivatives may be updated from the differential equation set and the auxiliary equations.

It can be obviously proposed to first predict and then correct, and if the two are not close enough, the correction could be repeated several times, using the latest estimate of the derivative, until no appreciable change occurs. Hamming (48) points out that, as a matter of principle, it is generally better to shorten the interval than to do repeated evaluations of the corrector formula (Eq. 89). During application in 1-DICOG, where the system is very dynamic and changing radically from one region to the other, it can be more economic to repeat the corrector for a few steps than to change the step size for an entire region. The trade-off is optimized by finding which requires the minimum number of derivative evaluations. 1-DICOG has been coded to allow the user to apply as many or as few correctors as desired. The sum of the derivatives of all particle energy equations (Eq. 6, Table 2) is monitored continuously and if this sum changes drastically from predictor to corrector then another corrector and another evaluation are applied. The test is performed again to determine if any more correctors should be applied. The user specifies the convergence criterion as well as the maximum number of correctors permissible. The particle energy equations are used since they have been found to be a sensitive measure of the stability of the whole system. It appears that the coupling through Q_{ig} is so tight that it reflects the first signs of instability. The number of correctors applied at each computational step is printed on the output to allow the user to evaluate his choice of step sizes.

This Adams-Moulton predictor-corrector method requires the derivatives at four back points before it can be initiated. This function and derivative information for the first four increments are obtained by a regular Runge-Kutta, fourth-order method (48) namely

$$k_1 = hy'(x_n, y_n)$$

$$k_2 = hy'(x_{n+h/2}, y_{n+k_1/2})$$

$$k_3 = hy'(x_{n+h/2}, y_{n+k_2/2})$$

$$k_4 = hy'(x_{n+h}, y_{n+k_3})$$

$$y_{n+1} = y_n + (k_1 + 2k_2 + 2k_3 + k_4)/6 \quad (90)$$

As soon as the first four increments have been completed the Adams-Moulton Predictor Corrector technique is initiated.

With appropriate step-size control discussed below this differential equation solution procedure is found to give accurate results with good stability.

B. TREATMENT FOR RADIATION

The approach for the calculation of radiant energy transfer within the reactor was introduced in the section entitled Radiative Heat Transfer. The radiative heat transfer and the recirculating fluid mechanics are the only mechanisms which require an iterative solution procedure. In some isolated cases where the radiation may be closely approximated by a diffusion process (see the Radiative Heat Transfer section) and where recirculation is not considered, then the differential equations may be recast (particularly Eqs. 5 and 6 of Table 2) and solved directly with the methods described in the previous section with no iteration.

The iterative technique is initiated by guessing initial profiles for each particle classification for temperature (T_i), number particle density (n_i), diameter (d_i) and the required recirculation parameters (h_{pg} , ω_{pgk}). The subroutine INPUT in the present version of 1-DICOG generates initial guesses for these profiles if a restart data set is not specified. The restart data set is an appropriately formatted output set these required variables from previous iterations or calculations of 1-DICOG. The user is thus allowed to stop 1-DICOG after any given iteration and continue without any penalty. This restart option also allows the user to find a previous computation to specify an initial guess for the new computation.

From these initial guessed profiles, the first estimate of radiative heat transfer is computed. The set of differential equations, with constitutive relations, is integrated along the reactor as described in the previous section. The resulting temperature profile and local properties are used to compute radiative transfer for the next iteration. This process is repeated until the user-specified convergence level is achieved. The convergence criterion is defined as a variation in the root mean square of the temperatures of each particle classification as follows:

$$\text{SUMSQ} = \left[\frac{1}{PJ} \sum_p \sum_j (T_{j\text{old}} - T_{j\text{new}})^2 \right]^{1/2} \quad (91)$$

where P is the total number of increments, J is the total number of particle types, $T_{j\text{old}}$ is the jth particle temperature of the last iteration, and $T_{j\text{new}}$ is the jth particle temperature of the present iteration. When SUMSQ has reached a user specified minimum the solution is considered converged. For this work a value of 5 Kelvin degrees was required for convergence. Figure 6 depicts the solution strategy outlined in these two sections.

C. STEP SIZE CONTROL

The zones required by the radiation treatment and the increments of the differential equation are not theoretically related. This section discusses how these step sizes are handled in 1-DICOG and how computational efficiency has been enhanced by using different step sizes at appropriate regions of the reactor.

1-DICOG is coded so that the reactor is initially divided into a userspecified number of equal-sized radiation zones or regions. These zones are used for computation of the radiation properties. Then, these radiation regions are further subdivided into equal sized steps for the ordinary differential equation (O.D.E.) solver. The user specifies the number of O.D.E. steps per radiation region. Although the functional values of each variable are computed at each O.D.E. step, they are only saved at each radiation region. The stored value of each variable is a spaceweighted average of all the O.D.E. steps within the radiation region. The final output contains the saved variables at each of the equally spaced radiation regions. This approach allows maximum versatility with a minimum amount of storage.

As mentioned in the Physical Properties Section, the calculation of the physical properties requires a great deal of summation arithmetic which could conceivably absorb an unacceptable share of the computational time. This is minimized by a user-specified variable, which controls the frequency of calculation of this tedious property updating. The user identifies the number of O.D.E. steps per property update; thus, variables, such as viscosity, thermal conductivity, and mass diffusivity are only calculated as frequently as deemed necessary.

Finally, physical characteristics of coal conversion processes help to identify regions in the reactor where numerical problems may arise. Often, there is a region of physical coal particle heat-up where very little is happening, followed by a region of dynamic exponential temperature and reaction rate growth due to rapid devolatilization. Usually this is followed by slower char oxidation and even complete particle burnout. It is apparent that a variable step size would be a great advantage for such a system. The predictor-corrector technique does not lend itself to a true variable step size approach since it is based on four equally spaced back points. 1-DICOG circumvents these difficulties by identifying four physical regions in the reactor and using different step sizes in the four regions but equal size steps for any given region. The four regions are: (1) initial particle heat-up,

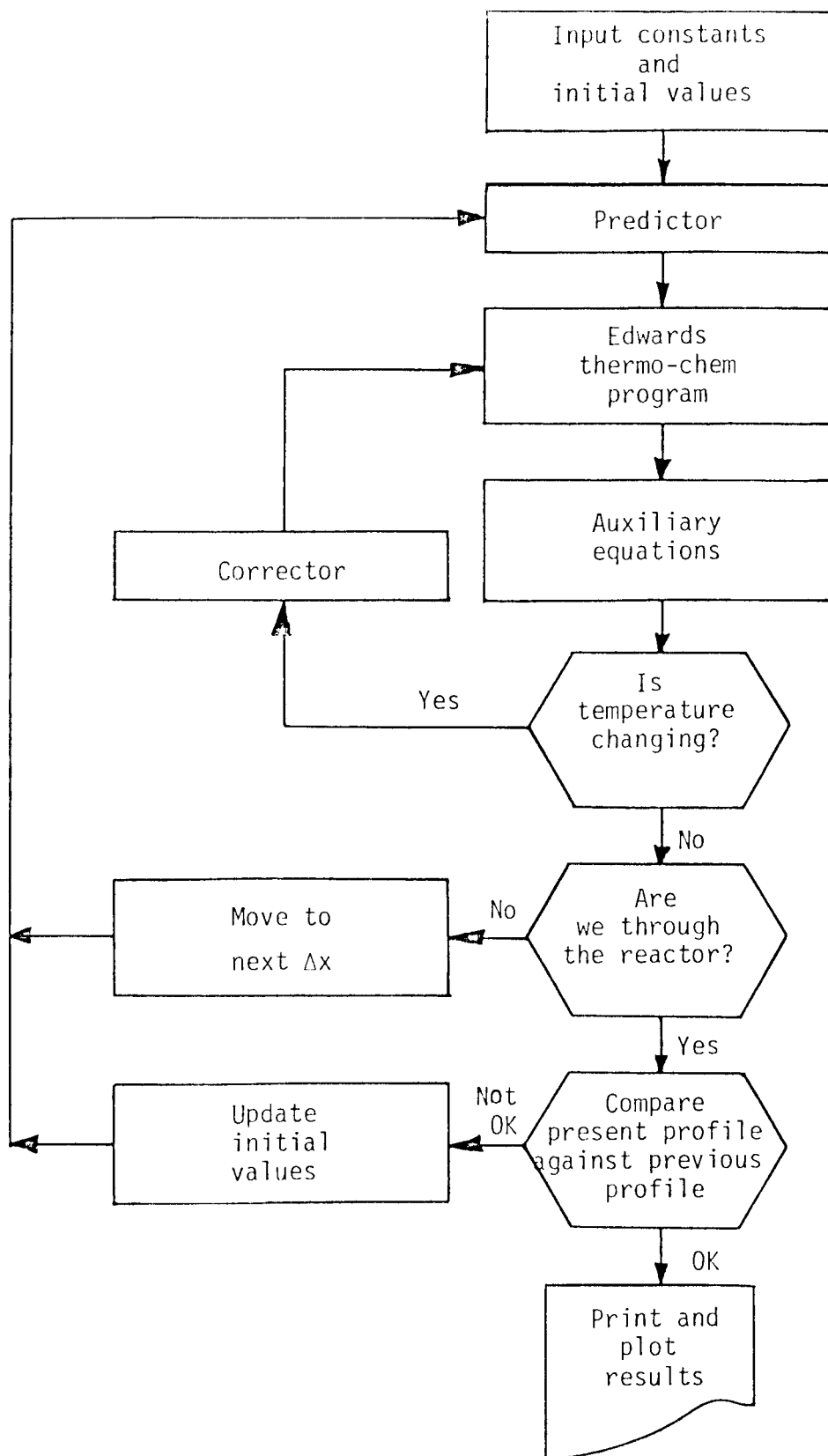


Figure 6. Information flow for 1-DICOG.

(2) devolatilization, (3) after devolatilization but during char burnout, (4) after char burnout. In this approach, the integration procedure proceeds until a flag is raised indicating a physical region border has been crossed (i.e. for the change between regions (1)-(2), a specified particle temperature is reached, for (2)-(3), volatiles are depleted from all the particle types, and for (3)-(4) all the char has been consumed). The existing step size is continued until a radiation region is reached. At that point the O.D.E. solution technique is terminated and reinitiated with the new step size. This means that the Runge-Kutta method is used for the next four O.D.E. steps then the Adams-Moulton predictor corrector method is reinitiated, all at the new step size. The user specifies the O.D.E. step size used in each region by specifying the initial number of O.D.E. steps per radiation region for region (1) above; then, by specifying what multiple of this will be used for each subsequent region. For region (4), where very little is happening, the specified factor is a division factor which allows the user to specify large steps to minimize computational time. A wise use of these step size control options permits extremely efficient use of the computational time spent on any given problem.

D. NUMERICAL STIFFNESS

In systems of differential equations, the term "stiff" has been classically used when such systems correspond to tight coupling between the driver and the driven in servo-mechanisms. This type of phenomenon is typical in such situations as control and kinetic systems. Indeed, all of the equations of Table 2 show signs of this kind of coupling. Luckily, the coupling is not too tight and a wise use of repeated correctors and of step size control is usually sufficient. Extensive experience with this set of equations uncovers one particularly difficult problem with stiffness. The problem occurs after or near complete burnout of the particle, the reaction rate is negligible and the energy of the system only changes due to heat transfer effects such as radiation and convection to the reactor walls, conduction between particles and gas, and particle-particle radiation within the reactor. A tight coupling is observed in the particle and gas energy differential equations (Eqs. 5 and 6 of Table 2) through the gas-particle conduction term. This problem does not occur to such an extent in regions where secondary mixing or recirculation are significant or in regions where the particle is reacting strongly. In such regions, these respective terms overshadow the gas-particle conduction term. 1-DICOG allows for the introduction of the pseudo steady-state approximation (pssa) for stiff differential systems (49). This approach need only be invoked after secondary mixing, recirculation and reaction rates become negligible and stiffness becomes severe.

The stiffness criterion is established by monitoring the value of the sum $(Q_{fj}Q_{rbj}-Q_j)$ for each particle type after secondary mixing and recirculation are complete. When this value drops to a user specified minimum (on the order of 10^{-2} - 10^{-3}), then the pssa is invoked for that particle classification. At this point, the particle and gas energy equations form the stiff differential set and the particle temperature is the particular stiff variable which is sought. The technique requires decomposition of each of the particle energy equations as they go stiff.

The pssa method calls for setting $d(w_j h_j)/dx=0$ resulting in Eq. 4 of Table 2 becoming an algebraic expression.

$$0 = m_{sj} h_{sj} + m_{ij} h_{i,j} + A(Q_{fj} - Q_{rbj} - Q_j - r_j h_j) \quad (92)$$

From this, the temperature of the j th particle type must be determined. At this point in the reactor, the first two terms are identically zero. The last reaction rate term will be very small but conceivably finite. This term is assumed to change insignificantly with temperature and is taken as the value at the immediately past O.D.E. step. The remaining terms are functions of T_j or $T_{i,j}$. With a little algebraic manipulation, an extremely fast iterative procedure is obtained for T_j . This value may then be used in the gas differential energy equation and the solution proceeds as normal. This technique is easily derived for radiation heat transfer (Q_{fj}) calculated from either the zone method or the diffusion method.

The success of the pssa method in this particular application can be explained on physical grounds. Stiffness is not a problem with the reaction rate terms. The Adams-Moulton predictor-corrector is sufficient to handle the heterogeneous reactions. Stiffness is a result of the particle-gas heat transfer but only towards the end of the reaction process. On physical grounds, this is when the derivative of the particle energy approaches zero, or in other words when the total particle energy stops changing. Thus, the "steady state solution" has been reached and pssa solves the equations efficiently.

This approach is an extremely powerful tool in increasing computational efficiency. By skillful use of the techniques outlined in the section on Solution Technique, computational time for 1-DICOG is on the order of 2 CPU minutes per particle type per length iteration on a relatively small DEC-SYSTEM 10 computer. Convergence requires usually about six iterations.

This code has been applied to the prediction of a large number of pulverized coal combustion and gasification systems. Predictions have included parametric studies of model parameters and combustor variables. Predicted results have been compared with measurements. These predictions and the comparisons with measurements are presented in Volume 1 of this final report.

IV. 1-DICOG CODE

A. GENERAL DESCRIPTION

1. Language and Availability

Every effort has been made to write 1-DICOG in ANS (American National Standard) FORTRAN-IV. Syntax should thus be compatible with most compilers. Plotting routines, which are used for convenience in interpreting the output, have been included. These routines were designed for use with a CALCOMP plotter. Plotting is not an essential feature of the output since all numbers plotted also appear in the written output. Plotting may be omitted by simply deleting lines 136 through 254 in subroutine OUTPUT and by omitting completely subroutines GRPH, ASCALE and LGND.

The total number of card images, including comment card as listed in Appendix B is 3340. Card decks punched in EBCID card format are available upon request from the authors for a specified cost.

2. Units

All input data to 1-DICOG must be in cgs units. All working variables within the program are either dimensionless or in cgs units. Units associated with all variables are given in the Nomenclature.

3. Debugging

Inevitably, problems will arise concerning the application of 1-DICOG to the individual needs of the user. A debugging feature in the code allows varying degrees of debugging output. The level desired is simply specified by setting the variable "BUG" in the input data to its corresponding value. BUG=0 is the normal operating condition. No extra debugging output is printed. All output will look like the output shown in the example calculation given in Appendix A. BUG=1 causes outprint of all previous output plus values of variables appearing in the differential equations as they are calculated. The variables output from each subroutine are as follows:

SOLVE: x, T_g, T_j

DIFF: v, n_j, A

RODEVL: $w_g, w_j, h_g, h_j, \alpha_k, \alpha_h, \alpha_w, \alpha_c, A$

AUX1: $\omega_c, \omega_h, \omega_w, \omega_a$

AUX3: $Q_{cb}, Q_{rbj}, Q_j, Q_f, r_{jk}, r_{cj}, r_{wj}, r_{jg}, r_j$

BUG=2 causes outprint of all previous output plus values of variables which have a significant impact upon the differential equations. The variables output from each subroutine are those of BUG=1 plus the following:

RINTS: I_{op}, I_{qt}
 AUX1: $C_{pcj}, C_{phj}, C_{paj}, C_{pj}, T_j, h_j, h_{old}, \rho_{cj}, \rho_{hj}, \rho_{wj},$
 $\rho_{wj}, \rho_j, h_h, h_w$
 AUX2PR: k_g, ω_g
 AUX3: $r_{hjm}, r_{cjm}, r_{hj\ell}, B_j, B_{mj}, r_{h\ell}, \sum r_{vjm}, \sum r_{hvjm}$
 EQUIL: $T_g, M_g, C_{pg}, X_i, C_{pi}, h_g, \rho_g, C_{ol}$

BUG=3 causes outprint of all previous output from each subroutine as listed under BUG=1 and BUG=2 plus the following:

SOLVE: $d(W_g^{\omega_p})/dx, d(W_j)/dx, d(W_g h_g)/dx, d(W_j h_j)/dx, d(vn_j A)/dx,$
 $d(W_g)/dx, d(\alpha_{cj})/dx, d(\alpha_{nj})/dx, d(\alpha_{wj})/dx, (W_g^{\omega_k}), W_j,$
 $(W_g h_g), (W_j h_j), \alpha_g, \alpha_{cj}, \alpha_{hj}, \alpha_{wj}$
 AUX2PR: k_j, μ_j
 AUX3: $k_{mj}, r_{vjm}, k_{\ell j}, C_g, A_j, P_{ej}, X_{wj}$

BUG=4 causes outprint of all previous variables plus additional information on the physical properties. The variables which are output are all of those listed under BUG=1 through BUG=3 plus the following:

AUX2PR: $\Omega_\mu, \Omega_D, \sigma_{ijk}, Re, Pr, h, D_{ij}, D_{om}$

BUG=5 causes output of all previous variables plus additional information on radiation. The variables which are output are all of those listed under BUG=1 through BUG=4 plus the following:

RINTS: $a_j, (a_j T^4), \sum I_{pg}$

BUG=6 is a special level designed for debugging the radiation subroutine RINTS only. All of the variables in RINTS are output then the program execution will terminate.

In the incremental technique employed in 1-DICOG, there could conceivably be several thousand increments in each iteration. Printing each variable for each iteration would generate several hundred pages of output. To help with paper conservation when debugging 1-DICOG, the user may specify the frequency of the debugging printout by setting the value of the variable "NPRINT" (see section entitled Input). For example, with NPRINT=1, each variable specified by the debug option BUG would be printed for every increment; whereas, if NPRINT=10 each variable would be printed only after every ten increments. The only exception to this rule is the printing of variables in subroutine SOLVE. This subroutine is not subject to restrictions by NPRINT and the output selected by the BUG option will be printed for every iteration. A little experience in debugging 1-DICOG will quickly show the wisdom behind this logic.

B. DESCRIPTION OF SUBROUTINES

Each of the subroutines in 1-DICOG is briefly described in this section. The listing of the program is given in Appendix B. Detailed descriptions of model equations and assumptions were given previously. The purpose of this section is to briefly acquaint potential users with the operations performed in each subroutine and thus present a rough overview of the program structure. Detailed understanding of subroutine operations can only come through careful study of the FORTRAN code.

MAIN. The main routine is only a short scheme which controls overall operation of the program. Control of the number of system iterations required for convergence of the temperature profiles for radiation is handled in MAIN. Step size control for different regions in the calculation is also managed in this routine.

ASCALE. This is a self-scaling subroutine used by GRPH to establish ordinate and abscissa values.

AUX1. This is the first of three subroutines which computes the values of each of the constitutive equations required in 1-DICOG. The order of solving these auxiliary-equations is chosen for convenience. Those equations solved in AUX1 are for the most part needed in AUX2PR and/or AUX3.

AUX2PR. All the gas phase physical property equations are modularized into this subroutine. This routine is only called after every NPROP ODE steps to save on computational time when desired.

AUX3. This is the final subroutine for evaluating the auxiliary equations. This routine concentrates mostly on the particle reaction equations. It includes an iterative scheme for calculating the total particle reaction rate r_j .

DIFF. This subroutine calculates the value of each of the differential equations in the system at each of the evaluation stages of the predictor corrector solution technique. This is actually done at the end of the subroutine. Performing this task requires updated values

for each variable. The first part of the routine obtains these values by controlling call statements to the appropriate subroutines.

EDWRDS. This is the main controlling routine for the thermochemical equilibrium calculations. This routine initializes required variables and calls the other thermochemical subroutines.

FIND. This is short extrapolation subroutine used by SIGMAM.

GRPH. The initial plotting routine for plotting the output on an available CALCOMP plotter with the BYU DEC-10 computer.

INPUT. This routine is rather long but only performs three functions. First, all of the input data are read into 1-DICOG through the subroutine INPUT. Secondly, default values of certain variables are established. Finally, all input variables are printed for review.

LGND. This is a small subroutine for printing a title or legend on the plot created by GRPH.

OPEN. This is a short subroutine used on the BYU DEC-10 to open the input data file on disc.

OUTPUT. This subroutine controls printing and plotting of all output information.

PROFIL. This subroutine saves all the profiles in their appropriate arrays in preparation for printout and plotting. In addition some of the profiles prepared here are used for the next pass through the reactor in calculating initial profiles for RINTS. It should be noted that values are only stored for the radiation regions. This means that the values calculated at each ODE step are averaged (linearly) to obtain values for the radiation region in question.

RESTR. This subroutine does all the work necessary for reading and writing information necessary for a restart.

RINTS. This subroutine is a compact calculation of all parameters needed for the radiation calculations within the reactor. It is for this subroutine that an initial or past temperature profile, particle number density profile, and diameter profile of the particles are needed. These initial profiles come from INPUT, or from RESTR, or of course, from the immediately past calculation in the iterative loop. The values calculated in RINTS are used in AUX1 and AUX3.

RODEV. This subroutine returns the value of each of the separate variables from the functions given by the predictor corrector calculations. For example SOLVE can calculate the value of $(w_j h_j)$ from Eq. 6 of Table 2, the particle energy equation. SOLVE also calculates w_j from the particle continuity equation. RODEVL takes this information and returns h_j .

SETUP1, EQUIL, TOY, SLE. These are other manipulative subroutines for the EDWARDS thermochemical equilibrium computations.

SIGMAD. This subroutine is used by AUX2PR for determining the value of the potential function needed for mass diffusivity as a function of the Lennard-Jones parameters and temperature.

SIGMAM. This is the routine used by AUX2R for determining the value of the potential function needed for viscosity and thermal conductivity as a function of the Stockmayer parameters and temperature.

SOLVE. This subroutine manages the Adams-Moulton predictor corrector solution technique. After some preliminary initialization the routine performs the Runge-Kutta fourth order computations for the first four ODE steps. It then switches to the Adams-Moulton predictor corrector computations. At each step the routine checks to see if a restart should be initiated due to completion of mixing or due to a step size change. The pssa method for stiff differential systems is monitored and controlled in this routine.

TIMET. This is a convenience subroutine used for running night batch on the BYU DEC-10 computer. This subroutine accepts a time of day and monitors the current run time. If run time is beyond the accepted time then this routine calls TRBLE.

TRBLE. This is a subroutine used by TIMET to get output and kill the program if it gets in trouble.

VALUE. This subroutine sets up all the initial values needed for the predictorcorrector differential equation solution performed in SOLVE. These values are stored in the dimensioned FORTRAN variable VALINT.

C. INPUT

The required set of data cards for input for 1-DICOG is shown in Table 10. Each punched card is identified within each group. The required format is also indicated. Table 11 gives a definition of the FORTRAN variables used in Table 10. A Group 1 of Table 10 contains comment cards that will be printed at the top of the output to identify the run, etc. Group 2 contains all of the variables pertaining to the numerical control of the computation. Group 3 contains the initial gas stream information. Group 4 contains all the data pertaining to each particle classification. This group must be repeated for as many times as there are particle classifications (presently a maximum of 5). Group 5 contains required data on each element to be used in the computation and is repeated for each element. Group 6 contains the information required for each species to be considered and is also repeated for each species. Finally, Group 7 contains reactor geometry and other miscellaneous parameters. At least one set of each group is required. Table 11 contains a detailed list of definitions of these program data variables together with further information on the requirements for each variable. Much of the thermochemical data required for Group 6 has been compiled for a number of species for the original EDWARDS thermochemical program (39) and is included in Appendix C.

TABLE 10
INPUT DATA FOR 1-DICOG

<u>GROUP</u>	<u>CARD</u>	<u>DATA ITEMS</u>	<u>FORMAT</u>
1	1	NCARD	I5
	2	COMENT (1,1), , COMENT (1,20)	20A4
		COMENT (2,1),	.
	NCARD+1	 COMENT (NCARD,20)	.
2	1	ODESTP, OSPRR, DYNAMO(1), DYNAMO(2), DYNAMO(3), NPRINT	6I5
	2	ELEMNT, SPECIE, PRTCLS, CRXN, HRXN, ICNVLM, ITRAMX	14I5
	3	NPROP, BUG, ISASUM, EUCKEN, KEQ, SHRINK, IRAD DYNTM, SQDIF, DELTPJ, DELRRJ, TTEST, STIFVAL, FUR	
3	1	GMW, HGAS, RHOG, WG, P	5E10.3
	2	SGH, SGMC(1), SGMC(2), SGMC(3)	4E10.3
	3	PGX, PGH, PGMC(1), PGMC(2), PGMC(3), PGMC(4)	6E10.3
4	1	DI(1), E(1), H(1), XI(1), W(1)	5E10.3
	2	ALPHAA(1), ALPHAC(1), PLPHAH(1), ALPHAW(1), HHO(1), HWO(1)	6E10.3
	3	TMIN(1), XBEGIN(1), TMAX(1), XCHNG(1)	4E10.3
	4	SJH(1), SJMC(1,1), SJMC(1,2), SJMC(1,3)	4E10.3
	5	PJX(1), PJH(1), PJMC(1,1), PJMC(1,2), PJMC(1,3), PJMC(1,4)	6E10.3
	6	AMJ(1,1), EMJ(1,1), YY(1,1)	3E10.3
	7	CPVC(1,1,1), CPVC(2,1,1), CPVC(3,1,1), HFV(1,1)	4E10.3
		Repeat Cards 6 & 7 for other m raw coal reactions, if any, up to CRXN	
	8	AL(1,1), EL(1,1), EMM(1,1)	3E10.3
		Repeat card 8 for other l char reactions, if any, up to HRXN	
	9	PHIJWK(1,1), , PHIJWK(1,ELEMNT)	9E10.3
	10	PHIVK (1,1,1), , PHIVK(1,1,CRXN)	5E10.3
		Repeat card 10 for each element to be considered up to ELEMNT	
	11	CCP(1,1,1), CCP(1,1,2), CCP(1,1,3)	3E10.4
	12	CCP(1,2,1),	
	13		
	14	 CCP(1,4,3)	
		Repeat Group 4 for other particle classifications, if any, up to PRTCLS	
	1	EDNAME(1), ATWT(1), OMEGAK(1), OSGKM(1), OPGKM(1)	2A4,2X, 3E10.3
	2	PHIKL(1,1),~PHIKL(1,2). , PHIKL(1,HRXN)	5E10.3
		Repeat Group 5 for each element in the computation up to ELEMNT	

TABLE 10 (Cont.)

<u>GROUP</u>	<u>CARD</u>	<u>DATA ITEMS</u>	<u>FORMAT</u>
6	1	NAME1(1), NAME2(1), S(1), EK(1), DELTA(1), YINT(1)	2A4,2X, 4E10.3
	2	A(1,1), A(1,2), , A(1,ELEMNT)	9E10.3
	3	HR(1), SR(1)	2E10.3
	4	Z(1,1), Z(1,2), , Z(1,5)	5E10.3
	5	Z(1,6), Z(1,7), , Z(1,10)	5E10.3
		Repeat Group 6 for each species to be considered in gaseous equilibrium computation up to SPECIE	
7	1	DDUCT, DS, ALEN, AGANGL, EB, TB	6E10.3
	2	ELAM, GAMMA, MG	3E10.3
	3	OXYD(1), OXYD(2), , OXYD(HRXN)	5J5
	4	PHIL(1), PHIL(2), , PHIL(HRXN)	5E10.3
	5	IVPFLG, VPRCOF(1), VPRCOF(2), , VPRCOF(5)	I5,5X, 5E10.3
	6	RSTRT	I5

Table 11
FORTRAN VARIABLE NOMENCLATURE

FORTRAN Variable	Type	Units	Description and Usual Symbol
A(K,JX)	real	-	Number of elements JX per species I
AGANGL	real	deg.	Area growth angle, θ
AL(J,L)	real	s^{-1}	Pre-exponential factor for the Lth char reaction for the Jth particle, $A_{j\ell}$
ALEN	real	cm	Reactor length
ALPHAA(J)	real	g	Mass of ash in Jth particle, α_{aj}
ALPHAC(J)	real	g	Mass of raw coal in Jth particle, α_{cj}
ALPHAH(J)	real	g	Mass of char in Jth particle, α_{nj}
ALPHAW(J)	real	g	Mass of moisture in Jth particle, α_{wj}
AMJ(J,M)	real	s^{-1}	Pre-exponential factor for the Mth devolatilization reaction for the Jth particle, A_{jm}
ATWT(K)	real	$gmol^{-1}$	Atomic, weight of the Kth element
BUG	integer	-	Debug level (see Debugging)
CCP(J,N,I)	real	$cal\ g^{-1}K^{-(I)}$	Quadratic heat capacity coefficients (I=1,3) for the Jth particle for: N=1, coal component; N=2, char component; N=3, moisture component; N=4 ash component
COMENT(I,N)	ASCII	-	Comment words for top of output
CPVC(I,J,M)	real	$cal\ g^{-1}K^{-(I)}$	Quadratic heat capacity coefficients (I=1,3) for the volatiles from the Mth devolatilization reaction for the jth particle
CRXN	integer	-	Number of raw coal devolatilization reactions, M
DI(J)	real	cm	Diameter of the Jth particle, d_j
DDUCT	real	cm	Diameter of the initial injection duct
DELRRJ	real	-	The fractional change tolerance for convergence of the total particle reaction rate (see AUX3, Section 4, Code Operation)

Table 11 (cont.)

<u>FORTTRAN Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
DELTA(I)	real	-	Stockmayer polar parameter of species I, δ
DELTPJ	real	-	Temperature change tolerance for convergence of particle temperature calculations (see AUX1, Section 4, Code Operation)
DS	real	cm	Diameter of reaction vessel, D_s
DYNAMO(I)	real	-	Multiplication factor (I=1,2) or division factor (I=3) for the number of O.D.E. steps per radiation region in the three regions following the first (see Section 4, Code Operation)
DYNTM	real	K	Temperature at which the second step size region will be initiated (see above)
ELAM	real	-	Absorption efficiency, E_λ
ELEMNT	integer	-	Number of elements in prediction
EMJ(J,M)	real	cal mol ⁻¹	Activation energy for the Mth devolatilization reaction for the Jth particle
E(J)	real	-	Emissivity of the Jth particle type, ϵ_j
EB	real	-	Emissivity of the reactor boundary or wall, ϵ_b
EDNAME(K)	ASCII	-	Name of the Kth element
EK(I)	real	-	Stockmayer Parameter for the Ith species, ϵ/k
EL(J,L)	real	cal mol ⁻¹	Activation energy for the Mth devolatilization reaction for the Jth particle
EMM(J,L)	real	-	Exponent on temperature in Equation 2-68 of Table 2-8, m
EUKEN	integer	-	If EUKEN=1 viscosity calculated from Euker equation - If EUKEN=0 viscosity calculated from Sage-Galloway equation

Table 11 (cont.)

<u>FORTTRAN Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
FUR	real	-	If $0.0 < \text{FUR} \leq 1.0$, underrelaxation factor for Adams-Moulton corrector equation If $0.0 > \text{FUR}$, or $\text{FUR} > 1.0$ then $\text{FUR} = 1.0$ (i.e. no underrelaxation)
GAMMA	real	-	Particle swelling parameter, γ
GMW	real	gmol^{-1}	Molecular weight of input gas phase, M_g
H(J)	real	cal g^{-1}	Initial enthalpy level of Jth particle
HRV(J,M)	real	cal g^{-1}	Heat of formation of the volatiles from the Mth devolatilization reaction in the Jth particle h_{vjm}
HGAS	real	cal g^{-1}	Initial enthalpy of the gaseous stream $h_g = \int_{298}^T C_{pg} dT + h_g^{\circ}$
HHO(J)	real	cal g^{-1}	Heat of formation of the char in the Jth particle, h_{hj}
HR(I)	real	kcal mol^{-1}	Enthalpy of species I at 1200 K $= \int_{298}^{1200} C_{pi} dT + h_{i, 298}^{\circ}$
HRXN	integer	-	Number of char oxidation reactions, L
HWO(J)	real	cal g^{-1}	Heat of formation of the moisture in the Jth particle, h_{wj}°
ICNVLM	integer	-	Maximum number of Adams-Moulton correctors
IRAD	integer	-	If $\text{IRAD}=1$ radiation is calculated as a diffusion process, if $\text{IRAD} \neq 1$ radiation is calculated by the zone method
ISASUM	integer	-	If $\text{ISASUM} < 0$ then the pssa method is not invoked; If $\text{ISASUM}=1$ the pssa method is introduced only when required after char burnout; If $\text{ISASUM}=2$ the pssa method is introduced when needed even if the char has not yet been completely reacted

Table 11 (cont.)

<u>FORTTRAN Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
ITRMAX	integer	-	Maximum number of system iterations
IVPFLG	integer	-	If IVPFLG=0 vapor pressure for moisture is calculated from Antoine Equation If IVPFLG $\neq$ 0 vapor pressure coefficients are used in a power series equation
KEQ	integer	-	If KEQ=1 the linear form of the Field (1969) char oxidation rate expression is used; If KEQ $\neq$ 1 normal Arrhenius form used
MH	real	gmol ⁻¹	Char molecular weight, M_h
NAME1(I)	ASCII	-	First four characters of the name of the Ith species
NAME2(I)	ASCII	-	Second four characters of the name of the Ith species
NCARD	integer	-	Number of comment cards to follow
NPROP	integer	-	Number of O.D.E. steps per property recalculation
ODESTP	integer	-	Initial number of O.D.E. steps
OPGKM(K)	real	-	Initial mass fraction of element K in the recirculation, ω_{gkp}
OSGKM(K)	real	-	Mass fraction of element K in the secondary gas, ω_{gks}
OSPRR	integer	-	Number of initial O.D.E. steps per radiation region
OMEGAK(K)	real	-	Initial mass fraction of element K in primary, ω_{gk}
OXYD(L)	integer	-	Identification number for the oxidizer for the Lth char oxidation reaction
P	real	atm	Pressure, P
PGH	real	cal g ⁻¹	Enthalpy of recirculation gas (initial guess), h_{pg}

Table 11 (Cont.)

FORTTRAN Variable	Type	Units	Description and Usual Symbol
PGMC(N)	real	$\text{g s}^{-1} \text{cm}^{-(N-1)}$	Nth coefficient for recirculation function, see Chapter 2 Recirculation
PGX	real	cm	Axial location for recirculation properties
PHIJWK(J,K)	real	-	Stoichiometric coefficient for Kth element in Jth particle with respect to moisture vaporization, ϕ_{jwk}
PHIKL(K,L)	real	-	Stoichiometric coefficient for Kth element with respect to the Lth char oxidation reaction, ϕ_{kl}
PHIL(L)	real	-	Stoichiometric coefficient for the oxidizer in the Lth char oxidation reaction, ϕ_l
PHIVK(J,K,M)	real	-	Stoichiometric coefficient for the Kth element in the Jth particle with respect to the Mth devolatilization reaction, ϕ_{vjkM}
PJH(J)	real	cal g^{-1}	Enthalpy of the Jth particle in the recirculation (initial guess), h_{pj}
PJMC(J,N)	real	$\text{g s}^{-1} \text{cm}^{-(N-1)}$	Nth coefficient for recirculation of the Jth particle type (see Chapter 2, Recirculation)
PJX(J)	real	cm	Location for properties of the Jth particle type in recirculation
PRTCLS	integer	-	Number of particle types in computation, J
RHOG	real	g cm^{-3}	Initial gas density, ρ_g
RSTRT	integer	-	If RSTRT=1 external restart information is used for initial guesses
S(I)	real	$\text{\AA}$	Stockmayer collision diameter, σ_i
SGH	real	cal g^{-1}	Enthalpy of secondary gas, h_{gs}
SGMC(N)	real	$\text{g s}^{-1} \text{cm}^{-(N-1)}$	Coefficients for secondary mass addition

Table 11 (Cont.)

<u>FORTTRAN Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Usual Symbol</u>
SHRINK	integer	-	If SHRINK=1 the shrinking particle model is used for char oxidation; If SHRINK $\neq$ 1 the constant diameter model is used
SJH(J)	real	cal g ⁻¹	Enthalpy of particle J in secondary stream, h_{js}
SJMC(J,N)	real	g s ⁻¹ cm ^{-(N-1)}	Nth coefficient for mass addition of Jth particle type by secondary stream
SPECIE	integer	-	Number of species to be included
SQDIF	real	K	The maximum acceptable root mean square temperature profile difference for convergence
SR(I)	real	cal mol ⁻¹ K ⁻¹	Entropy of species I at 1200 K
STIFVL	real	cal cm ⁻³ s ⁻¹	Value of stiffness criterion for initiation of pssa method (see Section 4, Code Operation)
TB	real	K	Reactor wall temperature, T_b
TMAX(J)	real	K	Initial guess at maximum Jth particle temperature
TMIN	real	K	Initial temperature of Jth particle group
TTEST	real	-	Fractional change in the sum of the slopes of all particle energy equations that is acceptable without applying another corrector
VPRCOF(N)	real	atm K ^{-(N-1)}	Nth coefficient of moisture partial pressure power series if JVPFLG $\neq$ 0
W(J)	real	g s ⁻¹	Initial mass flow rate of Jth particle group, w_j
WG	real	g s ⁻¹	Initial mass flow rate of gas stream, w_g
XBEGIN(J)	real	cm	Axial location for Jth particle phase for initial guess of temperature profile as shown in Figure 4-1

Table 11 (Cont.)

<u>FORTTRAN Variable</u>	<u>Type</u>	<u>Units</u>	<u>Description and Used Symbol</u>
XCHNG(J)	real	cm	Axial location for Jth particle phase for initial guess of temperature profile in Figure 4-1
XI(J)	real	-	Surface area factor for Jth particle type, ζ_j
YINT(I)	real	-	Rough order of magnitude initial guess for gas phase mole fractions
YY(J,M)	real	-	Stoichiometric coefficient for Jth particle with regards to Mth devolatilization reaction, Y_{jm}
Z(I,N)	real	-	Nth coefficient for Ith species heat capacity equation. For N=1-5 the temperature range of the heat capacity is 1200 K-6000 K and $C_p = \sum_{i=0}^4 Z_{i+1} \left(\frac{1000}{T}\right)^i$ where T is in Kelvin and C_p is cal g mol ⁻¹ K ⁻¹ . For N=6-10 ^p the temperature range of the heat capacity is 298 K - 1200 K and $C_p = \sum_{i=0}^4 Z_{i+6} \left(\frac{T}{1000}\right)^i$

A sample input file for a prediction of the BYU combustor (26) is shown in Appendix A. The card images, as indicated in Table 10, are shown as well as the echo output printed by 1-DICOG. This sample should also prove useful to the user in estimating what values to input for his particular application.

D. OUTPUT

The user has the ability to govern the extent of output obtained from 1-DICOG through the debugging options already discussed in the debugging section. Under normal operating procedure the debug switch would be turned off and the standard output would be received. Appendix A shows a sample input and output package.

The first section of the output is simply an echo of all the input parameters formatted as shown in Appendix A.

The next section of output is invaluable data regarding the numerical operation of the solution history. The ordered pair of the axial location and the number of correctors applied is given for each ordinary differential equation set. Section 3 discussed how the solution procedure uses multiple correctors when appropriate. The next section on Code Operation discusses how to use this information to optimize computational efficiency.

The last sections give the computational output. First, parameters for each individual particle phase are given for each radiation region through the reactor. Appendix A shows the sample output and the headings indicate the appropriate particle properties and their units for each particle phase as identified by its number j . The masses shown are for an individual particle of the given classification. Following each particle phase is a history of normalized compositions for the sum total of all particle phases. These are the numbers for the plots which follow. The final group is a printout of gas phase properties through the reactor. The mole fraction of each species is given for each radiation region through the reactor.

Appendix A also shows the plots which are obtained from the CALCOMP plotter when the plotting routines are included as discussed under Language and Availability. Particle and gas temperature histories are plotted. The mass history of each particle classification and of the total of all particles are also plotted. These plots show the normalized mass of each component of the particles (moisture, ash, char, raw coal, and the total of all components) at axial locations through the reactor. The final plot shows the gas phase mole fraction history of each gas phase species.

E. CODE OPERATION

The section on Input gave the user a description of all the variables needed for operating the computer code. This section is meant to give helpful insight into selection of the parameters that might be the most ambiguous, or that are the most important, in obtaining a successful converged computation.

As was discussed in Section 3 the solution procedure calls for iteration due to the zone method for solving the radiative heat transfer. Experience with the code has indicated that a large majority of combustion or gasification chambers are radiation stabilized. This physical insight indicates the important contribution of the radiative processes to the overall operation of these systems. Numerically, this importance is manifest in the need for a good guess on the temperature profile to initiate the radiation iteration. This guess is input for each jth particle classification on card 3 of group 4 in Table 10. The initial profile is schematically represented in Figure 7. If the parameters in this figure are not chosen carefully the first iteration will tend to cool the system temperatures such that ignition will not occur. Sometimes extreme cooling will be predicted even to the point of causing numerical instabilities. When this behavior is observed the user should try another guess for the particle temperature profile. The locations of XBEGIN and XCHNG are most crucial. It is obvious that when a restart is available from some previous computation it could prove extremely useful as a first guess for a similar prediction. The sample computation shown in Appendix A may prove helpful in giving the user some experience at guessing initial profiles.

Another important consideration in obtaining accurate predictions for coal combustion or gasification is a reasonable particle size distribution. If the discrete size distribution chosen by the user is not representative of the true continuous distribution, the prediction will not be realistic. Figure 8 shows the measured cumulative particle size distribution for the input coal of the sample prediction shown in Appendix A. The three particle size discretization chosen for this sample computation is also shown. If the user will perform a similar exercise for his particular case any difficulties from poor choice of particle size distribution should be alleviated. After the size classes have been picked, the user should assure himself that the discrete distribution has near the same mass mean particle diameter as the measured distribution.

Some of the more difficult input data to obtain, might be the species equilibrium input parameters of group 6 in Table 10. To help the user with these input variables, Appendix C contains a compilation of variables for selected species which might be important to combustion or gasification processes.

Group 2 of the Input Data shown in Table 10 contains the input variables which govern the numerics of the solution strategy. These were discussed in general terms in Section 3, but the successfully obtaining a solution in reasonable computational times is contingent on appropriate selection of these variables. Due to the sensitivity of these parameters to efficient operation a further discussion is presented here.

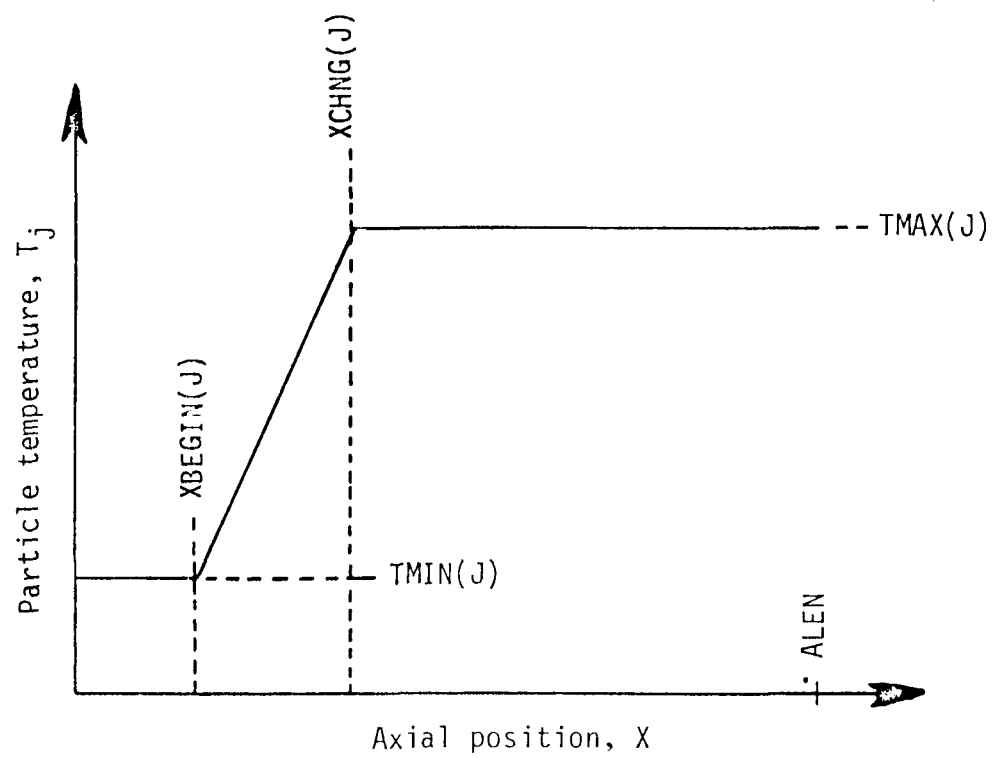


Figure 7. Initial guess at the j th particle type temperature profile.

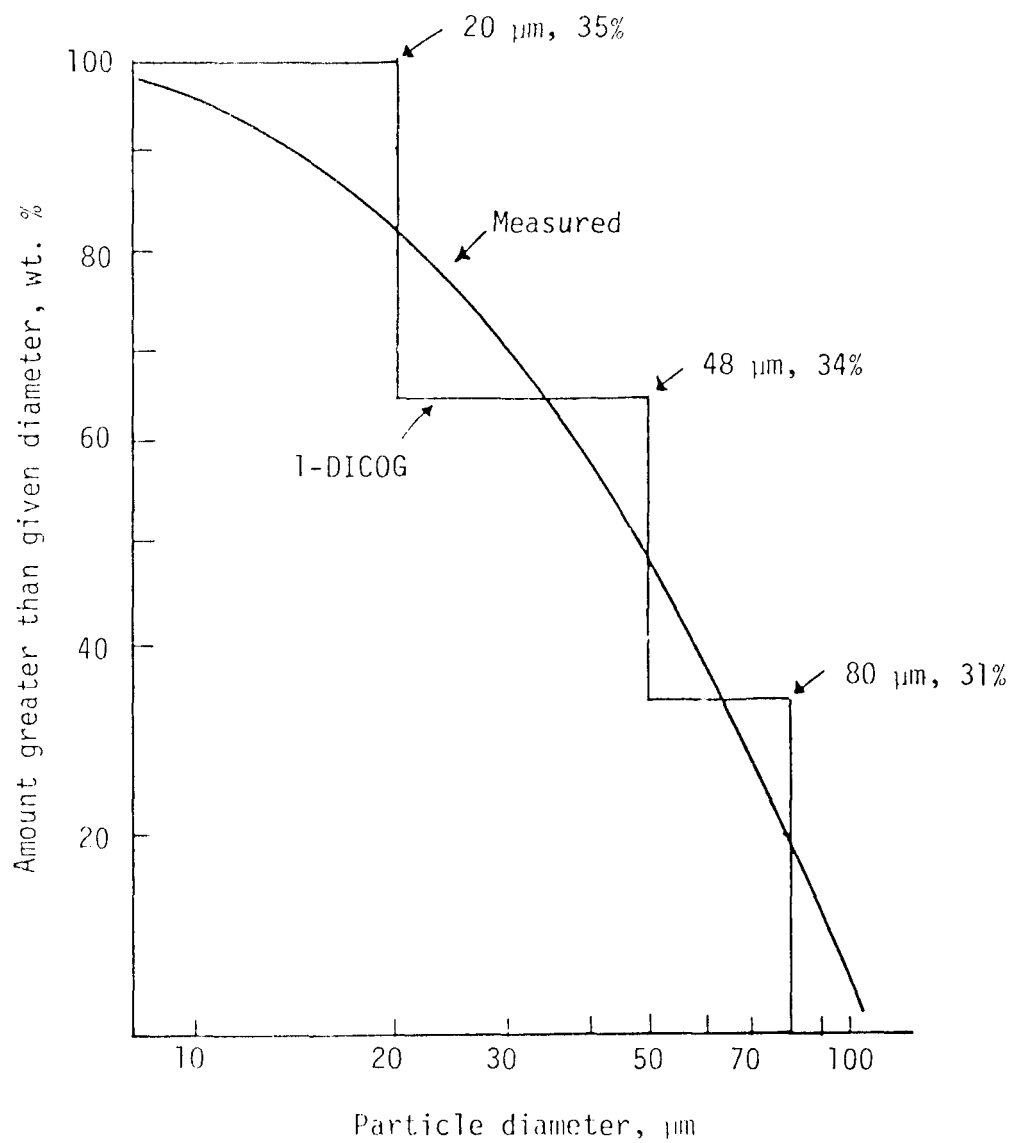


Figure 8. Particle size distribution used for the three increment poly-dispersed combustion calculation of Appendix A.

The variables on card 1 govern the step size in the reactor. These variables should be adjusted carefully for each particular application to insure the most efficient code operation. Trial and error is the best way of optimizing these parameters; however, some guidance is available. The output is structured to guide the user in this optimization (see Appendix A for sample). Immediately following the echo input a consolidated printout follows the progression of the ordinary differential equation steps. This output contains the ordered pair of the location in the reactor and the number of correctors applied at that location (see section 3). The difference between locations will tell the step size at that step. In general the step size should be adjusted (through the variables in card 1 of group 2, Table 10) to keep the number of correctors at 1 with an occasional 2 (see Appendix A for example). If the number of correctors is consistently greater than 1, more efficient operation can generally be achieved by decreasing the step size in that particular region. Just before the step size is about to change due to initiation of the dynamic region or completion of devolatilization, the number of correctors applied may increase for a few steps without any adverse effects on computational efficiency. The sample computation of Appendix A is operating quite efficiently and should be used as a pattern for efficient operation.

In selecting the numbers for these variables it is generally good practice to have about 250 radiation regions. Thus, after selecting the initial number of ordinary differential equation steps (ODESTP) the number of initial ordinary differential equation steps per radiation region (OSPRR) should be selected according to this criterion. The location of the first step size change is governed by the dynamic region initiation temperature (DYNTEM) which is usually selected around 800 K - 900 K. The size of the steps in each subsequent region should then be chosen by setting the three DYNAMO variables according to the criteria given in the preceding paragraph.

The convergence criteria of card 3 in group 3 are adjustable by the user. Suggested ranges are given below:

SQDIF = 5K - 20K
DELTPJ = 0.001K - 0.05K
DELRRJ = 1.0×10^{-7} - 1.0×10^{-6}
TTEST = 0.001 - 0.05
STIFVAL = 0.0001 - 0.010
FUR = 0.0

In preparing the input all other variables should be straightforward; however, some confusion has sometimes arisen regarding the stoichiometric

coefficients, PHIJK, PHIKL, PHIL, PHIK, and YY. To clarify the values to be used for these variables the following derivation is presented for the sample case shown in Appendix A. Table 12 shows the analysis of the coal used for these computations.

PHIJK(J,K) is the mass of element K per mass of water vapor. thus in virtually all cases PHIJK for hydrogen is 0.1111... and for oxygen it is 0.8888...

Next, the char composition must be defined by the user. In this example char was chosen to be pure carbon. Now PHIL(L) may be defined for each oxidizer with the help of Eq. 2. PHIL is the moles of char per mole of oxidizer. For the sample calculation only O_2 was considered as an oxidizer and the char was taken to be pure carbon. The gaseous products of Eq. 2-2 were taken to be only CO: thus, PHIL(1) is 2.

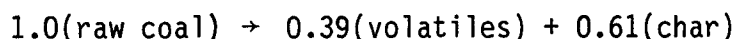
Now, since the char reaction is defined, the elemental stoichiometric coefficients PHIKL(K,L) can be computed. PHIKL(K,L) is the mass of element K given to the gas due to the char heterogeneous reaction per mass of gaseous product from the heterogeneous reaction. Thus for this sample, all PHIKL(K,L) will be zero, except for the element carbon, for which the value will be 1.0.

The PHIVK(J,K,M) are dependent on the coal analysis and the overall devolatilization stoichiometry (YY(J,M)). For the two step devolatilization mechanism suggested in Table 9 the YY (mass of volatile matter per mass of dry, ash free coal) are:

$$YY(J,1) = 0.39$$

$$YY(J,2) = 0.80$$

for all J. PHIVK(J,K,M) is the elemental stoichiometric coefficients for each devolatilization reaction and is defined as the mass of element K per total mass of volatiles from the mth reaction for the jth particle. In the sample calculation all of the J particles undergo the same two M reactions and have the same composition; thus for M = 1:



raw coal		Basis: 100 gms of DAF coal			
	gms	volatiles	gms	char	gms
H	6.0	H	6.0	C	61.0
C	79.9	C	18.9		
N	1.6	N	1.6		
S	0.6	S	0.6		
O	11.9	O	11.9		
total	100.0	total	39.0		

TABLE 12
COAL ANALYSIS FOR SAMPLE CALCULATION OF APPENDIX A

	<u>AS RECEIVED</u> <u>wt%</u>	<u>DAF</u> <u>wt%</u>
<u>Proximate Analysis</u>		
moisture	3.1	N/A
volatile matter	42.2	48.3
fixed carbon	45.2	51.7
ash	<u>9.5</u>	<u>N/A</u>
total	100.0	100.0
<u>Ultimate Analysis</u>		
hydrogen	5.6	6.0
carbon	69.8	79.9
nitrogen	1.4	1.6
sulfur	0.5	0.6
oxygen	13.2	11.9
ash	<u>9.5</u>	<u>N/A</u>
total	100.0	100.0

Which gives the following values for PHIVK(J,K,M):

<u>PHIVK(J,K,M)</u>	
H	0.15
C	0.48
N	0.04
S	0.02
O	0.31

The values of PHIVK for M = 2 are calculated in a similar manner and the results are shown in Appendix A.

Any further questions on code operation may be addressed to the authors directly.

REFERENCES

1. L. D. Smoot, and P. O. Hedman. "The Effect of Mixing on Kinetic Processes in Pulverized Coal Combustors." Final Report for Electric Power Research Institute, Contract No. RP-364-1, Brigham Young University. Provo, Utah: August, 1978.
2. A. D. Gosman, W. M. Pun, A. K. Ruchal, D. B. Spalding, and R. Wolfshtein. Heat and Mass Transfer in Recirculating Flows. London: Academic Press, 1969.
3. L. A. Vulis. Thermal Regimes of Combustion. New York: McGraw-Hill, 1961.
4. A. B. Hedley and W. E. Jackson. "Simplified Mathematical Model of a Pulverized Coal Flame Showing Effects of Recirculating on Combustion Rate." J. Inst. Fuel 39, 1966, p. 208.
5. G. Horn, J. Csaba, and D. J. Street. "Combustion Experiments Using a Pulverized Coal-Fired Superheater." J. Inst. Fuel 39, 1966, p. 521.
6. M. A. Field, D. W. Gill, B. B. Morgan, and P. G. W. Hawskley. Combustion of Pulverized Coal. The British Coal Utilization Research Association. Leatherhead, Surrey, England: 1967.
7. J. M. Beer, and K. B. Lee. "The Effect of Residence Time Distribution on the Performance and Efficiency of Combustion." 10th Symposium (International on Combustion, The Combustion Institute. Pittsburgh, PA: 1965, p. 1187-1202.
8. W. S. Lewellen, H. Segur, and A. K. Varma. "Modeling Two Phase Flow in a Swirl Combustor." Final Report, ERDA Contract No. EY-76-C-024062. Aeronautical Research Associates of Princeton, Inc.. Princeton, New Jersey: 1977.
9. W. Richter, and R. Quack. "A Mathematical Model of a Low-Volatile Pulverized Fuel Flame." Heat Transfer in Flames. Scripta Technica: 1974, p. 95.
10. M. M. Gibson, and B. B. Morgan. "Mathematical model of Combustion of Solid Particles in a Turulent Stream with Recirculation." Journal of the Institute of Fuel, 43, 1970, pp. 517-523.
11. H. R. Batchelder, R. M. Busche, and W. P. Armstrong. "Kinetics of Coal Gasification." Ind. and Eng. Chem 45, 1953, pp. 1856-1878.
12. A. K. Mehta. "Mathematical Modeling of Chemical Processes for Low BTU Gasification of Coal for Electric Power Generation." Final Report, ERDA Contract No. E(49-18)-1545, Combustion Engineering, Inc.. Windsor, Connecticut: August, 1976.
13. P. E. George, R. C. Lenzer, J. F. Thomas, J. S. Barnhard, and

- N. M. Laurendeau. "Gasification in Pulverized Coal Flames." Second Annual Progress Report, ERDA-FE-2029-6. West Lafayette, Indiana: The Combustion Laboratory, School of Mechanical Engineering, August, 1977.
14. P. Lewis, G. Simons, M. Finson, and E. Tomaszewski. "A Model for Entrained Flow Gasifiers." A paper presented at Fall Technical Meeting, Eastern Section, Combustion Institute, 1977.
 15. T. R. Blake. "Computer Modeling of Coal Gasification Reactors." QPR-FE1770-23, ERDA Contract EX-76-C-01-1770. System, Science and Software. La Jolla, CA: February, 1977.
 16. K. M. Sprouse. "Theory of Pulverized Coal Conversion in Entrained Flow." Technical Memorandum for U. S. Dept. of Energy, Contract No. EX-77-C-01-2518, Rockwell International, Rocketdyne Division. Canoga Park, California: December 1977.
 17. L. D. Smoot and D. T. Pratt (eds.). Pulverized Coal Combustion and Gasification. Plenum, New York: 1979.
 18. D. B. Stickler, F. E. Becker, and S. K. Ubhayakar. "Combustion of Pulverized Coal in High Temperature Preheated Air." Paper 79-0298, AIAA 17th Aerospace Science Meeting. New Orleans, LA: January, 1979.
 19. R. B. Bird, W. E. Stewart, and E. N. Lightfoot. Transport Phenomena. New York: John Wiley and Sons, 1960.
 20. A. S. Padia, A. F. Sarofim, and J. B. Howard. "The Behavior of Ash in Pulverized Coal, Under Simulated Combustion Conditions." Spring Meeting, Central States Section, Combustion Institute. Pittsburgh, PA: April 5, 1976.
 21. A. B. Ayling, M. F. R. Mulcahy, and I. W. Smith. "The Temperature of Burning Pulverized Fuel Particles." Investigation Report 88 of the Division of Mineral Chemistry, C.S.I.R.O. Sydney, New South Wales, Australia: May, 1971.
 22. C. F. Hirschfelder, and R. B. Bird. Molecular Theory of Gases and Liquids. New York: 1954.
 23. R. C. Reid, J. M. Prausnitz, and T. K. Sherwood. The Properties of Gases and Liquids, 3rd edition. New York: McGraw-Hill, 1977.
 24. D. Anson, F. D. Moles and P. J. Street. "Structure and Surface Areas of Pulverized Coal During Combustion." Comb. and Flame 16, 1971, p. 265.
 25. L. D. Smoot and M. D. Horton. "Exploratory Studies of Flame and Explosion Quenching." 3rd Interim Annual Reprt, Bureau of Mines Contract 10122052, Brigham Young University. Provo,

Utah: September 30, 1975.

26. J. R. Thurgood. "Mixing and Combustion of Pulverized Coal." Ph.D. Dissertation, Brigham Young University. Provo, Utah: 1979.
27. H. C. Hottel and A. F. Sarofim. Radiative Transfer. New York: McGraw-Hill, 1967.
28. J. F. Farnsworth and R. A. Glenn. "Status and Design Characteristics of BCR/OCR BI-GAS Pilot Plant." Vol. 15, No. 3, 162nd National Meeting of Am. Chem. Soc. Washington D. C.: 1971.
29. P. J. Smith. "Numerical Modeling of Coal and Gas Fired Turbulent Combustion and Gasification Processes." Ph.D. Dissertation, Department of Chemical Engineering. Brigham Young University. Provo, Utah: 1979.
30. F. Kreith. Principles of Heat Transfer, 3rd edition. New York: Intext Educational Publishers, 1973.
31. S. K. Ubhayakar, D. B. Stickler, C. W. von Rosenberg, and R. E. Gannon. "Rapid Devolatilization of Pulverized Coal in Hot Combustion Gas." 16th Symposium (International) on Combustion, The Combustion Institute. Pittsburgh, PA: 1976, pp. 427-436.
32. S. Badzioch, P. G. W. Hawksley and C. W. Peter. "Kinetics of Thermal Decomposition of Pulverized Coal Particles." Ind. Eng. Chem. Process Design and Development, 1970, pp. 521-530.
33. H. Reidelbach and M. Summerfield. "Kinetic Model for Coal Pyrolysis Optimization." Princeton University. Princeton, New Jersey: 1974.
34. M. A. Field. "Rate of Combustion of Size-Graded Fractions of Char from a Low-Rank Coal Between 1200 K." Combustion and Flame, 13, 1969, pp. 237-252.
35. A. M. Mayers. "The Rate of Reduction of Carbon Dioxide by Graphite." Am. Chem. Soc. J., 56, January, 1934, pp. 70-76.
36. A. M. Mayers. "The Rate of Oxidation of Graphite by Steam." Am. Chem. Soc. J., 56, September 1934, pp. 1879-1881.
37. W. B. White, S. M. Johnson, and G. B. Dantzig. "Chemical Equilibrium in Complex Mixtures." Journal of Chemical Physics, 28, 1958, p. 751.
38. S. Gordon and B. McBride. "Computer Program for Calculation of Complex Chemical Equilibrium Compositions." NASA SP-723, 1971.
39. C. Selph. "Generalized Thermochemical Equilibrium Program for Complex Mixtures." Rocket Propulsion Laboratory. Edwards Air Force Base, CA: 1965.

40. G. N. Abramovich. The Theory of Turbulent Jets. Cambridge, Massachusetts: M.I.T. Press, 1963.
41. M. W. Thring and M. P. Newby. "Combustion Length of Enclosed Turbulent Jet Flames." Fourth Symposium (International) on Combustion, The Combustion Institute. Pittsburgh, PA: 1953.
42. A. Craya and R. Curtet. "On the Spreading of a Confined Jet." Comptes-Rendus Academie des Sciences, Vol. 241, 1955, pp. 621-622.
43. M. Barchilon and R. Curtet. "Some Details of the Structure of an Axisymmetric Confined Jet with Backflow." Journal of Basic Engineering, 86D, 1964, pp. 777-787.
44. P. G. Hill. "Turbulent Jets in Ducted Streams." Journal of Fluid Mechanics, 22(1), 1965, pp. 161-186.
45. J. M. Beer and N. A. Chigier. Combustion Aerodynamics. London: Applied Science Publishers Ltd., 1972.
46. D. M. Brandon, Jr., "A New Single-Step Implicit Integration Algorithm with A Stability and Improved Accuracy." Simulation, July, 1974, p. 17.
47. P. L. Case and D. T. Pratt. "A New Integration Algorithm for Chemical Kinetics." Spring Meeting of the Western States Section, The Combustion Institute, 1977.
48. R. W. Hamming. Numerical Methods for Scientists and Engineers., 2nd edition. New York: McGraw-Hill, 1973.
49. L. Lapidus, R. C. Aiken, and Y. A. Liu. Stiff Differential Systems, (R. A. Willoughby, ed.). Plenum, New York: 1974.

1-DICOG SAMPLE CALCULATION

OUTPUT FOR SAMPLE COMPUTATION

```
*****
***** BRIGHAM YOUNG UNIVERSITY *****
***** 1 DIMENSIONAL COMBUSTION OR GASIFICATION *****
***** USER'S MANUAL EXAMPLE *****
***** 3 PARTICLE SIZES *****
*****
```

RUN PARAMETERS*****

```
INITIAL NUMBER OF O.D.E. STEPS          750
NUMBER OF INITIAL STEPS PER RADIATION REGION  3
DYNAMIC REGION MULTIPLICATION FACTOR      2
MULTIPLICATION FACTOR AFTER DEVOLATILIZATION 3
DIVISION FACTOR AFTER CHAR BURNOUT         3
NUMBER OF STEPS PER PRINT                 10
NUMBER OF ELEMENTS                        6
NUMBER OF SPECIES                         10
NUMBER OF PARTICLE TYPES/SIZES            3
NUMBER OF COAL REACTIONS                  2
NUMBER OF CHAR REACTIONS                   1
MAXIMUM NUMBER OF CORRECTORS               10
MAXIMUM NUMBER OF SYSTEM ITERATIONS        10
NUMBER OF STEPS PER PHY. PROP. CALCULATION 5
DEBUG LEVEL                               0
STIFF PARTICLE ENERGY EQUATION ASSUMPTION USED 2
THERMAL CONDUCTIVITY CALCULATIONS USE EUCKEN CORRECTION
THE K EQUATION OF FIELD ET. AL. IS USED FOR CHAR OXIDATION WITH O2
DYNAMIC REGION INITIATION TEMP.(DEGREES K) 800.00
MAXIMUM ACCEPTABLE ROOT MEAN SQUARE(DEGREES K) 10.00
TEMP. CHANGE TOLERANCE(DEGREES K)         0.01000000
TOTAL PARTICLE REACTION RATE CHANGE TOLERANCE 0.00000010
CORRECTOR CONVERGENCE SLOPE TOLERANCE      0.01000000
TOLERANCE FOR STIFF ASSUMPTION APPLICATION 0.00100000
```

GAS PARAMETERS*****

GAS MOLECULAR WEIGHT (G/GMOLE)	ENTHALPY OF THE GAS (CAL/G)	DENSITY OF THE GAS (G/CM**3)	MASS FLOW RATE (G/SEC)	PRESSURE (ATM)
29.5000	13.5900	0.98930E-03	5.6000	0.9252
	ENTHALPY OF THE SECONDARY (CAL/G)		MASS ADDITION RATE FROM SECONDARY (G/CM-SEC)	
	71.5400		0.0000X**2 + -0.0593X +	2.0691
DISTANCE FOR RECIRCULATION PROPERTIES (CM)	ENTHALPY OF RECIRCULATION (CAL/G)		MASS ADDITION RATE FROM RECIRCULATION (G/CM-SEC)	
26.0000	71.5400	0.0000X**3 +	0.0000X**2 + -0.0657X +	1.1463

PARAMETERS FOR THE NUMBER 1 PARTICLE PHASE*****

DIAMETER (CM)	EMISSIONITY	ENTHALPY (CAL/G)	SURFACE AREA FACTOR	MASS FLOW RATE (G/SEC)
0.0020	0.7000	-713.0000	0.10000E+01	1.3300

ASH MASS (G)	COAL MASS (G)	CHAR MASS (G)	WATER MASS (G)	CHAR REF. ENTHALPY (CAL/G)	WATER REF. ENTHALPY (CAL/G)
0.51700E-09	0.47600E-08	0.00000E+00	0.16900E-09	0.0000	-3185.4500

STARTING TEMPERATURE (K)	DISTANCE TEMP RISE BEGINS (CM)	INITIAL MAXIMUM TEMP IS REACHED (K)	DISTANCE INITIAL MAX (CM)
355.6000	80.0000	2100.0000	130.0000

ENTHALPY OF THE SECONDARY (CAL/G)	MASS ADDITION RATE FROM SECONDARY (G/CM-SEC)
0.0000	0.0000X**2 + 0.0000X + 0.0000

DISTANCE FOR RECIRCULATION PROPERTIES (CM)	ENTHALPY OF RECIRCULATION (CAL/G)	MASS ADDITION RATE FROM RECIRCULATION (G/CM-SEC)
17.0000	-600.0000	0.0000X**3 + 0.0000X**2 + 0.0000X + 0.0000

PARAMETERS FOR EACH COAL REACTION AND PARTICLE

REACTION	PYROLYSIS PRE- EXPONENTIAL FACTOR (1/SEC)	ACTIVATION ENERGY IN REACTION (CAL/GMOLE-K)	MASS FRACTION
1	0.37000E+06	17600.0000	0.3900
2	0.14600E+14	60000.0000	0.8000

CP COEFFICIENTS			H FVJ
	(CAL/G)		
0.174E+00	0.810E-03	0.000E+00	-807.000

CP COEFFICIENTS			H FVJ
	(CAL/G)		
0.543E+00	0.610E-03	0.000E+00	-394.000

PARAMETERS FOR EACH CHAR REACTION AND PARTICLE

REACTION	SURFACE REACTION PRE- EXPONENTIAL FACTOR (CM/SEC-K**M)	ACTIVATION ENERGY (CAL/GMOLE)	M
1	0.10051E+03	20400.0000	1.00

THE K EQUATION OF FIELD ET. AL. IS USED FOR CHAR OXIDATION WITH O2

STOICHIOMETRIC COEFFICIENT FOR JTH PARTICLE TO KTH ELEMENT IN MOISTURE EVAPORATION

ELEMENT	COEFFICIENT
C	0.0000
H	0.1111
N	0.0000
S	0.0000
O	0.8889
Ar	0.0000

STOICHIOMETRIC COEFFICIENT FOR JTH PARTICLE TO KTH ELEMENT IN MTH REACTION (DEVOLATILIZATION)

ELEMENT	REACTION	COEFFICIENT
C	1	0.4846
H	1	0.1538
N	1	0.0410
S	1	0.0154
O	1	0.3052
Ar	1	0.0000
C	2	0.7488
H	2	0.0750
N	2	0.0200
S	2	0.0075
O	2	0.1488
Ar	2	0.0000

COEFFICIENTS FOR QUADRATIC EQUATION OF HEAT CAPACITY

COAL PART	1	2	3
COAL	0.300E+00	0.000E+00	0.000E+00
CHAR	0.300E+00	0.000E+00	0.000E+00
WATER	0.100E+01	0.000E+00	0.000E+00
ASH	0.300E+00	0.000E+00	0.000E+00

PARAMETERS FOR THE NUMBER 2 PARTICLE PHASE*****

DIAMETER (CM) 0.0048	EMISSIVITY 0.7000	ENTHALPY (CAL/G) -713.0000	SURFACE AREA FACTOR 0.10000E+01	MASS FLOW RATE (G/SEC) 1.2900
ASH MASS (G) 0.71510E-08	COAL MASS (G) 0.65790E-07	CHAR MASS (G) 0.00000E+00	WATER MASS (G) 0.23340E-08	CHAR REF. ENTHALPY (CAL/G) 0.0000
				WATER REF. ENTHALPY (CAL/G) -3185.0000
STARTING TEMPERATURE (K) 355.6000	DISTANCE TEMP RISE BEGINS (CM) 80.0000	INITIAL MAXIMUM TEMP IS REACHED (K) 2100.0000	DISTANCE INITIAL MAX (CM) 130.0000	
	ENTHALPY OF THE SECONDARY (CAL/G) 0.0000		MASS ADDITON RATE FROM SECONDARY (G/CM=SEC) 0.0000X**2 + 0.0000X + 0.0000	
DISTANCE FOR RECIRCULATION PROPERTIES (CM) 0.0000	ENTHALPY OF RECIRCULATION (CAL/G) 0.0000	0.0000X**3 +	MASS ADDITION RATE FROM RECIRCULATION (G/CM=SEC) 0.0000X**2 + 0.0000X + 0.0000	

PARAMETERS FOR EACH COAL REACTION AND PARTICLE

REACTION	PYROLYSIS PRE- EXPONENTIAL FACTOR (1/SEC)	ACTIVATION ENERGY IN REACTION (CAL/GMOLE-K)	MASS FRACTION	
1	0.37000E+06	17600.0000	0.3900	
2	0.14600E+14	60000.0000	0.8000	
	CP COEFFICIENTS		H FVJ	
	0.174E+00	0.810E-03	0.000E+00	-807.000
	CP COEFFICIENTS		H FVJ	
	0.543E+00	0.610E-03	0.000E+00	-394.000

PARAMETERS FOR EACH CHAR REACTION AND PARTICLE

REACTION	SURFACE REACTION PRE- EXPONENTIAL FACTOR (CM/SEC-K**M)	ACTIVATION ENERGY (CAL/GMOLE)	M
1	0.10051E+03	20400.0000	1.00

THE K EQUATION OF FIELD ET. AL. IS USED FOR CHAR OXIDATION WITH O2

STOICHIOMETRIC COEFFICIENT FOR JTH PARTICLE TO KTH ELEMENT IN MOISTURE EVAPORATION

ELEMENT	COEFFICIENT
C	0.0000
H	0.1111
N	0.0000
S	0.0000
O	0.8889
Ar	0.0000

STOICHIOMETRIC COEFFICIENT FOR JTH PARTICLE TO KTH ELEMENT IN MTH REACTION (DEVOLATILIZATION)

ELEMENT	REACTION	COEFFICIENT
C	1	0.4846
H	1	0.1538
N	1	0.0410
S	1	0.0154
O	1	0.3052
Ar	1	0.0000
C	2	0.7488
H	2	0.0750
N	2	0.0200
S	2	0.0075
O	2	0.1488
Ar	2	0.0000

COEFFICIENTS FOR QUADRATIC EQUATION OF HEAT CAPACITY

COAL PART	1	2	3
COAL	0.300E+00	0.000E+00	0.000E+00
CHAR	0.300E+00	0.000E+00	0.000E+00
WATER	0.100E+01	0.000E+00	0.000E+00
ASH	0.300E+00	0.000E+00	0.000E+00

PARAMETERS FOR THE NUMBER 3 PARTICLE PHASE*****

DIAMETER (CM)	EMISSIVITY	ENTHALPY (CAL/G)	SURFACE AREA FACTOR	MASS FLOW RATE (G/SEC)
0.0080	0.7000	-713.0000	0.10000E+01	1.1800

ASH MASS (G)	COAL MASS (G)	CHAR MASS (G)	WATER MASS (G)	CHAR REF. ENTHALPY (CAL/G)	WATER REF. ENTHALPY (CAL/G)
0.33100E-07	0.30500E-06	0.00000E+00	0.10800E-07	0.0000	-3798.0000

STARTING TEMPERATURE (K)	DISTANCE TEMP RISE BEGINS (CM)	INITIAL MAXIMUM TEMP IS REACHED (K)	DISTANCE INITIAL MAX (CM)
355.6000	80.0000	2100.0000	130.0000

ENTHALPY OF THE SECONDARY (CAL/G)	MASS ADDITION RATE FROM SECONDARY (G/CM-SEC)
0.0000	0.0000X**2 + 0.0000X + 0.0000

DISTANCE FOR RECIRCULATION PROPERTIES (CM)	ENTHALPY OF RECIRCULATION (CAL/G)	MASS ADDITION RATE FROM RECIRCULATION (G/CM-SEC)
17.0000	300.0000	0.0000X**3 + 0.0000X**2 + 0.0000X + 0.0000

PARAMETERS FOR EACH COAL REACTION AND PARTICLE

REACTION	PYROLYSIS PRE- EXPONENTIAL FACTOR (1/SEC)	ACTIVATION ENERGY IN REACTION (CAL/GMOLE-K)	MASS FRACTION
1	0.37000E+06	17600.0000	0.3900
2	0.14600E+14	60000.0000	0.8000

CP COEFFICIENTS	H FVJ
(CAL/G)	
0.174E+00 0.810E-03 0.000E+00	-807.000

CP COEFFICIENTS	H FVJ
(CAL/G)	
0.543E+00 0.610E-03 0.000E+00	-394.000

PARAMETERS FOR EACH CHAR REACTION AND PARTICLE

REACTION	SURFACE REACTION PRE- EXPONENTIAL FACTOR (CM/SEC-K**M)	ACTIVATION ENERGY (CAL/GMOLE)	M
1	0.10051E+03	20400.0000	1.00

THE K EQUATION OF FIELD ET. AL. IS USED FOR CHAR OXIDATION WITH O2

STOICHIOMETRIC COEFFICIENT FOR JTH PARTICLE TO KTH ELEMENT IN MOISTURE EVAPORATION

ELEMENT	COEFFICIENT
C	0.0000
H	0.1111
N	0.0000
S	0.0000
O	0.8889
Ar	0.0000

STOICHIOMETRIC COEFFICIENT FOR JTH PARTICLE TO KTH ELEMENT IN MTH REACTION (DEVOLATILIZATION)

ELEMENT	REACTION	COEFFICIENT
C	1	0.4846
H	1	0.1538
N	1	0.0410
S	1	0.0154
O	1	0.3052
Ar	1	0.0000
C	2	0.7488
H	2	0.0750
N	2	0.0200
S	2	0.0075
O	2	0.1488
Ar	2	0.0000

COEFFICIENTS FOR QUADRATIC EQUATION OF HEAT CAPACITY

COAL PART	1	2	3
COAL	0.300E+00	0.000E+00	0.000E+00
CHAR	0.300E+00	0.000E+00	0.000E+00
WATER	0.100E+01	0.000E+00	0.000E+00
ASH	0.300E+00	0.000E+00	0.000E+00

ELEMENT PARAMETERS*****

ELEMENT	ATOMIC WT.	INITIAL MASS FRACTION	MASS FRACTION	MASS FRACTION	STOICHIOMETRIC COEFFICIENTS FROM LTH REACTION
			IN SEC. (G/CM-SEC)	IN RECIRC. (G/CM-SEC)	
C	12.00000	0.00000	0.00000	0.00000	1.00000
H	1.00000	0.00000	0.00000	0.00000	0.00000
N	14.00000	0.70120	0.75890	0.76000	0.00000
S	32.00000	0.00000	0.00000	0.00700	0.00000
O	16.00000	0.22180	0.23080	0.23080	0.00000
Ar	40.00000	0.07700	0.01030	0.01030	0.00000

SPECIES PARAMETERS*****

SPECIES	COLLISION DIAMETER	EPSILON/K	DELTA	MOL FRAC IN	NUMBER OF ELEMENTS IN A SPECIES					
					C	H	N	S	O	Ar
AR	3.41800	124.00000	0.00000	0.10000	0.	0.	0.	0.	0.	1.
CO	3.59000	110.00000	0.00000	0.10000	1.	0.	0.	0.	1.	0.
O2	3.43300	113.00000	0.00000	0.20000	0.	0.	0.	0.	2.	0.
N2	3.68100	91.50000	0.00000	1.00000	0.	0.	2.	0.	0.	0.
CO2	3.99600	190.00000	0.00000	0.10000	1.	0.	0.	0.	2.	0.
H2O	2.64100	809.10000	1.00000	0.20000	0.	2.	0.	0.	1.	0.
H2	2.91500	38.00000	0.00000	0.10000	0.	2.	0.	0.	0.	0.
CH4	3.82200	137.00000	0.00000	0.60000	1.	4.	0.	0.	0.	0.
SO2	4.29000	252.00000	0.42000	0.01000	0.	0.	0.	1.	2.	0.
NO	3.49200	116.70000	0.00000	0.00100	0.	0.	1.	0.	1.	0.

SPECIES	ENTHALPY	ENTROPY	HEAT CAPACITY COEFF. FOR EDWARDS				
AR	4.48700	43.90100	4.9870	0.0000	0.0000	0.0000	0.0000
			4.9870	0.0000	0.0000	0.0000	0.0000
CO	-19.62150	57.49990	9.6744	-4.2373	9.0746	-12.0826	5.6376
			7.5994	-4.8661	11.5395	-8.5080	2.1666
O2	7.11490	59.73200	10.9940	-1.0300	-16.8890	32.3940	-17.5193
			7.1663	-3.3897	12.9769	-12.1542	3.7360
N2	6.71870	55.95780	9.7325	-4.9604	11.2348	-15.2917	7.2889
			7.5309	-4.0828	8.9494	-5.9095	1.3277
CO2	-83.42260	66.75520	16.9476	-12.9426	31.5939	-40.9050	18.7665
			4.4269	19.8206	-19.3181	10.4840	-2.4332
H2O	-49.55700	57.44630	15.5208	-6.7693	0.7168	-2.1223	2.6974
			8.0455	-1.8538	7.2725	-4.7628	1.1489
H2	6.40480	41.03490	12.8548	-23.8674	52.9484	-61.0990	27.0132
			6.1563	4.6572	-9.6723	8.7834	-2.7044
CH4	-5.16060	62.43440					

			25.7473 7.4307	1.2222 -6.3982	-22.0015 44.3471	15.0340 -39.8204	-2.7867 11.5976
SD2	-60.07880	75.46430	16.0201 5.9938	-11.0806 14.2911	25.7165 -8.3110	-30.4358 0.0191	13.0862 1.0272
NO	28.54110	60.88110	9.6120 8.1959	-3.4797 -7.8995	7.1128 18.6061	-9.1987 -14.9907	4.1679 4.2114

PHYSICAL PARAMETERS*****

DIAMETER OF DUCT (CM)	DIAMETER OF CHAMBER (CM)	REACTOR LENGTH (CM)	GROWTH AREA ANGLE (DEGREES)	EMISSIVITY OF THE WALL	TEMPERATURE OF THE WALL (K)
1.5875	20.3200	152.4000	15.0000	1.0000	1200.0000

ABSORPTION EFFICIENCY	PARTICLE SWELLING	MOLECULAR WEIGHT OF CHAR (G/GMOLE)
1.0000	0.1000	12.0000

CHAR REACTION DATA*****

REACTION	OXYDIZER	STOICHIOMETRIC COEFFICIENT
1	O2	2.0000

THE ORDERED PAIR OF (X,# OF CORRECTORS APPLIED) FOLLOWS FOR EACH O,D,E, STEP

(1.22, 1)	(2.03, 1)	(2.24, 1)	(2.44, 1)	(2.64, 1)	(2.84, 1)	(3.66, 1)	(3.86, 1)	(4.06, 1)	(4.27, 1)	(4.47, 1)	(4.67, 1)
(4.88, 1)	(5.08, 1)	(5.28, 1)	(5.49, 1)	(5.69, 1)	(5.89, 1)	(6.10, 1)	(6.30, 1)	(6.50, 1)	(6.71, 1)	(6.91, 1)	(7.11, 1)
(7.32, 1)	(7.52, 1)	(7.72, 1)	(7.92, 1)	(8.13, 1)	(8.33, 1)	(8.53, 1)	(8.74, 1)	(8.94, 1)	(9.14, 1)	(9.35, 1)	(9.55, 1)
(9.75, 1)	(9.96, 1)	(10.16, 1)	(10.36, 1)	(10.57, 1)	(10.77, 1)	(10.97, 1)	(11.18, 1)	(11.38, 1)	(11.58, 1)	(11.79, 1)	(11.99, 1)
(12.19, 1)	(12.40, 1)	(12.60, 1)	(12.80, 1)	(13.00, 1)	(13.21, 1)	(13.41, 1)	(13.61, 1)	(13.82, 1)	(14.02, 1)	(14.22, 1)	(14.43, 1)
(14.63, 1)	(14.83, 1)	(15.04, 1)	(15.24, 1)	(15.44, 1)	(15.65, 1)	(15.85, 1)	(16.05, 1)	(16.26, 1)	(16.46, 1)	(16.66, 1)	(16.87, 1)
(17.07, 1)	(17.27, 1)	(17.48, 1)	(17.68, 1)	(17.88, 1)	(18.08, 1)	(18.29, 1)	(18.49, 1)	(18.69, 1)	(18.90, 1)	(19.10, 1)	(19.30, 1)
(19.51, 1)	(19.71, 1)	(19.91, 1)	(20.12, 1)	(20.32, 1)	(20.52, 1)	(20.73, 1)	(20.93, 1)	(21.13, 1)	(21.34, 1)	(21.54, 1)	(21.74, 1)
(21.95, 1)	(22.15, 1)	(22.35, 1)	(22.56, 1)	(22.76, 1)	(22.96, 1)	(23.16, 1)	(23.37, 1)	(23.57, 1)	(23.77, 1)	(23.98, 1)	(24.18, 1)
(24.38, 1)	(24.59, 1)	(24.79, 1)	(24.99, 1)	(25.20, 1)	(25.40, 1)	(25.60, 1)	(25.81, 1)	(26.01, 1)	(26.21, 1)	(26.42, 1)	(26.62, 1)
(26.82, 1)	(27.03, 1)	(27.23, 1)	(27.43, 1)	(27.64, 1)	(27.84, 1)	(28.04, 1)	(28.24, 1)	(28.45, 1)	(28.65, 1)	(28.85, 1)	(29.06, 1)
(29.26, 1)	(29.46, 1)	(29.67, 2)	(29.87, 2)	(30.07, 1)	(30.28, 1)	(30.48, 1)	(30.68, 2)	(30.89, 2)	(31.09, 1)	(31.29, 1)	(31.50, 1)
(31.70, 2)	(31.90, 2)	(32.11, 2)	(32.31, 1)	(32.51, 1)	(32.72, 2)	(32.92, 2)	(33.12, 2)	(33.32, 1)	(33.53, 1)	(33.73, 2)	(33.93, 2)
(34.14, 2)	(34.34, 1)	(34.54, 1)	(34.75, 2)	(34.95, 2)	(35.16, 4)	(35.37, 2)	(35.57, 2)	(35.78, 2)	(35.98, 1)	(36.19, 2)	(36.39, 2)
(36.59, 2)	(36.79, 1)	(36.99, 1)	(37.20, 2)	(37.40, 2)	(37.60, 2)	(37.81, 1)	(38.01, 1)	(38.21, 2)	(38.42, 2)	(38.62, 2)	(38.83, 1)
(39.03, 1)	(39.23, 2)	(39.43, 2)	(39.64, 2)	(39.84, 2)	(40.05, 2)	(40.25, 2)	(40.45, 2)	(40.66, 2)	(40.86, 2)	(41.07, 2)	(41.27, 2)
(41.47, 2)	(41.67, 2)	(41.88, 2)	(42.08, 2)	(42.28, 2)	(42.49, 2)	(42.69, 2)	(42.89, 2)	(43.10, 2)	(43.30, 2)	(43.51, 2)	(43.71, 2)
(43.92, 2)	(44.12, 2)	(44.33, 2)	(44.53, 2)	(44.74, 2)	(44.94, 2)	(45.15, 2)	(45.35, 2)	(45.56, 2)	(45.76, 2)	(45.97, 2)	(46.17, 2)
(46.37, 2)	(46.58, 2)	(46.78, 2)	(46.99, 2)	(47.19, 2)	(47.40, 2)	(47.60, 2)	(47.81, 2)	(48.01, 2)	(48.22, 2)	(48.42, 2)	(48.63, 2)
(48.83, 2)	(49.04, 2)	(49.24, 2)	(49.45, 2)	(49.65, 2)	(49.86, 2)	(50.06, 2)	(50.27, 2)	(50.47, 2)	(50.68, 2)	(50.88, 2)	(51.09, 2)
(51.29, 2)	(51.50, 2)	(51.70, 2)	(51.91, 2)	(52.11, 2)	(52.32, 2)	(52.52, 2)	(52.73, 2)	(52.93, 2)	(53.14, 2)	(53.34, 2)	(53.55, 2)
(53.75, 2)	(53.96, 2)	(54.16, 2)	(54.37, 2)	(54.57, 2)	(54.78, 2)	(54.98, 2)	(55.19, 2)	(55.39, 2)	(55.60, 2)	(55.80, 2)	(56.01, 2)
(56.21, 2)	(56.41, 2)	(56.62, 2)	(56.82, 2)	(57.03, 2)	(57.23, 2)	(57.44, 2)	(57.64, 2)	(57.85, 2)	(58.05, 2)	(58.26, 2)	(58.46, 2)
(58.67, 2)	(58.87, 2)	(59.08, 2)	(59.28, 2)	(59.49, 2)	(59.69, 2)	(59.90, 2)	(60.10, 2)	(60.31, 2)	(60.51, 2)	(60.72, 2)	(60.92, 2)
(61.13, 2)	(61.33, 2)	(61.54, 2)	(61.74, 2)	(61.95, 2)	(62.15, 2)	(62.36, 2)	(62.56, 2)	(62.77, 2)	(62.97, 2)	(63.18, 2)	(63.38, 2)
(63.58, 2)	(63.79, 2)	(63.99, 2)	(64.20, 2)	(64.40, 2)	(64.61, 2)	(64.81, 2)	(65.02, 2)	(65.22, 2)	(65.43, 2)	(65.63, 2)	(65.84, 2)
(66.04, 2)	(66.24, 2)	(66.45, 2)	(66.65, 2)	(66.86, 2)	(67.06, 2)	(67.27, 2)	(67.47, 2)	(67.67, 2)	(67.88, 2)	(68.08, 2)	(68.28, 2)
(68.49, 2)	(68.69, 2)	(68.89, 2)	(69.10, 2)	(69.30, 2)	(69.51, 2)	(69.71, 2)	(69.91, 2)	(70.12, 2)	(70.32, 2)	(70.53, 2)	(70.73, 2)
(70.94, 2)	(71.14, 2)	(71.35, 2)	(71.55, 2)	(71.75, 2)	(71.96, 2)	(72.16, 2)	(72.37, 2)	(72.57, 2)	(72.77, 2)	(72.98, 2)	(73.18, 2)
(73.38, 2)	(73.59, 2)	(73.79, 2)	(74.00, 2)	(74.20, 2)	(74.41, 2)	(74.61, 2)	(74.82, 2)	(75.02, 2)	(75.23, 2)	(75.43, 2)	(75.64, 2)
(75.84, 2)	(76.05, 2)	(76.25, 2)	(76.46, 2)	(76.66, 2)	(76.87, 2)	(77.07, 2)	(77.28, 2)	(77.48, 2)	(77.68, 2)	(77.89, 2)	(78.09, 2)
(78.30, 2)	(78.50, 2)	(78.71, 2)	(78.91, 2)	(79.12, 2)	(79.32, 2)	(79.53, 2)	(79.73, 2)	(79.94, 2)	(80.14, 2)	(80.35, 2)	(80.55, 2)
(80.76, 2)	(80.96, 2)	(81.17, 2)	(81.37, 2)	(81.58, 2)	(81.78, 2)	(81.99, 2)	(82.19, 2)	(82.40, 2)	(82.60, 2)	(82.81, 2)	(83.01, 2)
(83.22, 2)	(83.42, 2)	(83.63, 2)	(83.83, 2)	(84.04, 2)	(84.24, 2)	(84.45, 2)	(84.65, 2)	(84.86, 2)	(85.06, 2)	(85.27, 2)	(85.47, 2)
(85.68, 2)	(85.88, 2)	(86.08, 2)	(86.29, 2)	(86.49, 2)	(86.70, 2)	(86.90, 2)	(87.11, 2)	(87.31, 2)	(87.52, 2)	(87.72, 2)	(87.93, 2)
(88.13, 2)	(88.34, 2)	(88.54, 2)	(88.75, 2)	(88.95, 2)	(89.16, 2)	(89.36, 2)	(89.57, 2)	(89.77, 2)	(90.00, 2)	(90.20, 2)	(90.40, 2)
(90.60, 2)	(90.81, 2)	(91.01, 2)	(91.22, 2)	(91.42, 2)	(91.63, 2)	(91.83, 2)	(92.04, 2)	(92.24, 2)	(92.45, 2)	(92.65, 2)	(92.86, 2)
(93.06, 2)	(93.26, 2)	(93.47, 2)	(93.67, 2)	(93.88, 2)	(94.08, 2)	(94.29, 2)	(94.49, 2)	(94.70, 2)	(94.90, 2)	(95.11, 2)	(95.31, 2)
(95.52, 2)	(95.72, 2)	(95.93, 2)	(96.13, 2)	(96.34, 2)	(96.54, 2)	(96.75, 2)	(96.95, 2)	(97.16, 2)	(97.36, 2)	(97.57, 2)	(97.77, 2)
(97.98, 2)	(98.18, 2)	(98.39, 2)	(98.59, 2)	(98.80, 2)	(99.00, 2)	(99.21, 2)	(99.41, 2)	(99.62, 2)	(99.82, 2)	(100.03, 2)	(100.23, 2)
(100.44, 2)	(100.64, 2)	(100.85, 2)	(101.05, 2)	(101.26, 2)	(101.46, 2)	(101.67, 2)	(101.87, 2)	(102.08, 2)	(102.28, 2)	(102.48, 2)	(102.69, 2)
(102.89, 2)	(103.09, 2)	(103.30, 2)	(103.50, 2)	(103.71, 2)	(103.91, 2)	(104.12, 2)	(104.32, 2)	(104.53, 2)	(104.73, 2)	(104.94, 2)	(105.14, 2)
(105.35, 2)	(105.55, 2)	(105.76, 2)	(105.96, 2)	(106.17, 2)	(106.37, 2)	(106.58, 2)	(106.78, 2)	(106.99, 2)	(107.19, 2)	(107.40, 2)	(107.60, 2)
(107.81, 2)	(108.01, 2)	(108.22, 2)	(108.42, 2)	(108.63, 2)	(108.83, 2)	(109.04, 2)	(109.24, 2)	(109.45, 2)	(109.65, 2)	(109.86, 2)	(110.06, 2)
(110.27, 2)	(110.47, 2)	(110.68, 2)	(110.88, 2)	(111.09, 2)	(111.29, 2)	(111.50, 2)	(111.70, 2)	(111.91, 2)	(112.11, 2)	(112.32, 2)	(112.52, 2)
(112.73, 2)	(112.93, 2)	(113.14, 2)	(113.34, 2)	(113.55, 2)	(113.75, 2)	(113.96, 2)	(114.16, 2)	(114.37, 2)	(114.57, 2)	(114.78, 2)	(114.98, 2)
(115.19, 2)	(115.39, 2)	(115.60, 2)	(115.80, 2)	(116.01, 2)	(116.21, 2)	(116.42, 2)	(116.62, 2)	(116.83, 2)	(117.03, 2)	(117.24, 2)	(117.44, 2)
(117.65, 2)	(117.85, 2)	(118.06, 2)	(118.26, 2)	(118.47, 2)	(118.67, 2)	(118.88, 2)	(119.08, 2)	(119.29, 2)	(119.49, 2)	(119.70, 2)	(119.90, 2)
(120.11, 2)	(120.31, 2)	(120.52, 2)	(120.72, 2)	(120.93, 2)	(121.13, 2)	(121.34, 2)	(121.54, 2)	(121.75, 2)	(121.95, 2)	(122.16, 2)	(122.36, 2)
(122.57, 2)	(122.77, 2)	(122.98, 2)	(123.18, 2)	(123.39, 2)	(123.59, 2)	(123.80, 2)	(124.00, 2)	(124.21, 2)	(124.41, 2)	(124.62, 2)	(124.82, 2)
(125.03, 2)	(125.23, 2)	(125.44, 2)	(125.64, 2)	(125.85, 2)	(126.05, 2)	(126.26, 2)	(126.46, 2)	(126.67, 2)	(126.87, 2)	(127.08, 2)	(127.28, 2)
(127.48, 2)	(127.69, 2)	(127.89, 2)	(128.10, 2)	(128.30, 2)	(128.51, 2)	(128.71, 2)	(128.92, 2)	(129.12, 2)	(129.33, 2)	(129.53, 2)	(129.74, 2)
(129.94, 2)	(130.15, 2)	(130.35, 2)	(130.56, 2)	(130.76, 2)	(130.97, 2)	(131.17, 2)	(131.38, 2)	(131.58, 2)	(131.79, 2)	(131.99, 2)	(132.20, 2)
(132.40, 2)	(132.61, 2)	(132.81, 2)	(133.02, 2)	(133.22, 2)	(133.43, 2)	(133.63, 2)	(133.84, 2)	(134.04, 2)	(134.25, 2)	(134.45, 2)	(134.66, 2)
(134.86, 2)	(135.07, 2)	(135.27, 2)	(135.48, 2)	(135.68, 2)	(135.89, 2)	(136.09, 2)	(136.30, 2)	(136.50, 2)	(136.71, 2)	(136.91, 2)	(137.12, 2)
(137.32, 2)	(137.53, 2)	(137.73, 2)	(137.94, 2)	(138.14, 2)	(138.35, 2)	(138.55, 2)	(138.76, 2)	(138.96, 2)	(139.17, 2)	(139.37, 2)	(139.58, 2)
(139.78, 2)	(140.00, 2)	(140.20, 2)	(140.40, 2)	(140.60, 2)	(140.80, 2)	(141.01, 2)	(141.21, 2)	(141.42, 2)	(141.62, 2)	(141.83, 2)	(142.03, 2)
(142.24, 2)	(142.44, 2)	(142.65, 2)	(142.85, 2)	(143.06, 2)	(143.26, 2)	(143.47, 2)	(143.67, 2)	(143.88, 2)	(144.08, 2)	(144.29, 2)	(144.49, 2)
(144.70, 2)	(144.90, 2)	(145.11, 2)	(145.31, 2)	(145.52, 2)	(145.72, 2)	(145.93, 2)	(146.13, 2)	(146.34, 2)	(146.54, 2)	(146.75, 2)	(146.95, 2)
(147.16, 2)	(147.36, 2)	(147.57, 2)	(147.77, 2)	(147.98, 2)	(148.18, 2)	(148.39, 2)	(148.59, 2)	(148.80, 2)	(149.00, 2)	(149.21, 2)	(149.41, 2)
(149.62, 2)	(149.82, 2)	(150.03, 2)	(150.23, 2)	(150.44, 2)	(150.64, 2)	(150.85, 2)	(151.05, 2)	(151.26, 2)	(151.46, 2)	(151.67, 2)	(151.87, 2)
(152.08, 2)	(152.28, 2)	(152.48, 2)	(152.69, 2)	(152.89, 2)	(153.10, 2)	(153.30, 2)	(153.51, 2)	(153.71, 2)	(153.92, 2)	(154.12, 2)	(154.33, 2)
(154.53, 2)	(154.74, 2)	(154.94, 2)	(155.15, 2)	(155.35, 2)	(155.56, 2)	(155.76, 2)	(155.97, 2)	(156.17, 2)	(156.38, 2)	(156.58, 2)	(156.79, 2)
(156.99, 2)	(157.20, 2)	(157.40, 2)	(157.61, 2)	(157.81, 2)	(158.02, 2)	(158.22, 2)	(158.43, 2)	(158.63, 2)	(158.84, 2)	(159.04, 2)	(159.25, 2)
(159.45, 2)	(159.66, 2)	(159.86, 2)	(160.07, 2)	(160.27, 2)	(160.48, 2)	(160.68, 2)	(160.89, 2)	(161.09, 2)	(161.30, 2)	(161.50, 2)	(161.71, 2)
(161.91, 2)	(162.12, 2)	(162.32, 2)	(162.53, 2)	(162.73, 2)	(162.94, 2)	(163.14, 2)	(163.35, 2)	(163.55, 2)	(163.76, 2)	(163.96, 2)	(164.17, 2)
(164.37, 2)	(164.58, 2)	(164.78, 2)	(164.99, 2)	(165.19, 2)	(165.40, 2)	(165.60, 2)	(165.81, 2)	(166.01, 2)	(166.22, 2)	(166.42, 2)	(166.63, 2)
(166.83, 2)	(167.04, 2)	(167.24, 2)	(167.45, 2)	(167.65, 2)	(167.86, 2)	(168.06, 2)	(168.27, 2)	(168.47, 2)	(168.68, 2)	(168.88, 2)	(169.09, 2)
(169.29, 2)	(169.50, 2)	(169.70, 2)	(169.91, 2)	(170.11, 2)	(170.32, 2)	(170.52, 2)	(170.73, 2)	(170.93, 2)	(171.14, 2)	(171.34, 2)	(171.55, 2)
(171.75, 2)	(171.96, 2)	(172.16, 2)	(172.37, 2)	(172.57, 2)	(172.78, 2)	(172.98, 2)	(173.19, 2)	(173.39, 2)	(173.60, 2)	(173.80, 2)	(174.01, 2)
(174.21, 2)	(174.42, 2)	(174.62, 2)	(174.83, 2)	(175.03, 2)	(175.24, 2)	(175.44, 2)	(175.65, 2)	(175.85, 2)	(176.06, 2)	(176.26, 2)	(176.47, 2)
(176.67, 2)	(176.88, 2)	(177.08, 2)	(177.29, 2)	(177.49, 2)	(177.70, 2)	(177.90, 2)	(178.11, 2)	(178.31, 2)	(178.52, 2)	(178.72, 2)	(178.93, 2)
(179.13, 2)	(179.34, 2)	(179.54, 2)	(179.75, 2)	(179.95, 2)	(180.16, 2)	(180.36, 2)	(180.57, 2)	(180.77, 2)	(180.98, 2)	(181.18, 2)	(181.39, 2)
(181.59, 2)	(181.79, 2)	(182.00, 2)	(182.20, 2)	(182.41, 2)	(182.61, 2)	(182.82, 2)	(183.02, 2)	(183.23, 2			

THE STIFF PARTICLE ENERGY EQUATION ASSUMPTION IS INITIATED FOR PARTICLE NO. 2 AT 113.59 CM. DOWN THE REACTOR
 (113.66, 2)(113.72, 1)(113.79, 1)(113.86, 1)(113.93, 1)(114.00, 1)(114.06, 1)(114.13, 1)(114.20, 1)(114.27, 1)(114.33, 1)(114.40, 1)
 (114.47, 1)(114.54, 1)(114.60, 1)(114.67, 1)(114.74, 2)(114.81, 1)(114.88, 1)(114.94, 1)(115.01, 1)(115.08, 1)(115.15, 1)(115.21, 2)
 THE STIFF PARTICLE ENERGY EQUATION ASSUMPTION IS INITIATED FOR PARTICLE NO. 3 AT 115.21 CM. DOWN THE REACTOR
 (117.65, 1)(118.26, 1)(118.87, 1)(119.48, 1)(120.09, 1)(120.70, 1)(121.31, 1)(121.92, 1)(122.53, 1)(123.14, 1)(123.75, 1)(124.36, 1)
 (124.97, 1)(125.58, 1)(126.19, 1)(126.80, 1)(127.41, 1)(128.02, 1)(128.63, 1)(129.24, 1)(129.84, 1)(130.45, 1)(131.06, 1)(131.67, 1)
 (132.28, 1)(132.89, 1)(133.50, 1)(134.11, 1)(134.72, 1)(135.33, 1)(135.94, 1)(136.55, 1)(137.16, 1)(137.77, 1)(138.38, 1)(138.99, 1)
 (139.60, 1)(140.21, 1)(140.82, 1)(141.43, 1)(142.04, 1)(142.65, 1)(143.26, 1)(143.87, 1)(144.48, 1)(145.08, 1)(145.69, 1)(146.30, 1)
 (146.91, 1)(147.52, 1)(148.13, 1)(148.74, 1)(149.35, 1)(149.96, 1)(150.57, 1)(151.18, 1)(151.79, 1)(152.40, 1)(

AFTER 1 ITERATION(S) THROUGH THE REACTOR THE ROOT MEAN SQUARE OF ALL PARTICLE TEMPERATURES IS 535.742 DEGREES KELVIN

THE ORDERED PAIR OF (X,# OF CORRECTORS APPLIED) FOLLOWS FOR EACH O.D.E. STEP

(1.22, 1)	(2.03, 1)	(2.24, 1)	(2.44, 1)	(2.64, 1)	(2.84, 1)	(3.66, 1)	(3.86, 1)	(4.06, 1)	(4.27, 1)	(4.47, 1)	(4.67, 1)
(4.88, 1)	(5.08, 1)	(5.28, 1)	(5.49, 1)	(5.69, 1)	(5.89, 1)	(6.10, 1)	(6.30, 1)	(6.50, 1)	(6.71, 1)	(6.91, 1)	(7.11, 1)
(7.32, 1)	(7.52, 1)	(7.72, 1)	(7.92, 1)	(8.13, 1)	(8.33, 1)	(8.53, 1)	(8.74, 1)	(8.94, 1)	(9.14, 1)	(9.35, 1)	(9.55, 1)
(9.75, 1)	(9.96, 1)	(10.16, 1)	(10.36, 1)	(10.57, 1)	(10.77, 1)	(10.97, 1)	(11.18, 1)	(11.38, 1)	(11.58, 1)	(11.79, 1)	(11.99, 1)
(12.19, 1)	(12.40, 1)	(12.60, 1)	(12.80, 1)	(13.00, 1)	(13.21, 1)	(13.41, 1)	(13.61, 1)	(13.82, 1)	(14.02, 1)	(14.22, 1)	(14.43, 1)
(14.63, 1)	(14.83, 1)	(15.04, 1)	(15.24, 1)	(15.44, 1)	(15.65, 1)	(15.85, 1)	(16.05, 1)	(16.26, 1)	(16.46, 1)	(16.66, 1)	(16.87, 1)
(17.07, 1)	(17.27, 1)	(17.48, 1)	(17.68, 1)	(17.88, 1)	(18.08, 1)	(18.29, 1)	(18.49, 1)	(18.69, 1)	(18.90, 1)	(19.10, 1)	(19.30, 1)
(19.51, 1)	(19.71, 1)	(19.91, 1)	(20.12, 1)	(20.32, 1)	(20.52, 1)	(20.73, 1)	(20.93, 1)	(21.13, 1)	(21.34, 1)	(21.54, 1)	(21.74, 1)
(21.95, 1)	(22.15, 1)	(22.35, 1)	(22.56, 1)	(22.76, 1)	(22.96, 1)	(23.16, 1)	(23.37, 1)	(23.57, 1)	(23.77, 1)	(23.98, 1)	(24.18, 1)
(24.38, 1)	(24.59, 1)	(24.79, 1)	(24.99, 1)	(25.20, 1)	(25.40, 1)	(25.60, 1)	(25.81, 1)	(26.01, 1)	(26.21, 1)	(26.42, 1)	(26.62, 1)
(26.82, 1)	(27.03, 1)	(27.23, 1)	(27.43, 1)	(27.64, 1)	(27.84, 1)	(28.04, 1)	(28.24, 1)	(28.45, 1)	(28.65, 2)	(28.85, 2)	(29.06, 1)
(29.26, 1)	(29.46, 1)	(29.67, 1)	(29.87, 2)	(30.07, 1)	(30.28, 1)	(30.48, 1)	(30.68, 2)	(30.89, 2)	(31.09, 1)	(31.29, 1)	(31.50, 1)
(31.70, 2)	(31.90, 2)	(32.11, 2)	(32.31, 1)	(32.51, 1)	(32.72, 2)	(32.92, 2)	(33.12, 2)	(33.32, 1)	(33.53, 1)	(33.73, 2)	(33.93, 2)
(34.14, 2)	(34.34, 1)	(34.54, 1)	(34.75, 2)	(34.95, 2)	(35.16, 3)	(35.37, 3)	(35.57, 3)	(35.77, 2)	(35.98, 1)	(36.18, 2)	(36.38, 2)
(36.58, 2)	(36.78, 2)	(36.98, 2)	(37.19, 2)	(37.39, 2)	(37.59, 1)	(37.80, 2)	(38.00, 2)	(38.20, 2)	(38.41, 2)	(38.61, 2)	(38.81, 2)
(39.02, 1)	(39.22, 2)	(39.42, 2)	(39.62, 1)	(39.83, 2)	(40.03, 2)	(40.23, 2)	(40.44, 2)	(40.64, 1)	(40.84, 2)	(41.05, 3)	(41.25, 2)
(41.45, 1)	(41.66, 1)	(41.86, 2)	(42.06, 2)	(42.27, 2)	(42.47, 1)	(42.67, 1)	(42.88, 2)	(43.08, 2)	(43.28, 2)	(43.48, 2)	(43.69, 1)
(43.89, 2)	(44.09, 3)	(44.30, 2)	(44.50, 1)	(44.70, 1)	(44.91, 2)	(45.11, 2)	(45.31, 2)	(45.52, 1)	(45.72, 1)	(45.92, 1)	(46.13, 2)
(46.33, 2)	(46.53, 2)	(46.74, 2)	(46.94, 1)	(47.14, 2)	(47.35, 2)	(47.55, 2)	(47.75, 2)	(47.96, 1)	(48.16, 2)	(48.36, 2)	(48.56, 2)
(48.77, 1)	(48.97, 1)	(49.17, 2)	(49.38, 2)	(49.58, 2)	(49.78, 2)	(49.99, 1)	(50.19, 2)	(50.39, 2)	(50.60, 2)	(50.80, 2)	(51.00, 1)
(51.21, 2)	(51.41, 2)	(51.61, 2)	(51.82, 1)	(52.02, 1)	(52.22, 2)	(52.43, 2)	(52.63, 2)	(52.83, 2)	(53.04, 1)	(53.24, 2)	(53.44, 2)
(53.64, 2)	(53.85, 2)	(54.05, 1)	(54.25, 2)	(54.46, 2)	(54.66, 2)	(54.86, 1)	(55.07, 1)	(55.27, 2)	(55.47, 2)	(55.68, 2)	(55.88, 2)
(56.08, 1)	(56.29, 2)	(56.49, 2)	(56.69, 2)	(56.90, 2)	(57.10, 1)	(57.30, 2)	(57.51, 2)	(57.71, 2)	(57.91, 1)	(58.12, 1)	(58.32, 2)
(58.52, 2)	(58.72, 2)	(58.93, 1)	(59.13, 1)	(59.33, 2)	(59.54, 2)	(59.74, 2)	(59.94, 1)	(60.15, 1)	(60.35, 2)	(60.55, 2)	(60.76, 2)
(60.96, 1)	(61.16, 1)	(61.37, 2)	(61.57, 2)	(61.77, 2)	(61.98, 1)	(62.18, 1)	(62.38, 2)	(62.59, 2)	(62.79, 2)	(63.00, 2)	(63.20, 1)
(63.40, 2)	(63.60, 2)	(63.80, 2)	(64.01, 1)	(64.21, 1)	(64.41, 2)	(64.62, 2)	(64.82, 2)	(65.02, 1)	(65.23, 1)	(65.43, 2)	(65.63, 2)
(65.84, 2)	(66.04, 1)	(66.24, 1)	(66.45, 2)	(66.65, 2)	(66.85, 2)	(67.06, 1)	(67.26, 1)	(67.46, 2)	(67.67, 2)	(67.87, 2)	(68.07, 1)
(68.28, 1)	(68.48, 2)	(68.68, 2)	(68.88, 2)	(69.09, 1)	(69.29, 1)	(69.49, 2)	(69.70, 2)	(69.90, 1)	(70.10, 1)	(70.31, 1)	(70.51, 1)
(70.71, 1)	(70.92, 1)	(71.12, 1)	(71.32, 1)	(71.53, 1)	(71.73, 2)	(71.93, 1)	(72.14, 1)	(72.34, 1)	(72.54, 1)	(72.75, 1)	(72.95, 1)
(73.15, 1)	(73.36, 1)	(73.56, 1)	(73.76, 1)	(73.96, 1)	(74.17, 1)	(74.37, 1)	(74.57, 1)	(74.78, 1)	(74.98, 1)	(75.18, 1)	(75.39, 1)
(75.59, 1)	(75.79, 1)	(76.00, 1)	(76.20, 1)	(76.40, 1)	(76.61, 1)	(76.81, 1)	(77.01, 1)	(77.22, 1)	(77.42, 1)	(77.62, 1)	(77.83, 1)
(78.03, 1)	(78.23, 1)	(78.44, 1)	(78.64, 1)	(78.84, 1)	(79.04, 1)	(79.25, 1)	(79.45, 1)	(79.65, 1)	(79.86, 1)	(80.06, 1)	(80.26, 1)
(80.47, 1)	(80.67, 1)	(80.87, 1)	(81.08, 1)	(81.28, 1)	(81.48, 1)	(81.69, 1)	(81.89, 1)	(82.09, 1)	(82.30, 1)	(82.50, 1)	(82.70, 1)
(82.91, 1)	(83.11, 1)	(83.31, 1)	(83.51, 1)	(83.71, 1)	(83.92, 1)	(84.12, 1)	(84.32, 1)	(84.52, 1)	(84.72, 1)	(84.92, 1)	(85.12, 1)
(85.33, 1)	(85.53, 1)	(85.73, 1)	(85.93, 1)	(86.13, 1)	(86.33, 1)	(86.53, 1)	(86.73, 1)	(86.93, 1)	(87.13, 1)	(87.33, 1)	(87.53, 1)
(87.73, 1)	(87.93, 1)	(88.13, 1)	(88.33, 1)	(88.53, 1)	(88.73, 1)	(88.93, 1)	(89.13, 1)	(89.33, 1)	(89.53, 1)	(89.73, 1)	(89.93, 1)
(90.13, 1)	(90.33, 1)	(90.53, 1)	(90.73, 1)	(90.93, 1)	(91.13, 1)	(91.33, 1)	(91.53, 1)	(91.73, 1)	(91.93, 1)	(92.13, 1)	(92.33, 1)
(92.53, 1)	(92.73, 1)	(92.93, 1)	(93.13, 1)	(93.33, 1)	(93.53, 1)	(93.73, 1)	(93.93, 1)	(94.13, 1)	(94.33, 1)	(94.53, 1)	(94.73, 1)
(94.93, 1)	(95.13, 1)	(95.33, 1)	(95.53, 1)	(95.73, 1)	(95.93, 1)	(96.13, 1)	(96.33, 1)	(96.53, 1)	(96.73, 1)	(96.93, 1)	(97.13, 1)
(97.33, 1)	(97.53, 1)	(97.73, 1)	(97.93, 1)	(98.13, 1)	(98.33, 1)	(98.53, 1)	(98.73, 1)	(98.93, 1)	(99.13, 1)	(99.33, 1)	(99.53, 1)
(99.73, 1)	(100.00, 1)	(100.11, 2)	(100.25, 2)	(100.31, 1)	(100.38, 1)	(100.45, 1)	(100.52, 1)	(100.58, 1)	(100.65, 1)	(100.72, 2)	(100.79, 2)
(100.85, 2)	(100.92, 2)	(101.00, 2)	(101.06, 2)	(101.13, 2)	(101.19, 2)	(101.26, 2)	(101.33, 2)	(101.40, 3)	(101.46, 3)	(101.53, 1)	(101.60, 1)
(101.67, 1)	(101.74, 2)	(101.80, 3)	(101.87, 3)	(101.94, 4)	(102.01, 3)	(102.07, 1)	(102.14, 1)	(102.21, 1)	(102.28, 2)	(102.35, 3)	(102.41, 2)
(102.48, 3)	(102.55, 5)	(102.62, 4)	(102.68, 3)	(102.75, 3)	(102.82, 1)	(102.89, 3)	(102.95, 1)	(103.02, 1)	(103.09, 6)	(103.16, 9)	(103.23, 10)
(103.29, 10)	(103.36, 11)	(103.43, 11)	THE STIFF PARTICLE ENERGY EQUATION ASSUMPTION IS INITIATED FOR PARTICLE NO. 1 AT 103.84 CM. DOWN THE REACTOR								
(103.50, 1)	(103.56, 10)	(103.64, 11)	(103.70, 1)	(103.77, 1)	(103.84, 1)	(103.90, 1)	(103.97, 1)	(104.04, 1)	(104.11, 1)	(104.17, 1)	(104.24, 1)
(104.31, 1)	(104.38, 1)	(104.44, 1)	(104.51, 1)	(104.58, 1)	(104.65, 1)	(104.72, 1)	(104.78, 1)	(104.85, 1)	(104.92, 1)	(104.99, 1)	(105.05, 1)
(105.12, 1)	(105.19, 1)	(105.26, 1)	(105.33, 1)	(105.39, 1)	(105.46, 1)	(105.53, 1)	(105.60, 1)	(105.66, 1)	(105.73, 1)	(105.80, 1)	(105.87, 1)
(105.93, 1)	(106.00, 1)	(106.07, 1)	(106.14, 1)	(106.21, 1)	(106.27, 1)	(106.34, 1)	(106.41, 1)	(106.48, 1)	(106.54, 1)	(106.61, 1)	(106.68, 1)
(106.75, 1)	(106.82, 1)	(106.88, 1)	(106.95, 1)	(107.02, 1)	(107.09, 1)	(107.15, 1)	(107.22, 1)	(107.29, 1)	(107.36, 1)	(107.43, 1)	(107.49, 1)
(107.56, 1)	(107.63, 1)	(107.70, 1)	(107.76, 1)	(107.83, 1)	(107.90, 1)	(107.97, 1)	(108.03, 1)	(108.10, 1)	(108.17, 1)	(108.24, 1)	(108.31, 1)
(108.37, 1)	(108.44, 1)	(108.51, 1)									

(108.58, 1)(108.64, 1)(108.71, 1)(108.78, 1)(108.85, 1)(108.92, 1)(108.98, 1)(109.05, 1)(109.12, 1)(109.19, 1)(109.25, 1)(109.32, 1)
 (109.39, 1)(109.46, 1)(109.52, 1)(109.59, 1)(109.66, 1)(109.73, 1)(109.80, 1)(109.86, 1)(109.93, 1)(110.00, 1)(110.07, 1)(110.13, 1)
 (110.20, 1)(110.27, 1)(110.34, 1)(110.41, 1)(110.47, 1)(110.54, 1)(110.61, 1)(110.68, 1)(110.74, 1)(110.81, 1)(110.88, 1)(110.95, 1)
 (111.01, 1)(111.08, 1)(111.15, 1)(111.22, 1)(111.29, 1)(111.35, 1)(111.42, 1)(111.49, 1)(111.56, 1)(111.62, 1)(111.69, 1)(111.76, 1)
 (111.83, 1)(111.90, 1)(111.96, 1)(112.03, 1)(112.10, 1)(112.17, 1)(112.23, 1)(112.30, 1)(112.37, 1)(112.44, 1)(112.51, 1)(112.57, 1)
 (112.64, 1)(112.71, 1)(112.78, 1)(112.84, 1)(112.91, 1)(112.98, 1)(113.05, 1)(113.11, 1)(113.18, 1)(113.25, 1)(113.32, 1)(113.39, 1)
 THE STIFF PARTICLE ENERGY EQUATION ASSUMPTION IS INITIATED FOR PARTICLE NO. 2 AT 113.39 CM. DOWN THE REACTOR
 (113.45, 2)(113.52, 1)(113.59, 1)(113.66, 1)(113.72, 1)(113.79, 1)(113.86, 1)(113.93, 1)(114.00, 1)(114.06, 1)(114.13, 1)(114.20, 1)
 (114.27, 1)(114.33, 1)(114.40, 1)(114.47, 1)(114.54, 1)(114.60, 1)(114.67, 1)(114.74, 1)(114.81, 1)(114.88, 1)(114.94, 1)(115.01, 1)
 (115.08, 1)(115.15, 1)(115.21, 1)(115.28, 1)(115.35, 1)(115.42, 1)(115.49, 1)(115.55, 1)(115.62, 1)(115.69, 1)(115.76, 1)(115.82, 1)
 (115.89, 1)(115.96, 1)(116.03, 1)(116.10, 1)(116.16, 1)(116.23, 1)(116.30, 1)(116.37, 1)(116.43, 1)(116.50, 1)(116.57, 1)(116.64, 1)
 (116.70, 1)(116.77, 1)(116.84, 1)(116.91, 1)(116.98, 1)(117.04, 1)(117.11, 1)(117.18, 1)(117.25, 1)(117.31, 1)(117.38, 1)(117.45, 1)
 (117.52, 1)(117.59, 1)(117.65, 1)(117.72, 1)(117.79, 1)(117.86, 1)(117.92, 1)(117.99, 1)(118.06, 1)(118.13, 1)(118.19, 1)(118.26, 1)
 (118.33, 1)(118.40, 1)(118.47, 1)(118.53, 1)(118.60, 1)(118.67, 1)(118.74, 1)(118.80, 1)(118.87, 1)(118.94, 1)(119.01, 1)(119.08, 1)
 (119.14, 1)(119.21, 1)(119.28, 1)(119.35, 1)(119.41, 1)(119.48, 1)(119.55, 1)(119.62, 1)(119.68, 1)(119.75, 1)(119.82, 1)(119.89, 1)
 (119.96, 1)(120.02, 1)(120.09, 1)(120.16, 1)(120.23, 1)(120.29, 1)(120.36, 1)(120.43, 1)(120.50, 1)(120.57, 1)(120.63, 1)(120.70, 1)
 (120.77, 1)(120.84, 1)(120.90, 1)(120.97, 1)(121.04, 1)(121.11, 1)(121.18, 1)(121.24, 1)(121.31, 1)(121.38, 1)(121.45, 1)(121.51, 1)
 (121.58, 1)(121.65, 1)(121.72, 1)(121.78, 1)(121.85, 1)(121.92, 1)(121.99, 1)(122.06, 1)(122.12, 1)(122.19, 1)(122.26, 1)(122.33, 1)
 (122.39, 1)(122.46, 1)(122.53, 1)(122.60, 1)(122.67, 1)(122.73, 1)(122.80, 1)(122.87, 1)(122.94, 1)(123.00, 1)(123.07, 1)(123.14, 1)
 (123.21, 1)(123.27, 1)(123.34, 1)(123.41, 1)(123.48, 1)(123.55, 1)(123.61, 1)(123.68, 1)(123.75, 1)(123.82, 1)(123.88, 1)(123.95, 1)
 (124.02, 1)(124.09, 1)(124.16, 1)(124.22, 1)(124.29, 1)(124.36, 1)(124.43, 1)(124.49, 1)(124.56, 1)(124.63, 1)(124.70, 1)(124.76, 1)
 (124.83, 1)(124.90, 1)(124.97, 1)(125.04, 1)(125.10, 1)(125.17, 1)(125.24, 1)(125.31, 1)(125.37, 1)(125.44, 1)(125.51, 1)(125.58, 1)
 (125.65, 1)(125.71, 1)(125.78, 1)(125.85, 1)(125.92, 1)(125.98, 1)(126.05, 1)(126.12, 1)(126.19, 1)(126.26, 1)(126.32, 1)(126.39, 1)
 (126.46, 1)(126.53, 1)(126.59, 1)(126.66, 1)(126.73, 1)(126.80, 1)(126.86, 1)(126.93, 1)(127.00, 1)(127.07, 1)(127.14, 1)(127.20, 1)
 (127.27, 1)(127.34, 1)(127.41, 1)(127.47, 1)(127.54, 1)(127.61, 1)(127.68, 1)(127.75, 1)(127.81, 1)(127.88, 1)(127.95, 1)(128.02, 1)
 (128.08, 1)(128.15, 1)(128.22, 1)(128.29, 1)(128.35, 1)(128.42, 1)(128.49, 1)(128.56, 1)(128.63, 1)(128.69, 1)(128.76, 1)(128.83, 1)
 (128.90, 1)(128.96, 1)(129.03, 1)(129.10, 1)(129.17, 1)(129.24, 1)(129.30, 1)(129.37, 1)(129.44, 1)(129.51, 1)(129.57, 1)(129.64, 1)
 THE STIFF PARTICLE ENERGY EQUATION ASSUMPTION IS INITIATED FOR PARTICLE NO. 3 AT 130.18 CM. DOWN THE REACTOR
 (129.71, 1)(129.78, 1)(129.84, 1)(129.91, 1)(129.98, 1)(130.05, 1)(130.12, 1)(130.18, 1)(130.25, 1)(130.32, 1)(130.39, 1)(130.45, 1)
 (132.89, 1)(133.50, 1)(134.11, 1)(134.72, 1)(135.33, 1)(135.94, 1)(136.55, 1)(137.16, 1)(139.60, 1)(140.21, 1)(140.82, 1)(141.43, 1)
 (142.04, 1)(142.65, 1)(143.26, 1)(143.87, 1)(144.48, 1)(145.08, 1)(145.69, 1)(146.30, 1)(146.91, 1)(147.52, 1)(148.13, 1)(148.74, 1)
 (149.35, 1)(149.96, 1)(150.57, 1)(151.18, 1)(151.79, 1)(152.40, 1)

AFTER 2 ITERATION(S) THROUGH THE REACTOR THE ROOT MEAN SQUARE OF ALL PARTICLE TEMPERATURES IS 460.601 DEGREES KELVIN

THE ORDERED PAIR OF (X, # OF CORRECTORS APPLIED) FOLLOWS FOR EACH O.D.E. STEP

```

*****
( 1.22,1)( 2.03, 1)( 2.24, 1)( 2.44, 1)( 2.64, 1)( 3.45, 1)( 3.66, 1)( 3.86, 1)( 4.06, 1)( 4.27, 1)( 4.47, 1)( 4.67, 1)
( 4.88, 1)( 5.08, 1)( 5.28, 1)( 5.49, 1)( 5.69, 1)( 5.89, 1)( 6.10, 1)( 6.30, 1)( 6.50, 1)( 6.71, 1)( 6.91, 1)( 7.11, 1)
( 7.32, 1)( 7.52, 1)( 7.72, 1)( 7.92, 1)( 8.13, 1)( 8.33, 1)( 8.53, 1)( 8.74, 1)( 8.94, 1)( 9.14, 1)( 9.35, 1)( 9.55, 1)
( 9.75, 1)( 9.96, 1)( 10.16, 1)( 10.36, 1)( 10.57, 1)( 10.77, 1)( 10.97, 1)( 11.18, 1)( 11.38, 1)( 11.58, 1)( 11.79, 1)( 11.99, 1)
( 12.19, 1)( 12.40, 1)( 12.60, 1)( 12.80, 1)( 13.00, 1)( 13.21, 1)( 13.41, 1)( 13.61, 1)( 13.82, 1)( 14.02, 1)( 14.22, 1)( 14.43, 1)
( 14.63, 1)( 14.83, 1)( 15.04, 1)( 15.24, 1)( 15.44, 1)( 15.65, 1)( 15.85, 1)( 16.05, 1)( 16.26, 1)( 16.46, 1)( 16.66, 1)( 16.87, 1)
( 17.07, 1)( 17.27, 1)( 17.48, 1)( 17.68, 1)( 17.88, 1)( 18.08, 1)( 18.29, 1)( 18.49, 1)( 18.69, 1)( 18.90, 1)( 19.10, 1)( 19.30, 1)
( 19.51, 1)( 19.71, 1)( 19.91, 1)( 20.12, 1)( 20.32, 1)( 20.52, 1)( 20.73, 1)( 20.93, 1)( 21.13, 1)( 21.34, 1)( 21.54, 1)( 21.74, 1)
( 21.95, 1)( 22.15, 1)( 22.35, 1)( 22.56, 1)( 22.76, 1)( 22.96, 1)( 23.16, 1)( 23.37, 1)( 23.57, 1)( 23.77, 1)( 23.98, 1)( 24.18, 1)
( 24.38, 1)( 24.59, 1)( 24.79, 1)( 24.99, 1)( 25.20, 1)( 25.40, 1)( 25.60, 1)( 25.81, 2)( 26.01, 1)( 26.21, 1)( 26.42, 1)( 26.62, 2)
( 26.82, 2)( 27.03, 1)( 27.23, 1)( 27.43, 1)( 27.64, 1)( 27.84, 1)( 28.04, 1)( 28.24, 1)( 28.45, 1)( 28.65, 2)( 28.85, 2)( 29.06, 2)
( 29.26, 1)( 29.46, 1)( 29.67, 2)( 29.87, 2)( 30.07, 1)( 30.28, 1)( 30.48, 1)( 30.68, 2)( 30.89, 2)( 31.09, 1)( 31.29, 1)( 31.50, 1)
( 31.70, 2)( 31.90, 2)( 32.11, 2)( 32.31, 1)( 32.51, 1)( 32.72, 2)( 32.92, 2)( 33.12, 2)( 33.32, 1)( 33.53, 1)( 33.73, 2)( 33.93, 2)
( 34.14, 2)( 34.34, 2)( 34.54, 1)( 34.75, 2)( 34.95, 3)( 35.16, 3)( 35.37, 3)( 35.57, 2)( 35.78, 1)( 35.98, 1)( 36.18, 2)( 36.38, 2)
( 36.58, 2)( 36.79, 2)( 36.99, 2)( 37.19, 2)( 37.39, 2)( 37.59, 1)( 37.80, 2)( 38.00, 3)( 38.20, 2)( 38.40, 2)( 38.61, 1)( 38.81, 2)( 39.01, 2)( 39.22, 2)( 39.42, 1)
( 39.62, 1)( 39.83, 2)( 40.03, 2)( 40.23, 2)( 40.44, 2)( 40.64, 1)( 40.84, 2)( 41.05, 3)( 41.25, 2)( 41.45, 2)( 41.66, 1)( 41.86, 2)
( 42.06, 3)( 42.27, 2)( 42.47, 1)( 42.67, 1)( 42.88, 2)( 43.08, 2)( 43.28, 2)( 43.48, 2)( 43.69, 1)( 43.89, 2)( 44.09, 3)( 44.30, 2)
( 44.50, 2)( 44.70, 1)( 44.91, 2)( 45.11, 2)( 45.31, 2)( 45.52, 1)( 45.72, 1)( 45.92, 1)( 46.13, 2)( 46.33, 2)( 46.53, 2)( 46.74, 2)
( 46.94, 2)( 47.14, 2)( 47.35, 2)( 47.55, 2)( 47.75, 2)( 47.96, 1)( 48.16, 2)( 48.36, 2)( 48.56, 2)( 48.77, 1)( 48.97, 1)( 49.17, 2)
( 49.38, 2)( 49.58, 2)( 49.78, 2)( 49.99, 1)( 50.19, 2)( 50.39, 3)( 50.60, 2)( 50.80, 1)( 51.00, 2)( 51.21, 2)( 51.41, 3)( 51.61, 2)
( 51.82, 1)( 52.02, 1)( 52.22, 2)( 52.43, 2)( 52.63, 2)( 52.83, 2)( 53.04, 1)( 53.24, 2)( 53.44, 2)( 53.64, 2)( 53.85, 2)( 54.05, 1)
( 54.25, 2)( 54.46, 2)( 54.66, 2)( 54.86, 1)( 55.07, 1)( 55.27, 2)( 55.47, 2)( 55.68, 2)( 55.88, 2)( 56.08, 1)( 56.29, 2)( 56.49, 2)
( 56.69, 2)( 56.90, 2)( 57.10, 1)( 57.30, 2)( 57.51, 2)( 57.71, 2)( 57.91, 1)( 58.12, 1)( 58.32, 2)( 58.52, 2)( 58.72, 2)( 58.93, 1)
( 59.13, 1)( 59.33, 2)( 59.54, 2)( 59.74, 2)( 59.94, 2)( 60.15, 1)( 60.35, 2)( 60.55, 2)( 60.76, 2)( 60.96, 1)( 61.16, 1)( 61.37, 2)
( 61.57, 2)( 61.77, 2)( 61.98, 1)( 62.18, 1)( 62.38, 2)( 62.59, 2)( 62.79, 2)( 62.99, 1)( 63.20, 1)( 63.40, 2)( 63.60, 2)( 63.80, 2)
( 64.01, 1)( 64.21, 1)( 64.41, 2)( 64.62, 2)( 64.82, 2)( 65.02, 1)( 65.23, 1)( 65.43, 2)( 65.63, 2)( 65.84, 2)( 66.04, 1)( 66.24, 1)
( 66.45, 2)( 66.65, 2)( 66.85, 1)( 67.06, 1)( 67.26, 1)( 67.46, 1)( 67.67, 1)( 67.87, 1)( 68.07, 1)( 68.28, 1)( 68.48, 2)( 68.68, 2)
( 68.88, 2)( 69.09, 1)( 69.29, 1)( 69.49, 2)( 69.70, 2)( 69.90, 1)( 70.10, 1)( 70.31, 1)( 70.51, 1)( 70.71, 1)( 70.92, 1)( 71.12, 1)
( 71.32, 1)( 71.53, 1)( 71.73, 2)( 71.93, 1)( 72.14, 1)( 72.34, 1)( 72.54, 1)( 72.75, 1)( 72.95, 1)( 73.15, 1)( 73.36, 1)( 73.56, 1)
( 73.76, 1)( 73.96, 1)( 74.17, 1)( 74.37, 1)( 74.57, 1)( 74.78, 1)( 74.98, 1)( 75.18, 1)( 75.39, 1)( 75.59, 1)( 75.79, 1)( 76.00, 1)
( 76.20, 1)( 76.41, 1)( 76.61, 1)( 76.81, 1)( 77.01, 1)( 77.21, 1)( 77.42, 1)( 77.62, 1)( 77.82, 1)( 78.03, 1)( 78.23, 1)( 78.44, 1)
( 78.64, 1)( 78.84, 1)( 79.04, 1)( 79.25, 1)( 79.45, 1)( 79.65, 1)( 79.86, 1)( 79.96, 1)( 80.06, 1)
( 80.16, 1)( 80.26, 1)( 80.37, 1)( 80.47, 1)( 80.57, 1)( 80.67, 1)( 80.77, 1)( 80.87, 1)( 80.98, 1)( 81.08, 1)( 81.18, 1)( 81.28, 1)
( 81.38, 1)( 81.48, 1)( 81.58, 1)( 81.69, 1)( 81.79, 1)( 81.89, 1)( 81.99, 1)( 82.09, 1)( 82.19, 1)( 82.30, 1)( 82.40, 1)( 82.50, 1)
( 82.60, 1)( 82.70, 1)( 82.80, 1)( 82.91, 1)( 83.01, 1)( 83.11, 1)( 83.21, 1)( 83.31, 1)( 83.41, 1)( 83.52, 1)( 83.62, 1)( 83.72, 1)
( 83.82, 1)( 83.92, 1)( 84.02, 1)( 84.12, 1)( 84.23, 1)( 84.33, 1)( 84.43, 1)( 84.53, 1)( 84.63, 1)( 84.73, 1)( 84.84, 1)( 84.94, 1)
( 85.04, 1)( 85.14, 1)( 85.24, 1)( 85.34, 1)( 85.45, 1)( 85.55, 1)( 85.65, 1)( 85.75, 1)( 85.85, 1)( 85.95, 1)( 86.06, 1)( 86.16, 1)
( 86.26, 1)( 86.36, 1)( 86.46, 1)( 86.56, 1)( 86.66, 1)( 86.77, 1)( 86.87, 1)( 86.97, 1)( 87.07, 1)( 87.17, 1)( 87.27, 1)( 87.38, 1)
( 87.48, 1)( 87.58, 1)( 87.68, 2)( 87.78, 2)( 87.88, 1)( 88.29, 1)( 88.39, 1)( 88.49, 1)( 88.60, 1)( 88.70, 1)( 88.80, 1)( 88.90, 1)
( 89.31, 1)( 89.41, 1)( 89.51, 1)( 89.61, 1)( 89.71, 1)( 89.81, 1)( 89.92, 1)( 90.02, 1)( 90.12, 1)( 90.22, 1)( 90.32, 1)( 90.42, 1)
( 90.53, 1)( 90.63, 1)( 90.73, 1)( 90.83, 1)( 90.93, 1)( 91.03, 1)( 91.14, 1)( 91.24, 1)( 91.34, 1)( 91.44, 1)( 91.54, 1)( 91.65, 1)
( 92.05, 1)( 92.33, 1)( 92.39, 1)( 92.46, 1)( 92.52, 1)( 92.59, 1)( 92.66, 1)( 92.73, 1)( 92.79, 1)( 92.86, 1)( 92.93, 1)( 93.00, 1)
( 93.07, 1)( 93.13, 1)( 93.20, 1)( 93.27, 1)( 93.34, 1)( 93.40, 2)( 93.47, 2)( 93.54, 2)( 93.61, 2)( 93.68, 2)( 93.74, 2)( 93.81, 1)
( 93.88, 1)( 93.95, 2)( 94.01, 3)( 94.08, 3)( 94.15, 2)( 94.22, 1)( 94.28, 1)( 94.35, 1)( 94.42, 1)( 94.49, 1)( 94.56, 1)( 94.62, 3)
( 94.69, 3)( 94.76, 2)( 94.83, 1)( 94.89, 1)( 94.96, 1)( 95.03, 1)( 95.10, 1)( 95.17, 2)( 95.23, 4)( 95.30, 4)( 95.37, 4)( 95.44, 4)
( 95.50, 4)( 95.57, 4)( 95.64, 3)( 95.71, 1)( 95.77, 3)( 95.84, 4)( 95.91, 5)( 95.98, 5)( 96.05, 1)( 96.11, 3)( 96.18, 1)( 96.25, 4)
THE STIFF PARTICLE ENERGY EQUATION ASSUMPTION IS INITIATED FOR PARTICLE NO. 1 AT 97.20 CM. DOWN THE REACTOR
( 96.32, 6)( 96.38, 7)( 96.45, 1)( 96.52, 9)( 96.59, 10)( 96.66, 10)( 96.72, 11)( 96.79, 11)( 96.86, 8)( 96.93, 11)( 97.20, 1)( 97.27, 2)
( 97.33, 1)( 97.40, 1)( 97.47, 1)( 97.54, 1)( 97.60, 1)( 97.67, 1)( 97.74, 1)( 97.81, 1)( 97.87, 1)( 97.94, 1)( 98.01, 1)( 98.08, 1)
( 98.15, 1)( 98.21, 1)( 98.28, 1)( 98.35, 1)( 98.42, 1)( 98.48, 1)( 98.55, 1)( 98.62, 1)( 98.69, 1)( 98.76, 1)( 98.82, 1)( 98.89, 1)
( 98.96, 1)( 99.03, 1)( 99.09, 1)( 99.16, 1)( 99.23, 1)( 99.30, 1)( 99.36, 1)( 99.43, 1)( 99.50, 1)( 99.57, 1)( 99.64, 1)( 99.70, 1)
( 99.77, 1)( 99.84, 1)( 99.91, 1)( 99.97, 1)( 100.04, 1)( 100.11, 1)( 100.18, 1)( 100.25, 1)( 100.31, 1)( 100.38, 1)( 100.45, 1)( 100.52, 1)
( 100.58, 1)( 100.65, 1)( 100.72, 1)( 100.79, 1)( 100.85, 1)( 100.92, 1)( 100.99, 1)( 101.06, 1)( 101.13, 1)( 101.19, 1)( 101.26, 1)( 101.33, 1)
( 101.40, 1)( 101.46, 1)( 101.53, 1)( 101.60, 1)( 101.67, 1)( 101.74, 1)( 101.80, 1)( 101.87, 1)( 101.94, 1)( 102.01, 1)( 102.07, 1)( 102.14, 1)
( 102.21, 1)( 102.28, 1)( 102.35, 1)( 102.41, 1)( 102.48, 1)( 102.55, 1)( 102.62, 1)( 102.68, 1)( 102.75, 1)( 102.82, 1)( 102.89, 1)( 102.95, 1)
THE STIFF PARTICLE ENERGY EQUATION ASSUMPTION IS INITIATED FOR PARTICLE NO. 2 AT 103.02 CM. DOWN THE REACTOR
( 103.02, 1)( 103.09, 2)( 103.16, 1)( 103.23, 1)( 103.29, 1)( 103.36, 1)( 103.43, 1)( 103.50, 1)( 103.56, 1)( 103.63, 1)( 103.70, 1)( 103.77, 1)

```

(103.84, 1)(103.90, 1)(103.97, 1)(104.04, 1)(104.11, 1)(104.17, 1)(104.24, 1)(104.31, 2)(104.38, 1)(104.44, 1)(104.51, 1)(104.58, 1)
 (104.65, 1)(104.72, 1)(104.78, 1)(104.85, 1)(104.92, 1)(104.99, 1)(105.05, 1)(105.12, 1)(105.19, 1)(105.26, 1)(105.33, 1)(105.39, 1)
 (105.46, 1)(105.53, 1)(105.60, 1)(105.66, 1)(105.73, 1)(105.80, 1)(105.87, 1)(105.93, 1)(106.00, 1)(106.07, 1)(106.14, 1)(106.21, 1)
 (106.27, 1)(106.34, 1)(106.41, 1)(106.48, 1)(106.54, 1)(106.61, 1)(106.68, 1)(106.75, 1)(106.82, 1)(106.88, 1)(106.95, 1)(107.02, 1)
 (107.09, 1)(107.15, 1)(107.22, 1)(107.29, 1)(107.36, 1)(107.43, 1)(107.49, 1)(107.56, 1)(107.63, 1)(107.70, 1)(107.76, 1)(107.83, 1)
 (107.90, 1)(107.97, 1)(108.03, 1)(108.10, 1)(108.17, 1)(108.24, 1)(108.31, 1)(108.37, 1)(108.44, 1)(108.51, 1)(108.58, 1)(108.64, 1)
 (108.71, 1)(108.78, 1)(108.85, 1)(108.92, 1)(108.98, 1)(109.05, 1)(109.12, 1)(109.19, 1)(109.25, 1)(109.32, 1)(109.39, 1)(109.46, 1)
 (109.52, 1)(109.59, 1)(109.66, 1)(109.73, 1)(109.80, 1)(109.86, 1)(109.93, 1)(110.00, 1)(110.07, 1)(110.13, 1)(110.20, 1)(110.27, 1)
 (110.34, 1)(110.41, 1)(110.47, 1)(110.54, 1)(110.61, 1)(110.68, 1)(110.74, 1)(110.81, 1)(110.88, 1)(110.95, 1)(111.02, 1)(111.08, 1)
 (111.15, 1)(111.22, 1)(111.29, 1)(111.35, 1)(111.42, 1)(111.49, 1)(111.56, 1)(111.62, 1)(111.69, 1)(111.76, 1)(111.83, 1)(111.90, 1)
 (111.96, 1)(112.03, 1)(112.10, 1)(112.17, 1)(112.23, 1)(112.30, 1)(112.37, 1)(112.44, 1)(112.51, 1)(112.57, 1)(112.64, 1)(112.71, 1)
 (112.78, 1)(112.84, 1)(112.91, 1)(112.98, 1)(113.05, 1)(113.11, 1)(113.18, 1)(113.25, 1)(113.32, 1)(113.39, 1)(113.45, 1)(113.52, 1)
 (113.59, 1)(113.66, 1)(113.72, 1)(113.79, 1)(113.86, 1)(113.93, 1)(114.00, 1)(114.06, 1)(114.13, 1)(114.20, 1)(114.27, 1)(114.33, 1)
 THE STIFF PARTICLE ENERGY EQUATION ASSUMPTION IS INITIATED FOR PARTICLE NO. 3 AT 114.60 CM. DOWN THE REACTOR
 (114.40, 1)(114.47, 1)(114.54, 1)(114.60, 1)(117.04, 1)(117.65, 1)(118.26, 1)(118.87, 1)(119.48, 1)(120.09, 1)(120.70, 1)(121.31, 1)
 (121.92, 1)(122.53, 1)(123.14, 1)(123.75, 1)(124.36, 1)(124.97, 1)(125.58, 1)(126.19, 1)(126.80, 1)(127.41, 1)(128.02, 1)(128.63, 1)
 (129.24, 1)(129.84, 1)(130.45, 1)(132.89, 1)(133.50, 1)(134.11, 1)(134.72, 1)(135.33, 1)(135.94, 1)(136.55, 1)(137.16, 1)(137.77, 1)
 (138.38, 1)(138.99, 1)(139.60, 1)(140.21, 1)(140.82, 1)(141.43, 1)(142.04, 1)(142.65, 1)(143.26, 1)(143.87, 1)(144.48, 1)(145.08, 1)
 (145.69, 1)(146.30, 1)(146.91, 1)(147.52, 1)(148.13, 1)(148.74, 1)(149.35, 1)(149.96, 1)(150.57, 1)(151.18, 1)(151.79, 1)(152.40, 1)

AFTER 3 ITERATION(S) THROUGH THE REACTOR THE ROOT MEAN SQUARE OF ALL PARTICLE TEMPERATURES IS 247.644 DEGREES KELVIN

★ ★ ★ ★ ★

(1.22,1)(	2.03,1)(	2.24,1)(	2.44,1)(	2.64,1)(	3.45,1)(	3.66,1)(	3.86,1)(	4.06,1)(	4.27,1)(	4.47,1)(	4.67,1)(
(4.88,1)(	5.08,1)(	5.28,1)(	5.49,1)(	5.69,1)(	5.89,1)(	6.10,1)(	6.30,1)(	6.50,1)(	6.71,1)(	6.91,1)(	7.11,1)(
(7.32,1)(	7.52,1)(	7.72,1)(	7.92,1)(	8.13,1)(	8.33,1)(	8.53,1)(	8.74,1)(	8.94,1)(	9.14,1)(	9.35,1)(	9.55,1)(
(9.75,1)(	9.96,1)(	10.16,1)(	10.36,1)(	10.57,1)(	10.77,1)(	10.97,1)(	11.18,1)(	11.38,1)(	11.58,1)(	11.79,1)(	11.99,1)(
(12.19,1)(	12.40,1)(	12.60,1)(	12.80,1)(	13.00,1)(	13.21,1)(	13.41,1)(	13.61,1)(	13.82,1)(	14.02,1)(	14.22,1)(	14.43,1)(
(14.63,1)(	14.83,1)(	15.04,1)(	15.24,1)(	15.44,1)(	15.65,1)(	15.85,1)(	16.05,1)(	16.26,1)(	16.46,1)(	16.66,1)(	16.87,1)(
(17.07,1)(	17.27,1)(	17.48,1)(	17.68,1)(	17.88,1)(	18.08,1)(	18.29,1)(	18.49,1)(	18.69,1)(	18.90,1)(	19.10,1)(	19.30,1)(
(19.51,1)(	19.71,1)(	19.91,1)(	20.12,1)(	20.32,1)(	20.52,1)(	20.73,1)(	20.93,1)(	21.13,1)(	21.34,1)(	21.54,1)(	21.74,1)(
(21.95,1)(	22.15,1)(	22.35,1)(	22.56,1)(	22.76,1)(	22.96,1)(	23.16,1)(	23.37,1)(	23.57,1)(	23.77,1)(	23.98,1)(	24.18,1)(
(24.38,1)(	24.59,1)(	24.79,1)(	24.99,1)(	25.20,1)(	25.40,1)(	25.60,1)(	25.81,2)(	26.01,1)(	26.21,1)(	26.42,1)(	26.62,2)(
(26.82,2)(	27.03,1)(	27.23,1)(	27.43,1)(	27.64,1)(	27.84,1)(	28.04,1)(	28.24,1)(	28.45,1)(	28.65,2)(	28.85,2)(	29.06,2)(
(29.26,1)(	29.46,1)(	29.67,2)(	29.87,2)(	30.07,1)(	30.28,1)(	30.48,1)(	30.68,2)(	30.89,2)(	31.09,1)(	31.29,1)(	31.50,1)(
(31.70,2)(	31.90,2)(	32.11,2)(	32.31,1)(	32.51,1)(	32.72,2)(	32.92,2)(	33.12,2)(	33.32,1)(	33.53,1)(	33.73,2)(	33.93,2)(
(34.14,2)(	34.34,2)(	34.54,1)(	34.75,2)(	34.95,3)(	35.76,3)(	35.97,3)(	36.17,2)(	36.37,1)(	36.58,1)(	36.78,2)(	36.98,2)(
(37.19,2)(	37.39,2)(	37.59,1)(	37.80,2)(	38.00,3)(	38.20,2)(	38.40,2)(	38.61,1)(	38.81,2)(	39.01,3)(	39.22,2)(	39.42,1)(
(39.62,1)(	39.83,2)(	40.03,2)(	40.23,2)(	40.44,2)(	40.64,2)(	40.84,2)(	41.05,3)(	41.25,2)(	41.45,2)(	41.66,1)(	41.86,2)(
(42.06,3)(	42.27,2)(	42.47,1)(	42.67,1)(	42.88,2)(	43.08,2)(	43.28,2)(	43.48,2)(	43.69,2)(	43.89,2)(	44.09,3)(	44.30,2)(
(44.50,2)(	44.70,1)(	44.91,2)(	45.11,2)(	45.31,2)(	45.52,1)(	45.72,1)(	45.92,1)(	46.13,2)(	46.33,2)(	46.53,2)(	46.74,2)(
(46.94,2)(	47.14,2)(	47.35,3)(	47.55,2)(	47.75,2)(	47.96,1)(	48.16,2)(	48.36,2)(	48.56,2)(	48.77,1)(	48.97,1)(	49.17,2)(
(49.38,2)(	49.58,2)(	49.78,2)(	49.99,1)(	50.19,2)(	50.39,3)(	50.60,2)(	50.80,2)(	51.00,1)(	51.21,2)(	51.41,2)(	51.61,2)(
(51.82,1)(	52.02,1)(	52.22,2)(	52.43,2)(	52.63,2)(	52.83,2)(	53.04,1)(	53.24,2)(	53.44,2)(	53.64,2)(	53.85,2)(	54.05,1)(
(54.25,2)(	54.46,2)(	54.66,2)(	54.86,1)(	55.07,1)(	55.27,2)(	55.47,2)(	55.68,2)(	55.88,2)(	56.08,1)(	56.29,2)(	56.49,2)(
(56.69,2)(	56.90,2)(	57.10,1)(	57.30,2)(	57.51,2)(	57.71,2)(	57.91,1)(	58.12,1)(	58.32,2)(	58.52,2)(	58.72,2)(	58.93,1)(
(59.13,1)(	59.33,2)(	59.54,2)(	59.74,2)(	59.94,2)(	60.15,1)(	60.35,2)(	60.55,2)(	60.76,2)(	60.96,1)(	61.16,1)(	61.37,2)(
(61.57,2)(	61.77,2)(	61.98,1)(	62.18,1)(	62.38,2)(	62.59,2)(	62.79,2)(	62.99,1)(	63.20,1)(	63.40,2)(	63.60,2)(	63.80,2)(
(64.01,1)(	64.21,1)(	64.41,2)(	64.62,2)(	64.82,2)(	65.02,1)(	65.23,1)(	65.43,2)(				

(102.62, 1)(102.68, 1)(102.75, 1)(102.82, 1)(102.89, 1)(102.95, 1)(103.02, 1)(103.09, 2)(103.16, 1)(103.23, 1)(103.29, 1)(103.36, 1)
 (103.43, 1)(103.50, 1)(103.56, 1)(103.63, 1)(103.70, 1)(103.77, 1)(103.84, 1)(103.90, 1)(103.97, 1)(104.04, 1)(104.11, 1)(104.17, 1)
 (104.24, 1)(104.31, 1)(104.38, 1)(104.44, 1)(104.51, 1)(104.58, 1)(104.65, 1)(104.72, 1)(104.78, 1)(104.85, 1)(104.92, 1)(104.99, 1)
 (105.05, 1)(105.12, 1)(105.19, 1)(105.26, 1)(105.33, 1)(105.39, 1)(105.46, 1)(105.53, 1)(105.60, 1)(105.66, 1)(105.73, 1)(105.80, 1)
 (105.87, 1)(105.94, 1)(106.00, 1)(106.07, 1)(106.14, 1)(106.21, 1)(106.27, 1)(106.34, 1)(106.41, 1)(106.48, 1)(106.54, 1)(106.61, 1)
 (106.68, 1)(106.75, 1)(106.82, 1)(106.88, 1)(106.95, 1)(107.02, 1)(107.09, 1)(107.15, 1)(107.22, 1)(107.29, 1)(107.36, 1)(107.43, 1)
 (107.49, 1)(107.56, 1)(107.63, 1)(107.70, 1)(107.76, 1)(107.83, 1)(107.90, 1)(107.97, 1)(108.03, 1)(108.10, 1)(108.17, 1)(108.24, 1)
 (108.31, 1)(108.37, 1)(108.44, 1)(108.51, 1)(108.58, 1)(108.64, 1)(108.71, 1)(108.78, 1)(108.85, 1)(108.92, 1)(108.98, 1)(109.05, 1)
 (109.12, 1)(109.19, 1)(109.25, 1)(109.32, 1)(109.39, 1)(109.46, 1)(109.52, 1)(109.59, 1)(109.66, 1)(109.73, 1)(109.80, 1)(109.86, 1)
 (109.93, 1)(110.00, 1)(110.07, 1)(110.13, 1)(110.20, 1)(110.27, 1)(110.34, 1)(110.41, 1)(110.47, 1)(110.54, 1)(110.61, 1)(110.68, 1)
 (110.74, 1)(110.81, 1)(110.88, 1)(110.95, 1)(111.02, 1)(111.08, 1)(111.15, 1)(111.22, 1)(111.29, 1)(111.35, 1)(111.42, 1)(111.49, 1)
 (111.56, 1)(111.62, 1)(111.69, 1)(111.76, 1)(111.83, 1)(111.90, 1)(111.96, 1)(112.03, 1)(112.10, 1)(112.17, 1)(112.23, 1)(112.30, 1)
 (112.37, 1)(112.44, 1)(112.51, 1)(112.57, 1)(112.64, 1)(112.71, 1)(112.78, 1)(112.84, 1)(112.91, 1)(112.98, 1)(113.05, 1)(113.11, 1)
 THE STIFF PARTICLE ENERGY EQUATION ASSUMPTION IS INITIATED FOR PARTICLE NO. 3 AT 113.66 CM. DOWN THE REACTOR
 (113.18, 1)(113.25, 1)(113.32, 1)(113.39, 1)(113.45, 1)(113.52, 1)(113.59, 1)(113.66, 1)(113.72, 1)(113.79, 1)(113.86, 1)(113.93, 1)
 (114.00, 1)(116.43, 1)(117.04, 1)(117.65, 1)(118.26, 1)(118.87, 1)(119.48, 1)(120.09, 1)(120.70, 1)(121.31, 1)(121.92, 1)(122.53, 1)
 (123.14, 1)(123.75, 1)(124.36, 1)(124.97, 1)(125.58, 1)(126.19, 1)(126.80, 1)(127.41, 1)(128.02, 1)(128.63, 1)(129.24, 1)(131.67, 1)
 (132.28, 1)(132.89, 1)(133.50, 1)(134.11, 1)(134.72, 1)(135.33, 1)(135.94, 1)(136.55, 1)(137.16, 1)(137.77, 1)(138.38, 1)(138.99, 1)
 (139.60, 1)(140.21, 1)(140.82, 1)(141.43, 1)(142.04, 1)(142.65, 1)(143.26, 1)(143.87, 1)(144.48, 1)(145.08, 1)(145.69, 1)(146.30, 1)
 (146.91, 1)(147.52, 1)(148.13, 1)(148.74, 1)(149.35, 1)(149.96, 1)(150.57, 1)(151.18, 1)(151.79, 1)(152.40, 1)(

AFTER 4 ITERATION(S) THROUGH THE REACTOR THE ROOT MEAN SQUARE OF ALL PARTICLE TEMPERATURES IS 65.039 DEGREES KELVIN

THE ORDERED PAIR OF (X, # OF CORRECTORS APPLIED) FOLLOWS FOR EACH O.D.E. STEP

```

( 1.22, 1)( 2.03, 1)( 2.24, 1)( 2.44, 1)( 2.64, 1)( 3.45, 1)( 3.66, 1)( 4.06, 1)( 4.27, 1)( 4.47, 1)( 4.67, 1)
( 4.88, 1)( 5.08, 1)( 5.28, 1)( 5.49, 1)( 5.69, 1)( 5.89, 1)( 6.10, 1)( 6.30, 1)( 6.50, 1)( 6.71, 1)( 6.91, 1)( 7.11, 1)
( 7.32, 1)( 7.52, 1)( 7.72, 1)( 7.92, 1)( 8.13, 1)( 8.33, 1)( 8.53, 1)( 8.74, 1)( 8.94, 1)( 9.14, 1)( 9.35, 1)( 9.55, 1)
( 9.75, 1)( 9.96, 1)( 10.16, 1)( 10.36, 1)( 10.57, 1)( 10.77, 1)( 10.97, 1)( 11.18, 1)( 11.38, 1)( 11.58, 1)( 11.79, 1)( 11.99, 1)
( 12.19, 1)( 12.40, 1)( 12.60, 1)( 12.80, 1)( 13.00, 1)( 13.21, 1)( 13.41, 1)( 13.61, 1)( 13.82, 1)( 14.02, 1)( 14.22, 1)( 14.43, 1)
( 14.63, 1)( 14.83, 1)( 15.04, 1)( 15.24, 1)( 15.44, 1)( 15.65, 1)( 15.85, 1)( 16.05, 1)( 16.26, 1)( 16.46, 1)( 16.66, 1)( 16.87, 1)
( 17.07, 1)( 17.27, 1)( 17.48, 1)( 17.68, 1)( 17.88, 1)( 18.08, 1)( 18.29, 1)( 18.49, 1)( 18.69, 1)( 18.90, 1)( 19.10, 1)( 19.30, 1)
( 19.51, 1)( 19.71, 1)( 19.91, 1)( 20.12, 1)( 20.32, 1)( 20.52, 1)( 20.73, 1)( 20.93, 1)( 21.13, 1)( 21.34, 1)( 21.54, 1)( 21.74, 1)
( 21.95, 1)( 22.15, 1)( 22.35, 1)( 22.56, 1)( 22.76, 1)( 22.96, 1)( 23.16, 1)( 23.37, 1)( 23.57, 1)( 23.77, 1)( 23.98, 1)( 24.18, 1)
( 24.38, 1)( 24.59, 1)( 24.79, 1)( 24.99, 1)( 25.20, 1)( 25.40, 1)( 25.60, 1)( 25.81, 2)( 26.01, 1)( 26.21, 1)( 26.42, 1)( 26.62, 2)
( 26.82, 2)( 27.03, 1)( 27.23, 1)( 27.43, 1)( 27.64, 1)( 27.84, 1)( 28.04, 1)( 28.24, 1)( 28.45, 1)( 28.65, 2)( 28.85, 2)( 29.06, 2)
( 29.26, 1)( 29.46, 1)( 29.67, 2)( 29.87, 2)( 30.07, 1)( 30.28, 1)( 30.48, 1)( 30.68, 2)( 30.89, 2)( 31.09, 2)( 31.29, 1)( 31.50, 1)
( 31.70, 2)( 31.90, 2)( 32.11, 2)( 32.31, 1)( 32.51, 1)( 32.72, 2)( 32.92, 2)( 33.12, 2)( 33.32, 1)( 33.53, 1)( 33.73, 2)( 33.93, 2)
( 34.14, 2)( 34.34, 2)( 34.54, 1)( 34.75, 2)( 34.95, 3)( 35.16, 3)( 35.37, 3)( 35.57, 2)( 35.78, 2)( 35.98, 1)( 36.18, 2)( 36.38, 2)
( 36.58, 1)( 36.79, 2)( 36.99, 2)( 37.19, 2)( 37.39, 2)( 37.59, 1)( 37.80, 2)( 38.00, 3)( 38.20, 2)( 38.40, 2)( 38.61, 1)( 38.81, 2)( 39.01, 3)
( 39.22, 2)( 39.42, 1)( 39.62, 1)( 39.83, 2)( 40.03, 2)( 40.23, 2)( 40.44, 2)( 40.64, 2)( 40.84, 2)( 41.05, 3)( 41.25, 2)( 41.45, 2)( 41.66, 1)
( 41.86, 2)( 42.06, 3)( 42.27, 2)( 42.47, 1)( 42.67, 1)( 42.88, 2)( 43.08, 2)( 43.28, 2)( 43.48, 2)( 43.69, 2)( 43.89, 2)( 44.09, 3)( 44.30, 2)
( 44.50, 2)( 44.70, 1)( 44.91, 2)( 45.11, 2)( 45.31, 2)( 45.52, 1)( 45.72, 1)( 45.92, 1)( 46.13, 2)( 46.33, 2)( 46.53, 2)( 46.74, 2)
( 46.94, 2)( 47.14, 2)( 47.35, 3)( 47.55, 2)( 47.75, 2)( 47.96, 1)( 48.16, 2)( 48.36, 2)( 48.56, 2)( 48.77, 1)( 48.97, 1)( 49.17, 2)
( 49.38, 2)( 49.58, 2)( 49.78, 2)( 49.99, 1)( 50.19, 2)( 50.39, 3)( 50.60, 2)( 50.80, 2)( 51.00, 1)( 51.21, 2)( 51.41, 2)( 51.61, 2)
( 51.82, 1)( 52.02, 1)( 52.22, 2)( 52.43, 2)( 52.63, 2)( 52.83, 2)( 53.04, 1)( 53.24, 2)( 53.44, 2)( 53.64, 2)( 53.85, 2)( 54.05, 1)
( 54.25, 2)( 54.46, 2)( 54.66, 2)( 54.86, 1)( 55.07, 1)( 55.27, 2)( 55.47, 2)( 55.68, 2)( 55.88, 2)( 56.08, 1)( 56.29, 2)( 56.49, 2)
( 56.69, 2)( 56.90, 2)( 57.10, 1)( 57.30, 2)( 57.51, 2)( 57.71, 2)( 57.91, 1)( 58.12, 1)( 58.32, 2)( 58.52, 2)( 58.72, 2)( 58.93, 1)
( 59.13, 1)( 59.33, 2)( 59.54, 2)( 59.74, 2)( 59.94, 2)( 60.15, 1)( 60.35, 2)( 60.55, 2)( 60.76, 2)( 60.96, 1)( 61.16, 1)( 61.37, 2)
( 61.57, 2)( 61.77, 2)( 61.98, 1)( 62.18, 1)( 62.38, 2)( 62.59, 2)( 62.79, 2)( 62.99, 1)( 63.20, 1)( 63.40, 2)( 63.60, 2)( 63.80, 2)
( 64.01, 1)( 64.21, 1)( 64.41, 2)( 64.62, 2)( 64.82, 2)( 65.02, 1)( 65.23, 1)( 65.43, 2)( 65.63, 2)( 65.84, 2)( 66.04, 1)( 66.24, 1)
( 66.45, 2)( 66.65, 2)( 66.85, 1)( 67.06, 1)( 67.26, 1)( 67.46, 1)( 67.67, 1)( 67.87, 1)( 68.07, 1)( 68.28, 1)( 68.48, 1)( 68.68, 2)
( 68.88, 1)( 69.09, 1)( 69.29, 1)( 69.49, 2)( 69.70, 2)( 69.90, 1)( 70.10, 1)( 70.31, 1)( 70.51, 1)( 70.71, 1)( 70.92, 1)( 71.12, 1)
( 71.32, 1)( 71.53, 1)( 71.73, 1)( 71.93, 1)( 72.14, 1)( 72.34, 1)( 72.54, 1)( 72.75, 1)( 72.95, 1)( 73.15, 1)( 73.36, 1)( 73.56, 1)
( 73.76, 1)( 74.17, 1)( 74.27, 1)( 74.37, 1)( 74.47, 1)( 74.57, 1)( 74.68, 1)( 74.78, 1)( 74.88, 1)( 74.98, 1)( 75.08, 1)( 75.18, 1)
( 75.29, 1)( 75.39, 1)( 75.49, 1)( 75.59, 1)( 75.69, 1)( 75.79, 1)( 75.90, 1)( 76.00, 1)( 76.10, 1)( 76.20, 1)( 76.30, 1)( 76.40, 1)
( 76.50, 1)( 76.61, 1)( 76.71, 1)( 76.81, 1)( 76.91, 1)( 77.01, 1)( 77.11, 1)( 77.22, 1)( 77.32, 1)( 77.42, 1)( 77.52, 1)( 77.62, 1)
( 77.72, 1)( 77.83, 1)( 77.93, 1)( 78.03, 1)( 78.13, 1)( 78.23, 1)( 78.33, 1)( 78.44, 1)( 78.54, 1)( 78.64, 1)( 78.74, 1)( 78.84, 1)
( 78.94, 1)( 79.04, 1)( 79.15, 1)( 79.25, 1)( 79.35, 1)( 79.45, 1)( 79.55, 1)( 79.65, 1)( 79.76, 1)( 79.86, 1)( 79.96, 1)( 80.06, 1)
( 80.16, 1)( 80.26, 1)( 80.37, 1)( 80.47, 1)( 80.57, 1)( 80.67, 1)( 80.77, 1)( 80.87, 1)( 80.98, 1)( 81.08, 1)( 81.18, 1)( 81.28, 1)
( 81.38, 1)( 81.48, 1)( 81.58, 1)( 81.69, 1)( 81.79, 1)( 81.89, 1)( 81.99, 1)( 82.09, 1)( 82.19, 1)( 82.30, 1)( 82.40, 1)( 82.50, 1)
( 82.60, 1)( 82.70, 1)( 82.80, 1)( 82.91, 1)( 83.01, 1)( 83.11, 1)( 83.21, 1)( 83.31, 1)( 83.41, 1)( 83.52, 1)( 83.62, 1)( 83.72, 1)
( 83.82, 1)( 83.92, 1)( 84.02, 1)( 84.12, 1)( 84.23, 1)( 84.33, 1)( 84.43, 1)( 84.53, 1)( 84.63, 1)( 84.73, 1)( 84.84, 1)( 84.94, 1)
( 85.04, 1)( 85.14, 1)( 85.24, 1)( 85.34, 1)( 85.45, 1)( 85.55, 1)( 85.65, 1)( 85.75, 1)( 85.85, 2)( 86.26, 1)( 86.36, 1)( 86.46, 1)
( 86.56, 1)( 86.66, 1)( 86.77, 1)( 86.87, 2)( 86.97, 1)( 87.38, 1)( 87.48, 1)( 87.58, 1)( 87.68, 1)( 87.78, 1)( 87.88, 1)( 87.99, 1)
( 88.09, 2)( 88.19, 2)( 88.29, 1)( 88.39, 1)( 88.49, 1)( 88.60, 1)( 88.70, 1)( 88.80, 1)( 88.90, 1)( 89.00, 1)( 89.10, 2)( 89.20, 2)
( 89.31, 2)( 89.41, 2)( 89.51, 2)( 89.61, 1)( 89.88, 1)( 89.95, 1)( 90.02, 1)( 90.09, 1)( 90.15, 1)( 90.22, 1)( 90.29, 1)( 90.36, 1)
( 90.42, 1)( 90.49, 1)( 90.56, 1)( 90.63, 1)( 90.69, 1)( 90.76, 1)( 90.83, 1)( 90.90, 1)( 90.97, 2)( 91.03, 2)( 91.10, 1)( 91.17, 1)
( 91.24, 1)( 91.30, 1)( 91.37, 1)( 91.44, 1)( 91.51, 1)( 91.58, 1)( 91.64, 1)( 91.71, 1)( 91.78, 1)( 91.85, 1)( 91.91, 1)( 91.98, 1)
( 92.05, 1)( 92.12, 1)( 92.19, 2)( 92.25, 2)( 92.32, 2)( 92.39, 2)( 92.46, 2)( 92.52, 2)( 92.59, 1)( 92.66, 1)( 92.73, 2)( 92.79, 2)
( 92.86, 3)( 92.93, 2)( 93.00, 1)( 93.07, 1)( 93.13, 1)( 93.20, 1)( 93.27, 1)( 93.34, 1)( 93.40, 3)( 93.47, 3)( 93.54, 2)( 93.61, 2)
( 93.68, 3)( 93.74, 3)( 93.81, 1)( 93.88, 2)( 93.95, 4)( 94.01, 5)( 94.08, 6)( 94.15, 5)( 94.22, 4)( 94.28, 1)( 94.35, 3)( 94.42, 1)

```

THE STIFF PARTICLE ENERGY EQUATION ASSUMPTION IS INITIATED FOR PARTICLE NO. 1 AT 95.30 CM. DOWN THE REACTOR

```

( 94.49, 3)( 94.56, 3)( 94.62, 6)( 94.69, 9)( 94.76, 10)( 94.83, 10)( 94.89, 11)( 94.96, 11)( 95.03, 8)( 95.30, 10)( 95.37, 2)( 95.44, 1)
( 95.50, 1)( 95.57, 1)( 95.64, 1)( 95.71, 1)( 95.77, 1)( 95.84, 1)( 95.91, 1)( 95.98, 1)( 96.05, 1)( 96.11, 1)( 96.18, 1)( 96.25, 1)
( 96.32, 1)( 96.38, 1)( 96.45, 1)( 96.52, 1)( 96.59, 1)( 96.66, 1)( 96.72, 1)( 96.79, 1)( 96.86, 1)( 96.93, 1)( 96.99, 1)( 97.06, 1)
( 97.13, 1)( 97.20, 1)( 97.27, 1)( 97.33, 1)( 97.40, 1)( 97.47, 1)( 97.54, 1)( 97.60, 1)( 97.67, 1)( 97.74, 1)( 97.81, 1)( 97.87, 1)
( 97.94, 1)( 98.01, 1)( 98.08, 1)( 98.15, 1)( 98.21, 1)( 98.28, 1)( 98.35, 1)( 98.42, 1)( 98.48, 1)( 98.55, 1)( 98.62, 1)( 98.69, 1)
( 98.76, 1)( 98.82, 1)( 98.89, 1)( 98.96, 1)( 99.03, 1)( 99.09, 1)( 99.16, 1)( 99.23, 1)( 99.30, 1)( 99.36, 1)( 99.43, 1)( 99.50, 1)
( 99.57, 1)( 99.64, 1)( 99.70, 1)( 99.77, 1)( 99.84, 1)( 99.91, 1)( 99.97, 1)( 100.04, 1)( 100.11, 1)( 100.18, 1)( 100.25, 1)( 100.31, 1)
( 100.38, 1)( 100.45, 1)( 100.52, 1)( 100.58, 1)( 100.65, 1)( 100.72, 1)( 100.79, 1)( 100.85, 1)( 100.92, 1)( 100.99, 1)( 101.06, 1)( 101.13, 1)
( 101.19, 1)( 101.26, 1)( 101.33, 1)( 101.40, 1)( 101.46, 1)( 101.53, 1)( 101.60, 1)( 101.67, 1)( 101.74, 1)( 101.80, 1)( 101.87, 1)( 101.94, 1)
( 102.01, 1)( 102.07, 1)( 102.14, 1)( 102.21, 1)( 102.28, 1)( 102.35, 1)( 102.41, 1)( 102.48, 1)( 102.55, 1)( 102.62, 1)( 102.68, 1)( 102.75, 1)

```

THE STIFF PARTICLE ENERGY EQUATION ASSUMPTION IS INITIATED FOR PARTICLE NO. 2 AT 103.02 CM. DOWN THE REACTOR

(102.82, 1)(102.89, 1)(102.95, 1)(103.02, 1)(103.09, 2)(103.16, 1)(103.23, 1)(103.29, 1)(103.36, 1)(103.43, 1)(103.50, 1)(103.56, 1)
(103.63, 1)(103.70, 1)(103.77, 1)(103.84, 1)(103.90, 1)(103.97, 1)(104.04, 1)(104.11, 1)(104.17, 1)(104.24, 1)(104.31, 1)(104.38, 1)
(104.44, 1)(104.51, 1)(104.56, 1)(104.65, 1)(104.72, 1)(104.78, 1)(104.85, 1)(104.92, 1)(104.99, 1)(105.05, 1)(105.12, 1)(105.19, 1)
(105.26, 1)(105.33, 1)(105.39, 1)(105.46, 1)(105.53, 1)(105.60, 1)(105.66, 1)(105.73, 1)(105.80, 1)(105.87, 1)(105.94, 1)(106.00, 1)
(106.07, 1)(106.14, 1)(106.21, 1)(106.27, 1)(106.34, 1)(106.41, 1)(106.48, 1)(106.54, 1)(106.61, 1)(106.68, 1)(106.75, 1)(106.82, 1)
(106.88, 1)(106.95, 1)(107.02, 1)(107.09, 1)(107.15, 1)(107.22, 1)(107.29, 1)(107.36, 1)(107.43, 1)(107.49, 1)(107.56, 1)(107.63, 1)
(107.70, 1)(107.76, 1)(107.83, 1)(107.90, 1)(107.97, 1)(108.03, 1)(108.10, 1)(108.17, 1)(108.24, 1)(108.31, 1)(108.37, 1)(108.44, 1)
(108.51, 1)(108.58, 1)(108.64, 1)(108.71, 1)(108.78, 1)(108.85, 1)(108.92, 1)(108.98, 1)(109.05, 1)(109.12, 1)(109.19, 1)(109.25, 1)
(109.32, 1)(109.39, 1)(109.46, 1)(109.52, 1)(109.59, 1)(109.66, 1)(109.73, 1)(109.80, 1)(109.86, 1)(109.93, 1)(110.00, 1)(110.07, 1)
(110.13, 1)(110.20, 1)(110.27, 1)(110.34, 1)(110.41, 1)(110.47, 1)(110.54, 1)(110.61, 1)(110.68, 1)(110.74, 1)(110.81, 1)(110.88, 1)
(110.95, 1)(111.02, 1)(111.08, 1)(111.15, 1)(111.22, 1)(111.29, 1)(111.35, 1)(111.42, 1)(111.49, 1)(111.56, 1)(111.62, 1)(111.69, 1)
(111.76, 1)(111.83, 1)(111.90, 1)(111.96, 1)(112.03, 1)(112.10, 1)(112.17, 1)(112.23, 1)(112.30, 1)(112.37, 1)(112.44, 1)(112.51, 1)
(112.57, 1)(112.64, 1)(112.71, 1)(112.78, 1)(112.84, 1)(112.91, 1)(112.98, 1)(113.05, 1)(113.11, 1)(113.18, 1)(113.25, 1)(113.32, 1)

THE STIFF PARTICLE ENERGY EQUATION ASSUMPTION IS INITIATED FOR PARTICLE NO. 3 AT 113.39 CM. DOWN THE REACTOR

(113.39, 1)(115.82, 1)(116.43, 1)(117.04, 1)(117.65, 1)(118.26, 1)(118.87, 1)(119.48, 1)(120.09, 1)(120.70, 1)(121.31, 1)(121.92, 1)
(122.53, 1)(123.14, 1)(123.75, 1)(124.36, 1)(124.97, 1)(125.58, 1)(126.19, 1)(126.80, 1)(127.41, 1)(128.02, 1)(128.63, 1)(129.24, 1)
(131.67, 1)(132.28, 1)(132.89, 1)(133.50, 1)(134.11, 1)(134.72, 1)(135.33, 1)(135.94, 1)(136.55, 1)(137.16, 1)(137.77, 1)(138.38, 1)
(138.99, 1)(139.60, 1)(140.21, 1)(140.82, 1)(141.43, 1)(142.04, 1)(142.65, 1)(143.26, 1)(143.87, 1)(144.48, 1)(145.08, 1)(145.69, 1)
(146.30, 1)(146.91, 1)(147.52, 1)(148.13, 1)(148.74, 1)(149.35, 1)(149.96, 1)(150.57, 1)(151.18, 1)(151.79, 1)(152.40, 1)

AFTER 5 ITERATION(S) THROUGH THE REACTOR THE ROOT MEAN SQUARE OF ALL PARTICLE TEMPERATURES IS 13.091 DEGREES KELVIN

THE ORDERED PAIR OF (X,# OF CORRECTORS APPLIED) FOLLOWS FOR EACH O.D.E. STEP

(1.22,11)	(2.03, 1)	(2.24, 1)	(2.44, 1)	(2.64, 1)	(3.45, 1)	(3.66, 1)	(3.86, 1)	(4.06, 1)	(4.27, 1)	(4.47, 1)	(4.67, 1)
(4.88, 1)	(5.08, 1)	(5.28, 1)	(5.49, 1)	(5.69, 1)	(5.89, 1)	(6.10, 1)	(6.30, 1)	(6.50, 1)	(6.71, 1)	(6.91, 1)	(7.11, 1)
(7.32, 1)	(7.52, 1)	(7.72, 1)	(7.92, 1)	(8.13, 1)	(8.33, 1)	(8.53, 1)	(8.74, 1)	(8.94, 1)	(9.14, 1)	(9.35, 1)	(9.55, 1)
(9.75, 1)	(9.96, 1)	(10.16, 1)	(10.36, 1)	(10.57, 1)	(10.77, 1)	(10.97, 1)	(11.18, 1)	(11.38, 1)	(11.58, 1)	(11.79, 1)	(11.99, 1)
(12.19, 1)	(12.40, 1)	(12.60, 1)	(12.80, 1)	(13.00, 1)	(13.21, 1)	(13.41, 1)	(13.61, 1)	(13.82, 1)	(14.02, 1)	(14.22, 1)	(14.43, 1)
(14.63, 1)	(14.83, 1)	(15.04, 1)	(15.24, 1)	(15.44, 1)	(15.65, 1)	(15.85, 1)	(16.05, 1)	(16.26, 1)	(16.46, 1)	(16.66, 1)	(16.87, 1)
(17.07, 1)	(17.27, 1)	(17.48, 1)	(17.68, 1)	(17.88, 1)	(18.08, 1)	(18.29, 1)	(18.49, 1)	(18.69, 1)	(18.90, 1)	(19.10, 1)	(19.30, 1)
(19.51, 1)	(19.71, 1)	(19.91, 1)	(20.12, 1)	(20.32, 1)	(20.52, 1)	(20.73, 1)	(20.93, 1)	(21.13, 1)	(21.34, 1)	(21.54, 1)	(21.74, 1)
(21.95, 1)	(22.15, 1)	(22.35, 1)	(22.56, 1)	(22.76, 1)	(22.96, 1)	(23.16, 1)	(23.37, 1)	(23.57, 1)	(23.77, 1)	(23.98, 1)	(24.18, 1)
(24.38, 1)	(24.59, 1)	(24.79, 1)	(24.99, 1)	(25.20, 1)	(25.40, 1)	(25.60, 1)	(25.81, 2)	(26.01, 1)	(26.21, 1)	(26.42, 1)	(26.62, 2)
(26.82, 2)	(27.03, 1)	(27.23, 1)	(27.43, 1)	(27.64, 1)	(27.84, 1)	(28.04, 1)	(28.24, 1)	(28.45, 1)	(28.65, 2)	(28.85, 2)	(29.06, 2)
(29.26, 1)	(29.46, 1)	(29.67, 2)	(29.87, 2)	(30.07, 1)	(30.28, 1)	(30.48, 1)	(30.68, 2)	(30.89, 2)	(31.09, 2)	(31.29, 1)	(31.50, 1)
(31.70, 2)	(31.90, 2)	(32.11, 2)	(32.31, 1)	(32.51, 1)	(32.72, 2)	(32.92, 2)	(33.12, 2)	(33.32, 1)	(33.53, 1)	(33.73, 2)	(33.93, 2)
(34.14, 2)	(34.34, 2)	(34.54, 1)	(34.75, 2)	(34.95, 3)	(35.16, 3)	(35.37, 3)	(35.57, 2)	(35.78, 1)	(35.98, 1)	(36.19, 2)	(36.39, 2)
(36.59, 2)	(36.79, 2)	(36.99, 1)	(37.20, 2)	(37.40, 3)	(37.60, 2)	(37.81, 1)	(38.01, 2)	(38.21, 2)	(38.41, 3)	(38.61, 2)	(38.81, 1)
(39.02, 1)	(39.22, 2)	(39.42, 2)	(39.62, 2)	(39.82, 2)	(40.03, 2)	(40.23, 2)	(40.44, 2)	(40.64, 2)	(40.84, 2)	(41.05, 3)	(41.25, 2)
(41.45, 2)	(41.66, 1)	(41.86, 2)	(42.06, 3)	(42.27, 2)	(42.47, 1)	(42.67, 1)	(42.88, 2)	(43.08, 2)	(43.28, 2)	(43.48, 2)	(43.69, 2)
(43.89, 2)	(44.09, 3)	(44.30, 2)	(44.50, 2)	(44.70, 1)	(44.91, 2)	(45.11, 3)	(45.31, 2)	(45.52, 1)	(45.72, 1)	(45.92, 1)	(46.13, 2)
(46.33, 2)	(46.53, 2)	(46.74, 2)	(46.94, 2)	(47.14, 2)	(47.35, 3)	(47.55, 2)	(47.75, 2)	(47.96, 1)	(48.16, 2)	(48.36, 2)	(48.56, 2)
(48.77, 1)	(48.97, 1)	(49.17, 2)	(49.38, 2)	(49.58, 2)	(49.78, 2)	(49.99, 1)	(50.19, 2)	(50.39, 3)	(50.60, 2)	(50.80, 2)	(51.00, 1)
(51.21, 2)	(51.41, 1)	(51.61, 2)	(51.82, 1)	(52.02, 1)	(52.22, 2)	(52.43, 2)	(52.63, 2)	(52.83, 2)	(53.04, 1)	(53.24, 2)	(53.44, 2)
(53.64, 2)	(53.85, 2)	(54.05, 1)	(54.25, 2)	(54.46, 2)	(54.66, 2)	(54.86, 1)	(55.07, 1)	(55.27, 2)	(55.47, 2)	(55.68, 2)	(55.88, 2)
(56.08, 1)	(56.29, 2)	(56.49, 2)	(56.69, 2)	(56.90, 2)	(57.10, 1)	(57.30, 2)	(57.51, 2)	(57.71, 2)	(57.91, 1)	(58.12, 1)	(58.32, 2)
(58.52, 2)	(58.72, 2)	(58.93, 1)	(59.13, 1)	(59.33, 2)	(59.54, 2)	(59.74, 2)	(59.94, 2)	(60.15, 1)	(60.35, 2)	(60.55, 2)	(60.76, 2)
(60.96, 1)	(61.16, 1)	(61.37, 2)	(61.57, 2)	(61.77, 2)	(61.98, 2)	(62.18, 1)	(62.38, 2)	(62.59, 2)	(62.79, 2)	(62.99, 1)	(63.20, 1)
(63.40, 1)	(63.60, 2)	(63.80, 2)	(64.01, 1)	(64.21, 1)	(64.41, 2)	(64.62, 2)	(64.82, 2)	(65.02, 1)	(65.23, 1)	(65.43, 2)	(65.63, 2)
(65.84, 2)	(66.04, 1)	(66.24, 1)	(66.45, 2)	(66.65, 2)	(66.85, 1)	(67.06, 1)	(67.26, 1)	(67.46, 1)	(67.67, 1)	(67.87, 1)	(68.07, 1)
(68.28, 1)	(68.48, 1)	(68.68, 2)	(68.88, 1)	(69.09, 1)	(69.29, 1)	(69.49, 2)	(69.70, 2)	(69.90, 1)	(70.10, 1)	(70.31, 1)	(70.51, 1)
(70.71, 1)	(70.92, 1)	(71.12, 1)	(71.32, 1)	(71.53, 1)	(71.73, 1)	(71.93, 1)	(72.14, 1)	(72.34, 1)	(72.54, 1)	(72.75, 1)	(72.95, 1)
(73.15, 1)	(73.36, 1)	(73.56, 1)	(73.76, 1)	(73.97, 1)	(74.17, 1)	(74.37, 1)	(74.57, 1)	(74.78, 1)	(74.98, 1)	(75.18, 1)	(75.38, 1)
(75.59, 1)	(75.79, 1)	(75.99, 1)	(76.19, 1)	(76.39, 1)	(76.59, 1)	(76.79, 1)	(76.99, 1)	(77.19, 1)	(77.39, 1)	(77.59, 1)	(77.79, 1)
(77.99, 1)	(78.19, 1)	(78.39, 1)	(78.59, 1)	(78.79, 1)	(78.99, 1)	(79.19, 1)	(79.39, 1)	(79.59, 1)	(79.79, 1)	(79.99, 1)	(80.19, 1)
(80.39, 1)	(80.59, 1)	(80.79, 1)	(80.99, 1)	(81.19, 1)	(81.39, 1)	(81.59, 1)	(81.79, 1)	(81.99, 1)	(82.19, 1)	(82.39, 1)	(82.59, 1)
(82.79, 1)	(82.99, 1)	(83.19, 1)	(83.39, 1)	(83.59, 1)	(83.79, 1)	(83.99, 1)	(84.19, 1)	(84.39, 1)	(84.59, 1)	(84.79, 1)	(84.99, 1)
(85.19, 1)	(85.39, 1)	(85.59, 1)	(85.79, 1)	(85.99, 1)	(86.19, 1)	(86.39, 1)	(86.59, 1)	(86.79, 1)	(86.99, 1)	(87.19, 1)	(87.39, 1)
(87.59, 1)	(87.79, 1)	(87.99, 1)	(88.19, 1)	(88.39, 1)	(88.59, 1)	(88.79, 1)	(88.99, 1)	(89.19, 1)	(89.39, 1)	(89.59, 1)	(89.79, 1)
(89.99, 1)	(90.19, 1)	(90.39, 1)	(90.59, 1)	(90.79, 1)	(90.99, 1)	(91.19, 1)	(91.39, 1)	(91.59, 1)	(91.79, 1)	(91.99, 1)	(92.19, 1)
(92.39, 1)	(92.59, 1)	(92.79, 1)	(92.99, 1)	(93.19, 1)	(93.39, 1)	(93.59, 1)	(93.79, 1)	(93.99, 1)	(94.19, 1)	(94.39, 1)	(94.59, 1)
(94.79, 1)	(94.99, 1)	(95.19, 1)	(95.39, 1)	(95.59, 1)	(95.79, 1)	(95.99, 1)	(96.19, 1)	(96.39, 1)	(96.59, 1)	(96.79, 1)	(96.99, 1)
(97.19, 1)	(97.39, 1)	(97.59, 1)	(97.79, 1)	(97.99, 1)	(98.19, 1)	(98.39, 1)	(98.59, 1)	(98.79, 1)	(98.99, 1)	(99.19, 1)	(99.39, 1)
(99.59, 1)	(99.79, 1)	(99.99, 1)	(100.19, 1)	(100.39, 1)	(100.59, 1)	(100.79, 1)	(100.99, 1)	(101.19, 1)	(101.39, 1)	(101.59, 1)	(101.79, 1)
(101.99, 1)	(102.19, 1)	(102.39, 1)	(102.59, 1)	(102.79, 1)	(102.99, 1)	(103.19, 1)	(103.39, 1)	(103.59, 1)	(103.79, 1)	(103.99, 1)	(104.19, 1)
(104.39, 1)	(104.59, 1)	(104.79, 1)	(104.99, 1)	(105.19, 1)	(105.39, 1)	(105.59, 1)	(105.79, 1)	(105.99, 1)	(106.19, 1)	(106.39, 1)	(106.59, 1)
(106.79, 1)	(106.99, 1)	(107.19, 1)	(107.39, 1)	(107.59, 1)	(107.79, 1)	(107.99, 1)	(108.19, 1)	(108.39, 1)	(108.59, 1)	(108.79, 1)	(108.99, 1)
(109.19, 1)	(109.39, 1)	(109.59, 1)	(109.79, 1)	(109.99, 1)	(110.19, 1)	(110.39, 1)	(110.59, 1)	(110.79, 1)	(110.99, 1)	(111.19, 1)	(111.39, 1)
(111.59, 1)	(111.79, 1)	(111.99, 1)	(112.19, 1)	(112.39, 1)	(112.59, 1)	(112.79, 1)	(112.99, 1)	(113.19, 1)	(113.39, 1)	(113.59, 1)	(113.79, 1)
(113.99, 1)	(114.19, 1)	(114.39, 1)	(114.59, 1)	(114.79, 1)	(114.99, 1)	(115.19, 1)	(115.39, 1)	(115.59, 1)	(115.79, 1)	(115.99, 1)	(116.19, 1)
(116.39, 1)	(116.59, 1)	(116.79, 1)	(116.99, 1)	(117.19, 1)	(117.39, 1)	(117.59, 1)	(117.79, 1)	(117.99, 1)	(118.19, 1)	(118.39, 1)	(118.59, 1)
(118.79, 1)	(118.99, 1)	(119.19, 1)	(119.39, 1)	(119.59, 1)	(119.79, 1)	(119.99, 1)	(120.19, 1)	(120.39, 1)	(120.59, 1)	(120.79, 1)	(120.99, 1)
(121.19, 1)	(121.39, 1)	(121.59, 1)	(121.79, 1)	(121.99, 1)	(122.19, 1)	(122.39, 1)	(122.59, 1)	(122.79, 1)	(122.99, 1)	(123.19, 1)	(123.39, 1)
(123.59, 1)	(123.79, 1)	(123.99, 1)	(124.19, 1)	(124.39, 1)	(124.59, 1)	(124.79, 1)	(124.99, 1)	(125.19, 1)	(125.39, 1)	(125.59, 1)	(125.79, 1)
(125.99, 1)	(126.19, 1)	(126.39, 1)	(126.59, 1)	(126.79, 1)	(126.99, 1)	(127.19, 1)	(127.39, 1)	(127.59, 1)	(127.79, 1)	(127.99, 1)	(128.19, 1)
(128.39, 1)	(128.59, 1)	(128.79, 1)	(128.99, 1)	(129.19, 1)	(129.39, 1)	(129.59, 1)	(129.79, 1)	(129.99, 1)	(130.19, 1)	(130.39, 1)	(130.59, 1)
(130.79, 1)	(130.99, 1)	(131.19, 1)	(131.39, 1)	(131.59, 1)	(131.79, 1)	(131.99, 1)	(132.19, 1)	(132.39, 1)	(132.59, 1)	(132.79, 1)	(132.99, 1)
(133.19, 1)	(133.39, 1)	(133.59, 1)	(133.79, 1)	(133.99, 1)	(134.19, 1)	(134.39, 1)	(134.59, 1)	(134.79, 1)	(134.99, 1)	(135.19, 1)	(135.39, 1)
(135.59, 1)	(135.79, 1)	(135.99, 1)	(136.19, 1)	(136.39, 1)	(136.59, 1)	(136.79, 1)	(136.99, 1)	(137.19, 1)	(137.39, 1)	(137.59, 1)	(137.79, 1)
(137.99, 1)	(138.19, 1)	(138.39, 1)	(138.59, 1)	(138.79, 1)	(138.99, 1)	(139.19, 1)	(139.39, 1)	(139.59, 1)	(139.79, 1)	(139.99, 1)	(140.19, 1)
(140.39, 1)	(140.59, 1)	(140.79, 1)	(140.99, 1)	(141.19, 1)	(141.39, 1)	(141.59, 1)	(141.79, 1)	(141.99, 1)	(142.19, 1)	(142.39, 1)	(142.59, 1)
(142.79, 1)	(142.99, 1)	(143.19, 1)	(143.39, 1)	(143.59, 1)	(143.79, 1)	(143.99, 1)	(144.19, 1)	(144.39, 1)	(144.59, 1)	(144.79, 1)	(144.99, 1)
(145.19, 1)	(145.39, 1)	(145.59, 1)	(145.79, 1)	(145.99, 1)	(146.19, 1)	(146.39, 1)	(146.59, 1)	(146.79, 1)	(146.99, 1)	(147.19, 1)	(147.39, 1)
(147.59, 1)	(147.79, 1)	(147.99, 1)	(148.19, 1)	(148.39, 1)	(148.59, 1)	(148.79, 1)	(148.99, 1)	(149.19, 1)	(149.39, 1)	(149.59, 1)	(149.79, 1)
(149.99, 1)	(150.19, 1)	(150.39, 1)	(150.59, 1)	(150.79, 1)	(150.99, 1)	(151.19, 1)	(151.39, 1)	(151.59, 1)	(151.79, 1)	(151.99, 1)	(152.19, 1)
(152.39, 1)	(152.59, 1)	(152.79, 1)	(152.99, 1)	(153.19, 1)	(153.39, 1)	(153.59, 1)	(153.79, 1)	(153.99, 1)	(154.19, 1)	(154.39, 1)	(154.59, 1)
(154.79, 1)	(154.99, 1)	(155.19, 1)	(155.39, 1)	(155.59, 1)	(155.79, 1)	(155.99, 1)	(156.19, 1)	(156.39, 1)	(156.59, 1)	(156.79, 1)	(156.99, 1)
(157.19, 1)	(157.39, 1)	(157.59, 1)	(157.79, 1)	(157.99, 1)	(158.19, 1)	(158.39, 1)	(158.59, 1)	(158.79, 1)	(158.99, 1)	(159.19, 1)	(159.39, 1)
(159.59, 1)	(159.79, 1)	(159.99, 1)	(160.19, 1)	(160.39, 1)	(160.59, 1)	(160.79, 1)	(160.99, 1)	(161.19, 1)	(161.39, 1)	(161.59, 1)	(161.79, 1)
(161.99, 1)	(162.19, 1)	(162.39, 1)	(162.59, 1)	(162.79, 1)	(162.99, 1)	(163.19, 1)	(163.39, 1)	(163.59, 1)	(163.79, 1)	(163.99, 1)	(164.19, 1)
(164.39, 1)	(164.59, 1)	(164.79, 1)	(164.99, 1)	(165.19, 1)	(165.39, 1)	(165.59, 1)	(165.79, 1)	(165.99, 1)	(166.19, 1)	(166.39, 1)	(166.59, 1)
(166.79, 1)	(166.99, 1)	(167.19, 1)	(167.39, 1)	(167.59, 1)	(167.79, 1)	(167.99, 1)	(168.19, 1)	(168.39, 1)	(168.59, 1)	(168.79, 1)	(168.99, 1)
(169.19, 1)	(169.39, 1)										

THE STIFF PARTICLE ENERGY EQUATION ASSUMPTION IS INITIATED FOR PARTICLE NO. 2 AT 103.02 CM. DOWN THE REACTOR

(102.95, 1)(103.02, 1)(103.09, 2)(103.16, 1)(103.23, 1)(103.29, 1)(103.36, 1)(103.43, 1)(103.50, 1)(103.56, 1)(103.63, 1)(103.70, 1)
 (103.77, 1)(103.84, 1)(103.90, 1)(103.97, 1)(104.04, 1)(104.11, 1)(104.17, 1)(104.24, 1)(104.31, 1)(104.38, 1)(104.44, 1)(104.51, 1)
 (104.58, 1)(104.65, 1)(104.72, 1)(104.78, 1)(104.85, 1)(104.92, 1)(104.99, 1)(105.05, 1)(105.12, 1)(105.19, 1)(105.26, 1)(105.33, 1)
 (105.39, 1)(105.46, 1)(105.53, 1)(105.60, 1)(105.66, 1)(105.73, 1)(105.80, 1)(105.87, 1)(105.94, 1)(106.00, 1)(106.07, 1)(106.14, 1)
 (106.21, 1)(106.27, 1)(106.34, 1)(106.41, 1)(106.48, 1)(106.54, 1)(106.61, 1)(106.68, 1)(106.75, 1)(106.82, 1)(106.88, 1)(106.95, 1)
 (107.02, 1)(107.09, 1)(107.15, 1)(107.22, 1)(107.29, 1)(107.36, 1)(107.43, 1)(107.49, 1)(107.56, 1)(107.63, 1)(107.70, 1)(107.76, 1)
 (107.83, 1)(107.90, 1)(107.97, 1)(108.03, 1)(108.10, 1)(108.17, 1)(108.24, 1)(108.31, 1)(108.37, 1)(108.44, 1)(108.51, 1)(108.58, 1)
 (108.64, 1)(108.71, 1)(108.78, 1)(108.85, 1)(108.92, 1)(108.98, 1)(109.05, 1)(109.12, 1)(109.19, 1)(109.25, 1)(109.32, 1)(109.39, 1)
 (109.46, 1)(109.52, 1)(109.59, 1)(109.66, 1)(109.73, 1)(109.80, 1)(109.86, 1)(109.93, 1)(110.00, 1)(110.07, 1)(110.13, 1)(110.20, 1)
 (110.27, 1)(110.34, 1)(110.41, 1)(110.47, 1)(110.54, 1)(110.61, 1)(110.68, 1)(110.74, 1)(110.81, 1)(110.88, 1)(110.95, 1)(111.02, 1)
 (111.08, 1)(111.15, 1)(111.22, 1)(111.29, 1)(111.35, 1)(111.42, 1)(111.49, 1)(111.56, 1)(111.62, 1)(111.69, 1)(111.76, 1)(111.83, 1)
 (111.90, 1)(111.96, 1)(112.03, 1)(112.10, 1)(112.17, 1)(112.23, 1)(112.30, 1)(112.37, 1)(112.44, 1)(112.51, 1)(112.57, 1)(112.64, 1)

THE STIFF PARTICLE ENERGY EQUATION ASSUMPTION IS INITIATED FOR PARTICLE NO. 3 AT 113.39 CM. DOWN THE REACTOR

(112.71, 1)(112.78, 1)(112.84, 1)(112.91, 1)(112.98, 1)(113.05, 1)(113.11, 1)(113.18, 1)(113.25, 1)(113.32, 1)(113.39, 1)(115.82, 1)
 (116.43, 1)(117.04, 1)(117.65, 1)(118.26, 1)(118.87, 1)(119.48, 1)(120.09, 1)(120.70, 1)(121.31, 1)(121.92, 1)(122.53, 1)(123.14, 1)
 (123.75, 1)(124.36, 1)(124.97, 1)(125.58, 1)(126.19, 1)(126.80, 1)(127.41, 1)(128.02, 1)(128.63, 1)(129.24, 1)(131.67, 1)(132.28, 1)
 (132.89, 1)(133.50, 1)(134.11, 1)(134.72, 1)(135.33, 1)(135.94, 1)(136.55, 1)(137.16, 1)(137.77, 1)(138.38, 1)(138.99, 1)(139.60, 1)
 (140.21, 1)(140.82, 1)(141.43, 1)(142.04, 1)(142.65, 1)(143.26, 1)(143.87, 1)(144.48, 1)(145.08, 1)(145.69, 1)(146.30, 1)(146.91, 1)
 (147.52, 1)(148.13, 1)(148.74, 1)(149.35, 1)(149.96, 1)(150.57, 1)(151.18, 1)(151.79, 1)(152.40, 1)(

AFTER 6 ITERATION(S) THROUGH THE REACTOR THE ROOT MEAN SQUARE OF ALL PARTICLE TEMPERATURES IS 2.480 DEGREES KELVIN

BYU -- ONE Dimensional Combustion Or Gasification model (1-DICOG): particle number 1

23-May-79

DISTANCE	GAS	PARTICLE	VELOCITY	PARTICLE	PARTICLE	COAL	CHAR	H2O	ASH	PART
(cm)	TEMP	TEMP	(cm/sec)	NO. DENS	DIA.	MASS	MASS	MASS	MASS	MASS
	(kelvin)	(kelvin)		(#/cc)	(cm)	(gr)	(gr)	(gr)	(gr)	(gr)

0.00	356.6	355.6	2.86E+03	4.31E+04	2.00E-03	4.76E-09	0.00E+00	1.69E-10	5.17E-10	5.45E-09
0.61	366.7	357.2	2.70E+03	3.17E+04	2.00E-03	4.76E-09	2.32E-18	6.89E-12	5.17E-10	5.28E-09
1.22	361.3	359.8	2.49E+03	2.50E+04	2.00E-03	4.76E-09	6.56E-18	0.00E+00	5.17E-10	5.28E-09
1.83	357.3	361.8	2.27E+03	2.08E+04	2.00E-03	4.76E-09	1.21E-17	0.00E+00	5.17E-10	5.28E-09
2.44	355.9	363.6	2.08E+03	1.78E+04	2.00E-03	4.76E-09	1.90E-17	0.00E+00	5.17E-10	5.28E-09
3.05	356.8	365.4	1.92E+03	1.56E+04	2.00E-03	4.76E-09	2.75E-17	0.00E+00	5.17E-10	5.28E-09
3.66	359.7	367.5	1.79E+03	1.38E+04	2.00E-03	4.76E-09	3.81E-17	0.00E+00	5.17E-10	5.28E-09
4.27	363.3	369.9	1.68E+03	1.24E+04	2.00E-03	4.76E-09	5.12E-17	0.00E+00	5.17E-10	5.28E-09
4.88	367.1	372.9	1.57E+03	1.12E+04	2.00E-03	4.76E-09	6.80E-17	0.00E+00	5.17E-10	5.28E-09
5.49	370.8	376.2	1.48E+03	1.03E+04	2.00E-03	4.76E-09	9.00E-17	0.00E+00	5.17E-10	5.28E-09
6.10	374.6	379.9	1.39E+03	9.47E+03	2.00E-03	4.76E-09	1.19E-16	0.00E+00	5.17E-10	5.28E-09
6.71	378.1	383.8	1.32E+03	8.79E+03	2.00E-03	4.76E-09	1.58E-16	0.00E+00	5.17E-10	5.28E-09
7.32	381.6	387.8	1.25E+03	8.22E+03	2.00E-03	4.76E-09	2.11E-16	0.00E+00	5.17E-10	5.28E-09
7.92	384.9	392.0	1.18E+03	7.72E+03	2.00E-03	4.76E-09	2.82E-16	0.00E+00	5.17E-10	5.28E-09
8.53	388.1	396.1	1.12E+03	7.29E+03	2.00E-03	4.76E-09	3.77E-16	0.00E+00	5.17E-10	5.28E-09
9.14	391.2	400.2	1.07E+03	6.92E+03	2.00E-03	4.76E-09	5.04E-16	0.00E+00	5.17E-10	5.28E-09
9.75	394.1	404.2	1.02E+03	6.58E+03	2.00E-03	4.76E-09	6.71E-16	0.00E+00	5.17E-10	5.28E-09
10.36	397.0	408.1	9.70E+02	6.29E+03	2.00E-03	4.76E-09	8.88E-16	0.00E+00	5.17E-10	5.28E-09
10.97	399.8	411.8	9.26E+02	6.02E+03	2.00E-03	4.76E-09	1.17E-15	0.00E+00	5.17E-10	5.28E-09
11.58	402.5	415.4	8.84E+02	5.79E+03	2.00E-03	4.76E-09	1.52E-15	0.00E+00	5.17E-10	5.28E-09
12.19	405.2	418.8	8.46E+02	5.58E+03	2.00E-03	4.76E-09	1.96E-15	0.00E+00	5.17E-10	5.28E-09
12.80	407.7	422.1	8.09E+02	5.38E+03	2.00E-03	4.76E-09	2.51E-15	0.00E+00	5.17E-10	5.28E-09
13.41	410.3	425.2	7.75E+02	5.21E+03	2.00E-03	4.76E-09	3.19E-15	0.00E+00	5.17E-10	5.28E-09
14.02	412.8	428.2	7.43E+02	5.05E+03	2.00E-03	4.76E-09	4.00E-15	0.00E+00	5.17E-10	5.28E-09
14.63	415.2	431.2	7.13E+02	4.91E+03	2.00E-03	4.76E-09	4.99E-15	0.00E+00	5.17E-10	5.28E-09
15.24	417.7	434.0	6.84E+02	4.78E+03	2.00E-03	4.76E-09	6.16E-15	0.00E+00	5.17E-10	5.28E-09
15.85	420.1	436.7	6.57E+02	4.66E+03	2.00E-03	4.76E-09	7.56E-15	0.00E+00	5.17E-10	5.28E-09
16.46	422.5	439.4	6.31E+02	4.55E+03	2.00E-03	4.76E-09	9.21E-15	0.00E+00	5.17E-10	5.28E-09
17.07	424.9	442.1	6.07E+02	4.45E+03	2.00E-03	4.76E-09	1.12E-14	0.00E+00	5.17E-10	5.28E-09
17.68	427.3	444.7	5.84E+02	4.35E+03	2.00E-03	4.76E-09	1.34E-14	0.00E+00	5.17E-10	5.28E-09
18.29	429.8	447.3	5.62E+02	4.27E+03	2.00E-03	4.76E-09	1.61E-14	0.00E+00	5.17E-10	5.28E-09
18.90	432.2	449.9	5.41E+02	4.19E+03	2.00E-03	4.76E-09	1.92E-14	0.00E+00	5.17E-10	5.28E-09
19.51	434.7	452.4	5.21E+02	4.12E+03	2.00E-03	4.76E-09	2.28E-14	0.00E+00	5.17E-10	5.28E-09
20.12	437.1	455.0	5.01E+02	4.05E+03	2.00E-03	4.76E-09	2.70E-14	0.00E+00	5.17E-10	5.28E-09
20.73	439.7	457.6	4.83E+02	3.99E+03	2.00E-03	4.76E-09	3.19E-14	0.00E+00	5.17E-10	5.28E-09
21.34	442.2	460.2	4.66E+02	3.94E+03	2.00E-03	4.76E-09	3.75E-14	0.00E+00	5.17E-10	5.28E-09
21.95	444.9	462.8	4.49E+02	3.89E+03	2.00E-03	4.76E-09	4.40E-14	0.00E+00	5.17E-10	5.28E-09
22.56	447.5	465.5	4.33E+02	3.84E+03	2.00E-03	4.76E-09	5.16E-14	0.00E+00	5.17E-10	5.28E-09
23.16	450.3	468.3	4.18E+02	3.80E+03	2.00E-03	4.76E-09	6.03E-14	0.00E+00	5.17E-10	5.28E-09
23.77	453.1	471.1	4.03E+02	3.76E+03	2.00E-03	4.76E-09	7.05E-14	0.00E+00	5.17E-10	5.28E-09
24.38	456.0	474.0	3.89E+02	3.72E+03	2.00E-03	4.76E-09	8.23E-14	0.00E+00	5.17E-10	5.28E-09
24.99	459.0	476.9	3.75E+02	3.69E+03	2.00E-03	4.76E-09	9.60E-14	0.00E+00	5.17E-10	5.28E-09
25.60	462.0	480.0	3.62E+02	3.66E+03	2.00E-03	4.76E-09	1.12E-13	0.00E+00	5.17E-10	5.28E-09
26.21	465.2	483.1	3.50E+02	3.64E+03	2.00E-03	4.76E-09	1.31E-13	0.00E+00	5.17E-10	5.28E-09
26.82	468.5	486.3	3.37E+02	3.62E+03	2.00E-03	4.76E-09	1.52E-13	0.00E+00	5.17E-10	5.28E-09
27.43	471.9	489.7	3.26E+02	3.60E+03	2.00E-03	4.76E-09	1.78E-13	0.00E+00	5.17E-10	5.28E-09
28.04	475.5	493.2	3.15E+02	3.58E+03	2.00E-03	4.76E-09	2.08E-13	0.00E+00	5.17E-10	5.28E-09

28.65	479.2	496.8	3.04E+02	3.57E+03	2.00E-03	4.76E-09	2.44E-13	0.00E+00	5.17E-10	5.28E-09
29.26	483.1	500.6	2.93E+02	3.56E+03	2.00E-03	4.76E-09	2.45E-13	0.00E+00	5.17E-10	5.28E-09
29.87	487.2	504.5	2.83E+02	3.55E+03	2.00E-03	4.76E-09	3.35E-13	0.00E+00	5.17E-10	5.28E-09
30.48	491.5	508.7	2.73E+02	3.54E+03	2.00E-03	4.76E-09	3.95E-13	0.00E+00	5.17E-10	5.28E-09
31.09	496.0	513.1	2.64E+02	3.54E+03	2.00E-03	4.76E-09	4.66E-13	0.00E+00	5.17E-10	5.28E-09
31.70	500.7	517.7	2.55E+02	3.54E+03	2.00E-03	4.76E-09	5.52E-13	0.00E+00	5.17E-10	5.28E-09
32.31	505.7	522.5	2.46E+02	3.54E+03	2.00E-03	4.76E-09	6.56E-13	0.00E+00	5.17E-10	5.28E-09
32.92	511.0	527.6	2.37E+02	3.54E+03	2.00E-03	4.76E-09	7.83E-13	0.00E+00	5.17E-10	5.28E-09
33.53	516.7	533.1	2.29E+02	3.55E+03	2.00E-03	4.76E-09	9.38E-13	0.00E+00	5.17E-10	5.28E-09
34.14	522.7	538.8	2.21E+02	3.56E+03	2.00E-03	4.76E-09	1.13E-12	0.00E+00	5.17E-10	5.28E-09
34.75	529.1	545.0	2.13E+02	3.57E+03	2.00E-03	4.76E-09	1.37E-12	0.00E+00	5.17E-10	5.28E-09
35.36	534.4	551.0	2.11E+02	3.57E+03	2.00E-03	4.76E-09	1.66E-12	0.00E+00	5.17E-10	5.28E-09
35.97	537.0	554.5	2.12E+02	3.56E+03	2.00E-03	4.76E-09	2.01E-12	0.00E+00	5.17E-10	5.28E-09
36.58	539.6	557.1	2.13E+02	3.54E+03	2.00E-03	4.76E-09	2.38E-12	0.00E+00	5.17E-10	5.28E-09
37.19	542.1	559.6	2.14E+02	3.52E+03	2.00E-03	4.76E-09	2.77E-12	0.00E+00	5.17E-10	5.28E-09
37.80	544.7	562.2	2.15E+02	3.51E+03	2.00E-03	4.75E-09	3.20E-12	0.00E+00	5.17E-10	5.27E-09
38.40	547.4	564.7	2.16E+02	3.49E+03	2.00E-03	4.75E-09	3.65E-12	0.00E+00	5.17E-10	5.27E-09
39.01	550.0	567.3	2.17E+02	3.47E+03	2.00E-03	4.75E-09	4.13E-12	0.00E+00	5.17E-10	5.27E-09
39.62	552.7	570.0	2.18E+02	3.46E+03	2.00E-03	4.75E-09	4.65E-12	0.00E+00	5.17E-10	5.27E-09
40.23	555.4	572.6	2.19E+02	3.44E+03	2.00E-03	4.75E-09	5.20E-12	0.00E+00	5.17E-10	5.27E-09
40.84	558.1	575.3	2.20E+02	3.42E+03	2.00E-03	4.75E-09	5.79E-12	0.00E+00	5.17E-10	5.27E-09
41.45	560.9	578.0	2.21E+02	3.41E+03	2.00E-03	4.75E-09	6.43E-12	0.00E+00	5.17E-10	5.27E-09
42.06	563.6	580.6	2.22E+02	3.39E+03	2.00E-03	4.75E-09	7.10E-12	0.00E+00	5.17E-10	5.27E-09
42.67	566.4	583.4	2.23E+02	3.37E+03	2.00E-03	4.75E-09	7.82E-12	0.00E+00	5.17E-10	5.27E-09
43.28	569.1	586.1	2.24E+02	3.36E+03	2.00E-03	4.75E-09	8.59E-12	0.00E+00	5.17E-10	5.27E-09
43.89	571.9	588.8	2.26E+02	3.34E+03	2.00E-03	4.74E-09	9.41E-12	0.00E+00	5.17E-10	5.27E-09
44.50	574.7	591.6	2.27E+02	3.32E+03	2.00E-03	4.74E-09	1.03E-11	0.00E+00	5.17E-10	5.27E-09
45.11	577.6	594.4	2.28E+02	3.31E+03	2.00E-03	4.74E-09	1.12E-11	0.00E+00	5.17E-10	5.27E-09
45.72	580.4	597.2	2.29E+02	3.29E+03	2.00E-03	4.74E-09	1.22E-11	0.00E+00	5.17E-10	5.27E-09
46.33	583.3	600.0	2.30E+02	3.27E+03	2.00E-03	4.74E-09	1.33E-11	0.00E+00	5.17E-10	5.27E-09
46.94	586.2	602.8	2.31E+02	3.26E+03	2.00E-03	4.74E-09	1.44E-11	0.00E+00	5.17E-10	5.27E-09
47.55	589.1	605.6	2.32E+02	3.24E+03	2.00E-03	4.73E-09	1.56E-11	0.00E+00	5.17E-10	5.27E-09
48.16	592.0	608.5	2.33E+02	3.23E+03	2.00E-03	4.73E-09	1.69E-11	0.00E+00	5.17E-10	5.27E-09
48.77	595.0	611.4	2.35E+02	3.21E+03	2.00E-03	4.73E-09	1.83E-11	0.00E+00	5.17E-10	5.27E-09
49.38	597.9	614.3	2.36E+02	3.19E+03	2.00E-03	4.73E-09	1.98E-11	0.00E+00	5.17E-10	5.26E-09
49.99	601.0	617.3	2.37E+02	3.18E+03	2.00E-03	4.73E-09	2.13E-11	0.00E+00	5.17E-10	5.26E-09
50.60	604.0	620.2	2.38E+02	3.16E+03	2.00E-03	4.72E-09	2.30E-11	0.00E+00	5.17E-10	5.26E-09
51.21	607.1	623.2	2.39E+02	3.14E+03	2.00E-03	4.72E-09	2.47E-11	0.00E+00	5.17E-10	5.26E-09
51.82	610.2	626.3	2.41E+02	3.13E+03	2.00E-03	4.72E-09	2.66E-11	0.00E+00	5.17E-10	5.26E-09
52.43	613.3	629.4	2.42E+02	3.11E+03	2.00E-03	4.71E-09	2.86E-11	0.00E+00	5.17E-10	5.26E-09
53.04	616.5	632.5	2.43E+02	3.10E+03	2.00E-03	4.71E-09	3.08E-11	0.00E+00	5.17E-10	5.26E-09
53.64	619.7	635.6	2.45E+02	3.08E+03	2.00E-03	4.71E-09	3.30E-11	0.00E+00	5.17E-10	5.26E-09
54.25	623.0	638.8	2.46E+02	3.06E+03	2.00E-03	4.70E-09	3.55E-11	0.00E+00	5.17E-10	5.25E-09
54.86	626.3	642.0	2.47E+02	3.05E+03	2.00E-03	4.70E-09	3.80E-11	0.00E+00	5.17E-10	5.25E-09
55.47	629.6	645.3	2.48E+02	3.03E+03	2.00E-03	4.69E-09	4.08E-11	0.00E+00	5.17E-10	5.25E-09
56.08	633.0	648.6	2.50E+02	3.01E+03	2.00E-03	4.69E-09	4.37E-11	0.00E+00	5.17E-10	5.25E-09
56.69	636.5	652.0	2.51E+02	3.00E+03	2.00E-03	4.68E-09	4.69E-11	0.00E+00	5.17E-10	5.25E-09
57.30	640.0	655.4	2.53E+02	2.98E+03	2.00E-03	4.68E-09	5.02E-11	0.00E+00	5.17E-10	5.24E-09
57.91	643.6	658.9	2.54E+02	2.96E+03	2.00E-03	4.67E-09	5.38E-11	0.00E+00	5.17E-10	5.24E-09
58.52	647.3	662.5	2.56E+02	2.95E+03	2.00E-03	4.67E-09	5.76E-11	0.00E+00	5.17E-10	5.24E-09
59.13	651.0	666.1	2.57E+02	2.93E+03	2.00E-03	4.66E-09	6.16E-11	0.00E+00	5.17E-10	5.24E-09
59.74	654.8	669.8	2.59E+02	2.91E+03	2.00E-03	4.65E-09	6.59E-11	0.00E+00	5.17E-10	5.23E-09
60.35	658.7	673.6	2.60E+02	2.90E+03	2.00E-03	4.64E-09	7.06E-11	0.00E+00	5.17E-10	5.23E-09
60.96	662.6	677.4	2.62E+02	2.88E+03	2.01E-03	4.64E-09	7.55E-11	0.00E+00	5.17E-10	5.23E-09
61.57	666.7	681.4	2.63E+02	2.86E+03	2.01E-03	4.63E-09	8.08E-11	0.00E+00	5.17E-10	5.23E-09
62.18	670.9	685.4	2.65E+02	2.84E+03	2.01E-03	4.62E-09	8.64E-11	0.00E+00	5.17E-10	5.22E-09
62.79	675.2	689.5	2.67E+02	2.82E+03	2.01E-03	4.61E-09	9.25E-11	0.00E+00	5.17E-10	5.22E-09
63.40	679.5	693.8	2.68E+02	2.81E+03	2.01E-03	4.60E-09	9.90E-11	0.00E+00	5.17E-10	5.21E-09
64.01	684.1	698.2	2.70E+02	2.79E+03	2.01E-03	4.59E-09	1.06E-10	0.00E+00	5.17E-10	5.21E-09
64.62	688.7	702.7	2.72E+02	2.77E+03	2.01E-03	4.57E-09	1.13E-10	0.00E+00	5.17E-10	5.20E-09

65.23	693.5	707.3	2.74E+02	2.75E+03	2.01E-03	4.56E-09	1.22E-10	0.00E+00	5.17E-10	5.20E-09
65.84	698.5	712.1	2.76E+02	2.73E+03	2.01E-03	4.55E-09	1.30E-10	0.00E+00	5.17E-10	5.19E-09
66.45	703.6	717.1	2.78E+02	2.71E+03	2.01E-03	4.53E-09	1.39E-10	0.00E+00	5.17E-10	5.19E-09
67.06	708.9	722.2	2.80E+02	2.69E+03	2.01E-03	4.51E-09	1.50E-10	0.00E+00	5.17E-10	5.18E-09
67.67	714.5	727.5	2.83E+02	2.66E+03	2.01E-03	4.50E-09	1.60E-10	0.00E+00	5.17E-10	5.17E-09
68.28	720.2	733.1	2.85E+02	2.64E+03	2.01E-03	4.48E-09	1.72E-10	0.00E+00	5.17E-10	5.17E-09
68.88	726.2	738.8	2.87E+02	2.62E+03	2.01E-03	4.46E-09	1.85E-10	0.00E+00	5.17E-10	5.16E-09
69.49	732.4	744.8	2.90E+02	2.60E+03	2.01E-03	4.43E-09	1.99E-10	0.00E+00	5.17E-10	5.15E-09
70.10	739.0	751.1	2.93E+02	2.57E+03	2.01E-03	4.41E-09	2.14E-10	0.00E+00	5.17E-10	5.14E-09
70.71	745.8	757.6	2.95E+02	2.55E+03	2.02E-03	4.38E-09	2.30E-10	0.00E+00	5.17E-10	5.13E-09
71.32	753.0	764.5	2.98E+02	2.52E+03	2.02E-03	4.35E-09	2.48E-10	0.00E+00	5.17E-10	5.12E-09
71.93	760.6	771.7	3.01E+02	2.50E+03	2.02E-03	4.32E-09	2.67E-10	0.00E+00	5.17E-10	5.11E-09
72.54	768.6	779.3	3.05E+02	2.47E+03	2.02E-03	4.29E-09	2.89E-10	0.00E+00	5.17E-10	5.09E-09
73.15	777.1	787.4	3.08E+02	2.44E+03	2.02E-03	4.25E-09	3.12E-10	0.00E+00	5.17E-10	5.08E-09
73.76	786.1	796.0	3.12E+02	2.42E+03	2.02E-03	4.21E-09	3.38E-10	0.00E+00	5.17E-10	5.06E-09
74.37	794.9	804.3	3.15E+02	2.39E+03	2.03E-03	4.16E-09	3.65E-10	0.00E+00	5.17E-10	5.04E-09
74.98	805.1	814.0	3.20E+02	2.36E+03	2.03E-03	4.11E-09	3.96E-10	0.00E+00	5.17E-10	5.02E-09
75.59	816.0	824.3	3.24E+02	2.32E+03	2.03E-03	4.05E-09	4.31E-10	0.00E+00	5.17E-10	5.00E-09
76.20	827.8	835.5	3.29E+02	2.29E+03	2.03E-03	3.99E-09	4.71E-10	0.00E+00	5.17E-10	4.98E-09
76.81	840.5	847.4	3.34E+02	2.25E+03	2.04E-03	3.92E-09	5.15E-10	0.00E+00	5.17E-10	4.95E-09
77.42	854.3	860.4	3.40E+02	2.22E+03	2.04E-03	3.84E-09	5.64E-10	0.00E+00	5.17E-10	4.92E-09
78.03	869.4	874.6	3.46E+02	2.18E+03	2.04E-03	3.74E-09	6.20E-10	0.00E+00	5.17E-10	4.88E-09
78.64	885.9	890.0	3.53E+02	2.13E+03	2.05E-03	3.64E-09	6.83E-10	0.00E+00	5.17E-10	4.84E-09
79.25	904.0	907.0	3.61E+02	2.09E+03	2.05E-03	3.52E-09	7.56E-10	0.00E+00	5.17E-10	4.79E-09
79.86	924.0	925.7	3.69E+02	2.04E+03	2.06E-03	3.39E-09	8.38E-10	0.00E+00	5.17E-10	4.74E-09
80.47	946.3	946.5	3.78E+02	1.99E+03	2.06E-03	3.23E-09	9.33E-10	0.00E+00	5.17E-10	4.68E-09
81.08	971.1	969.6	3.89E+02	1.94E+03	2.07E-03	3.05E-09	1.04E-09	0.00E+00	5.17E-10	4.61E-09
81.69	999.0	995.6	4.01E+02	1.88E+03	2.08E-03	2.84E-09	1.17E-09	0.00E+00	5.17E-10	4.53E-09
82.30	1030.6	1024.9	4.14E+02	1.82E+03	2.09E-03	2.60E-09	1.31E-09	0.00E+00	5.17E-10	4.43E-09
82.91	1066.8	1058.3	4.29E+02	1.75E+03	2.10E-03	2.32E-09	1.48E-09	0.00E+00	5.17E-10	4.31E-09
83.52	1109.2	1097.2	4.47E+02	1.68E+03	2.12E-03	1.99E-09	1.66E-09	0.00E+00	5.17E-10	4.17E-09
84.12	1161.0	1144.1	4.69E+02	1.60E+03	2.13E-03	1.60E-09	1.88E-09	0.00E+00	5.17E-10	3.99E-09
84.73	1229.7	1204.7	4.99E+02	1.51E+03	2.15E-03	1.10E-09	2.11E-09	0.00E+00	5.17E-10	3.73E-09
85.34	1328.3	1291.1	5.41E+02	1.39E+03	2.18E-03	4.56E-10	2.34E-09	0.00E+00	5.17E-10	3.32E-09
85.95	1435.6	1398.5	5.87E+02	1.28E+03	2.20E-03	2.97E-11	2.41E-09	0.00E+00	5.17E-10	2.96E-09
86.56	1523.3	1487.9	6.24E+02	1.21E+03	2.20E-03	0.00E+00	2.31E-09	0.00E+00	5.17E-10	2.83E-09
87.17	1587.8	1556.8	6.52E+02	1.16E+03	2.20E-03	0.00E+00	2.17E-09	0.00E+00	5.17E-10	2.69E-09
87.78	1644.2	1610.6	6.76E+02	1.11E+03	2.20E-03	0.00E+00	2.02E-09	0.00E+00	5.17E-10	2.53E-09
88.39	1703.1	1666.9	7.01E+02	1.07E+03	2.20E-03	0.00E+00	1.85E-09	0.00E+00	5.17E-10	2.37E-09
89.00	1748.7	1714.0	7.20E+02	1.05E+03	2.20E-03	0.00E+00	1.68E-09	0.00E+00	5.17E-10	2.20E-09
89.61	1778.4	1744.7	7.32E+02	1.03E+03	2.20E-03	0.00E+00	1.51E-09	0.00E+00	5.17E-10	2.03E-09
90.22	1804.4	1769.4	7.43E+02	1.01E+03	2.20E-03	0.00E+00	1.35E-09	0.00E+00	5.17E-10	1.86E-09
90.83	1831.1	1794.6	7.54E+02	9.99E+02	2.20E-03	0.00E+00	1.18E-09	0.00E+00	5.17E-10	1.69E-09
91.44	1857.6	1819.6	7.65E+02	9.85E+02	2.20E-03	0.00E+00	1.01E-09	0.00E+00	5.17E-10	1.53E-09
92.05	1883.7	1844.2	7.76E+02	9.71E+02	2.20E-03	0.00E+00	8.41E-10	0.00E+00	5.17E-10	1.36E-09
92.66	1909.2	1868.2	7.86E+02	9.58E+02	2.20E-03	0.00E+00	6.77E-10	0.00E+00	5.17E-10	1.19E-09
93.27	1934.0	1891.4	7.96E+02	9.46E+02	2.20E-03	0.00E+00	5.14E-10	0.00E+00	5.17E-10	1.03E-09
93.88	1958.1	1913.9	8.06E+02	9.34E+02	2.20E-03	0.00E+00	3.55E-10	0.00E+00	5.17E-10	8.72E-10
94.49	1981.3	1935.7	8.16E+02	9.23E+02	2.20E-03	0.00E+00	1.99E-10	0.00E+00	5.17E-10	7.16E-10
95.10	2003.0	1956.3	8.25E+02	9.13E+02	2.20E-03	0.00E+00	4.91E-11	0.00E+00	5.17E-10	5.66E-10
95.71	2010.9	1964.4	8.28E+02	9.09E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
96.32	2014.0	1967.3	8.30E+02	9.08E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
96.93	2017.2	1970.2	8.31E+02	9.06E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
97.54	2020.3	1973.1	8.32E+02	9.05E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
98.15	2023.5	1975.9	8.33E+02	9.04E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
98.76	2026.5	1978.7	8.35E+02	9.02E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
99.36	2029.6	1981.5	8.36E+02	9.01E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
99.97	2032.5	1984.2	8.37E+02	8.99E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
100.58	2035.4	1986.8	8.38E+02	8.98E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
101.19	2038.2	1989.3	8.40E+02	8.97E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10

101.80	2040.9	1991.8	8.41E+02	8.96E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
102.41	2043.6	1994.2	8.42E+02	8.95E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
103.02	2046.1	1996.6	8.43E+02	8.93E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
103.63	2048.7	1999.0	8.44E+02	8.92E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
104.24	2051.4	2001.3	8.45E+02	8.91E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
104.85	2053.9	2003.7	8.46E+02	8.90E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
105.46	2056.4	2005.9	8.47E+02	8.89E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
106.07	2058.8	2008.1	8.48E+02	8.88E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
106.68	2061.1	2010.2	8.49E+02	8.87E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
107.29	2063.3	2012.2	8.50E+02	8.86E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
107.90	2065.5	2014.2	8.51E+02	8.85E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
108.51	2067.6	2016.1	8.52E+02	8.84E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
109.12	2069.6	2017.9	8.53E+02	8.83E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
109.73	2071.5	2019.7	8.53E+02	8.82E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
110.34	2073.4	2021.3	8.54E+02	8.82E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
110.95	2075.2	2023.0	8.55E+02	8.81E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
111.56	2076.9	2024.5	8.56E+02	8.80E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
112.17	2078.6	2026.0	8.56E+02	8.79E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
112.78	2080.1	2027.5	8.57E+02	8.79E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
113.39	2081.7	2028.9	8.58E+02	8.78E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
114.00	2083.8	2030.8	8.59E+02	8.77E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
114.60	2085.2	2032.1	8.59E+02	8.76E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
115.21	2086.6	2033.3	8.60E+02	8.76E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
115.82	2087.9	2034.5	8.60E+02	8.75E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
116.43	2089.1	2035.6	8.61E+02	8.75E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
117.04	2090.3	2036.6	8.61E+02	8.74E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
117.65	2091.4	2037.6	8.62E+02	8.74E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
118.26	2092.5	2038.6	8.62E+02	8.73E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
118.87	2093.5	2039.5	8.63E+02	8.73E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
119.48	2094.4	2040.4	8.63E+02	8.72E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
120.09	2095.3	2041.2	8.64E+02	8.72E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
120.70	2096.1	2041.9	8.64E+02	8.72E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
121.31	2096.9	2042.6	8.64E+02	8.71E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
121.92	2097.6	2043.3	8.65E+02	8.71E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
122.53	2098.3	2043.9	8.65E+02	8.71E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
123.14	2098.9	2044.4	8.65E+02	8.71E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
123.75	2099.5	2044.9	8.65E+02	8.70E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
124.36	2100.0	2045.4	8.66E+02	8.70E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
124.97	2100.5	2045.8	8.66E+02	8.70E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
125.58	2100.9	2046.2	8.66E+02	8.70E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
126.19	2101.3	2046.6	8.66E+02	8.70E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
126.80	2101.6	2046.8	8.66E+02	8.69E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
127.41	2101.9	2047.1	8.66E+02	8.69E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
128.02	2102.1	2047.3	8.66E+02	8.69E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
128.63	2102.3	2047.5	8.67E+02	8.69E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
129.24	2102.5	2047.7	8.67E+02	8.69E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
129.84	2099.8	2045.3	8.66E+02	8.70E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
130.45	2097.2	2042.9	8.64E+02	8.71E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
131.06	2094.5	2040.6	8.63E+02	8.72E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
131.67	2091.9	2038.1	8.62E+02	8.73E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
132.28	2089.2	2035.7	8.61E+02	8.75E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
132.89	2086.6	2033.4	8.60E+02	8.76E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
133.50	2084.0	2031.1	8.59E+02	8.77E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
134.11	2081.4	2028.5	8.58E+02	8.78E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
134.72	2078.8	2026.2	8.57E+02	8.79E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
135.33	2076.2	2023.9	8.56E+02	8.80E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
135.94	2073.6	2021.5	8.55E+02	8.81E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
136.55	2071.0	2019.2	8.53E+02	8.82E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
137.16	2068.4	2016.7	8.52E+02	8.83E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
137.77	2065.9	2014.4	8.51E+02	8.85E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10

138.38	2063.3	2012.1	8.50E+02	8.86E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
138.99	2060.8	2009.8	8.49E+02	8.87E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
139.60	2058.2	2007.6	8.48E+02	8.88E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
140.21	2055.7	2005.1	8.47E+02	8.89E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
140.82	2053.1	2002.8	8.46E+02	8.90E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
141.43	2050.6	2000.6	8.45E+02	8.91E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
142.04	2048.1	1998.3	8.44E+02	8.92E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
142.65	2045.6	1996.1	8.43E+02	8.93E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
143.26	2043.1	1993.6	8.42E+02	8.95E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
143.87	2040.6	1991.4	8.41E+02	8.96E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
144.48	2038.1	1989.2	8.40E+02	8.97E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
145.08	2035.7	1986.9	8.39E+02	8.98E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
145.69	2033.2	1984.7	8.38E+02	8.99E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
146.30	2030.7	1982.3	8.37E+02	9.00E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
146.91	2028.3	1980.1	8.36E+02	9.01E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
147.52	2025.8	1977.9	8.35E+02	9.02E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
148.13	2023.4	1975.7	8.34E+02	9.03E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
148.74	2021.0	1973.5	8.33E+02	9.04E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
149.35	2018.6	1971.2	8.32E+02	9.06E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
149.96	2016.1	1969.0	8.31E+02	9.07E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
150.57	2013.7	1966.8	8.30E+02	9.08E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
151.18	2011.3	1964.7	8.29E+02	9.09E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
151.79	2008.9	1962.5	8.28E+02	9.10E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10
152.40	2006.6	1960.1	8.27E+02	9.11E+02	2.20E-03	0.00E+00	0.00E+00	0.00E+00	5.17E-10	5.17E-10

BYU -- ONE DIMENSIONAL Combustion Or Gasification model (1-DICOG): particle number 2

23-May-79

DISTANCE	GAS	PARTICLE	VELOCITY	PARTICLE	PARTICLE	COAL	CHAR	H2O	ASH	PART
(cm)	TEMP	TEMP	(cm/sec)	NO. DENS	DIA.	MASS	MASS	MASS	MASS	MASS
	(kelvin)	(kelvin)		(#/cc)	(cm)	(gr)	(gr)	(gr)	(gr)	(gr)

0.00	356.6	355.6	2.86E+03	3.03E+03	4.80E-03	6.58E-08	0.00E+00	2.33E-09	7.15E-09	7.53E-08
0.61	366.7	356.2	2.70E+03	2.22E+03	4.80E-03	6.58E-08	3.09E-17	1.62E-09	7.15E-09	7.46E-08
1.22	361.3	357.3	2.49E+03	1.75E+03	4.80E-03	6.58E-08	8.26E-17	4.28E-10	7.15E-09	7.34E-08
1.83	357.3	358.4	2.27E+03	1.46E+03	4.80E-03	6.58E-08	1.44E-16	0.00E+00	7.15E-09	7.29E-08
2.44	355.9	359.6	2.08E+03	1.25E+03	4.80E-03	6.58E-08	2.19E-16	0.00E+00	7.15E-09	7.29E-08
3.05	356.8	360.9	1.92E+03	1.09E+03	4.80E-03	6.58E-08	3.07E-16	0.00E+00	7.15E-09	7.29E-08
3.66	359.7	362.4	1.79E+03	9.68E+02	4.80E-03	6.58E-08	4.13E-16	0.00E+00	7.15E-09	7.29E-08
4.27	363.3	364.1	1.68E+03	8.68E+02	4.80E-03	6.58E-08	5.39E-16	0.00E+00	7.15E-09	7.29E-08
4.88	367.1	366.0	1.57E+03	7.87E+02	4.80E-03	6.58E-08	6.92E-16	0.00E+00	7.15E-09	7.29E-08
5.49	370.8	368.0	1.48E+03	7.20E+02	4.80E-03	6.58E-08	8.79E-16	0.00E+00	7.15E-09	7.29E-08
6.10	374.6	370.3	1.39E+03	6.64E+02	4.80E-03	6.58E-08	1.11E-15	0.00E+00	7.15E-09	7.29E-08
6.71	378.1	372.9	1.32E+03	6.17E+02	4.80E-03	6.58E-08	1.39E-15	0.00E+00	7.15E-09	7.29E-08
7.32	381.6	375.6	1.25E+03	5.77E+02	4.80E-03	6.58E-08	1.75E-15	0.00E+00	7.15E-09	7.29E-08
7.92	384.9	378.5	1.18E+03	5.42E+02	4.80E-03	6.58E-08	2.20E-15	0.00E+00	7.15E-09	7.29E-08
8.53	388.1	381.6	1.12E+03	5.12E+02	4.80E-03	6.58E-08	2.77E-15	0.00E+00	7.15E-09	7.29E-08
9.14	391.2	384.9	1.07E+03	4.85E+02	4.80E-03	6.58E-08	3.51E-15	0.00E+00	7.15E-09	7.29E-08
9.75	394.1	388.4	1.02E+03	4.62E+02	4.80E-03	6.58E-08	4.46E-15	0.00E+00	7.15E-09	7.29E-08
10.36	397.0	392.0	9.70E+02	4.41E+02	4.80E-03	6.58E-08	5.69E-15	0.00E+00	7.15E-09	7.29E-08
10.97	399.8	395.8	9.26E+02	4.23E+02	4.80E-03	6.58E-08	7.28E-15	0.00E+00	7.15E-09	7.29E-08
11.58	402.5	399.6	8.84E+02	4.06E+02	4.80E-03	6.58E-08	9.36E-15	0.00E+00	7.15E-09	7.29E-08
12.19	405.2	403.6	8.46E+02	3.91E+02	4.80E-03	6.58E-08	1.21E-14	0.00E+00	7.15E-09	7.29E-08
12.80	407.7	407.7	8.09E+02	3.78E+02	4.80E-03	6.58E-08	1.56E-14	0.00E+00	7.15E-09	7.29E-08
13.41	410.3	411.9	7.75E+02	3.66E+02	4.80E-03	6.58E-08	2.02E-14	0.00E+00	7.15E-09	7.29E-08
14.02	412.8	416.1	7.43E+02	3.55E+02	4.80E-03	6.58E-08	2.61E-14	0.00E+00	7.15E-09	7.29E-08
14.63	415.2	420.4	7.13E+02	3.44E+02	4.80E-03	6.58E-08	3.39E-14	0.00E+00	7.15E-09	7.29E-08
15.24	417.7	424.7	6.84E+02	3.35E+02	4.80E-03	6.58E-08	4.39E-14	0.00E+00	7.15E-09	7.29E-08
15.85	420.1	429.0	6.57E+02	3.27E+02	4.80E-03	6.58E-08	5.68E-14	0.00E+00	7.15E-09	7.29E-08
16.46	422.5	433.3	6.31E+02	3.19E+02	4.80E-03	6.58E-08	7.33E-14	0.00E+00	7.15E-09	7.29E-08
17.07	424.9	437.6	6.07E+02	3.12E+02	4.80E-03	6.58E-08	9.43E-14	0.00E+00	7.15E-09	7.29E-08
17.68	427.3	441.8	5.84E+02	3.06E+02	4.80E-03	6.58E-08	1.21E-13	0.00E+00	7.15E-09	7.29E-08
18.29	429.8	446.1	5.62E+02	3.00E+02	4.80E-03	6.58E-08	1.55E-13	0.00E+00	7.15E-09	7.29E-08
18.90	432.2	450.3	5.41E+02	2.94E+02	4.80E-03	6.58E-08	1.97E-13	0.00E+00	7.15E-09	7.29E-08
19.51	434.7	454.4	5.21E+02	2.89E+02	4.80E-03	6.58E-08	2.50E-13	0.00E+00	7.15E-09	7.29E-08
20.12	437.1	458.5	5.01E+02	2.84E+02	4.80E-03	6.58E-08	3.15E-13	0.00E+00	7.15E-09	7.29E-08
20.73	439.7	462.6	4.83E+02	2.80E+02	4.80E-03	6.58E-08	3.95E-13	0.00E+00	7.15E-09	7.29E-08
21.34	442.2	466.6	4.66E+02	2.76E+02	4.80E-03	6.58E-08	4.94E-13	0.00E+00	7.15E-09	7.29E-08
21.95	444.9	470.5	4.49E+02	2.73E+02	4.80E-03	6.58E-08	6.14E-13	0.00E+00	7.15E-09	7.29E-08
22.56	447.5	474.4	4.33E+02	2.69E+02	4.80E-03	6.58E-08	7.60E-13	0.00E+00	7.15E-09	7.29E-08
23.16	450.3	478.2	4.18E+02	2.66E+02	4.80E-03	6.58E-08	9.37E-13	0.00E+00	7.15E-09	7.29E-08
23.77	453.1	482.0	4.03E+02	2.64E+02	4.80E-03	6.58E-08	1.15E-12	0.00E+00	7.15E-09	7.29E-08
24.38	456.0	485.8	3.89E+02	2.61E+02	4.80E-03	6.58E-08	1.40E-12	0.00E+00	7.15E-09	7.29E-08
24.99	459.0	489.5	3.75E+02	2.59E+02	4.80E-03	6.58E-08	1.70E-12	0.00E+00	7.15E-09	7.29E-08
25.60	462.0	493.3	3.62E+02	2.57E+02	4.80E-03	6.58E-08	2.07E-12	0.00E+00	7.15E-09	7.29E-08
26.21	465.2	497.0	3.50E+02	2.55E+02	4.80E-03	6.58E-08	2.49E-12	0.00E+00	7.15E-09	7.29E-08
26.82	468.5	500.8	3.37E+02	2.54E+02	4.80E-03	6.58E-08	3.00E-12	0.00E+00	7.15E-09	7.29E-08
27.43	471.9	504.5	3.26E+02	2.52E+02	4.80E-03	6.58E-08	3.60E-12	0.00E+00	7.15E-09	7.29E-08
28.04	475.5	508.3	3.15E+02	2.51E+02	4.80E-03	6.58E-08	4.31E-12	0.00E+00	7.15E-09	7.29E-08

65.23	693.5	720.5	2.74E+02	1.93E+02	4.83E-03	6.20E-08	2.34E-09	0.00E+00	7.15E-09	7.14E-08
65.84	698.5	724.9	2.76E+02	1.91E+02	4.83E-03	6.17E-08	2.49E-09	0.00E+00	7.15E-09	7.14E-08
66.45	703.6	729.4	2.78E+02	1.90E+02	4.83E-03	6.15E-08	2.64E-09	0.00E+00	7.15E-09	7.13E-08
67.06	708.9	734.0	2.80E+02	1.88E+02	4.83E-03	6.12E-08	2.81E-09	0.00E+00	7.15E-09	7.11E-08
67.67	714.5	738.8	2.83E+02	1.87E+02	4.84E-03	6.09E-08	2.99E-09	0.00E+00	7.15E-09	7.10E-08
68.28	720.2	743.8	2.85E+02	1.85E+02	4.84E-03	6.06E-08	3.18E-09	0.00E+00	7.15E-09	7.09E-08
68.88	726.2	748.9	2.87E+02	1.84E+02	4.84E-03	6.02E-08	3.38E-09	0.00E+00	7.15E-09	7.08E-08
69.49	732.4	754.3	2.90E+02	1.82E+02	4.84E-03	5.99E-08	3.60E-09	0.00E+00	7.15E-09	7.06E-08
70.10	739.0	759.9	2.93E+02	1.81E+02	4.85E-03	5.95E-08	3.84E-09	0.00E+00	7.15E-09	7.05E-08
70.71	745.8	765.7	2.95E+02	1.79E+02	4.85E-03	5.91E-08	4.09E-09	0.00E+00	7.15E-09	7.03E-08
71.32	753.0	771.8	2.98E+02	1.77E+02	4.85E-03	5.86E-08	4.36E-09	0.00E+00	7.15E-09	7.02E-08
71.93	760.6	778.1	3.01E+02	1.75E+02	4.86E-03	5.82E-08	4.65E-09	0.00E+00	7.15E-09	7.00E-08
72.54	768.6	784.8	3.05E+02	1.73E+02	4.86E-03	5.77E-08	4.96E-09	0.00E+00	7.15E-09	6.98E-08
73.15	777.1	791.9	3.08E+02	1.72E+02	4.86E-03	5.71E-08	5.30E-09	0.00E+00	7.15E-09	6.96E-08
73.76	786.1	799.3	3.12E+02	1.69E+02	4.87E-03	5.65E-08	5.67E-09	0.00E+00	7.15E-09	6.93E-08
74.37	794.9	806.5	3.15E+02	1.68E+02	4.87E-03	5.59E-08	6.04E-09	0.00E+00	7.15E-09	6.91E-08
74.98	805.1	814.8	3.20E+02	1.65E+02	4.88E-03	5.52E-08	6.47E-09	0.00E+00	7.15E-09	6.88E-08
75.59	816.0	823.6	3.24E+02	1.63E+02	4.88E-03	5.44E-08	6.94E-09	0.00E+00	7.15E-09	6.85E-08
76.20	827.8	833.1	3.29E+02	1.61E+02	4.89E-03	5.36E-08	7.46E-09	0.00E+00	7.15E-09	6.82E-08
76.81	840.5	843.2	3.34E+02	1.58E+02	4.90E-03	5.26E-08	8.02E-09	0.00E+00	7.15E-09	6.78E-08
77.42	854.3	854.1	3.40E+02	1.55E+02	4.90E-03	5.16E-08	8.65E-09	0.00E+00	7.15E-09	6.74E-08
78.03	869.4	865.9	3.46E+02	1.53E+02	4.91E-03	5.05E-08	9.34E-09	0.00E+00	7.15E-09	6.70E-08
78.64	885.9	878.6	3.53E+02	1.50E+02	4.92E-03	4.92E-08	1.01E-08	0.00E+00	7.15E-09	6.65E-08
79.25	904.0	892.6	3.61E+02	1.47E+02	4.93E-03	4.78E-08	1.09E-08	0.00E+00	7.15E-09	6.59E-08
79.86	924.0	907.9	3.69E+02	1.43E+02	4.94E-03	4.63E-08	1.19E-08	0.00E+00	7.15E-09	6.53E-08
80.47	946.3	924.7	3.78E+02	1.40E+02	4.96E-03	4.45E-08	1.30E-08	0.00E+00	7.15E-09	6.46E-08
81.08	971.1	943.3	3.89E+02	1.36E+02	4.97E-03	4.26E-08	1.41E-08	0.00E+00	7.15E-09	6.39E-08
81.69	999.0	964.1	4.01E+02	1.32E+02	4.99E-03	4.04E-08	1.55E-08	0.00E+00	7.15E-09	6.30E-08
82.30	1030.6	987.3	4.14E+02	1.28E+02	5.00E-03	3.79E-08	1.70E-08	0.00E+00	7.15E-09	6.20E-08
82.91	1066.8	1013.6	4.29E+02	1.23E+02	5.02E-03	3.50E-08	1.87E-08	0.00E+00	7.15E-09	6.09E-08
83.52	1109.2	1043.6	4.47E+02	1.18E+02	5.05E-03	3.18E-08	2.06E-08	0.00E+00	7.15E-09	5.96E-08
84.12	1161.0	1078.6	4.69E+02	1.13E+02	5.08E-03	2.80E-08	2.28E-08	0.00E+00	7.15E-09	5.80E-08
84.73	1229.7	1121.1	4.99E+02	1.06E+02	5.11E-03	2.37E-08	2.53E-08	0.00E+00	7.15E-09	5.61E-08
85.34	1328.3	1176.2	5.41E+02	9.78E+01	5.15E-03	1.82E-08	2.80E-08	0.00E+00	7.15E-09	5.34E-08
85.95	1435.6	1247.8	5.87E+02	9.01E+01	5.20E-03	1.09E-08	3.10E-08	0.00E+00	7.15E-09	4.91E-08
86.56	1523.3	1330.2	6.24E+02	8.47E+01	5.26E-03	2.93E-09	3.35E-08	0.00E+00	7.15E-09	4.36E-08
87.17	1587.8	1417.8	6.52E+02	8.11E+01	5.28E-03	8.32E-11	3.40E-08	0.00E+00	7.15E-09	4.13E-08
87.78	1644.2	1492.6	6.76E+02	7.82E+01	5.28E-03	0.00E+00	3.36E-08	0.00E+00	7.15E-09	4.07E-08
88.39	1703.1	1557.1	7.01E+02	7.54E+01	5.28E-03	0.00E+00	3.31E-08	0.00E+00	7.15E-09	4.02E-08
89.00	1748.7	1613.3	7.20E+02	7.34E+01	5.28E-03	0.00E+00	3.25E-08	0.00E+00	7.15E-09	3.96E-08
89.61	1778.4	1658.1	7.32E+02	7.22E+01	5.28E-03	0.00E+00	3.18E-08	0.00E+00	7.15E-09	3.90E-08
90.22	1804.4	1692.0	7.43E+02	7.11E+01	5.28E-03	0.00E+00	3.12E-08	0.00E+00	7.15E-09	3.83E-08
90.83	1831.1	1721.4	7.54E+02	7.01E+01	5.28E-03	0.00E+00	3.05E-08	0.00E+00	7.15E-09	3.77E-08
91.44	1857.6	1747.7	7.65E+02	6.91E+01	5.28E-03	0.00E+00	2.99E-08	0.00E+00	7.15E-09	3.70E-08
92.05	1883.7	1772.2	7.76E+02	6.81E+01	5.28E-03	0.00E+00	2.92E-08	0.00E+00	7.15E-09	3.64E-08
92.66	1909.2	1795.6	7.86E+02	6.72E+01	5.28E-03	0.00E+00	2.86E-08	0.00E+00	7.15E-09	3.58E-08
93.27	1934.0	1818.1	7.96E+02	6.64E+01	5.28E-03	0.00E+00	2.80E-08	0.00E+00	7.15E-09	3.51E-08
93.88	1958.1	1839.7	8.06E+02	6.55E+01	5.28E-03	0.00E+00	2.74E-08	0.00E+00	7.15E-09	3.45E-08
94.49	1981.3	1860.6	8.16E+02	6.48E+01	5.28E-03	0.00E+00	2.68E-08	0.00E+00	7.15E-09	3.39E-08
95.10	2003.0	1880.5	8.25E+02	6.41E+01	5.28E-03	0.00E+00	2.62E-08	0.00E+00	7.15E-09	3.33E-08
95.71	2010.9	1896.4	8.28E+02	6.38E+01	5.28E-03	0.00E+00	2.56E-08	0.00E+00	7.15E-09	3.28E-08
96.32	2014.0	1905.5	8.30E+02	6.37E+01	5.28E-03	0.00E+00	2.50E-08	0.00E+00	7.15E-09	3.22E-08
96.93	2017.2	1911.0	8.31E+02	6.36E+01	5.28E-03	0.00E+00	2.44E-08	0.00E+00	7.15E-09	3.16E-08
97.54	2020.3	1914.9	8.32E+02	6.35E+01	5.28E-03	0.00E+00	2.39E-08	0.00E+00	7.15E-09	3.10E-08
98.15	2023.5	1918.1	8.33E+02	6.34E+01	5.28E-03	0.00E+00	2.33E-08	0.00E+00	7.15E-09	3.05E-08
98.76	2026.5	1921.0	8.35E+02	6.33E+01	5.28E-03	0.00E+00	2.27E-08	0.00E+00	7.15E-09	2.99E-08
99.36	2029.6	1923.7	8.36E+02	6.32E+01	5.28E-03	0.00E+00	2.22E-08	0.00E+00	7.15E-09	2.93E-08
99.97	2032.5	1926.3	8.37E+02	6.31E+01	5.28E-03	0.00E+00	2.16E-08	0.00E+00	7.15E-09	2.88E-08
100.58	2035.4	1928.8	8.38E+02	6.30E+01	5.28E-03	0.00E+00	2.11E-08	0.00E+00	7.15E-09	2.82E-08
101.19	2038.2	1931.2	8.40E+02	6.29E+01	5.28E-03	0.00E+00	2.05E-08	0.00E+00	7.15E-09	2.77E-08

101.80	2040.9	1933.6	8.41E+02	6.29E+01	5.28E-03	0.00E+00	2.00E-08	0.00E+00	7.15E-09	2.71E-08
102.41	2043.6	1935.9	8.42E+02	6.28E+01	5.28E-03	0.00E+00	1.95E-08	0.00E+00	7.15E-09	2.66E-08
103.02	2046.1	1938.1	8.43E+02	6.27E+01	5.28E-03	0.00E+00	1.89E-08	0.00E+00	7.15E-09	2.61E-08
103.63	2048.7	1957.7	8.44E+02	6.26E+01	5.28E-03	0.00E+00	1.84E-08	0.00E+00	7.15E-09	2.56E-08
104.24	2051.4	1959.6	8.45E+02	6.25E+01	5.28E-03	0.00E+00	1.79E-08	0.00E+00	7.15E-09	2.50E-08
104.85	2053.9	1961.6	8.46E+02	6.25E+01	5.28E-03	0.00E+00	1.74E-08	0.00E+00	7.15E-09	2.45E-08
105.46	2056.4	1963.4	8.47E+02	6.24E+01	5.28E-03	0.00E+00	1.68E-08	0.00E+00	7.15E-09	2.40E-08
106.07	2058.8	1965.2	8.48E+02	6.23E+01	5.28E-03	0.00E+00	1.63E-08	0.00E+00	7.15E-09	2.35E-08
106.68	2061.1	1966.9	8.49E+02	6.22E+01	5.28E-03	0.00E+00	1.58E-08	0.00E+00	7.15E-09	2.30E-08
107.29	2063.3	1968.6	8.50E+02	6.22E+01	5.28E-03	0.00E+00	1.53E-08	0.00E+00	7.15E-09	2.25E-08
107.90	2065.5	1970.2	8.51E+02	6.21E+01	5.28E-03	0.00E+00	1.48E-08	0.00E+00	7.15E-09	2.20E-08
108.51	2067.6	1971.7	8.52E+02	6.20E+01	5.28E-03	0.00E+00	1.43E-08	0.00E+00	7.15E-09	2.15E-08
109.12	2069.6	1973.2	8.53E+02	6.20E+01	5.28E-03	0.00E+00	1.38E-08	0.00E+00	7.15E-09	2.10E-08
109.73	2071.5	1974.7	8.53E+02	6.19E+01	5.28E-03	0.00E+00	1.33E-08	0.00E+00	7.15E-09	2.05E-08
110.34	2073.4	1976.0	8.54E+02	6.19E+01	5.28E-03	0.00E+00	1.29E-08	0.00E+00	7.15E-09	2.00E-08
110.95	2075.2	1977.4	8.55E+02	6.18E+01	5.28E-03	0.00E+00	1.24E-08	0.00E+00	7.15E-09	1.95E-08
111.56	2076.9	1978.6	8.56E+02	6.18E+01	5.28E-03	0.00E+00	1.19E-08	0.00E+00	7.15E-09	1.91E-08
112.17	2078.6	1979.8	8.56E+02	6.17E+01	5.28E-03	0.00E+00	1.15E-08	0.00E+00	7.15E-09	1.86E-08
112.78	2080.1	1981.0	8.57E+02	6.17E+01	5.28E-03	0.00E+00	1.10E-08	0.00E+00	7.15E-09	1.81E-08
113.39	2081.7	1982.1	8.58E+02	6.16E+01	5.28E-03	0.00E+00	1.05E-08	0.00E+00	7.15E-09	1.77E-08
114.00	2083.8	1983.7	8.59E+02	6.15E+01	5.28E-03	0.00E+00	9.89E-09	0.00E+00	7.15E-09	1.70E-08
114.60	2085.2	1984.6	8.59E+02	6.15E+01	5.28E-03	0.00E+00	9.44E-09	0.00E+00	7.15E-09	1.66E-08
115.21	2086.6	1985.6	8.60E+02	6.15E+01	5.28E-03	0.00E+00	9.00E-09	0.00E+00	7.15E-09	1.62E-08
115.82	2087.9	1986.5	8.60E+02	6.14E+01	5.28E-03	0.00E+00	8.57E-09	0.00E+00	7.15E-09	1.57E-08
116.43	2089.1	1987.4	8.61E+02	6.14E+01	5.28E-03	0.00E+00	8.14E-09	0.00E+00	7.15E-09	1.53E-08
117.04	2090.3	1988.2	8.61E+02	6.13E+01	5.28E-03	0.00E+00	7.71E-09	0.00E+00	7.15E-09	1.49E-08
117.65	2091.4	1988.9	8.62E+02	6.13E+01	5.28E-03	0.00E+00	7.29E-09	0.00E+00	7.15E-09	1.44E-08
118.26	2092.5	1989.6	8.62E+02	6.13E+01	5.28E-03	0.00E+00	6.87E-09	0.00E+00	7.15E-09	1.40E-08
118.87	2093.5	1990.5	8.63E+02	6.13E+01	5.28E-03	0.00E+00	6.45E-09	0.00E+00	7.15E-09	1.36E-08
119.48	2094.4	1991.1	8.63E+02	6.12E+01	5.28E-03	0.00E+00	6.04E-09	0.00E+00	7.15E-09	1.32E-08
120.09	2095.3	1991.7	8.64E+02	6.12E+01	5.28E-03	0.00E+00	5.64E-09	0.00E+00	7.15E-09	1.28E-08
120.70	2096.1	1992.2	8.64E+02	6.12E+01	5.28E-03	0.00E+00	5.23E-09	0.00E+00	7.15E-09	1.24E-08
121.31	2096.9	1992.7	8.64E+02	6.11E+01	5.28E-03	0.00E+00	4.84E-09	0.00E+00	7.15E-09	1.20E-08
121.92	2097.6	1993.3	8.65E+02	6.11E+01	5.28E-03	0.00E+00	4.44E-09	0.00E+00	7.15E-09	1.16E-08
122.53	2098.3	1993.7	8.65E+02	6.11E+01	5.28E-03	0.00E+00	4.05E-09	0.00E+00	7.15E-09	1.12E-08
123.14	2098.9	1994.1	8.65E+02	6.11E+01	5.28E-03	0.00E+00	3.66E-09	0.00E+00	7.15E-09	1.08E-08
123.75	2099.5	1994.4	8.65E+02	6.11E+01	5.28E-03	0.00E+00	3.28E-09	0.00E+00	7.15E-09	1.04E-08
124.36	2100.0	1994.7	8.66E+02	6.11E+01	5.28E-03	0.00E+00	2.90E-09	0.00E+00	7.15E-09	1.01E-08
124.97	2100.5	1995.0	8.66E+02	6.10E+01	5.28E-03	0.00E+00	2.53E-09	0.00E+00	7.15E-09	9.68E-09
125.58	2100.9	1995.3	8.66E+02	6.10E+01	5.28E-03	0.00E+00	2.16E-09	0.00E+00	7.15E-09	9.31E-09
126.19	2101.3	1995.5	8.66E+02	6.10E+01	5.28E-03	0.00E+00	1.79E-09	0.00E+00	7.15E-09	8.94E-09
126.80	2101.6	1995.6	8.66E+02	6.10E+01	5.28E-03	0.00E+00	1.43E-09	0.00E+00	7.15E-09	8.58E-09
127.41	2101.9	1995.7	8.66E+02	6.10E+01	5.28E-03	0.00E+00	1.07E-09	0.00E+00	7.15E-09	8.22E-09
128.02	2102.1	1995.8	8.66E+02	6.10E+01	5.28E-03	0.00E+00	7.11E-10	0.00E+00	7.15E-09	7.86E-09
128.63	2102.3	1995.9	8.67E+02	6.10E+01	5.28E-03	0.00E+00	3.58E-10	0.00E+00	7.15E-09	7.51E-09
129.24	2102.5	1996.5	8.67E+02	6.10E+01	5.28E-03	0.00E+00	8.85E-12	0.00E+00	7.15E-09	7.16E-09
129.84	2099.8	1985.2	8.66E+02	6.11E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
130.45	2097.2	1983.1	8.64E+02	6.11E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
131.06	2094.5	1981.0	8.63E+02	6.12E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
131.67	2091.9	1978.7	8.62E+02	6.13E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
132.28	2089.2	1976.7	8.61E+02	6.14E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
132.89	2086.6	1974.6	8.60E+02	6.14E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
133.50	2084.0	1972.5	8.59E+02	6.15E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
134.11	2081.4	1970.0	8.58E+02	6.16E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
134.72	2078.8	1968.0	8.57E+02	6.17E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
135.33	2076.2	1965.9	8.56E+02	6.18E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
135.94	2073.6	1963.9	8.55E+02	6.18E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
136.55	2071.0	1961.8	8.53E+02	6.19E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
137.16	2068.4	1959.4	8.52E+02	6.20E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
137.77	2065.9	1957.3	8.51E+02	6.21E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09

138.38	2063.3	1955.3	8.50E+02	6.22E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
138.99	2060.8	1953.3	8.49E+02	6.22E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
139.60	2058.2	1951.3	8.48E+02	6.23E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
140.21	2055.7	1948.8	8.47E+02	6.24E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
140.82	2053.1	1946.8	8.46E+02	6.25E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
141.43	2050.6	1944.8	8.45E+02	6.25E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
142.04	2048.1	1942.8	8.44E+02	6.26E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
142.65	2045.6	1940.9	8.43E+02	6.27E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
143.26	2043.1	1938.5	8.42E+02	6.28E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
143.87	2040.6	1936.5	8.41E+02	6.28E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
144.48	2038.1	1934.5	8.40E+02	6.29E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
145.08	2035.7	1932.5	8.39E+02	6.30E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
145.69	2033.2	1930.6	8.38E+02	6.31E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
146.30	2030.7	1928.2	8.37E+02	6.32E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
146.91	2028.3	1926.2	8.36E+02	6.32E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
147.52	2025.8	1924.3	8.35E+02	6.33E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
148.13	2023.4	1922.3	8.34E+02	6.34E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
148.74	2021.0	1920.4	8.33E+02	6.35E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
149.35	2018.6	1918.1	8.32E+02	6.35E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
149.96	2016.1	1916.1	8.31E+02	6.36E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
150.57	2013.7	1914.2	8.30E+02	6.37E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
151.18	2011.3	1912.3	8.29E+02	6.38E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
151.79	2008.9	1910.4	8.28E+02	6.38E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09
152.40	2006.6	1908.0	8.27E+02	6.39E+01	5.28E-03	0.00E+00	0.00E+00	0.00E+00	7.15E-09	7.15E-09

BYU -- ONE Dimensional Combustion Or Gasification model (1-DICOG) particle number 3

23-May-79

DISTANCE	GAS	PARTICLE	VELOCITY	PARTICLE	PARTICLE	COAL	CHAR	H2O	ASH	PART
(cm)	TEMP	TEMP	(cm/sec)	NO. DENS	DIA.	MASS	MASS	MASS	MASS	MASS
	(kelvin)	(kelvin)		(#/cc)	(cm)	(gr)	(gr)	(gr)	(gr)	(gr)

0.00	356.6	355.6	2.86E+03	5.97E+02	8.00E-03	3.05E-07	0.00E+00	1.08E-08	3.31E-08	3.49E-07
0.61	366.7	356.0	2.70E+03	4.39E+02	8.00E-03	3.05E-07	1.42E-16	9.62E-09	3.31E-08	3.48E-07
1.22	361.3	356.6	2.49E+03	3.46E+02	8.00E-03	3.05E-07	3.74E-16	7.69E-09	3.31E-08	3.46E-07
1.83	357.3	357.3	2.27E+03	2.88E+02	8.00E-03	3.05E-07	6.43E-16	5.47E-09	3.31E-08	3.44E-07
2.44	355.9	358.0	2.08E+03	2.47E+02	8.00E-03	3.05E-07	9.56E-16	2.90E-09	3.31E-08	3.41E-07
3.05	356.8	358.9	1.92E+03	2.16E+02	8.00E-03	3.05E-07	1.32E-15	3.32E-10	3.31E-08	3.38E-07
3.66	359.7	359.9	1.79E+03	1.91E+02	8.00E-03	3.05E-07	1.74E-15	0.00E+00	3.31E-08	3.3AE-07
4.27	363.3	360.9	1.68E+03	1.71E+02	8.00E-03	3.05E-07	2.22E-15	0.00E+00	3.31E-08	3.3AE-07
4.88	367.1	362.1	1.57E+03	1.55E+02	8.00E-03	3.05E-07	2.78E-15	0.00E+00	3.31E-08	3.38E-07
5.49	370.8	363.4	1.48E+03	1.42E+02	8.00E-03	3.05E-07	3.44E-15	0.00E+00	3.31E-08	3.38E-07
6.10	374.6	364.9	1.39E+03	1.31E+02	8.00E-03	3.05E-07	4.20E-15	0.00E+00	3.31E-08	3.38E-07
6.71	378.1	366.5	1.32E+03	1.22E+02	8.00E-03	3.05E-07	5.09E-15	0.00E+00	3.31E-08	3.38E-07
7.32	381.6	368.2	1.25E+03	1.14E+02	8.00E-03	3.05E-07	6.15E-15	0.00E+00	3.31E-08	3.38E-07
7.92	384.9	370.0	1.18E+03	1.07E+02	8.00E-03	3.05E-07	7.41E-15	0.00E+00	3.31E-08	3.38E-07
8.53	388.1	372.0	1.12E+03	1.01E+02	8.00E-03	3.05E-07	8.92E-15	0.00E+00	3.31E-08	3.38E-07
9.14	391.2	374.1	1.07E+03	9.58E+01	8.00E-03	3.05E-07	1.07E-14	0.00E+00	3.31E-08	3.38E-07
9.75	394.1	376.4	1.02E+03	9.12E+01	8.00E-03	3.05E-07	1.29E-14	0.00E+00	3.31E-08	3.3AE-07
10.36	397.0	378.7	9.70E+02	8.71E+01	8.00E-03	3.05E-07	1.56E-14	0.00E+00	3.31E-08	3.38E-07
10.97	399.8	381.3	9.26E+02	8.34E+01	8.00E-03	3.05E-07	1.88E-14	0.00E+00	3.31E-08	3.3AE-07
11.58	402.5	383.9	8.84E+02	8.01E+01	8.00E-03	3.05E-07	2.28E-14	0.00E+00	3.31E-08	3.38E-07
12.19	405.2	386.7	8.46E+02	7.72E+01	8.00E-03	3.05E-07	2.77E-14	0.00E+00	3.31E-08	3.38E-07
12.80	407.7	389.7	8.09E+02	7.46E+01	8.00E-03	3.05E-07	3.38E-14	0.00E+00	3.31E-08	3.3AE-07
13.41	410.3	392.7	7.75E+02	7.22E+01	8.00E-03	3.05E-07	4.14E-14	0.00E+00	3.31E-08	3.38E-07
14.02	412.8	395.9	7.43E+02	7.00E+01	8.00E-03	3.05E-07	5.09E-14	0.00E+00	3.31E-08	3.38E-07
14.63	415.2	399.2	7.13E+02	6.80E+01	8.00E-03	3.05E-07	6.29E-14	0.00E+00	3.31E-08	3.38E-07
15.24	417.7	402.7	6.84E+02	6.62E+01	8.00E-03	3.05E-07	7.79E-14	0.00E+00	3.31E-08	3.38E-07
15.85	420.1	406.2	6.57E+02	6.45E+01	8.00E-03	3.05E-07	9.68E-14	0.00E+00	3.31E-08	3.38E-07
16.46	422.5	409.9	6.31E+02	6.30E+01	8.00E-03	3.05E-07	1.21E-13	0.00E+00	3.31E-08	3.38E-07
17.07	424.9	413.7	6.07E+02	6.16E+01	8.00E-03	3.05E-07	1.51E-13	0.00E+00	3.31E-08	3.38E-07
17.68	427.3	417.5	5.84E+02	6.03E+01	8.00E-03	3.05E-07	1.90E-13	0.00E+00	3.31E-08	3.38E-07
18.29	429.8	421.5	5.62E+02	5.91E+01	8.00E-03	3.05E-07	2.38E-13	0.00E+00	3.31E-08	3.38E-07
18.90	432.2	425.6	5.41E+02	5.80E+01	8.00E-03	3.05E-07	3.01E-13	0.00E+00	3.31E-08	3.38E-07
19.51	434.7	429.8	5.21E+02	5.71E+01	8.00E-03	3.05E-07	3.80E-13	0.00E+00	3.31E-08	3.38E-07
20.12	437.1	434.1	5.01E+02	5.61E+01	8.00E-03	3.05E-07	4.80E-13	0.00E+00	3.31E-08	3.38E-07
20.73	439.7	438.4	4.83E+02	5.53E+01	8.00E-03	3.05E-07	6.08E-13	0.00E+00	3.31E-08	3.38E-07
21.34	442.2	442.9	4.66E+02	5.45E+01	8.00E-03	3.05E-07	7.71E-13	0.00E+00	3.31E-08	3.38E-07
21.95	444.9	447.4	4.49E+02	5.38E+01	8.00E-03	3.05E-07	9.77E-13	0.00E+00	3.31E-08	3.38E-07
22.56	447.5	451.9	4.33E+02	5.32E+01	8.00E-03	3.05E-07	1.24E-12	0.00E+00	3.31E-08	3.38E-07
23.16	450.3	456.6	4.18E+02	5.26E+01	8.00E-03	3.05E-07	1.57E-12	0.00E+00	3.31E-08	3.38E-07
23.77	453.1	461.3	4.03E+02	5.21E+01	8.00E-03	3.05E-07	1.99E-12	0.00E+00	3.31E-08	3.38E-07
24.38	456.0	466.1	3.89E+02	5.16E+01	8.00E-03	3.05E-07	2.52E-12	0.00E+00	3.31E-08	3.38E-07
24.99	459.0	470.9	3.75E+02	5.11E+01	8.00E-03	3.05E-07	3.19E-12	0.00E+00	3.31E-08	3.38E-07
25.60	462.0	475.8	3.62E+02	5.07E+01	8.00E-03	3.05E-07	4.03E-12	0.00E+00	3.31E-08	3.38E-07
26.21	465.2	480.7	3.50E+02	5.04E+01	8.00E-03	3.05E-07	5.09E-12	0.00E+00	3.31E-08	3.38E-07
26.82	468.5	485.7	3.37E+02	5.01E+01	8.00E-03	3.05E-07	6.41E-12	0.00E+00	3.31E-08	3.38E-07
27.43	471.9	490.8	3.26E+02	4.98E+01	8.00E-03	3.05E-07	8.07E-12	0.00E+00	3.31E-08	3.38E-07
28.04	475.5	495.9	3.15E+02	4.96E+01	8.00E-03	3.05E-07	1.01E-11	0.00E+00	3.31E-08	3.38E-07

28.65	479.2	501.0	3.04E+02	4.94E+01	8.00E-03	3.05E-07	1.27E-11	0.00E+00	3.31E-08	3.38E-07
29.26	483.1	506.3	2.93E+02	4.92E+01	8.00E-03	3.05E-07	1.59E-11	0.00E+00	3.31E-08	3.38E-07
29.87	487.2	511.6	2.83E+02	4.91E+01	8.00E-03	3.05E-07	1.99E-11	0.00E+00	3.31E-08	3.38E-07
30.48	491.5	516.9	2.73E+02	4.90E+01	8.00E-03	3.05E-07	2.48E-11	0.00E+00	3.31E-08	3.38E-07
31.09	496.0	522.4	2.64E+02	4.90E+01	8.00E-03	3.05E-07	3.10E-11	0.00E+00	3.31E-08	3.38E-07
31.70	500.7	527.9	2.55E+02	4.90E+01	8.00E-03	3.05E-07	3.85E-11	0.00E+00	3.31E-08	3.38E-07
32.31	505.7	533.5	2.46E+02	4.90E+01	8.00E-03	3.05E-07	4.79E-11	0.00E+00	3.31E-08	3.38E-07
32.92	511.0	539.3	2.37E+02	4.91E+01	8.00E-03	3.05E-07	5.95E-11	0.00E+00	3.31E-08	3.38E-07
33.53	516.7	545.2	2.29E+02	4.91E+01	8.00E-03	3.05E-07	7.39E-11	0.00E+00	3.31E-08	3.38E-07
34.14	522.7	551.3	2.21E+02	4.93E+01	8.00E-03	3.05E-07	9.17E-11	0.00E+00	3.31E-08	3.38E-07
34.75	529.1	557.6	2.13E+02	4.94E+01	8.00E-03	3.05E-07	1.14E-10	0.00E+00	3.31E-08	3.38E-07
35.36	534.4	564.0	2.11E+02	4.95E+01	8.00E-03	3.05E-07	1.41E-10	0.00E+00	3.31E-08	3.38E-07
35.97	537.0	570.1	2.12E+02	4.93E+01	8.00E-03	3.05E-07	1.74E-10	0.00E+00	3.31E-08	3.38E-07
36.58	539.6	575.7	2.13E+02	4.90E+01	8.00E-03	3.05E-07	2.12E-10	0.00E+00	3.31E-08	3.38E-07
37.19	542.1	580.9	2.14E+02	4.88E+01	8.00E-03	3.05E-07	2.56E-10	0.00E+00	3.31E-08	3.38E-07
37.80	544.7	585.7	2.15E+02	4.86E+01	8.00E-03	3.04E-07	3.06E-10	0.00E+00	3.31E-08	3.38E-07
38.40	547.4	590.2	2.16E+02	4.83E+01	8.00E-03	3.04E-07	3.62E-10	0.00E+00	3.31E-08	3.38E-07
39.01	550.0	594.5	2.17E+02	4.81E+01	8.00E-03	3.04E-07	4.24E-10	0.00E+00	3.31E-08	3.38E-07
39.62	552.7	598.5	2.18E+02	4.79E+01	8.00E-03	3.04E-07	4.92E-10	0.00E+00	3.31E-08	3.38E-07
40.23	555.4	602.3	2.19E+02	4.76E+01	8.00E-03	3.04E-07	5.68E-10	0.00E+00	3.31E-08	3.38E-07
40.84	558.1	606.0	2.20E+02	4.74E+01	8.00E-03	3.04E-07	6.49E-10	0.00E+00	3.31E-08	3.38E-07
41.45	560.9	609.5	2.21E+02	4.72E+01	8.00E-03	3.04E-07	7.38E-10	0.00E+00	3.31E-08	3.38E-07
42.06	563.6	612.9	2.22E+02	4.69E+01	8.00E-03	3.04E-07	8.34E-10	0.00E+00	3.31E-08	3.38E-07
42.67	566.4	616.1	2.23E+02	4.67E+01	8.00E-03	3.03E-07	9.37E-10	0.00E+00	3.31E-08	3.38E-07
43.28	569.1	619.3	2.24E+02	4.65E+01	8.00E-03	3.03E-07	1.05E-09	0.00E+00	3.31E-08	3.37E-07
43.89	571.9	622.4	2.26E+02	4.62E+01	8.01E-03	3.03E-07	1.17E-09	0.00E+00	3.31E-08	3.37E-07
44.50	574.7	625.5	2.27E+02	4.60E+01	8.01E-03	3.03E-07	1.29E-09	0.00E+00	3.31E-08	3.37E-07
45.11	577.6	628.4	2.28E+02	4.58E+01	8.01E-03	3.03E-07	1.43E-09	0.00E+00	3.31E-08	3.37E-07
45.72	580.4	631.4	2.29E+02	4.56E+01	8.01E-03	3.02E-07	1.57E-09	0.00E+00	3.31E-08	3.37E-07
46.33	583.3	634.3	2.30E+02	4.53E+01	8.01E-03	3.02E-07	1.72E-09	0.00E+00	3.31E-08	3.37E-07
46.94	586.2	637.1	2.31E+02	4.51E+01	8.01E-03	3.02E-07	1.88E-09	0.00E+00	3.31E-08	3.37E-07
47.55	589.1	640.0	2.32E+02	4.49E+01	8.01E-03	3.02E-07	2.05E-09	0.00E+00	3.31E-08	3.37E-07
48.16	592.0	642.8	2.33E+02	4.47E+01	8.01E-03	3.01E-07	2.23E-09	0.00E+00	3.31E-08	3.37E-07
48.77	595.0	645.6	2.35E+02	4.44E+01	8.01E-03	3.01E-07	2.42E-09	0.00E+00	3.31E-08	3.37E-07
49.38	597.9	648.4	2.36E+02	4.42E+01	8.01E-03	3.01E-07	2.62E-09	0.00E+00	3.31E-08	3.36E-07
49.99	601.0	651.2	2.37E+02	4.40E+01	8.01E-03	3.00E-07	2.83E-09	0.00E+00	3.31E-08	3.36E-07
50.60	604.0	654.0	2.38E+02	4.38E+01	8.01E-03	3.00E-07	3.05E-09	0.00E+00	3.31E-08	3.36E-07
51.21	607.1	656.8	2.39E+02	4.36E+01	8.01E-03	3.00E-07	3.28E-09	0.00E+00	3.31E-08	3.36E-07
51.82	610.2	659.6	2.41E+02	4.33E+01	8.02E-03	2.99E-07	3.53E-09	0.00E+00	3.31E-08	3.36E-07
52.43	613.3	662.4	2.42E+02	4.31E+01	8.02E-03	2.99E-07	3.79E-09	0.00E+00	3.31E-08	3.36E-07
53.04	616.5	665.3	2.43E+02	4.29E+01	8.02E-03	2.98E-07	4.06E-09	0.00E+00	3.31E-08	3.36E-07
53.64	619.7	668.1	2.45E+02	4.27E+01	8.02E-03	2.98E-07	4.34E-09	0.00E+00	3.31E-08	3.35E-07
54.25	623.0	671.0	2.46E+02	4.24E+01	8.02E-03	2.97E-07	4.64E-09	0.00E+00	3.31E-08	3.35E-07
54.86	626.3	673.8	2.47E+02	4.22E+01	8.02E-03	2.97E-07	4.96E-09	0.00E+00	3.31E-08	3.35E-07
55.47	629.6	676.8	2.48E+02	4.20E+01	8.02E-03	2.96E-07	5.29E-09	0.00E+00	3.31E-08	3.35E-07
56.08	633.0	679.7	2.50E+02	4.17E+01	8.02E-03	2.96E-07	5.64E-09	0.00E+00	3.31E-08	3.34E-07
56.69	636.5	682.7	2.51E+02	4.15E+01	8.03E-03	2.95E-07	6.00E-09	0.00E+00	3.31E-08	3.34E-07
57.30	640.0	685.7	2.53E+02	4.13E+01	8.03E-03	2.95E-07	6.39E-09	0.00E+00	3.31E-08	3.34E-07
57.91	643.6	688.7	2.54E+02	4.11E+01	8.03E-03	2.94E-07	6.79E-09	0.00E+00	3.31E-08	3.34E-07
58.52	647.3	691.8	2.56E+02	4.08E+01	8.03E-03	2.93E-07	7.22E-09	0.00E+00	3.31E-08	3.33E-07
59.13	651.0	694.9	2.57E+02	4.06E+01	8.03E-03	2.92E-07	7.66E-09	0.00E+00	3.31E-08	3.33E-07
59.74	654.8	698.0	2.59E+02	4.03E+01	8.03E-03	2.92E-07	8.13E-09	0.00E+00	3.31E-08	3.33E-07
60.35	658.7	701.3	2.60E+02	4.01E+01	8.04E-03	2.91E-07	8.62E-09	0.00E+00	3.31E-08	3.33E-07
60.96	662.6	704.5	2.62E+02	3.99E+01	8.04E-03	2.90E-07	9.13E-09	0.00E+00	3.31E-08	3.32E-07
61.57	666.7	707.8	2.63E+02	3.96E+01	8.04E-03	2.89E-07	9.68E-09	0.00E+00	3.31E-08	3.32E-07
62.18	670.9	711.2	2.65E+02	3.94E+01	8.04E-03	2.88E-07	1.02E-08	0.00E+00	3.31E-08	3.32E-07
62.79	675.2	714.7	2.67E+02	3.91E+01	8.05E-03	2.87E-07	1.08E-08	0.00E+00	3.31E-08	3.31E-07
63.40	679.5	718.2	2.68E+02	3.88E+01	8.05E-03	2.86E-07	1.15E-08	0.00E+00	3.31E-08	3.31E-07
64.01	684.1	721.8	2.70E+02	3.86E+01	8.05E-03	2.85E-07	1.21E-08	0.00E+00	3.31E-08	3.30E-07
64.62	688.7	725.4	2.72E+02	3.83E+01	8.06E-03	2.84E-07	1.28E-08	0.00E+00	3.31E-08	3.30E-07

65.23	693.5	729.2	2.74E+02	3.80E+01	8.06E-03	2.83E-07	1.36E-08	0.00E+00	3.31E-08	3.29E-07
65.84	698.5	733.0	2.76E+02	3.78E+01	8.06E-03	2.81E-07	1.43E-08	0.00E+00	3.31E-08	3.29E-07
66.45	703.6	737.0	2.78E+02	3.75E+01	8.07E-03	2.80E-07	1.52E-08	0.00E+00	3.31E-08	3.28E-07
67.06	708.9	741.0	2.80E+02	3.72E+01	8.07E-03	2.79E-07	1.60E-08	0.00E+00	3.31E-08	3.28E-07
67.67	714.5	745.2	2.83E+02	3.69E+01	8.07E-03	2.77E-07	1.69E-08	0.00E+00	3.31E-08	3.27E-07
68.28	720.2	749.5	2.85E+02	3.66E+01	8.08E-03	2.76E-07	1.79E-08	0.00E+00	3.31E-08	3.27E-07
68.88	726.2	753.9	2.87E+02	3.63E+01	8.08E-03	2.74E-07	1.89E-08	0.00E+00	3.31E-08	3.26E-07
69.49	732.4	758.5	2.90E+02	3.60E+01	8.09E-03	2.72E-07	1.99E-08	0.00E+00	3.31E-08	3.25E-07
70.10	739.0	763.3	2.93E+02	3.56E+01	8.09E-03	2.70E-07	2.11E-08	0.00E+00	3.31E-08	3.25E-07
70.71	745.8	768.2	2.95E+02	3.53E+01	8.10E-03	2.68E-07	2.23E-08	0.00E+00	3.31E-08	3.24E-07
71.32	753.0	773.3	2.98E+02	3.50E+01	8.10E-03	2.66E-07	2.35E-08	0.00E+00	3.31E-08	3.23E-07
71.93	760.6	778.6	3.01E+02	3.46E+01	8.11E-03	2.64E-07	2.49E-08	0.00E+00	3.31E-08	3.22E-07
72.54	768.6	784.2	3.05E+02	3.42E+01	8.11E-03	2.62E-07	2.63E-08	0.00E+00	3.31E-08	3.21E-07
73.15	777.1	790.0	3.08E+02	3.38E+01	8.12E-03	2.59E-07	2.78E-08	0.00E+00	3.31E-08	3.20E-07
73.76	786.1	796.1	3.12E+02	3.34E+01	8.13E-03	2.57E-07	2.94E-08	0.00E+00	3.31E-08	3.19E-07
74.37	794.9	801.9	3.15E+02	3.31E+01	8.13E-03	2.54E-07	3.10E-08	0.00E+00	3.31E-08	3.18E-07
74.98	805.1	808.6	3.20E+02	3.26E+01	8.14E-03	2.51E-07	3.28E-08	0.00E+00	3.31E-08	3.17E-07
75.59	816.0	815.7	3.24E+02	3.22E+01	8.15E-03	2.48E-07	3.48E-08	0.00E+00	3.31E-08	3.16E-07
76.20	827.8	823.2	3.29E+02	3.17E+01	8.16E-03	2.45E-07	3.69E-08	0.00E+00	3.31E-08	3.15E-07
76.81	840.5	831.2	3.34E+02	3.12E+01	8.17E-03	2.41E-07	3.91E-08	0.00E+00	3.31E-08	3.13E-07
77.42	854.3	839.7	3.40E+02	3.07E+01	8.18E-03	2.37E-07	4.16E-08	0.00E+00	3.31E-08	3.12E-07
78.03	869.4	848.8	3.46E+02	3.01E+01	8.19E-03	2.33E-07	4.42E-08	0.00E+00	3.31E-08	3.10E-07
78.64	885.9	858.5	3.53E+02	2.95E+01	8.20E-03	2.28E-07	4.70E-08	0.00E+00	3.31E-08	3.08E-07
79.25	904.0	869.1	3.61E+02	2.89E+01	8.22E-03	2.23E-07	5.01E-08	0.00E+00	3.31E-08	3.06E-07
79.86	924.0	880.5	3.69E+02	2.83E+01	8.23E-03	2.17E-07	5.34E-08	0.00E+00	3.31E-08	3.04E-07
80.47	946.3	893.0	3.78E+02	2.76E+01	8.25E-03	2.12E-07	5.70E-08	0.00E+00	3.31E-08	3.02E-07
81.08	971.1	906.6	3.89E+02	2.68E+01	8.26E-03	2.05E-07	6.10E-08	0.00E+00	3.31E-08	2.99E-07
81.69	999.0	921.5	4.01E+02	2.60E+01	8.28E-03	1.98E-07	6.53E-08	0.00E+00	3.31E-08	2.96E-07
82.30	1030.6	938.1	4.14E+02	2.52E+01	8.30E-03	1.90E-07	7.01E-08	0.00E+00	3.31E-08	2.93E-07
82.91	1066.8	956.5	4.29E+02	2.43E+01	8.32E-03	1.81E-07	7.54E-08	0.00E+00	3.31E-08	2.90E-07
83.52	1109.2	977.1	4.47E+02	2.33E+01	8.35E-03	1.72E-07	8.12E-08	0.00E+00	3.31E-08	2.86E-07
84.12	1161.0	1000.6	4.69E+02	2.22E+01	8.38E-03	1.61E-07	8.77E-08	0.00E+00	3.31E-08	2.82E-07
84.73	1229.7	1028.0	4.99E+02	2.09E+01	8.41E-03	1.49E-07	9.48E-08	0.00E+00	3.31E-08	2.77E-07
85.34	1328.3	1061.4	5.41E+02	1.93E+01	8.44E-03	1.36E-07	1.03E-07	0.00E+00	3.31E-08	2.71E-07
85.95	1435.6	1102.6	5.87E+02	1.78E+01	8.49E-03	1.20E-07	1.12E-07	0.00E+00	3.31E-08	2.65E-07
86.56	1523.3	1149.3	6.24E+02	1.67E+01	8.54E-03	1.00E-07	1.22E-07	0.00E+00	3.31E-08	2.55E-07
87.17	1587.8	1198.0	6.52E+02	1.60E+01	8.60E-03	7.55E-08	1.34E-07	0.00E+00	3.31E-08	2.42E-07
87.78	1644.2	1246.8	6.76E+02	1.54E+01	8.68E-03	4.59E-08	1.46E-07	0.00E+00	3.31E-08	2.25E-07
88.39	1703.1	1299.2	7.01E+02	1.49E+01	8.75E-03	1.80E-08	1.55E-07	0.00E+00	3.31E-08	2.06E-07
89.00	1748.7	1360.2	7.20E+02	1.45E+01	8.79E-03	2.63E-09	1.59E-07	0.00E+00	3.31E-08	1.95E-07
89.61	1778.4	1424.7	7.32E+02	1.42E+01	8.80E-03	3.93E-11	1.59E-07	0.00E+00	3.31E-08	1.92E-07
90.22	1804.4	1481.0	7.43E+02	1.40E+01	8.80E-03	0.00E+00	1.58E-07	0.00E+00	3.31E-08	1.92E-07
90.83	1831.1	1531.7	7.54E+02	1.38E+01	8.80E-03	0.00E+00	1.58E-07	0.00E+00	3.31E-08	1.91E-07
91.44	1857.6	1576.3	7.65E+02	1.36E+01	8.80E-03	0.00E+00	1.57E-07	0.00E+00	3.31E-08	1.90E-07
92.05	1883.7	1616.1	7.76E+02	1.34E+01	8.80E-03	0.00E+00	1.55E-07	0.00E+00	3.31E-08	1.89E-07
92.66	1909.2	1651.8	7.86E+02	1.33E+01	8.80E-03	0.00E+00	1.54E-07	0.00E+00	3.31E-08	1.87E-07
93.27	1934.0	1684.1	7.96E+02	1.31E+01	8.80E-03	0.00E+00	1.53E-07	0.00E+00	3.31E-08	1.86E-07
93.88	1958.1	1713.7	8.06E+02	1.29E+01	8.80E-03	0.00E+00	1.52E-07	0.00E+00	3.31E-08	1.85E-07
94.49	1981.3	1740.9	8.16E+02	1.28E+01	8.80E-03	0.00E+00	1.51E-07	0.00E+00	3.31E-08	1.84E-07
95.10	2003.0	1766.1	8.25E+02	1.26E+01	8.80E-03	0.00E+00	1.50E-07	0.00E+00	3.31E-08	1.83E-07
95.71	2010.9	1788.2	8.28E+02	1.26E+01	8.80E-03	0.00E+00	1.49E-07	0.00E+00	3.31E-08	1.82E-07
96.32	2014.0	1806.2	8.30E+02	1.26E+01	8.80E-03	0.00E+00	1.48E-07	0.00E+00	3.31E-08	1.81E-07
96.93	2017.2	1820.6	8.31E+02	1.26E+01	8.80E-03	0.00E+00	1.47E-07	0.00E+00	3.31E-08	1.80E-07
97.54	2020.3	1832.3	8.32E+02	1.25E+01	8.80E-03	0.00E+00	1.45E-07	0.00E+00	3.31E-08	1.78E-07
98.15	2023.5	1841.8	8.33E+02	1.25E+01	8.80E-03	0.00E+00	1.44E-07	0.00E+00	3.31E-08	1.77E-07
98.76	2026.5	1849.6	8.35E+02	1.25E+01	8.80E-03	0.00E+00	1.43E-07	0.00E+00	3.31E-08	1.76E-07
99.36	2029.6	1856.2	8.36E+02	1.25E+01	8.80E-03	0.00E+00	1.42E-07	0.00E+00	3.31E-08	1.75E-07
99.97	2032.5	1861.7	8.37E+02	1.25E+01	8.80E-03	0.00E+00	1.41E-07	0.00E+00	3.31E-08	1.74E-07
100.58	2035.4	1866.5	8.38E+02	1.24E+01	8.80E-03	0.00E+00	1.40E-07	0.00E+00	3.31E-08	1.73E-07
101.19	2038.2	1870.6	8.40E+02	1.24E+01	8.80E-03	0.00E+00	1.39E-07	0.00E+00	3.31E-08	1.72E-07

101.80	2040.9	1874.2	8.41E+02	1.24E+01	8.80E-03	0.00E+00	1.36E-07	0.00E+00	3.31E-08	1.71E-07
102.41	2043.6	1877.5	8.42E+02	1.24E+01	8.80E-03	0.00E+00	1.37E-07	0.00E+00	3.31E-08	1.70E-07
103.02	2046.1	1880.4	8.43E+02	1.24E+01	8.80E-03	0.00E+00	1.35E-07	0.00E+00	3.31E-08	1.69E-07
103.63	2048.7	1883.2	8.44E+02	1.24E+01	8.80E-03	0.00E+00	1.34E-07	0.00E+00	3.31E-08	1.68E-07
104.24	2051.4	1885.7	8.45E+02	1.23E+01	8.80E-03	0.00E+00	1.33E-07	0.00E+00	3.31E-08	1.66E-07
104.85	2053.9	1888.1	8.46E+02	1.23E+01	8.80E-03	0.00E+00	1.32E-07	0.00E+00	3.31E-08	1.65E-07
105.46	2056.4	1890.4	8.47E+02	1.23E+01	8.80E-03	0.00E+00	1.31E-07	0.00E+00	3.31E-08	1.64E-07
106.07	2058.8	1892.6	8.48E+02	1.23E+01	8.80E-03	0.00E+00	1.30E-07	0.00E+00	3.31E-08	1.63E-07
106.68	2061.1	1894.7	8.49E+02	1.23E+01	8.80E-03	0.00E+00	1.29E-07	0.00E+00	3.31E-08	1.62E-07
107.29	2063.3	1896.7	8.50E+02	1.23E+01	8.80E-03	0.00E+00	1.28E-07	0.00E+00	3.31E-08	1.61E-07
107.90	2065.5	1898.6	8.51E+02	1.23E+01	8.80E-03	0.00E+00	1.27E-07	0.00E+00	3.31E-08	1.60E-07
108.51	2067.6	1900.4	8.52E+02	1.22E+01	8.80E-03	0.00E+00	1.26E-07	0.00E+00	3.31E-08	1.59E-07
109.12	2069.6	1902.2	8.53E+02	1.22E+01	8.80E-03	0.00E+00	1.25E-07	0.00E+00	3.31E-08	1.58E-07
109.73	2071.5	1903.9	8.53E+02	1.22E+01	8.80E-03	0.00E+00	1.24E-07	0.00E+00	3.31E-08	1.57E-07
110.34	2073.4	1905.6	8.54E+02	1.22E+01	8.80E-03	0.00E+00	1.23E-07	0.00E+00	3.31E-08	1.56E-07
110.95	2075.2	1907.1	8.55E+02	1.22E+01	8.80E-03	0.00E+00	1.22E-07	0.00E+00	3.31E-08	1.56E-07
111.56	2076.9	1908.6	8.56E+02	1.22E+01	8.80E-03	0.00E+00	1.21E-07	0.00E+00	3.31E-08	1.55E-07
112.17	2078.6	1910.1	8.56E+02	1.22E+01	8.80E-03	0.00E+00	1.21E-07	0.00E+00	3.31E-08	1.54E-07
112.78	2080.1	1911.5	8.57E+02	1.22E+01	8.80E-03	0.00E+00	1.20E-07	0.00E+00	3.31E-08	1.53E-07
113.39	2081.7	1912.8	8.58E+02	1.22E+01	8.80E-03	0.00E+00	1.19E-07	0.00E+00	3.31E-08	1.52E-07
114.00	2083.8	1933.0	8.59E+02	1.21E+01	8.80E-03	0.00E+00	1.17E-07	0.00E+00	3.31E-08	1.50E-07
114.60	2085.2	1933.8	8.59E+02	1.21E+01	8.80E-03	0.00E+00	1.16E-07	0.00E+00	3.31E-08	1.50E-07
115.21	2086.6	1934.6	8.60E+02	1.21E+01	8.80E-03	0.00E+00	1.16E-07	0.00E+00	3.31E-08	1.49E-07
115.82	2087.9	1935.5	8.60E+02	1.21E+01	8.80E-03	0.00E+00	1.15E-07	0.00E+00	3.31E-08	1.48E-07
116.43	2089.1	1936.2	8.61E+02	1.21E+01	8.80E-03	0.00E+00	1.14E-07	0.00E+00	3.31E-08	1.47E-07
117.04	2090.3	1936.9	8.61E+02	1.21E+01	8.80E-03	0.00E+00	1.13E-07	0.00E+00	3.31E-08	1.46E-07
117.65	2091.4	1937.6	8.62E+02	1.21E+01	8.80E-03	0.00E+00	1.12E-07	0.00E+00	3.31E-08	1.45E-07
118.26	2092.5	1938.2	8.62E+02	1.21E+01	8.80E-03	0.00E+00	1.11E-07	0.00E+00	3.31E-08	1.44E-07
118.87	2093.5	1938.9	8.63E+02	1.21E+01	8.80E-03	0.00E+00	1.10E-07	0.00E+00	3.31E-08	1.44E-07
119.48	2094.4	1939.5	8.63E+02	1.21E+01	8.80E-03	0.00E+00	1.10E-07	0.00E+00	3.31E-08	1.43E-07
120.09	2095.3	1940.0	8.64E+02	1.21E+01	8.80E-03	0.00E+00	1.09E-07	0.00E+00	3.31E-08	1.42E-07
120.70	2096.1	1940.4	8.64E+02	1.21E+01	8.80E-03	0.00E+00	1.08E-07	0.00E+00	3.31E-08	1.41E-07
121.31	2096.9	1940.8	8.64E+02	1.21E+01	8.80E-03	0.00E+00	1.07E-07	0.00E+00	3.31E-08	1.40E-07
121.92	2097.6	1941.4	8.65E+02	1.21E+01	8.80E-03	0.00E+00	1.06E-07	0.00E+00	3.31E-08	1.39E-07
122.53	2098.3	1941.7	8.65E+02	1.21E+01	8.80E-03	0.00E+00	1.06E-07	0.00E+00	3.31E-08	1.39E-07
123.14	2098.9	1942.0	8.65E+02	1.21E+01	8.80E-03	0.00E+00	1.05E-07	0.00E+00	3.31E-08	1.38E-07
123.75	2099.5	1942.3	8.65E+02	1.21E+01	8.80E-03	0.00E+00	1.04E-07	0.00E+00	3.31E-08	1.37E-07
124.36	2100.0	1942.5	8.66E+02	1.20E+01	8.80E-03	0.00E+00	1.03E-07	0.00E+00	3.31E-08	1.36E-07
124.97	2100.5	1942.8	8.66E+02	1.20E+01	8.80E-03	0.00E+00	1.02E-07	0.00E+00	3.31E-08	1.36E-07
125.58	2100.9	1943.0	8.66E+02	1.20E+01	8.80E-03	0.00E+00	1.02E-07	0.00E+00	3.31E-08	1.35E-07
126.19	2101.3	1943.2	8.66E+02	1.20E+01	8.80E-03	0.00E+00	1.01E-07	0.00E+00	3.31E-08	1.34E-07
126.80	2101.6	1943.3	8.66E+02	1.20E+01	8.80E-03	0.00E+00	1.00E-07	0.00E+00	3.31E-08	1.33E-07
127.41	2101.9	1943.4	8.66E+02	1.20E+01	8.80E-03	0.00E+00	9.95E-08	0.00E+00	3.31E-08	1.33E-07
128.02	2102.1	1943.5	8.66E+02	1.20E+01	8.80E-03	0.00E+00	9.87E-08	0.00E+00	3.31E-08	1.32E-07
128.63	2102.3	1943.5	8.67E+02	1.20E+01	8.80E-03	0.00E+00	9.80E-08	0.00E+00	3.31E-08	1.31E-07
129.24	2102.5	1943.6	8.67E+02	1.20E+01	8.80E-03	0.00E+00	9.73E-08	0.00E+00	3.31E-08	1.30E-07
129.84	2099.8	1941.6	8.66E+02	1.20E+01	8.80E-03	0.00E+00	9.66E-08	0.00E+00	3.31E-08	1.30E-07
130.45	2097.2	1939.8	8.64E+02	1.21E+01	8.80E-03	0.00E+00	9.59E-08	0.00E+00	3.31E-08	1.29E-07
131.06	2094.5	1937.9	8.63E+02	1.21E+01	8.80E-03	0.00E+00	9.52E-08	0.00E+00	3.31E-08	1.28E-07
131.67	2091.9	1935.8	8.62E+02	1.21E+01	8.80E-03	0.00E+00	9.45E-08	0.00E+00	3.31E-08	1.28E-07
132.28	2089.2	1933.9	8.61E+02	1.21E+01	8.80E-03	0.00E+00	9.38E-08	0.00E+00	3.31E-08	1.27E-07
132.89	2086.6	1932.0	8.60E+02	1.21E+01	8.80E-03	0.00E+00	9.31E-08	0.00E+00	3.31E-08	1.26E-07
133.50	2084.0	1930.3	8.59E+02	1.21E+01	8.80E-03	0.00E+00	9.24E-08	0.00E+00	3.31E-08	1.26E-07
134.11	2081.4	1927.8	8.58E+02	1.22E+01	8.80E-03	0.00E+00	9.17E-08	0.00E+00	3.31E-08	1.25E-07
134.72	2078.8	1925.9	8.57E+02	1.22E+01	8.80E-03	0.00E+00	9.11E-08	0.00E+00	3.31E-08	1.24E-07
135.33	2076.2	1924.1	8.56E+02	1.22E+01	8.80E-03	0.00E+00	9.04E-08	0.00E+00	3.31E-08	1.23E-07
135.94	2073.6	1922.2	8.55E+02	1.22E+01	8.80E-03	0.00E+00	8.97E-08	0.00E+00	3.31E-08	1.23E-07
136.55	2071.0	1920.5	8.53E+02	1.22E+01	8.80E-03	0.00E+00	8.90E-08	0.00E+00	3.31E-08	1.22E-07
137.16	2068.4	1918.0	8.52E+02	1.22E+01	8.80E-03	0.00E+00	8.83E-08	0.00E+00	3.31E-08	1.21E-07
137.77	2065.9	1916.2	8.51E+02	1.23E+01	8.80E-03	0.00E+00	8.77E-08	0.00E+00	3.31E-08	1.21E-07

138.38	2063.3	1914.4	8.50E+02	1.23E+01	8.80E-03	0.00E+00	8.70E-08	0.00E+00	3.31E-08	1.20E-07
138.99	2060.8	1912.6	8.49E+02	1.23E+01	8.80E-03	0.00E+00	8.63E-08	0.00E+00	3.31E-08	1.19E-07
139.60	2058.2	1910.8	8.48E+02	1.23E+01	8.80E-03	0.00E+00	8.56E-08	0.00E+00	3.31E-08	1.19E-07
140.21	2055.7	1908.4	8.47E+02	1.23E+01	8.80E-03	0.00E+00	8.50E-08	0.00E+00	3.31E-08	1.18E-07
140.82	2053.1	1906.6	8.46E+02	1.23E+01	8.80E-03	0.00E+00	8.43E-08	0.00E+00	3.31E-08	1.17E-07
141.43	2050.6	1904.8	8.45E+02	1.23E+01	8.80E-03	0.00E+00	8.36E-08	0.00E+00	3.31E-08	1.17E-07
142.04	2048.1	1903.0	8.44E+02	1.24E+01	8.80E-03	0.00E+00	8.30E-08	0.00E+00	3.31E-08	1.16E-07
142.65	2045.6	1901.2	8.43E+02	1.24E+01	8.80E-03	0.00E+00	8.23E-08	0.00E+00	3.31E-08	1.15E-07
143.26	2043.1	1898.8	8.42E+02	1.24E+01	8.80E-03	0.00E+00	8.17E-08	0.00E+00	3.31E-08	1.15E-07
143.87	2040.6	1897.1	8.41E+02	1.24E+01	8.80E-03	0.00E+00	8.10E-08	0.00E+00	3.31E-08	1.14E-07
144.48	2038.1	1895.3	8.40E+02	1.24E+01	8.80E-03	0.00E+00	8.04E-08	0.00E+00	3.31E-08	1.13E-07
145.08	2035.7	1893.5	8.39E+02	1.24E+01	8.80E-03	0.00E+00	7.97E-08	0.00E+00	3.31E-08	1.13E-07
145.69	2033.2	1891.8	8.38E+02	1.24E+01	8.80E-03	0.00E+00	7.91E-08	0.00E+00	3.31E-08	1.12E-07
146.30	2030.7	1889.4	8.37E+02	1.25E+01	8.80E-03	0.00E+00	7.84E-08	0.00E+00	3.31E-08	1.12E-07
146.91	2028.3	1887.6	8.36E+02	1.25E+01	8.80E-03	0.00E+00	7.78E-08	0.00E+00	3.31E-08	1.11E-07
147.52	2025.8	1885.9	8.35E+02	1.25E+01	8.80E-03	0.00E+00	7.71E-08	0.00E+00	3.31E-08	1.10E-07
148.13	2023.4	1884.1	8.34E+02	1.25E+01	8.80E-03	0.00E+00	7.65E-08	0.00E+00	3.31E-08	1.10E-07
148.74	2021.0	1882.4	8.33E+02	1.25E+01	8.80E-03	0.00E+00	7.59E-08	0.00E+00	3.31E-08	1.09E-07
149.35	2018.6	1880.1	8.32E+02	1.25E+01	8.80E-03	0.00E+00	7.52E-08	0.00E+00	3.31E-08	1.08E-07
149.96	2016.1	1878.3	8.31E+02	1.26E+01	8.80E-03	0.00E+00	7.46E-08	0.00E+00	3.31E-08	1.08E-07
150.57	2013.7	1876.6	8.30E+02	1.26E+01	8.80E-03	0.00E+00	7.40E-08	0.00E+00	3.31E-08	1.07E-07
151.18	2011.3	1874.8	8.29E+02	1.26E+01	8.80E-03	0.00E+00	7.34E-08	0.00E+00	3.31E-08	1.06E-07
151.79	2008.9	1873.1	8.28E+02	1.26E+01	8.80E-03	0.00E+00	7.27E-08	0.00E+00	3.31E-08	1.06E-07
152.40	2006.6	1870.8	8.27E+02	1.26E+01	8.80E-03	0.00E+00	7.21E-08	0.00E+00	3.31E-08	1.05E-07

BYU == ONE Dimensional Combustion Or Gasification model (1-DICOG); total particle phase

23-May-79

DISTANCE (cm)	COAL	CHAR (component mass/initial particle mass)	H2O	ASH	TOTAL
0.00	.87407	.00000	.03100	.09494	1.00000
0.61	.87407	0.00000	.01630	.09494	.98530
1.22	.87134	0.00000	.00875	.09494	.97502
1.83	.87039	0.00000	.00485	.09494	.97018
2.44	.86994	0.00000	.00257	.09494	.96745
3.05	.86970	0.00000	.00029	.09494	.96492
3.66	.86948	0.00000	.00000	.09494	.96442
4.27	.86932	0.00000	.00000	.09494	.96425
4.88	.86919	0.00000	.00000	.09494	.96412
5.49	.86909	0.00000	.00000	.09494	.96402
6.10	.86901	0.00000	.00000	.09494	.96395
6.71	.86895	0.00000	.00000	.09494	.96388
7.32	.86890	0.00000	.00000	.09494	.96383
7.92	.86886	0.00000	.00000	.09494	.96379
8.53	.86883	0.00000	.00000	.09494	.96376
9.14	.86880	0.00000	.00000	.09494	.96373
9.75	.86877	0.00000	.00000	.09494	.96371
10.36	.86876	0.00000	.00000	.09494	.96369
10.97	.86874	0.00000	.00000	.09494	.96367
11.58	.86873	0.00000	.00000	.09494	.96366
12.19	.86871	0.00000	.00000	.09494	.96365
12.80	.86870	0.00000	.00000	.09494	.96364
13.41	.86869	0.00000	.00000	.09494	.96363
14.02	.86869	0.00000	.00000	.09494	.96362
14.63	.86868	0.00000	.00000	.09494	.96361
15.24	.86867	0.00000	.00000	.09494	.96361
15.85	.86867	0.00000	.00000	.09494	.96360
16.46	.86866	0.00000	.00000	.09494	.96360
17.07	.86866	0.00000	.00000	.09494	.96359
17.68	.86865	0.00000	.00000	.09494	.96359
18.29	.86865	0.00000	.00000	.09494	.96359
18.90	.86865	0.00000	.00000	.09494	.96358
19.51	.86864	0.00000	.00000	.09494	.96358
20.12	.86864	0.00000	.00000	.09494	.96358
20.73	.86864	0.00000	.00000	.09494	.96358
21.34	.86863	.00001	.00000	.09494	.96357
21.95	.86863	.00001	.00000	.09494	.96357
22.56	.86863	.00001	.00000	.09494	.96357
23.16	.86862	.00001	.00000	.09494	.96357
23.77	.86862	.00001	.00000	.09494	.96356
24.38	.86861	.00001	.00000	.09494	.96356
24.99	.86861	.00002	.00000	.09494	.96356
25.60	.86860	.00002	.00000	.09494	.96356
26.21	.86859	.00002	.00000	.09494	.96355
26.82	.86858	.00003	.00000	.09494	.96355
27.43	.86857	.00003	.00000	.09494	.96354
28.04	.86856	.00004	.00000	.09494	.96354
28.65	.86855	.00005	.00000	.09494	.96353

29.26	.86853	.00006	.00000	.09494	.96353
29.87	.86851	.00007	.00000	.09494	.96352
30.48	.86849	.00009	.00000	.09494	.96351
31.09	.86846	.00010	.00000	.09494	.96350
31.70	.86843	.00012	.00000	.09494	.96349
32.31	.86838	.00015	.00000	.09494	.96347
32.92	.86833	.00018	.00000	.09494	.96345
33.53	.86827	.00022	.00000	.09494	.96343
34.14	.86820	.00027	.00000	.09494	.96340
34.75	.86810	.00032	.00000	.09494	.96336
35.36	.86799	.00039	.00000	.09494	.96331
35.97	.86785	.00048	.00000	.09494	.96326
36.58	.86770	.00057	.00000	.09494	.96320
37.19	.86753	.00067	.00000	.09494	.96314
37.80	.86734	.00079	.00000	.09494	.96306
38.40	.86713	.00092	.00000	.09494	.96298
39.01	.86691	.00105	.00000	.09494	.96289
39.62	.86666	.00120	.00000	.09494	.96280
40.23	.86640	.00136	.00000	.09494	.96270
40.84	.86612	.00153	.00000	.09494	.96259
41.45	.86581	.00172	.00000	.09494	.96247
42.06	.86549	.00192	.00000	.09494	.96234
42.67	.86514	.00213	.00000	.09494	.96221
43.28	.86477	.00235	.00000	.09494	.96206
43.89	.86438	.00259	.00000	.09494	.96191
44.50	.86396	.00285	.00000	.09494	.96174
45.11	.86351	.00312	.00000	.09494	.96157
45.72	.86304	.00341	.00000	.09494	.96138
46.33	.86253	.00372	.00000	.09494	.96119
46.94	.86200	.00405	.00000	.09494	.96098
47.55	.86143	.00439	.00000	.09494	.96076
48.16	.86083	.00476	.00000	.09494	.96052
48.77	.86020	.00514	.00000	.09494	.96028
49.38	.85953	.00555	.00000	.09494	.96002
49.99	.85882	.00599	.00000	.09494	.95974
50.60	.85806	.00645	.00000	.09494	.95945
51.21	.85727	.00693	.00000	.09494	.95914
51.82	.85643	.00744	.00000	.09494	.95881
52.43	.85554	.00798	.00000	.09494	.95846
53.04	.85460	.00856	.00000	.09494	.95810
53.64	.85361	.00916	.00000	.09494	.95771
54.25	.85257	.00980	.00000	.09494	.95730
54.86	.85146	.01047	.00000	.09494	.95687
55.47	.85029	.01119	.00000	.09494	.95641
56.08	.84906	.01194	.00000	.09494	.95593
56.69	.84775	.01274	.00000	.09494	.95542
57.30	.84637	.01358	.00000	.09494	.95489
57.91	.84491	.01447	.00000	.09494	.95432
58.52	.84337	.01541	.00000	.09494	.95371
59.13	.84174	.01640	.00000	.09494	.95308
59.74	.84001	.01746	.00000	.09494	.95241
60.35	.83819	.01857	.00000	.09494	.95169
60.96	.83626	.01975	.00000	.09494	.95094
61.57	.83421	.02100	.00000	.09494	.95014
62.18	.83204	.02232	.00000	.09494	.94930
62.79	.82974	.02372	.00000	.09494	.94840
63.40	.82730	.02521	.00000	.09494	.94745
64.01	.82472	.02679	.00000	.09494	.94644
64.62	.82197	.02846	.00000	.09494	.94537
65.23	.81905	.03025	.00000	.09494	.94423

65.84	.81594	.03214	.00000	.09494	.94302
66.45	.81263	.03416	.00000	.09494	.94173
67.06	.80911	.03631	.00000	.09494	.94035
67.67	.80535	.03860	.00000	.09494	.93889
68.28	.80134	.04105	.00000	.09494	.93732
68.88	.79704	.04367	.00000	.09494	.93565
69.49	.79245	.04647	.00000	.09494	.93386
70.10	.78752	.04948	.00000	.09494	.93193
70.71	.78223	.05271	.00000	.09494	.92987
71.32	.77654	.05618	.00000	.09494	.92765
71.93	.77040	.05992	.00000	.09494	.92526
72.54	.76378	.06396	.00000	.09494	.92268
73.15	.75662	.06833	.00000	.09494	.91988
73.76	.74885	.07307	.00000	.09494	.91686
74.37	.74113	.07778	.00000	.09494	.91385
74.98	.73200	.08335	.00000	.09494	.91028
75.59	.72201	.08944	.00000	.09494	.90639
76.20	.71107	.09612	.00000	.09494	.90212
76.81	.69904	.10346	.00000	.09494	.89743
77.42	.68576	.11156	.00000	.09494	.89225
78.03	.67106	.12052	.00000	.09494	.88651
78.64	.65471	.13049	.00000	.09494	.88013
79.25	.63646	.14162	.00000	.09494	.87301
79.86	.61600	.15408	.00000	.09494	.86502
80.47	.59298	.16809	.00000	.09494	.85601
81.08	.56698	.18390	.00000	.09494	.84581
81.69	.53751	.20176	.00000	.09494	.83420
82.30	.50397	.22199	.00000	.09494	.82090
82.91	.46567	.24487	.00000	.09494	.80547
83.52	.42160	.27070	.00000	.09494	.78724
84.12	.37015	.29970	.00000	.09494	.76479
84.73	.30799	.33201	.00000	.09494	.73494
85.34	.23076	.36629	.00000	.09494	.69199
85.95	.15663	.39213	.00000	.09494	.64370
86.56	.10186	.40588	.00000	.09494	.60267
87.17	.06715	.40940	.00000	.09494	.57148
87.78	.04059	.40806	.00000	.09494	.54359
88.39	.01591	.40355	.00000	.09494	.51439
89.00	.00233	.39385	.00000	.09494	.49111
89.61	.00003	.38020	.00000	.09494	.47517
90.22	.00000	.36607	.00000	.09494	.46100
90.83	.00000	.35143	.00000	.09494	.44636
91.44	.00000	.33680	.00000	.09494	.43173
92.05	.00000	.32227	.00000	.09494	.41720
92.66	.00000	.30790	.00000	.09494	.40283
93.27	.00000	.29374	.00000	.09494	.38867
93.88	.00000	.27982	.00000	.09494	.37475
94.49	.00000	.26617	.00000	.09494	.36111
95.10	.00000	.25300	.00000	.09494	.34793
95.71	.00000	.24030	.00000	.09494	.33424
96.32	.00000	.22723	.00000	.09494	.32066
96.93	.00000	.21395	.00000	.09494	.30709
97.54	.00000	.20059	.00000	.09494	.29352
98.15	.00000	.18705	.00000	.09494	.27998
98.76	.00000	.17353	.00000	.09494	.26647
99.36	.00000	.16004	.00000	.09494	.25297
99.97	.00000	.14657	.00000	.09494	.23951
100.58	.00000	.13314	.00000	.09494	.22607
101.19	.00000	.11973	.00000	.09494	.21267
101.80	.00000	.10636	.00000	.09494	.20029

102.41	.00000	.20801	.00000	.09494	.30294
103.02	.00000	.20469	.00000	.09494	.29963
103.63	.00000	.20138	.00000	.09494	.29632
104.24	.00000	.19808	.00000	.09494	.29302
104.85	.00000	.19481	.00000	.09494	.28975
105.46	.00000	.19157	.00000	.09494	.28651
106.07	.00000	.18837	.00000	.09494	.28330
106.68	.00000	.18519	.00000	.09494	.28013
107.29	.00000	.18205	.00000	.09494	.27698
107.90	.00000	.17893	.00000	.09494	.27387
108.51	.00000	.17585	.00000	.09494	.27078
109.12	.00000	.17279	.00000	.09494	.26773
109.73	.00000	.16977	.00000	.09494	.26470
110.34	.00000	.16677	.00000	.09494	.26171
110.95	.00000	.16381	.00000	.09494	.25874
111.56	.00000	.16087	.00000	.09494	.25581
112.17	.00000	.15796	.00000	.09494	.25290
112.78	.00000	.15508	.00000	.09494	.25002
113.39	.00000	.15223	.00000	.09494	.24717
114.00	.00000	.14815	.00000	.09494	.24309
114.60	.00000	.14536	.00000	.09494	.24029
115.21	.00000	.14260	.00000	.09494	.23753
115.82	.00000	.13986	.00000	.09494	.23479
116.43	.00000	.13715	.00000	.09494	.23208
117.04	.00000	.13446	.00000	.09494	.22940
117.65	.00000	.13181	.00000	.09494	.22674
118.26	.00000	.12918	.00000	.09494	.22411
118.87	.00000	.12658	.00000	.09494	.22151
119.48	.00000	.12400	.00000	.09494	.21893
120.09	.00000	.12145	.00000	.09494	.21638
120.70	.00000	.11892	.00000	.09494	.21386
121.31	.00000	.11642	.00000	.09494	.21136
121.92	.00000	.11395	.00000	.09494	.20888
122.53	.00000	.11150	.00000	.09494	.20643
123.14	.00000	.10907	.00000	.09494	.20400
123.75	.00000	.10667	.00000	.09494	.20160
124.36	.00000	.10429	.00000	.09494	.19923
124.97	.00000	.10194	.00000	.09494	.19687
125.58	.00000	.09961	.00000	.09494	.19454
126.19	.00000	.09730	.00000	.09494	.19224
126.80	.00000	.09502	.00000	.09494	.18996
127.41	.00000	.09276	.00000	.09494	.18770
128.02	.00000	.09052	.00000	.09494	.18546
128.63	.00000	.08831	.00000	.09494	.18324
129.24	.00000	.08612	.00000	.09494	.18105
129.84	.00000	.08545	.00000	.09494	.18039
130.45	.00000	.08483	.00000	.09494	.17977
131.06	.00000	.08421	.00000	.09494	.17915
131.67	.00000	.08360	.00000	.09494	.17853
132.28	.00000	.08298	.00000	.09494	.17791
132.89	.00000	.08236	.00000	.09494	.17730
133.50	.00000	.08175	.00000	.09494	.17669
134.11	.00000	.08114	.00000	.09494	.17608
134.72	.00000	.08054	.00000	.09494	.17547
135.33	.00000	.07993	.00000	.09494	.17486
135.94	.00000	.07933	.00000	.09494	.17426
136.55	.00000	.07872	.00000	.09494	.17366
137.16	.00000	.07812	.00000	.09494	.17306
137.77	.00000	.07753	.00000	.09494	.17246
138.38	.00000	.07693	.00000	.09494	.17187

139.99	.00000	.07634	.00000	.09494	.17127
139.60	.00000	.07574	.00000	.09494	.17068
140.21	.00000	.07515	.00000	.09494	.17009
140.82	.00000	.07457	.00000	.09494	.16950
141.43	.00000	.07398	.00000	.09494	.16892
142.04	.00000	.07340	.00000	.09494	.16833
142.65	.00000	.07282	.00000	.09494	.16775
143.26	.00000	.07224	.00000	.09494	.16717
143.87	.00000	.07166	.00000	.09494	.16659
144.48	.00000	.07108	.00000	.09494	.16602
145.08	.00000	.07051	.00000	.09494	.16544
145.69	.00000	.06994	.00000	.09494	.16487
146.30	.00000	.06937	.00000	.09494	.16430
146.91	.00000	.06880	.00000	.09494	.16374
147.52	.00000	.06823	.00000	.09494	.16317
148.13	.00000	.06767	.00000	.09494	.16260
148.74	.00000	.06711	.00000	.09494	.16204
149.35	.00000	.06655	.00000	.09494	.16148
149.96	.00000	.06599	.00000	.09494	.16092
150.57	.00000	.06543	.00000	.09494	.16037
151.18	.00000	.06488	.00000	.09494	.15981
151.79	.00000	.06432	.00000	.09494	.15926
152.40	.00000	.06377	.00000	.09494	.15871

BYU -- ONE Dimensional Combustion Or Gasification model (1-DICOG): gas phase mole fractions

23-May-79

DISTANCE (cm)	FLOW RATE (cc/sec)	AR	CO	O2	N2	CO2	H2O	H2	CH4	SO2	NO
0.61	7.76E+03	.04684	.00000	.20185	.73481	.00000	.01650	.00000	.00000	.00000	.00000
1.22	9.80E+03	.03804	.00000	.20231	.74180	.00000	.01785	.00000	.00000	.00000	.00000
1.83	1.18E+04	.03262	.00000	.20294	.74744	.00000	.01700	.00000	.00000	.00000	.00000
2.44	1.37E+04	.02893	.00000	.20353	.75190	.00000	.01563	.00000	.00000	.00000	.00000
3.05	1.57E+04	.02626	.00000	.20401	.75531	.00000	.01442	.00000	.00000	.00000	.00000
3.66	1.77E+04	.02424	.00000	.20451	.75838	.00000	.01287	.00000	.00000	.00000	.00000
4.27	1.98E+04	.02265	.00000	.20489	.76080	.00000	.01166	.00000	.00000	.00000	.00000
4.88	2.18E+04	.02137	.00000	.20521	.76274	.00000	.01067	.00000	.00000	.00000	.00000
5.49	2.38E+04	.02032	.00000	.20546	.76435	.00000	.00987	.00000	.00000	.00000	.00000
6.10	2.58E+04	.01944	.00000	.20568	.76569	.00000	.00919	.00000	.00000	.00000	.00000
6.71	2.78E+04	.01869	.00000	.20586	.76682	.00000	.00862	.00000	.00000	.00000	.00000
7.32	2.97E+04	.01805	.00000	.20602	.76779	.00000	.00813	.00000	.00000	.00000	.00000
7.92	3.16E+04	.01750	.00000	.20615	.76863	.00000	.00771	.00000	.00000	.00000	.00000
8.53	3.35E+04	.01702	.00000	.20627	.76937	.00000	.00734	.00000	.00000	.00000	.00000
9.14	3.53E+04	.01660	.00000	.20637	.77001	.00000	.00701	.00000	.00000	.00000	.00000
9.75	3.71E+04	.01622	.00000	.20647	.77058	.00000	.00673	.00000	.00000	.00000	.00000
10.36	3.89E+04	.01589	.00000	.20655	.77109	.00000	.00647	.00000	.00000	.00000	.00000
10.97	4.05E+04	.01559	.00000	.20662	.77154	.00000	.00624	.00000	.00000	.00000	.00000
11.58	4.22E+04	.01533	.00000	.20668	.77194	.00000	.00604	.00000	.00000	.00000	.00000
12.19	4.38E+04	.01509	.00000	.20674	.77231	.00000	.00586	.00000	.00000	.00000	.00000
12.80	4.54E+04	.01487	.00000	.20680	.77264	.00000	.00569	.00000	.00000	.00000	.00000
13.41	4.69E+04	.01468	.00000	.20684	.77293	.00000	.00554	.00000	.00000	.00000	.00000
14.02	4.83E+04	.01450	.00000	.20689	.77320	.00000	.00541	.00000	.00000	.00000	.00000
14.63	4.98E+04	.01434	.00000	.20693	.77344	.00000	.00529	.00000	.00000	.00000	.00000
15.24	5.11E+04	.01420	.00000	.20696	.77366	.00000	.00517	.00000	.00000	.00000	.00000
15.85	5.24E+04	.01407	.00000	.20699	.77386	.00000	.00507	.00000	.00000	.00000	.00000
16.46	5.37E+04	.01395	.00000	.20702	.77405	.00000	.00498	.00000	.00000	.00000	.00000
17.07	5.49E+04	.01384	.00000	.20705	.77421	.00000	.00490	.00000	.00000	.00000	.00000
17.68	5.61E+04	.01374	.00000	.20707	.77436	.00000	.00483	.00000	.00000	.00000	.00000
18.29	5.72E+04	.01365	.00000	.20709	.77449	.00000	.00476	.00000	.00000	.00000	.00000
18.90	5.83E+04	.01358	.00000	.20711	.77461	.00000	.00470	.00000	.00000	.00000	.00000
19.51	5.93E+04	.01350	.00000	.20713	.77472	.00000	.00464	.00000	.00000	.00000	.00000
20.12	6.02E+04	.01344	.00000	.20714	.77481	.00000	.00460	.00000	.00000	.00000	.00000
20.73	6.12E+04	.01339	.00000	.20716	.77490	.00000	.00455	.00000	.00000	.00000	.00000
21.34	6.20E+04	.01334	.00000	.20717	.77497	.00000	.00452	.00000	.00000	.00000	.00000
21.95	6.28E+04	.01330	.00000	.20718	.77504	.00000	.00448	.00000	.00000	.00000	.00000
22.56	6.36E+04	.01326	.00000	.20719	.77509	.00000	.00446	.00000	.00000	.00000	.00000
23.16	6.43E+04	.01323	.00000	.20720	.77513	.00000	.00444	.00000	.00000	.00000	.00000
23.77	6.50E+04	.01321	.00000	.20720	.77517	.00000	.00442	.00000	.00000	.00000	.00000
24.38	6.56E+04	.01319	.00000	.20721	.77520	.00000	.00440	.00000	.00000	.00000	.00000
24.99	6.61E+04	.01318	.00000	.20721	.77521	.00000	.00440	.00000	.00000	.00000	.00000
25.60	6.67E+04	.01317	.00000	.20721	.77522	.00000	.00439	.00000	.00000	.00000	.00000
26.21	6.71E+04	.01317	.00000	.20721	.77522	.00000	.00439	.00000	.00000	.00000	.00000
26.82	6.75E+04	.01318	.00000	.20721	.77521	.00000	.00440	.00000	.00000	.00000	.00000
27.43	6.79E+04	.01319	.00000	.20720	.77520	.00000	.00441	.00000	.00000	.00000	.00000
28.04	6.82E+04	.01321	.00000	.20720	.77517	.00000	.00442	.00000	.00000	.00000	.00000
28.65	6.85E+04	.01323	.00000	.20719	.77513	.00000	.00444	.00000	.00000	.00000	.00000
29.26	6.87E+04	.01326	.00000	.20718	.77509	.00000	.00446	.00000	.00000	.00000	.00000

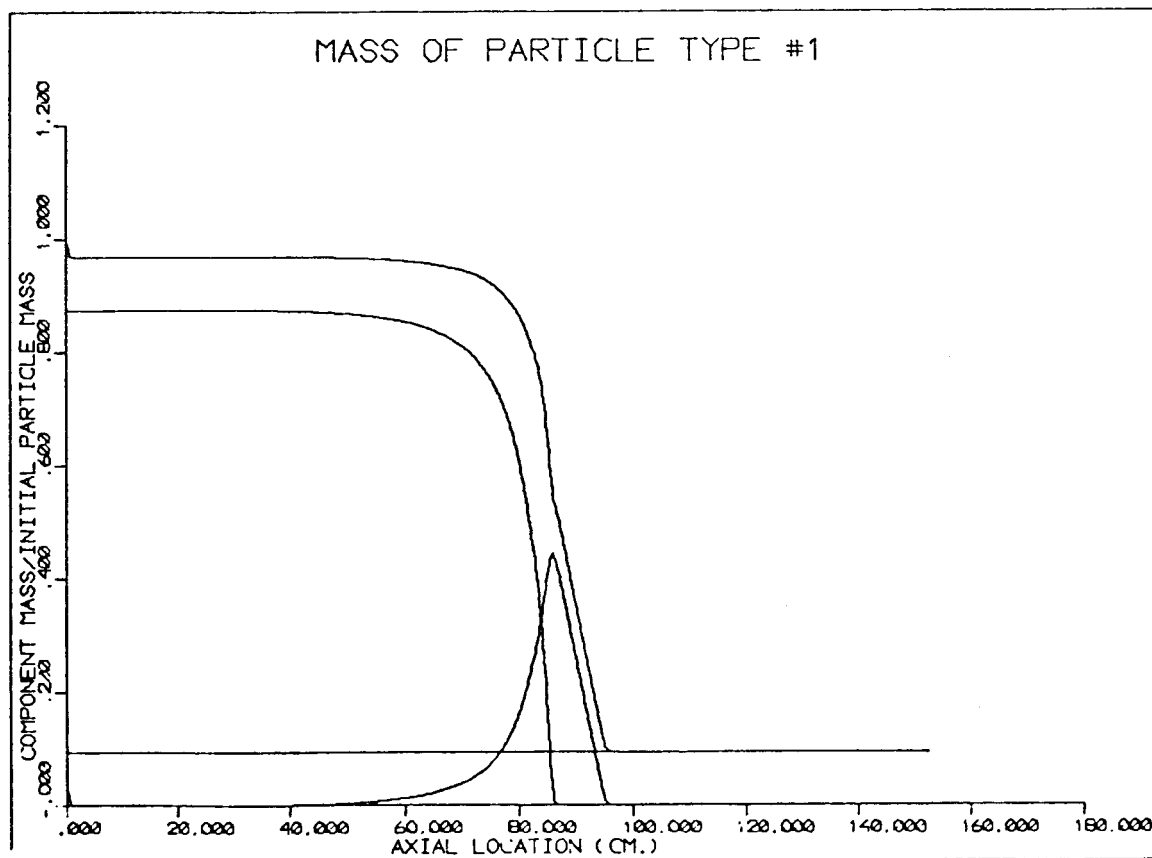
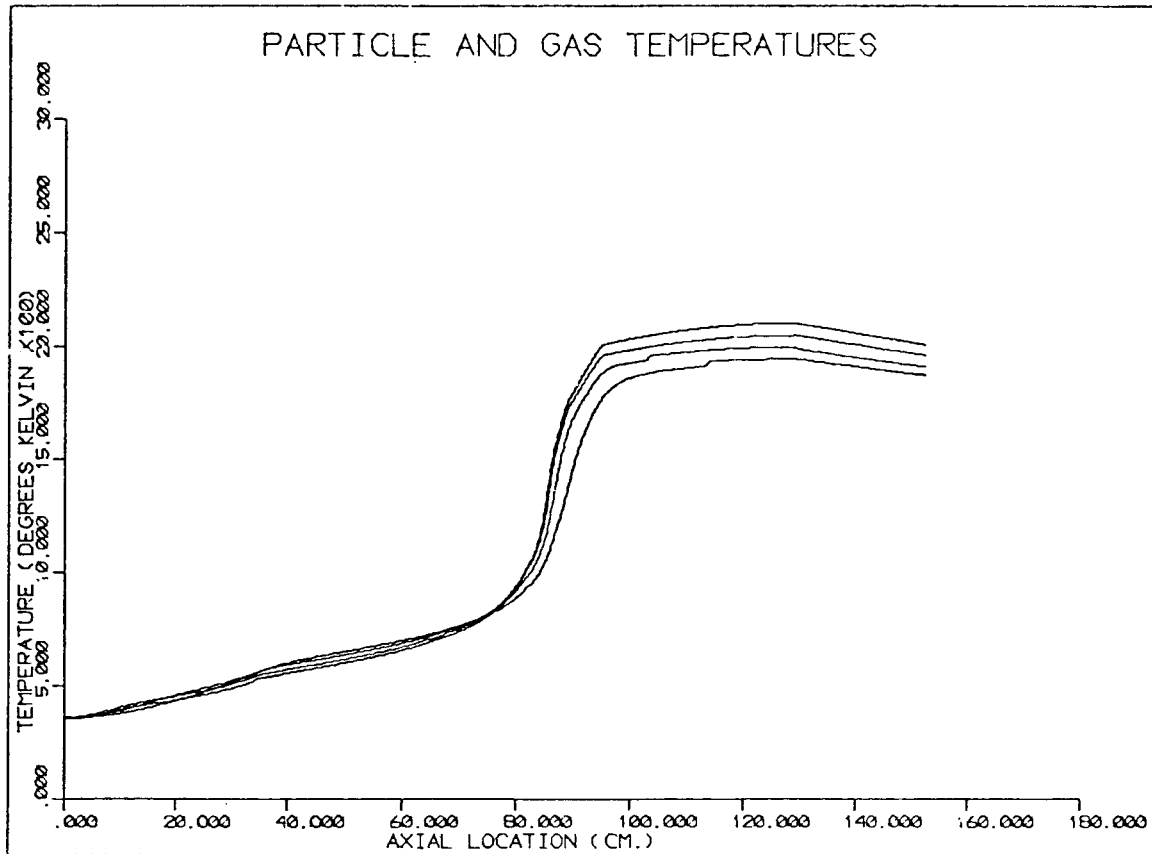
29.87	6.86E+04	.01329	.00000	.20717	.77504	.00000	.00449	.00000	.00000	.00000	.00000
30.48	6.90E+04	.01333	.00000	.20716	.77497	.00001	.00452	.00000	.00000	.00000	.00000
31.09	6.90E+04	.01338	.00000	.20715	.77490	.00001	.00456	.00000	.00000	.00000	.00000
31.70	6.90E+04	.01344	.00000	.20713	.77481	.00001	.00461	.00000	.00000	.00000	.00000
32.31	6.90E+04	.01350	.00000	.20711	.77472	.00001	.00466	.00000	.00000	.00000	.00000
32.92	6.89E+04	.01357	.00000	.20709	.77461	.00001	.00472	.00000	.00000	.00000	.00000
33.53	6.88E+04	.01365	.00000	.20707	.77449	.00001	.00478	.00000	.00000	.00000	.00000
34.14	6.87E+04	.01374	.00000	.20704	.77435	.00002	.00485	.00000	.00000	.00000	.00000
34.75	6.84E+04	.01383	.00000	.20701	.77420	.00002	.00494	.00000	.00000	.00000	.00000
35.36	6.84E+04	.01390	.00000	.20698	.77409	.00003	.00500	.00000	.00000	.00000	.00000
35.97	6.87E+04	.01391	.00000	.20697	.77407	.00003	.00502	.00000	.00000	.00000	.00000
36.58	6.90E+04	.01391	.00000	.20696	.77407	.00004	.00503	.00000	.00000	.00000	.00000
37.19	6.93E+04	.01391	.00000	.20694	.77406	.00005	.00504	.00000	.00000	.00000	.00000
37.80	6.96E+04	.01391	.00000	.20693	.77405	.00005	.00506	.00000	.00000	.00000	.00000
38.40	7.00E+04	.01391	.00000	.20691	.77405	.00006	.00507	.00000	.00000	.00000	.00000
39.01	7.03E+04	.01391	.00000	.20689	.77404	.00007	.00509	.00000	.00000	.00000	.00000
39.62	7.07E+04	.01391	.00000	.20687	.77403	.00008	.00511	.00000	.00000	.00000	.00000
40.23	7.10E+04	.01391	.00000	.20685	.77402	.00009	.00513	.00000	.00000	.00000	.00000
40.84	7.14E+04	.01391	.00000	.20683	.77401	.00010	.00515	.00000	.00000	.00000	.00000
41.45	7.17E+04	.01391	.00000	.20680	.77400	.00012	.00518	.00000	.00000	.00000	.00000
42.06	7.21E+04	.01391	.00000	.20677	.77398	.00013	.00520	.00000	.00000	.00000	.00000
42.67	7.24E+04	.01391	.00000	.20675	.77397	.00015	.00523	.00000	.00000	.00000	.00000
43.28	7.28E+04	.01391	.00000	.20671	.77396	.00016	.00526	.00000	.00000	.00000	.00000
43.89	7.31E+04	.01391	.00000	.20668	.77394	.00018	.00529	.00000	.00000	.00000	.00000
44.50	7.35E+04	.01391	.00000	.20665	.77393	.00020	.00532	.00000	.00000	.00000	.00000
45.11	7.39E+04	.01390	.00000	.20661	.77391	.00021	.00536	.00000	.00000	.00000	.00000
45.72	7.42E+04	.01390	.00000	.20657	.77389	.00023	.00540	.00000	.00000	.00000	.00000
46.33	7.46E+04	.01390	.00000	.20653	.77387	.00025	.00544	.00000	.00000	.00000	.00000
46.94	7.50E+04	.01390	.00000	.20649	.77385	.00028	.00548	.00000	.00000	.00000	.00000
47.55	7.53E+04	.01390	.00000	.20644	.77383	.00030	.00552	.00000	.00000	.00000	.00000
48.16	7.57E+04	.01390	.00000	.20639	.77381	.00033	.00557	.00000	.00000	.00000	.00000
48.77	7.61E+04	.01390	.00000	.20634	.77378	.00035	.00562	.00000	.00000	.00000	.00000
49.38	7.65E+04	.01390	.00000	.20628	.77376	.00038	.00568	.00000	.00000	.00000	.00000
49.99	7.69E+04	.01390	.00000	.20622	.77373	.00041	.00573	.00000	.00000	.00000	.00000
50.60	7.73E+04	.01390	.00000	.20616	.77370	.00044	.00579	.00000	.00000	.00001	.00000
51.21	7.77E+04	.01390	.00000	.20609	.77367	.00047	.00585	.00000	.00000	.00001	.00000
51.82	7.81E+04	.01390	.00000	.20602	.77364	.00051	.00592	.00000	.00000	.00001	.00000
52.43	7.85E+04	.01390	.00000	.20595	.77361	.00055	.00599	.00000	.00000	.00001	.00000
53.04	7.89E+04	.01390	.00000	.20587	.77357	.00059	.00606	.00000	.00000	.00001	.00000
53.64	7.93E+04	.01390	.00000	.20579	.77353	.00063	.00614	.00000	.00000	.00001	.00000
54.25	7.97E+04	.01390	.00000	.20571	.77349	.00067	.00623	.00000	.00000	.00001	.00000
54.86	8.01E+04	.01390	.00000	.20561	.77345	.00072	.00631	.00000	.00000	.00001	.00000
55.47	8.06E+04	.01390	.00000	.20552	.77341	.00077	.00641	.00000	.00000	.00001	.00000
56.08	8.10E+04	.01389	.00000	.20542	.77336	.00082	.00650	.00000	.00000	.00001	.00000
56.69	8.15E+04	.01389	.00000	.20531	.77331	.00087	.00661	.00000	.00000	.00001	.00000
57.30	8.19E+04	.01389	.00000	.20519	.77326	.00093	.00672	.00000	.00000	.00001	.00000
57.91	8.24E+04	.01389	.00000	.20507	.77320	.00099	.00683	.00000	.00000	.00001	.00000
58.52	8.29E+04	.01389	.00000	.20495	.77314	.00105	.00695	.00000	.00000	.00001	.00000
59.13	8.33E+04	.01389	.00000	.20481	.77308	.00112	.00708	.00000	.00000	.00001	.00000
59.74	8.38E+04	.01389	.00000	.20467	.77302	.00119	.00722	.00000	.00000	.00001	.00000
60.35	8.43E+04	.01389	.00000	.20452	.77295	.00127	.00736	.00000	.00000	.00002	.00000
60.96	8.49E+04	.01389	.00000	.20436	.77287	.00135	.00752	.00000	.00000	.00002	.00000
61.57	8.54E+04	.01388	.00000	.20419	.77280	.00144	.00768	.00000	.00000	.00002	.00000
62.18	8.59E+04	.01388	.00000	.20401	.77271	.00153	.00785	.00000	.00000	.00002	.00000
62.79	8.65E+04	.01388	.00000	.20382	.77263	.00162	.00803	.00000	.00000	.00002	.00000
63.40	8.71E+04	.01388	.00000	.20362	.77253	.00172	.00822	.00000	.00000	.00002	.00000
64.01	8.77E+04	.01388	.00000	.20341	.77244	.00183	.00843	.00000	.00000	.00002	.00000
64.62	8.83E+04	.01388	.00000	.20318	.77233	.00194	.00865	.00000	.00000	.00002	.00000
65.23	8.89E+04	.01387	.00000	.20294	.77222	.00207	.00888	.00000	.00000	.00002	.00000
65.84	8.95E+04	.01387	.00000	.20268	.77210	.00220	.00912	.00000	.00000	.00003	.00000

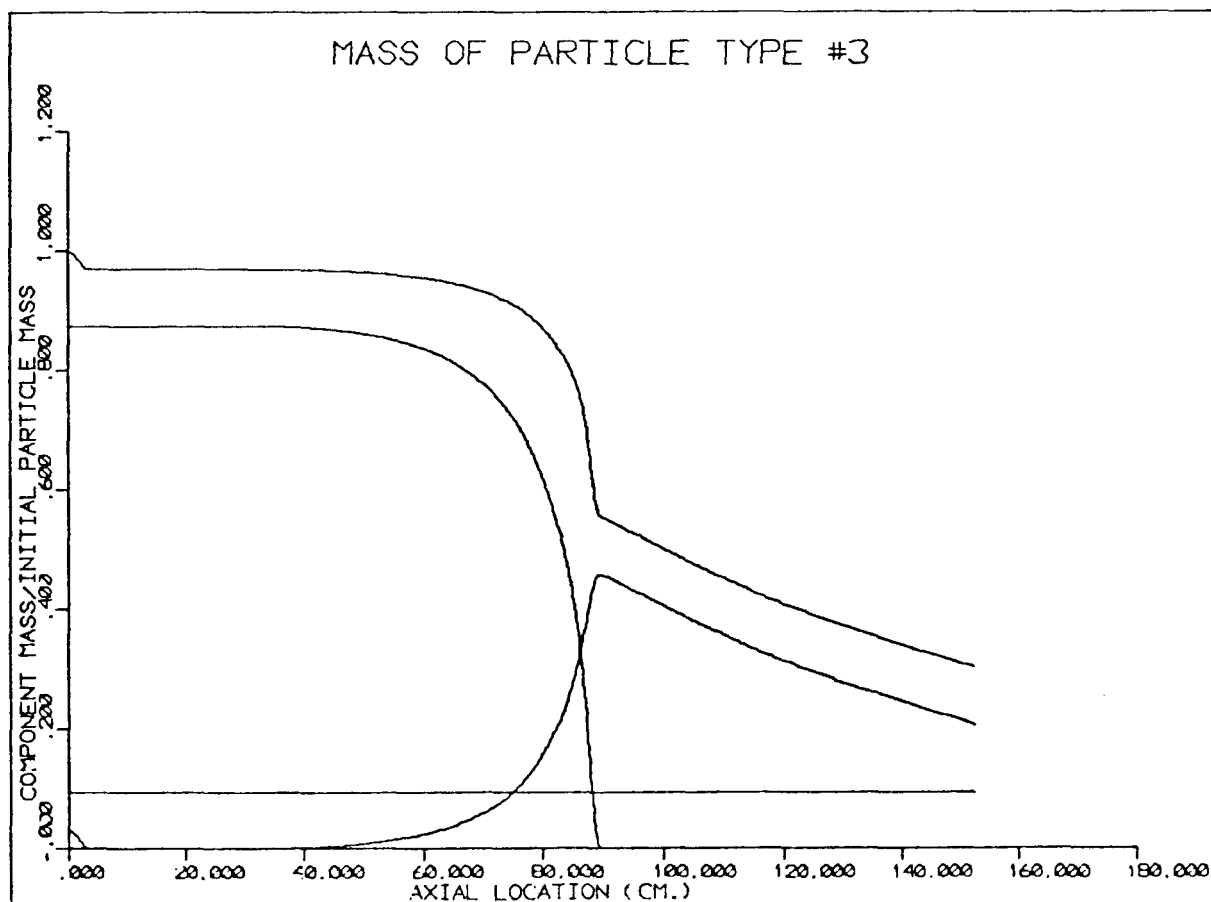
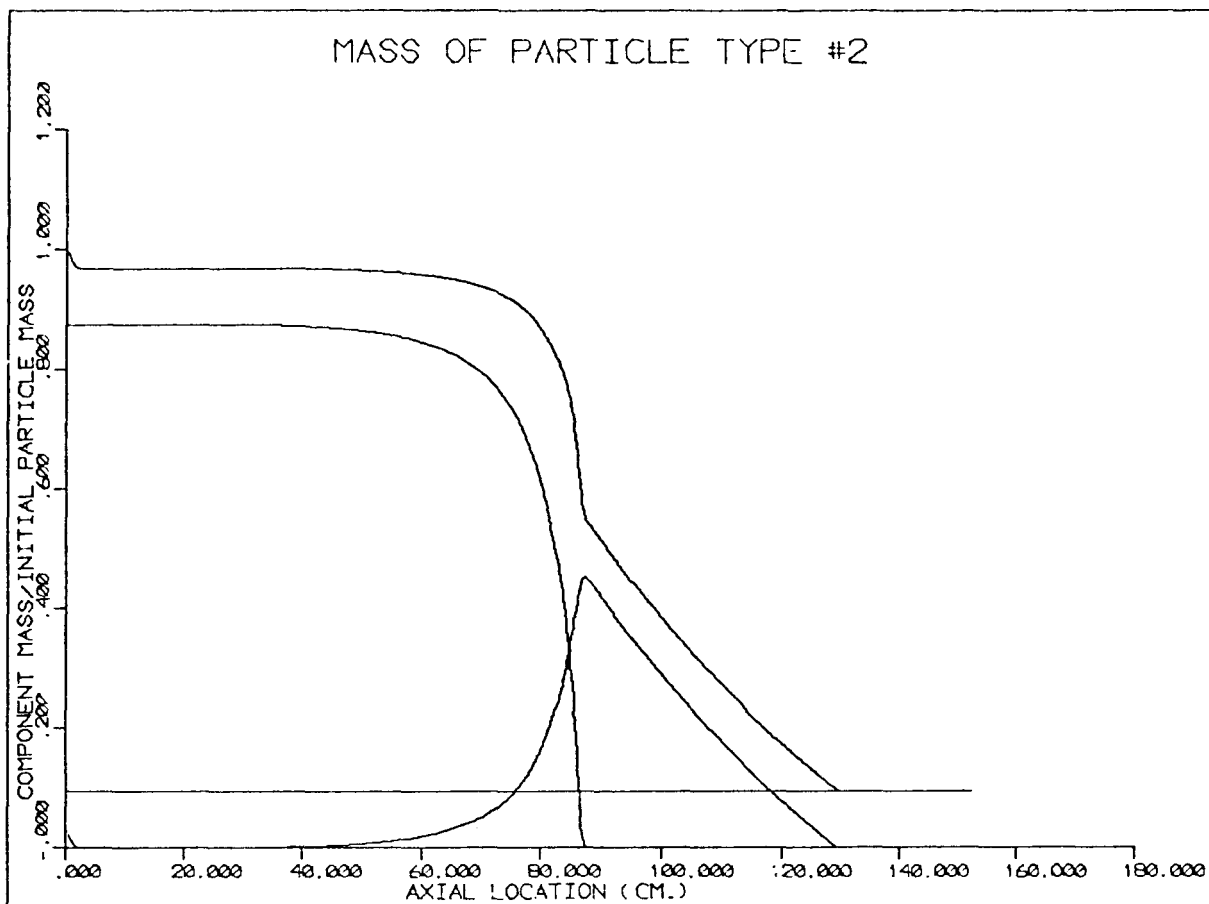
66.45	9.02E+04	.01387	.00000	.20241	.77199	.00233	.00938	.00000	.00000	.00003	.00000
67.06	9.09E+04	.01387	.00000	.20212	.77184	.00248	.00966	.00000	.00000	.00003	.00000
67.67	9.16E+04	.01386	.00000	.20181	.77170	.00264	.00996	.00000	.00000	.00003	.00000
68.28	9.24E+04	.01386	.00000	.20148	.77155	.00280	.01027	.00000	.00000	.00003	.00000
68.88	9.32E+04	.01386	.00000	.20113	.77139	.00298	.01061	.00000	.00000	.00004	.00000
69.49	9.40E+04	.01385	.00000	.20075	.77121	.00317	.01097	.00000	.00000	.00004	.00000
70.10	9.49E+04	.01385	.00000	.20035	.77103	.00337	.01136	.00000	.00000	.00004	.00000
70.71	9.58E+04	.01385	.00000	.19991	.77083	.00359	.01178	.00000	.00000	.00004	.00000
71.32	9.67E+04	.01384	.00000	.19945	.77061	.00383	.01222	.00000	.00000	.00005	.00000
71.93	9.77E+04	.01384	.00000	.19894	.77038	.00408	.01270	.00000	.00000	.00005	.00000
72.54	9.88E+04	.01383	.00000	.19840	.77013	.00436	.01322	.00000	.00000	.00005	.00000
73.15	9.99E+04	.01383	.00000	.19781	.76986	.00465	.01379	.00000	.00000	.00006	.00000
73.76	1.01E+05	.01382	.00000	.19718	.76957	.00497	.01439	.00000	.00000	.00006	.00000
74.37	1.02E+05	.01382	.00000	.19655	.76928	.00529	.01500	.00000	.00000	.00006	.00000
74.98	1.04E+05	.01381	.00000	.19580	.76893	.00567	.01571	.00000	.00000	.00007	.00000
75.59	1.05E+05	.01380	.00000	.19498	.76856	.00608	.01649	.00000	.00000	.00007	.00000
76.20	1.07E+05	.01380	.00000	.19409	.76815	.00653	.01735	.00000	.00000	.00008	.00000
76.81	1.08E+05	.01379	.00000	.19311	.76770	.00703	.01829	.00000	.00000	.00008	.00000
77.42	1.10E+05	.01378	.00000	.19203	.76720	.00757	.01932	.00000	.00000	.00009	.00001
78.03	1.12E+05	.01377	.00000	.19084	.76665	.00817	.02047	.00000	.00000	.00010	.00001
78.64	1.14E+05	.01376	.00000	.18951	.76604	.00885	.02174	.00000	.00000	.00011	.00001
79.25	1.17E+05	.01375	.00000	.18803	.76536	.00959	.02315	.00000	.00000	.00011	.00001
79.86	1.20E+05	.01373	.00000	.18637	.76460	.01043	.02473	.00000	.00000	.00012	.00001
80.47	1.23E+05	.01371	.00000	.18451	.76374	.01137	.02651	.00000	.00000	.00014	.00002
81.08	1.26E+05	.01370	.00000	.18240	.76278	.01244	.02851	.00000	.00000	.00015	.00002
81.69	1.30E+05	.01368	.00000	.18000	.76169	.01366	.03078	.00000	.00000	.00016	.00003
82.30	1.34E+05	.01365	.00000	.17727	.76045	.01507	.03334	.00000	.00000	.00018	.00004
82.91	1.39E+05	.01363	.00000	.17410	.75903	.01671	.03627	.00000	.00000	.00020	.00006
83.52	1.45E+05	.01360	.00000	.17036	.75741	.01871	.03961	.00000	.00000	.00022	.00009
84.12	1.52E+05	.01356	.00000	.16575	.75552	.02128	.04351	.00000	.00000	.00024	.00014
84.73	1.62E+05	.01352	.00000	.15961	.75323	.02496	.04818	.00000	.00000	.00027	.00023
85.34	1.75E+05	.01347	.00000	.15072	.75035	.03077	.05395	.00000	.00000	.00031	.00043
85.95	1.90E+05	.01342	.00000	.14077	.74756	.03771	.05943	.00000	.00000	.00034	.00077
86.56	2.02E+05	.01338	.00000	.13228	.74544	.04394	.06344	.00000	.00000	.00037	.00115
87.17	2.11E+05	.01336	.00000	.12575	.74405	.04899	.06598	.00000	.00000	.00038	.00149
87.78	2.19E+05	.01334	.00000	.11986	.74294	.05370	.06792	.00000	.00000	.00040	.00184
88.39	2.27E+05	.01333	.00001	.11366	.74187	.05876	.06971	.00000	.00000	.00041	.00224
89.00	2.33E+05	.01332	.00002	.10868	.74122	.06305	.07070	.00001	.00000	.00041	.00259
89.61	2.37E+05	.01332	.00003	.10521	.74101	.06631	.07086	.00001	.00000	.00041	.00283
90.22	2.41E+05	.01332	.00005	.10212	.74090	.06929	.07086	.00001	.00000	.00041	.00304
90.83	2.45E+05	.01332	.00007	.09892	.74078	.07237	.07086	.00002	.00000	.00041	.00327
91.44	2.48E+05	.01332	.00009	.09572	.74065	.07544	.07085	.00002	.00000	.00041	.00350
92.05	2.52E+05	.01332	.00013	.09255	.74052	.07848	.07084	.00003	.00000	.00041	.00373
92.66	2.55E+05	.01332	.00017	.08941	.74039	.08147	.07084	.00003	.00000	.00041	.00396
93.27	2.58E+05	.01332	.00022	.08633	.74025	.08441	.07082	.00004	.00000	.00041	.00418
93.88	2.62E+05	.01331	.00029	.08331	.74012	.08729	.07081	.00005	.00000	.00041	.00440
94.49	2.65E+05	.01331	.00037	.08036	.73998	.09009	.07080	.00007	.00000	.00041	.00461
95.10	2.68E+05	.01331	.00047	.07757	.73984	.09274	.07078	.00008	.00000	.00041	.00480
95.71	2.69E+05	.01331	.00051	.07628	.73979	.09398	.07077	.00008	.00000	.00041	.00487
96.32	2.69E+05	.01331	.00053	.07552	.73977	.09471	.07077	.00009	.00000	.00041	.00486
96.93	2.69E+05	.01331	.00055	.07477	.73976	.09545	.07077	.00009	.00000	.00041	.00490
97.54	2.70E+05	.01331	.00057	.07402	.73974	.09618	.07076	.00009	.00000	.00041	.00492
98.15	2.70E+05	.01331	.00059	.07327	.73972	.09690	.07076	.00009	.00000	.00041	.00493
98.76	2.71E+05	.01331	.00062	.07253	.73970	.09762	.07076	.00010	.00000	.00041	.00495
99.36	2.71E+05	.01331	.00064	.07180	.73969	.09834	.07075	.00010	.00000	.00041	.00496
99.97	2.72E+05	.01331	.00066	.07107	.73967	.09904	.07075	.00010	.00000	.00041	.00497
100.58	2.72E+05	.01331	.00069	.07035	.73966	.09975	.07074	.00010	.00000	.00041	.00499
101.19	2.72E+05	.01331	.00071	.06964	.73964	.10044	.07074	.00011	.00000	.00041	.00500
101.80	2.73E+05	.01331	.00074	.06893	.73962	.10113	.07074	.00011	.00000	.00041	.00501
102.41	2.73E+05	.01331	.00076	.06823	.73961	.10181	.07073	.00011	.00000	.00041	.00502

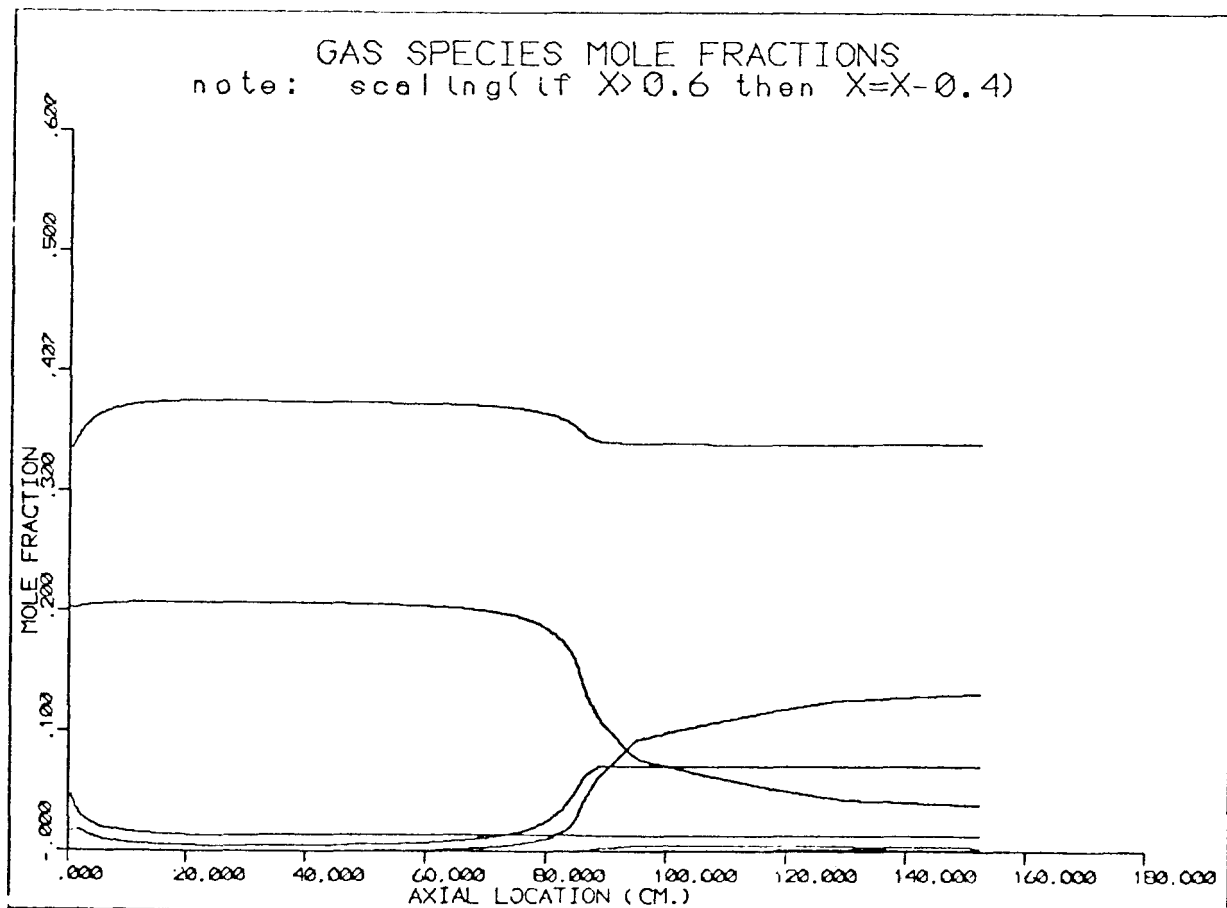
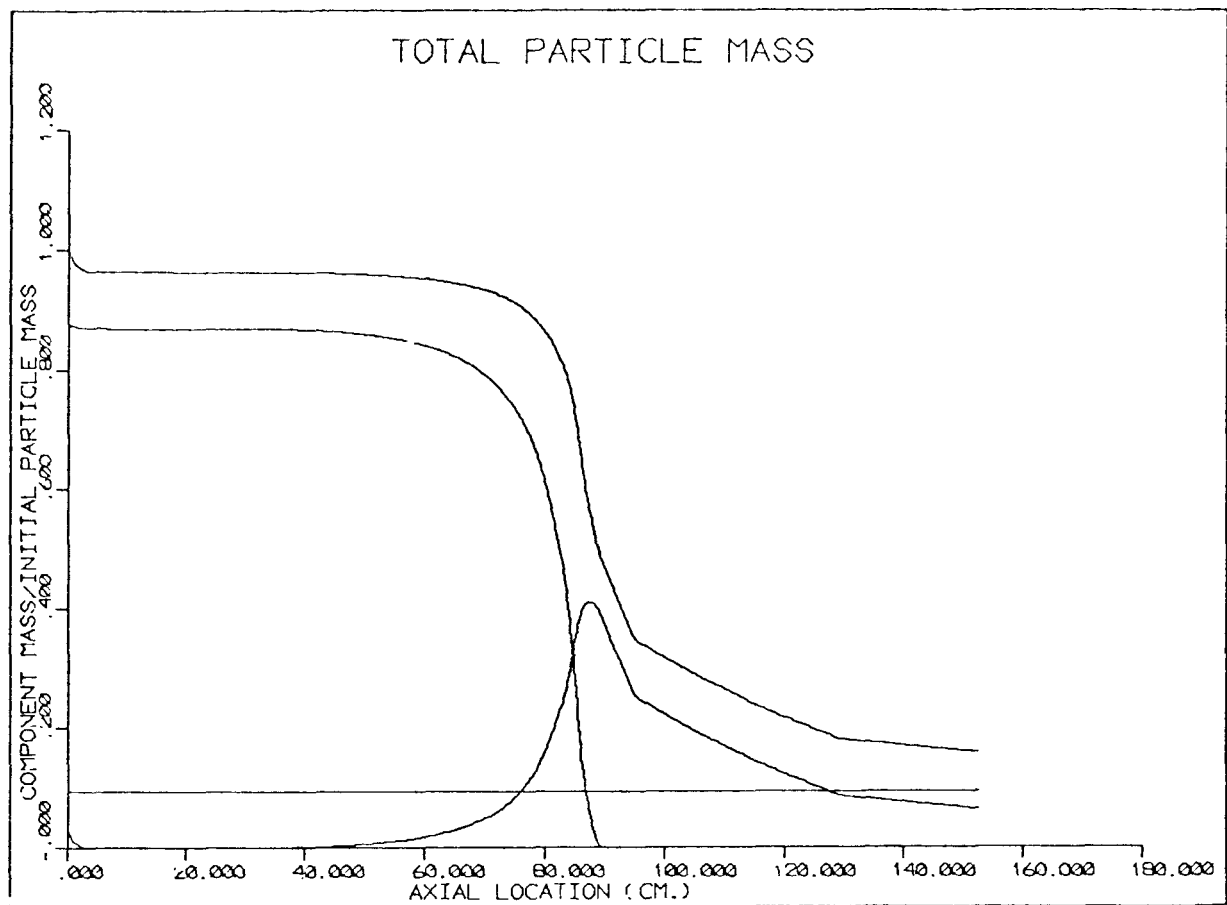
103.02	2.73E+05	.01331	.00079	.06754	.73960	.10249	.07073	.00012	.00000	.00041	.00502
103.63	2.74E+05	.01331	.00081	.06685	.73958	.10316	.07073	.00012	.00000	.00041	.00503
104.24	2.74E+05	.01331	.00084	.06616	.73957	.10383	.07072	.00012	.00000	.00041	.00504
104.85	2.74E+05	.01331	.00087	.06548	.73955	.10449	.07072	.00012	.00000	.00041	.00505
105.46	2.75E+05	.01331	.00089	.06480	.73954	.10515	.07071	.00013	.00000	.00041	.00505
106.07	2.75E+05	.01331	.00092	.06414	.73952	.10580	.07071	.00013	.00000	.00041	.00506
106.68	2.75E+05	.01331	.00095	.06348	.73951	.10644	.07071	.00013	.00000	.00041	.00506
107.29	2.76E+05	.01331	.00098	.06282	.73950	.10708	.07070	.00014	.00000	.00041	.00506
107.90	2.76E+05	.01331	.00100	.06218	.73949	.10771	.07070	.00014	.00000	.00041	.00507
108.51	2.76E+05	.01331	.00103	.06154	.73947	.10833	.07069	.00014	.00000	.00041	.00507
109.12	2.77E+05	.01331	.00106	.06091	.73946	.10895	.07069	.00014	.00000	.00041	.00507
109.73	2.77E+05	.01331	.00109	.06028	.73945	.10956	.07069	.00015	.00000	.00041	.00506
110.34	2.77E+05	.01331	.00111	.05967	.73944	.11016	.07068	.00015	.00000	.00041	.00506
110.95	2.77E+05	.01331	.00114	.05905	.73943	.11076	.07068	.00015	.00000	.00041	.00506
111.56	2.78E+05	.01331	.00117	.05845	.73942	.11135	.07068	.00015	.00000	.00041	.00506
112.17	2.78E+05	.01331	.00120	.05785	.73941	.11194	.07067	.00016	.00000	.00041	.00505
112.78	2.78E+05	.01331	.00122	.05726	.73941	.11252	.07067	.00016	.00000	.00041	.00504
113.39	2.78E+05	.01331	.00125	.05667	.73940	.11309	.07067	.00016	.00000	.00041	.00504
114.00	2.78E+05	.01331	.00129	.05584	.73939	.11391	.07066	.00017	.00000	.00041	.00503
114.60	2.79E+05	.01331	.00132	.05526	.73938	.11447	.07066	.00017	.00000	.00041	.00502
115.21	2.79E+05	.01331	.00135	.05470	.73937	.11503	.07065	.00017	.00000	.00041	.00501
115.82	2.79E+05	.01331	.00137	.05414	.73937	.11558	.07065	.00017	.00000	.00041	.00500
116.43	2.79E+05	.01331	.00140	.05358	.73936	.11612	.07065	.00018	.00000	.00041	.00499
117.04	2.79E+05	.01331	.00143	.05303	.73936	.11666	.07064	.00018	.00000	.00041	.00498
117.65	2.79E+05	.01331	.00145	.05249	.73935	.11720	.07064	.00018	.00000	.00041	.00497
118.26	2.80E+05	.01331	.00148	.05196	.73935	.11772	.07064	.00018	.00000	.00041	.00495
118.87	2.80E+05	.01331	.00150	.05143	.73934	.11825	.07063	.00018	.00000	.00041	.00494
119.48	2.80E+05	.01331	.00153	.05090	.73934	.11877	.07063	.00019	.00000	.00041	.00493
120.09	2.80E+05	.01331	.00155	.05038	.73934	.11928	.07063	.00019	.00000	.00041	.00491
120.70	2.80E+05	.01331	.00158	.04987	.73934	.11979	.07062	.00019	.00000	.00041	.00490
121.31	2.80E+05	.01330	.00160	.04936	.73933	.12029	.07062	.00019	.00000	.00041	.00488
121.92	2.80E+05	.01330	.00163	.04886	.73933	.12079	.07062	.00019	.00000	.00041	.00487
122.53	2.80E+05	.01330	.00165	.04836	.73933	.12128	.07061	.00020	.00000	.00041	.00485
123.14	2.81E+05	.01330	.00167	.04787	.73933	.12177	.07061	.00020	.00000	.00041	.00483
123.75	2.81E+05	.01330	.00170	.04738	.73933	.12225	.07061	.00020	.00000	.00041	.00481
124.36	2.81E+05	.01330	.00172	.04690	.73933	.12273	.07061	.00020	.00000	.00041	.00480
124.97	2.81E+05	.01330	.00174	.04642	.73933	.12321	.07060	.00020	.00000	.00041	.00478
125.58	2.81E+05	.01330	.00176	.04595	.73933	.12368	.07060	.00021	.00000	.00041	.00476
126.19	2.81E+05	.01330	.00178	.04548	.73934	.12414	.07060	.00021	.00000	.00041	.00474
126.80	2.81E+05	.01330	.00180	.04502	.73934	.12460	.07060	.00021	.00000	.00041	.00472
127.41	2.81E+05	.01330	.00182	.04456	.73934	.12506	.07060	.00021	.00000	.00041	.00470
128.02	2.81E+05	.01330	.00184	.04411	.73934	.12551	.07059	.00021	.00000	.00041	.00467
128.63	2.81E+05	.01330	.00186	.04366	.73935	.12596	.07059	.00021	.00000	.00041	.00465
129.24	2.81E+05	.01330	.00188	.04322	.73935	.12640	.07059	.00021	.00000	.00041	.00463
129.84	2.81E+05	.01330	.00185	.04309	.73938	.12657	.07059	.00021	.00000	.00041	.00459
130.45	2.80E+05	.01330	.00181	.04296	.73941	.12674	.07060	.00021	.00000	.00041	.00456
131.06	2.80E+05	.01330	.00178	.04283	.73945	.12690	.07060	.00020	.00000	.00041	.00452
131.67	2.80E+05	.01330	.00175	.04270	.73948	.12706	.07061	.00020	.00000	.00041	.00449
132.28	2.79E+05	.01330	.00172	.04257	.73950	.12723	.07061	.00020	.00000	.00041	.00445
132.89	2.79E+05	.01330	.00169	.04244	.73954	.12739	.07062	.00019	.00000	.00041	.00441
133.50	2.79E+05	.01330	.00166	.04232	.73957	.12755	.07062	.00019	.00000	.00041	.00438
134.11	2.78E+05	.01330	.00163	.04219	.73959	.12771	.07063	.00019	.00000	.00041	.00434
134.72	2.78E+05	.01330	.00161	.04206	.73962	.12787	.07063	.00018	.00000	.00041	.00431
135.33	2.77E+05	.01331	.00158	.04194	.73965	.12802	.07063	.00018	.00000	.00041	.00427
135.94	2.77E+05	.01331	.00155	.04181	.73968	.12818	.07064	.00018	.00000	.00041	.00424
136.55	2.77E+05	.01331	.00152	.04169	.73971	.12834	.07064	.00018	.00000	.00041	.00421
137.16	2.76E+05	.01331	.00150	.04156	.73974	.12849	.07065	.00017	.00000	.00041	.00417
137.77	2.76E+05	.01331	.00147	.04144	.73976	.12865	.07065	.00017	.00000	.00041	.00414
138.38	2.76E+05	.01331	.00145	.04132	.73979	.12880	.07065	.00017	.00000	.00041	.00411
138.99	2.75E+05	.01331	.00142	.04119	.73982	.12895	.07066	.00016	.00000	.00041	.00407

139.60	2.75E+05	.01331	.00140	.04107	.73984	.12910	.07066	.00016	.00000	.00041	.00404
140.21	2.75E+05	.01331	.00137	.04095	.73967	.12925	.07066	.00016	.00000	.00041	.00401
140.82	2.74E+05	.01331	.00135	.04083	.73989	.12940	.07067	.00016	.00000	.00041	.00398
141.43	2.74E+05	.01331	.00133	.04071	.73992	.12955	.07067	.00015	.00000	.00041	.00395
142.04	2.74E+05	.01331	.00130	.04059	.73994	.12970	.07067	.00015	.00000	.00041	.00392
142.65	2.73E+05	.01331	.00128	.04047	.73997	.12985	.07068	.00015	.00000	.00041	.00388
143.26	2.73E+05	.01331	.00126	.04035	.73999	.12999	.07068	.00015	.00000	.00041	.00385
143.87	2.73E+05	.01331	.00124	.04023	.74002	.13014	.07068	.00014	.00000	.00041	.00382
144.48	2.72E+05	.01331	.00122	.04011	.74004	.13028	.07069	.00014	.00000	.00041	.00379
145.08	2.72E+05	.01331	.00120	.04000	.74007	.13043	.07069	.00014	.00000	.00041	.00376
145.69	2.72E+05	.01331	.00117	.03988	.74009	.13057	.07069	.00014	.00000	.00041	.00373
146.30	2.71E+05	.01331	.00115	.03976	.74011	.13071	.07070	.00013	.00000	.00041	.00370
146.91	2.71E+05	.01331	.00113	.03965	.74013	.13085	.07070	.00013	.00000	.00041	.00368
147.52	2.71E+05	.01331	.00112	.03953	.74016	.13100	.07070	.00013	.00000	.00041	.00365
148.13	2.70E+05	.01331	.00110	.03942	.74018	.13113	.07071	.00013	.00000	.00041	.00362
148.74	2.70E+05	.01331	.00108	.03930	.74020	.13127	.07071	.00013	.00000	.00041	.00359
149.35	2.70E+05	.01331	.00106	.03919	.74022	.13141	.07071	.00012	.00000	.00041	.00356
149.96	2.69E+05	.01331	.00104	.03907	.74024	.13155	.07071	.00012	.00000	.00041	.00353
150.57	2.69E+05	.01331	.00102	.03896	.74027	.13169	.07072	.00012	.00000	.00041	.00351
151.18	2.69E+05	.01331	.00100	.03885	.74029	.13182	.07072	.00012	.00000	.00041	.00348
151.79	2.68E+05	.01331	.00099	.03873	.74031	.13196	.07072	.00012	.00000	.00041	.00345
152.40	2.68E+05	.01331	.00097	.03862	.74033	.13209	.07072	.00011	.00000	.00041	.00342

OUTPUT PLOTS FOR SAMPLE CALCULATIONS







Appendix B

1-DICOG PROGRAM FORTRAN LISTING

MAIN.FOR

24-May-79 13:18

PAGE 1

```

00001      COMMON/EDNUM/RHOG,CPG,TG,CPI(20),X(20),CO(5),HGAS,EDNAME(9),
00002      1OXYD(5),GMW,QMASS(9,20),WTM(20)
00003      COMMON/TRUBLE/INDX,ITRBLE
00004      COMMON /RADI/T0(255,5),N0(5),D0(5),SIGMA,PI,E(5),IT(255),H0(5)
00005      1,NUMRDR,DEL,IRAD,T0OLD(5)
00006      COMMON /GENRAL/ALPHA(5),S(20),KG,MUG,DS,
00007      1TPJJ(5),YY(5,5),PRTCLS,SPECIE,
00008      2ELEMNT,CRXN,HRXN,HH(5),HW(5),RGC
00009      COMMON /LAST/GASTMN,TMIN(5),IQ0J(255,5)
00010      COMMON /DIFEGN/OMEGAK(9),ALPHA(5),ALPHAC(5),ALPHAH(5),
00011      1ALPHAW(5),N(5),H(5),QF(5),QCB,QZ(5),P,V,HG(5),RK(5,9),
00012      2RL(5,20),RM(5,20),RC(5),RH(5),RW(5),RR(5),W(5),WG,AREA,PRESSR
00013      COMMON /ODEVAL/XDIS,XTRMNL,VALINT(42),ODESTP
00014      COMMON /APR77/DELTPJ,DELRRJ,ALEN,JFAR,HM,DIFMW,ICNVLM,
00015      1TTEST,SUMSQ,ITRSYS,GAST(255),OSPRR,NPROP,ARMAX,AMIN,SQDIF
00016      COMMON/CONVER/ITRMAX,DYNAMO(3),DYNTM,DYNFLG,DYNFLO
00017      REAL N,N0
00018      INTEGER PRTCLS,ELEMNT,CRXN,BUG,ODESTP,DYNAMO,DYNFLG,DYNFLO
00019      1,OSPRR,ODEST0,OSPRR0
00020      C
00021      C
00022      C*****INITIALIZATION
00023      C
00024          ITRBLE=0
00025          CALL INPUT
00026          CALL VALUE
00027          ITRSYS=0
00028          ODEST0=ODESTP
00029          OSPRR0=OSPRR
00030          HGAS0=HGAS
00031          GMW0=GMW
00032      C
00033      C*****INITIALIZATION AND REINITIALIZATION FOR SECOND ITERATION OR MORE
00034      C
00035      20      ITRSYS=ITRSYS+1
00036              IDISP=0
00037              SUMSQ=0.0
00038              XDIS=0.0
00039              DYNFLG=0
00040              DYNFLO=DYNFLG
00041              ODESTP=ODEST0
00042              OSPRR=OSPRR0
00043              HGAS=HGAS0
00044              GMW=GMW0
00045              IF(IRAD.NE.1)CALL RINTS
00046              DO 25 J=1,PRTCLS
00047                  N(J)=N0(J)
00048                  TPJJ(J)=TMIN(J)
00049      25      H(J)=H0(J)
00050              P=PRESSR
00051      30      CALL SOLVE(IDISP,JX)
00052      C
00053      C*****RESTART INFORMATION WHEN CHANGING STEP SIZE OR SIMPLY RESTARTING

```

```
00054 C
00055 IF(JX.GT.3)JX=JX-1
00056 IDISP=IDISP+JX
00057 IF(DYNFLO.NE.0.OR.DYNFLG.NE.1)GO TO 35
00058 DYNFLO=DYNFLG
00059 ODESTP=ODEST0*DYNAMO(1)
00060 OSPRR=OSPRR0*DYNAMO(1)
00061 IDISP=IDISP*DYNAMO(1)
00062 35 IF(DYNFLO.NE.1.OR.DYNFLG.NE.2)GO TO 40
00063 DYNFLO=DYNFLG
00064 ODESTP=ODEST0*DYNAMO(2)
00065 OSPRR=OSPRR0*DYNAMO(2)
00066 IDISP=(IDISP/DYNAMO(1))*DYNAMO(2)
00067 40 IF(DYNFLO.NE.2.OR.DYNFLG.NE.3)GO TO 45
00068 DYNFLO=DYNFLG
00069 ODESTP=ODEST0/DYNAMO(3)
00070 OSPRR=OSPRR0/DYNAMO(3)
00071 IDISP=(IDISP/DYNAMO(2))/DYNAMO(3)
00072 45 IF(IDISP.LT.(ODESTP-1))GO TO 30
00073 C
00074 C*****TERMINATION
00075 C
00076 SUMSQ=SQRT(SUMSQ/(FLOAT(NUMRDR)+FLOAT(PRTCLS)))
00077 WRITE(3,100)ITRSYS,SUMSQ
00078 CALL RESTR(0)
00079 IF(SUMSQ.GT.SQDIF.AND.ITRSYS.LT.ITRMAX)GO TO 20
00080 CALL OUTPUT
00081 STOP
00082 100 FORMAT(7H0AFTER ,I2,86H ITERATION(S) THROUGH THE REACTOR THE ROOT
00083 1 MEAN SQUARE OF ALL PARTICLE TEMPERATURES IS,F9.3,15H DEGREES
00084 2 KELVIN)
00085 END
```

```
00001      SUBROUTINE ASCALE(X,N,S,XIV,DX,XFV)
00002  C   SCALE IS INCREMENTED IN MULTIPLES OF 1,2,5 OR 6 FROM .01 TO 600
00003  C   OVERRANGE MAKES DX.LT.0.0
00004      DIMENSION X(N)
00005  C   FIND THE MAX AND MIN VALUES OF THE DATA
00006      XMAX=X(1)
00007      XMIN=X(1)
00008      DO 10 I=2,N
00009      IF(X(I).GT.XMAX) XMAX=X(I)
00010      IF(X(I).LT.XMIN) XMIN=X(I)
00011 10     CONTINUE
00012  C   CALCULATE MINIMUM SCALE VALUE AND SCALE INCREMENT
00013      XIV=AINT(XMIN)
00014      DX=.0001
00015      DO 20 I=1,7
00016      DO 15 J=1,5
00017      XI=XIV
00018      IF(J.EQ.2) DX=2.*DX
00019      IF(J.EQ.3) DX=(DX/2.)*2.5
00020      IF(J.EQ.4) DX=(DX/2.5)*5.
00021      IF(J.EQ.5) DX=(DX/5.)*6.
00022      Y=AINT(XI/DX)
00023      XI=Y*DX
00024      IF(Y.EQ.0.0) XI=DX
00025      IF(XI.GT.XMIN) XI=XI-DX
00026      IF(XI+S*DX.GE.XMAX) GOTO 30
00027 15     CONTINUE
00028 20     DX=(DX/6.0)*10.0
00029 30     XIV=XI
00030      IF(DX.LT.1000.0) GO TO 101
00031      DX=-1*DX/2.
00032 101    XFV=XIV+S*DX
00033      RETURN
00034      END
```

```

00001      SUBROUTINE AUX1
00002      COMMON/STIFF/ISASUM,ISTIFF(5),STIFVL
00003      COMMON /LAST/GASTMN,TMIN(5),IQOJ(255,5)
00004      COMMON/EDNUM/RHOG,CPG,TG,CPI(20),X(20),CO(5),HGAS,EDNAME(9),
00005      10XYD(5),GMW,QMASS(9,20),WTM(20)
00006      COMMON /APR77/DELTPJ,DELRRJ,ALEN,JFAR,HM,DIFMW,ICNVLM,
00007      1TTEST,SUMSQ,ITRSYS,GAST(255),OSPRR,NPROP,ARMAX,AMIN,SQDIF
00008      COMMON /IO/DDUCT,DYDXM,AGSTPD,CPVC(3,5,5),HFV(5,5),DELHV(5,5),
00009      1INTCPV(5,5),QRBJ(5)
00010      COMMON/MORE/D01(255,5),N01(255,5),ALFA0(255,5),ALFA0C(255,5),
00011      1ALFA0H(255,5),ALFA0W(255,5),ALFA0A(255,5),X0(255,20),WVG(255)
00012      COMMON /ADD/CCP(5,4,3)
00013      COMMON /AREA13/ALFAC0(5),GAMMA,EK(20),XI(5),AMJ(5,5),
00014      1EMJ(5,5),KVD(5,5),TB,D(5),RHOC(5),RHO(5),DELTA(20),DIFM(20)
00015      2,ALFAH0(5),ALFAW0(5),ALFAA0(5)
00016      COMMON /AREA2/K(20),MU(20),SHRINK,HH0(5),HW0(5),EB,ELAM,
00017      1EUCKEN
00018      COMMON /AREA4/AL(5,5),EL(5,5),MH,PHIJWK(5,9),
00019      1PHIL(5),PHIKL(9,5),PHIVK(5,9,5),KEQ,EMM(5,5)
00020      COMMON /AREA5/NPRINT,TNIRP,CHECK,BUG
00021      COMMON /RADI/T0(255,5),N0(5),D0(5),SIGMA,PI,E(5),IT(255),H0(5)
00022      1,NUMRDR,DEL,IRAD,TOOLD(5)
00023      COMMON /GENRAL/ALPHA(5),S(20),KG,MUG,DS,
00024      1TPJJ(5),YY(5,5),PRTCLS,SPECIE,
00025      2ELEMNT,CRXN,HRXN,HH(5),HW(5),RGC
00026      COMMON/GNRL2/NAME1(20),NAME2(20)
00027      COMMON /DIFEQN/OMEGAK(9),ALPHA(5),ALPHAC(5),ALPHAH(5),
00028      1ALPHAW(5),N(5),H(5),QF(5),QCB,QZ(5),P,V,HG(5),RK(5,9),
00029      2RL(5,20),RM(5,20),RC(5),RH(5),RW(5),RR(5),W(5),WG,AREA,PRESSR
00030      COMMON /ODEVAL/XDIS,XTRMNL,VALINT(42),ODESTP
00031      INTEGER PRTCLS,ELEMNT,SPECIE,BUG,CRXN,SHRINK,ODESTP,OSPRR
00032      REAL IT,IQOJ,N,N0,MH,N01,HOLD,INTCPV,CP(5)
00033      DIMENSION HOLD(5),RHOSIG(5)
00034      C
00035      C*****RADIATION REGIONS
00036      C
00037      IQ=IFIX(FLOAT(JFAR)/FLOAT(OSPRR))+1
00038      IF(JFAR.EQ.ODESTP)IQ=NUMRDR
00039      IF(IRAD.NE.1)GO TO 2
00040      SAJ=0.0
00041      DO 1 J=1,PRTCLS
00042      IF(XDIS.EQ.0.0)D(J)=D0(J)
00043      AJ=(PI/4.0)*E(J)*N(J)*D(J)**2
00044      1   SAJ=AJ+SAJ
00045      2   CONTINUE
00046      C
00047      C*****TOTAL PARTICLE COMPONENT MASS
00048      C
00049      DO 50 J=1,PRTCLS
00050      ALPHA(J)=ALPHAC(J)+ALPHAH(J)+ALPHAW(J)+ALPHA(J)
00051      C
00052      C*****PARTICLE DIAMETER
00053      C

```

```

00054      IF(ALFAC0(J).NE.0.0)D(J)=D0(J)*(1.0+GAMMA*((ALFAC0(J)=
00055      1ALPHAC(J))/ALFAC0(J)))
00056      IF(ALFAC0(J).EQ.0.0)D(J)=D0(J)
00057      IF(SHRINK.EQ.1.AND.ALFAC0(J).EQ.0.0)RHOSIG(J)=
00058      16.0*(ALFAH0(J)+ALFAW0(J)+ALFAA0(J))/(PI*D0(J)**3)
00059      IF(SHRINK.EQ.1.AND.ALPHAC(J).NE.0.0)RHOSIG(J)=6.0*ALPHA(J)/(PI
00060      1*D(J)**3)
00061      IF(SHRINK.EQ.1.AND.ALPHAC(J).EQ.0.0)D(J)=(6.0*ALPHA(J)/(PI
00062      1*RHOSIG(J)))*(1./3.)
00063      IF(ALFAA0(J).EQ.0.0.AND.D(J).LT.1.0E-12)D(J)=1.0E-12
00064      C
00065      C*****PARTICLE DENSITY
00066      C
00067      RHOC(J)=ALPHAC(J)*N(J)
00068      RHOHJ=ALPHAH(J)*N(J)
00069      RHOAJ=ALPHAH(J)*N(J)
00070      RHOAJ=ALPHAH(J)*N(J)
00071      RHO(J)=RHOC(J)+RHOHJ+RHOAJ
00072      C
00073      C*****PARTICLE MASS FRACTIONS
00074      C
00075      OMEGAC=ALPHAC(J)/ALPHA(J)
00076      OMEGAH=ALPHAH(J)/ALPHA(J)
00077      OMEGAW=ALPHAH(J)/ALPHA(J)
00078      OMEGAA=ALPHAH(J)/ALPHA(J)
00079      C
00080      C*****RADIATIVE HEAT TRANSFER WITHIN THE REACTOR
00081      C
00082      QF(J)=PI/4.0*IT(IQ)*N(J)*D(J)**2*E(J)=IQ0J(IQ,J)/
00083      1 ALEN*FLOAT(NUMRDR)
00084      IF(IRAD.NE.1) GO TO 3
00085      IF(IQ.LT.NUMRDR)DTDX=(T0(IQ+1,J)-T00LD(J))*NUMRDR/ALEN
00086      QF(J)=-16.0*SIGMA*T00LD(J)**3*DTDX/(3.0*SAJ*ALEN/FLOAT(NUMRDR))
00087      3 CONTINUE
00088      C
00089      C*****PARTICLE TEMPERATURE -- DOWN TO STATEMENT NUMBER 30
00090      C      NOTE: THE FOLLOWING DO LOOP IS NECCESARY AS A TRIAL AND ERROR
00091      C      APPROACH TO GETTING THE PARTICLE TEMPERATURE SINCE THE
00092      C      HEAT CAPACITY MUST BE KNOWN FIRST AND SINCE HEAT CAPACITY
00093      C      IS A FUNCTION OF TEMPERATURE.
00094      C
00095      TMP=TPJJ(J)
00096      TJ0=TMP
00097      C
00098      C*****STIFF EQUATION ASSUMPTION?
00099      C
00100      IF(ISA$UM.LE.0.OR.ISTIFF(J).NE.1) GO TO 5
00101      C=QZ(J)/(TJ0-TG0)
00102      R=(4.*SIGMA*EB/DS)*(1.-EXP(-ELAM*(PI/4.)*(DS/2.)*N(J)*D(J)**2))
00103      F=QF(J)+R*TB**4+C*TG=RR(J)*HOLD(J)
00104      CC=F/C
00105      DD=R/C
00106      DO 4 L=1,20

```

```
00107      TPJJ0=TMP
00108      TMP=CC-DD*TMP**4
00109      IF (ABS(TMP-TPJJ0).LE.DELTPJ)GO TO 5
00110  4      CONTINUE
00111  5      DO 10 L=1,20
00112      TPJJ0=TMP
00113  C
00114  C*****HEAT CAPACITIES
00115  C
00116      CPCJ=CCP(J,1,1)+CCP(J,1,2)*TMP+CCP(J,1,3)*TMP**2
00117      CPHJ=CCP(J,2,1)+CCP(J,2,2)*TMP+CCP(J,2,3)*TMP**2
00118      CPWJ=CCP(J,3,1)+CCP(J,3,2)*TMP+CCP(J,3,3)*TMP**2
00119      CPAJ=CCP(J,4,1)+CCP(J,4,2)*TMP+CCP(J,4,3)*TMP**2
00120      CP(J)=OMEGAC*CPCJ+OMEGAH*CPHJ+OMEGAW*CPWJ+OMEGAA*CPAJ
00121  C
00122  C*****INITIALIZING PAST PARTICLE ENTHALPY
00123  C
00124      IF(XDIS.LE.0.0)HOLD(J)=H(J)
00125  C
00126  C*****CALCULATING PARTICLE ENTHALPY WHEN THE PSSA STIFF ASSUMPTION IS USED
00127  C
00128      IF(ISASUM.GT.0.AND.ISTIFF(J).EQ.1)H(J)=HOLD(J)+CP(J)*(TMP-TJ0)
00129  C
00130  C*****PARTICLE TEMPERATURE
00131  C
00132      TMP=TJ0+(H(J)-HOLD(J))/CP(J)
00133  C
00134  C*****DEBUG
00135  C
00136      IF (TNIRP.EQ.1.0.AND.BUG.GE.2)
00137  1      WRITE(3,340)CPCJ,CPHJ,CPWJ,CPAJ,CP(J)
00138      IF (TNIRP.EQ.1.0.AND.BUG.GE.2)
00139  1      WRITE(3,350)TMP,H(J),HOLD(J)
00140  C
00141  C*****TEST FOR CONVERGENCE
00142  C
00143      IF (ABS(TMP-TPJJ0).LE.DELTPJ)GO TO 20
00144  10      CONTINUE
00145  20      TPJJ(J)=TMP
00146  C
00147  C*****DEBUG
00148  C
00149      IF (TNIRP.EQ.1.0.AND.BUG.GE.2)
00150  1WRITE(3,310) J,RHOC(J),RHOHJ,RHOWJ,RHOAJ,RHO(J)
00151      IF (TNIRP.EQ.1.0.AND.BUG.GE.1)
00152  1WRITE(3,330) OMEGAC,OMEGAH,OMEGAW,OMEGAA
00153  C
00154  C*****RESETTING OLD ENTHALPY
00155  C
00156  30      HOLD(J)=H(J)
00157  C
00158  C*****CHAR AND WATER ENTHALPY
00159  C
```

```
00160      T1=298.0
00161      T2=TPJJ(J)
00162      DT1=T2-T1
00163      DT2=(T2**2-T1**2)/2.0
00164      DT3=(T2**3-T1**3)/3.0
00165      HH(J)=CCP(J,2,1)*DT1+CCP(J,2,2)*DT2+CCP(J,2,3)*DT3+HH0(J)
00166      HW(J)=CCP(J,3,1)*DT1+CCP(J,3,2)*DT2+CCP(J,3,3)*DT3+HW0(J)
00167      C
00168      C*****INTEGRAL OF HEAT CAPACITY FROM 298KTO PRESENT TEMPERATURE
00169      C      TO BE USED IN AUX3
00170      C
00171      DO 40 M1=1,CRXN
00172      40      INTCPV(J,M1)=CPVC(1,J,M1)*DT1+CPVC(2,J,M1)*DT2+CPVC(3,J,M1)*DT3
00173      C
00174      C*****RADIATIVE HEAT TRANSFER TO SURROUNDINGS
00175      C
00176      QRB(J)=4.0*SIGMA*EB*(TPJJ(J)**4-TB**4)/DS*(1.0-EXP(-ELAM*PI/
00177      14.0*DS/2.0*N(J)*D(J)**2))
00178      C
00179      C*****DEBUG
00180      C
00181      IF(TNIRP.EQ.1.0.AND.BUG.GE.1)WRITE(3,370)J,QRB(J),QF(J)
00182      IF(TNIRP.EQ.1.0.AND.BUG.GE.2)WRITE(3,360)J,HH(J),HW(J)
00183      50      CONTINUE
00184      C
00185      C*****SAVING OLD GAS TEMPERATURE
00186      C
00187      TG0=TG
00188      C
00189      C*****FORMAT STATEMENTS
00190      C
00191      310      FORMAT(1H ,3HJ =,I2,4X,9HRHOC(J) =,E12.5,4X,9HRHOH(J) =,E12.5,4X,
00192      19HRHOW(J) =,E12.5,4X,9HRHOA(J) =,E12.5,4X,4X,9HRHO(J) = ,E12.5)
00193      320      FORMAT(1H0,10X,6HSUMI =,E12.4,10X,6HSUMK =,E12.4)
00194      330      FORMAT(8H OMEGAC=,E12.5,8H OMEGAH=,E12.5,8H OMEGAW=,E12.5,
00195      18H OMEGAA=,E12.5)
00196      340      FORMAT(6H CPCJ=,E12.5,6H CPHJ=,E12.5,6H CPWJ=,E12.5,6H CPAJ=,
00197      1E12.5,7H CP(J)=,E12.5)
00198      350      FORMAT(6H T(J)=,E12.5,6H H(J)=,E12.5,8H HOLD(J),E12.5)
00199      360      FORMAT(4H J =,I2,4X,4X,7HHH(J) =,E12.5,4X,7HHW(J) =,E12.5)
00200      370      FORMAT(4H J =,I2,8X,10HQRB(J) = ,E12.5,8X,8HQF(J) = ,E12.5)
00201      RETURN
00202      END
```

```

00001      SUBROUTINE AUX2PR
00002      C
00003      C*****NOTE:  AUX2PR IS A MODULAR SUBROUTINE WHICH CALCULATES THE PHYSICAL
00004      C      PROPERTIES, TRANSPORT DATA, ETC. THAT DO NOT CHANGE SIGNIFICANTLY
00005      C      FROM ONE POINT TO THE NEXT THROUGH THE REACTOR.  THIS ALLOWS UPDATING
00006      C      TO TAKE PLACE ONLY PERIODICALLY (AS SPECIFIED BY INPUT) AND NOT
00007      C      NECESSARILY AT EVERY O.D.E. STEP.
00008      C
00009      COMMON /APR77/DELTPJ,DELRRJ,ALEN,JFAR,HM,DIFMW,ICNVLM,
00010      1TTEST,SUMSQ,ITRSYS,GAST(255),OSPRR,NPROP,ARMAX,AMIN,SQDIF
00011      COMMON /IO/DDUCT,DYDXM,AGSTPD,CPVC(3,5,5),HFV(5,5),DELHV(5,5),
00012      1INTCPV(5,5),QRB(5)
00013      COMMON/MORE/D01(255,5),N01(255,5),ALFA0(255,5),ALFA0C(255,5),
00014      1ALFA0H(255,5),ALFA0W(255,5),ALFA0A(255,5),X0(255,20),WVG(255)
00015      COMMON /ADD/CCP(5,4,3)
00016      COMMON /AREA13/ALFAC0(5),GAMMA,EK(20),XI(5),AMJ(5,5),
00017      1EMJ(5,5),KVD(5,5),TB,D(5),RHOC(5),RHO(5),DELTA(20),DIFM(20)
00018      2,ALFAH0(5),ALFAW0(5),ALFAA0(5)
00019      COMMON /AREA2/K(20),MU(20),SHRINK,HH0(5),HW0(5),EB,ELAM,
00020      1EUCKEN
00021      COMMON /AREA4/AL(5,5),EL(5,5),MH,PHIJWK(5,9),
00022      1PHIL(5),PHIKL(9,5),PHIVK(5,9,5),KEQ,EMM(5,5)
00023      COMMON /AREA5/NPRINT,TNIRP,CHECK,BUG
00024      COMMON /GENRAL/ALPHA(5),S(20),KG,MUG,DS,
00025      1TPJJ(5),YY(5,5),PRTCLS,SPECIE,
00026      2ELEMNT,CRXN,HRXN,HH(5),HW(5),RGC
00027      COMMON/GNRL2/NAME1(20),NAME2(20)
00028      COMMON /DIFCON/OMEGAK(9),ALPHA(5),ALPHAC(5),ALPHAH(5),
00029      1ALPHAW(5),N(5),H(5),QF(5),QCB,QZ(5),P,V,HG(5),RK(5,9),
00030      2RL(5,20),RM(5,20),RC(5),RH(5),RW(5),RR(5),W(5),WG,AREA,PRESSR
00031      COMMON /EDNUM/RHOG,CPG,TG,CPI(20),X(20),CO(5),HGAS,EDNAME(9),
00032      1OXYD(5),GMW,GMASS(9,20),WTM(20)
00033      INTEGER PRTCLS,SPECIE,EUCKEN,BUG,EDNAME,H2O,CO2,O2
00034      REAL KG,MUG,K,MU,MH,N
00035      DATA H2O/'H2O'/,CO2/'CO2'/,O2/'O2'/
00036      C
00037      C*****COLLISION INTEGRAL FOR VISCOSITY
00038      C
00039      DO 10 I1=1,SPECIE
00040      TEK=TG/EK(I1)
00041      COLMU=SIGMAM(TEK,DELTA(I1))
00042      C
00043      C*****DEBUG
00044      C
00045      IF (TNIRP.EQ.1.0.AND.BUG.GE.4) WRITE(3,410) NAME1(I1),NAME2(I1),
00046      1COLMU
00047      C
00048      C*****SPECIE VISCOSITY AND THERMAL CONDUCTIVITY
00049      C
00050      MU(I1)=2.67E-05*SQRT(WTM(I1)*TG)/(S(I1)**2*COLMU)
00051      K(I1)=1.25*(CPI(I1)+RGC/(2.0*WTM(I1)))*MU(I1)
00052      IF (EUCKEN.EQ.1) K(I1)=(CPI(I1)+1.25*RGC/WTM(I1))*MU(I1)
00053      C

```

```
00054 C*****DEBUG
00055 C
00056 10 IF (TNIRP.EQ.1.0.AND.BUG.GE.3) WRITE(3,310) NAME1(I1),NAME2(I1),
00057 1K(I1),MU(I1)
00058 C
00059 C*****MIXTURE VISCOSITY AND THERMAL CONDUCTIVITY
00060 C
00061 SUMXMU=0.0
00062 SUMXK=0.0
00063 DO 20 I2=1,SPECIE
00064 SUMXFI=0.0
00065 DO 30 K1=1,SPECIE
00066 PHI1K=.3535534*SQRT(1.0/((1.0+WTM(I2)/WTM(K1))))*(1.0+SQRT(MU(I2)
00067 1/MU(K1)))*(WTM(K1)/WTM(I2))**(0.25))**2
00068 C
00069 C*****DEBUG
00070 C
00071 IF (TNIRP.EQ.1.0.AND.BUG.GE.4) WRITE(3,420) I2,K1,PHI1K
00072 30 SUMXFI=SUMXFI+X(K1)*PHI1K
00073 IF(X(I2).LT.1.0E-30)GO TO 20
00074 SUMXK=SUMXK+X(I2)*K(I2)/SUMXFI
00075 SUMXMU=SUMXMU+X(I2)*MU(I2)/SUMXFI
00076 20 CONTINUE
00077 KG=SUMXK
00078 MUG=SUMXMU
00079 C
00080 C*****DEBUG
00081 C
00082 IF (TNIRP.EQ.1.0.AND.BUG.GE.2)WRITE(3,220)KG,MUG
00083 C
00084 C*****CONVECTIVE HEAT TRANSFER COEFICIENT FROM GAS TO WALL
00085 C
00086 REG=DS*WG/(ARMAX*MUG)
00087 PRG=CPG*MUG/KG
00088 HM=0.023*KG/DS*REG**(0.8)*PRG**(1.0/3.0)
00089 C
00090 C*****DEBUG
00091 C
00092 IF (TNIRP.EQ.1.0.AND.BUG.GE.4) WRITE(3,440) PRG,REG,HM
00093 C
00094 C*****DIFFUSIVITIES
00095 C
00096 DIFMW=0.0
00097 DO 50 I1=1,SPECIE
00098 IF(NAME1(I1).NE.H2O.AND.NAME1(I1).NE.CO2.AND.
00099 1NAME1(I1).NE.O2)GO TO 50
00100 SUMXD=0.0
00101 DO 40 KI=1,SPECIE
00102 IF (I1.EQ.KI) GO TO 40
00103 TEK=TG/SQRT(EK(I1)*EK(KI))
00104 COLDIF=SIGMAD(TEK)
00105 DIF=0.00186*TG**(1.5)*SQRT(1.0/WTM(I1)+1.0/WTM(KI))/(P*((S(I1)+
00106 1S(KI))/2.0)**2*COLDIF)
```

```
00107      IF(TNIRP.EQ.1.0.AND.BUG.GE.4)WRITE(3,S10)NAME1(I1),NAME2(I1),
00108      1NAME1(KI),NAME2(KI),COLDIF,DIF
00109      SUMXD=SUMXD+X(KI)/DIF
00110  40      CONTINUE
00111      DIFM(I1)=(1.0-X(I1))/SUMXD
00112      IF(TNIRP.EQ.1.0.AND.BUG.GE.4)WRITE(3,S15)NAME1(I1),NAME2(I1),
00113      1DIFM(I1)
00114      IF(NAME1(I1).NE.H2O)GO TO 50
00115      DIFMW=DIFM(I1)
00116  50      CONTINUE
00117  410      FORMAT(1H ,2A6,10X,30HVISCOSITY COLLISION INTEGRAL =,F10,4)
00118  420      FORMAT(1H ,3HI =,I4,4X,3HK =,I4,4X,23HINTERACTION PARAMETER =,
00119      1E12,5)
00120  440      FORMAT(1H ,16HPRANDTL NUMBER =,E12,5,10X,17HREYNOLDS NUMBER =,E12,
00121      15,10X,6HHBAR =,E12,5)
00122  310      FORMAT(1H ,2A6,10X,22HTHERMAL CONDUCTIVITY =,E12,5,10X,
00123      11HVISCOSITY =,E12,5)
00124  510      FORMAT(1H ,4A6,32HDIFFUSIVITY COLLISION INTEGRAL =,F10,4,4X,5HDIF
00125      1=,E12,5)
00126  515      FORMAT(1H ,2A6,24HDIFFUSIVITY IN MIXTURE= ,E12,5)
00127  220      FORMAT(1H ,3HKG=,E12,5,5H MUG=,E12,5)
00128      RETURN
00129      END
```

```

00001      SUBROUTINE AUX3
00002      COMMON /APR77/DELTPJ,DELRRJ,ALEN,JFAR,HM,DIFMW,ICNVLN,
00003      1TTEST,SUMSQ,ITRYS,GAST(255),OSPRR,NPROP,ARMAX,AMIN,SQDIF
00004      COMMON /IO/DDUCT,DYDXM,AGSTPD,CPVC(3,5,5),HFV(5,5),DELHV(5,5),
00005      1INTCPV(5,5),QRB(5)
00006      COMMON /H2OP/IVPFLG,VPRCOF(5)
00007      COMMON /ADD/CCP(5,4,3)
00008      COMMON /AREA13/ALFAC(5),GAMMA,EK(20),XI(5),AMJ(5,5),
00009      1EMJ(5,5),KVD(5,5),TB,D(5),RHOC(5),RHO(5),DELTA(20),DIFM(20)
00010      2,ALFAH(5),ALFAW(5),ALFAA(5)
00011      COMMON /AREA4/AL(5,5),EL(5,5),MH,PHIJWK(5,9),
00012      1PHIL(5),PHIKL(9,5),PHIVK(5,9,5),KEQ,EMM(5,5)
00013      COMMON /AREA5/NPRINT,TNIRP,CHECK,BUG
00014      COMMON /ODEVAL/XDIS,XTRMNL,VALINT(42),ODESTP
00015      COMMON /EDNUM/RHOG,CPG,TG,CPI(20),X(20),CO(5),HGAS,EDNAME(9),
00016      1OXYD(5),GMW,QMASS(9,20),WTM(20)
00017      COMMON /RADI/TO(255,5),NO(5),DO(5),SIGMA,PI,E(5),IT(255),HO(5)
00018      1,NUMRDR,DEL,IRAD,TOOLD(5)
00019      COMMON /DIFEQN/OMEGAK(9),ALPHA(5),ALPHAC(5),ALPHAH(5),
00020      1ALPHAW(5),N(5),H(5),QF(5),QCB,QZ(5),P,V,HG(5),RK(5,9),
00021      2RL(5,20),RM(5,20),RC(5),RH(5),RW(5),RR(5),W(5),WG,AREA,PRESSR
00022      COMMON /GENRAL/ALPHA(5),S(20),KG,MUG,DS,
00023      1TPJJ(5),YY(5,5),PRTCLS,SPECIE,
00024      2ELEMNT,CRXN,HRXN,HH(5),HW(5),RGC
00025      COMMON/GNRAL2/NAME1(20),NAME2(20)
00026      INTEGER PRTCLS,SPECIE,BUG,HRXN,CRXN,EDNAME,ELEMNT,ODESTP,
00027      1OXYD,OSPRR
00028      DOUBLE PRECISION DENOM,BJJ,BJM,BJWJ
00029      REAL KCJ(5),KVD,N,KG,KMJ,NAME1,NAME2,NJ,MHC,KL,MH,INTCPV
00030      DIMENSION RCJ(5),RHJL(5),RVJ(5)
00031      DATA H2O/4HH2O /,CO2/4HCO2 /,O2/4HO2 /
00032      C
00033      C*****PICKING OUT H2O MOLE FRACTION
00034      C
00035          XM=0.0
00036          DO 5 I=1,SPECIE
00037              IF(NAME1(I).NE.H2O)GO TO 5
00038              XM=X(I)
00039      5      CONTINUE
00040      C
00041      C*****HEAT TRANSFER TO THE WALL BY CONVECTION
00042      C
00043          QCB=4.0*HM*(TG-TB)/DS
00044          IF(TNIRP.EQ.1.0.AND.BUG.GE.1)WRITE(3,200)QCB
00045      C
00046      C*****IDEAL GAS CONCENTRATION
00047      C
00048          CG=P/(82.057*TG)
00049          IF (TNIRP.EQ.1.0.AND.BUG.GE.3) WRITE(3,420) CG
00050      C
00051      C*****THE REMAINDER OF THE CALCULATIONS IN THIS SUBROUTINE ARE DONE FOR
00052      C      EACH PARTICLE.
00053      C

```

```
00054      DO 10 J=1,PRTCLS
00055      C
00056      C*****COMPUTATIONAL INITIALIZATION
00057      C
00058          DJ=D(J)
00059          NJ=N(J)
00060          TJ=TPJJ(J)
00061          RRJ=RR(J)
00062          IF(XDIS.EQ.0.0)RRJ=0.0
00063          RHOJ=RHO(J)
00064      C
00065      C*****PARTICLE AREA
00066      C
00067          AJ=PI*DJ**2
00068      C
00069      C*****MORE INITIALIZATION
00070      C
00071          SRHJM=0.0
00072          SRVJM=0.0
00073          SRHVJM=0.0
00074          RC(J)=0.0
00075      C
00076      C*****COAL REACTION RATES (PYROLYSIS)
00077      C
00078          IF(ALPHAC(J).LE.0.0)GO TO 21
00079          DO 20 M1=1,CRXN
00080              KMJ=AMJ(J,M1)*EXP(-EMJ(J,M1)/(RGC*TJ))
00081              RVJ(M1)=KMJ*YY(J,M1)*RHOC(J)
00082              IF (TNIRP.EQ.1.0.AND.BUG.GE.3) WRITE(3,440) J,M1,KMJ,RVJ(M1)
00083              RHJM=RVJ(M1)*(1.0-YY(J,M1))/YY(J,M1)
00084              RCJM= (RHJM+RVJ(M1))
00085              IF (TNIRP.EQ.1.0.AND.BUG.GE.2) WRITE(3,311) J,M1,RHJM,RCJM
00086              SRHJM=SRHJM+RHJM
00087              SRVJM=SRVJM+RVJ(M1)
00088              SRHVJM=SRHVJM+(RVJ(M1)*(INTCPV(J,M1)+HFV(J,M1)))
00089      20      RC(J)=RC(J)-RCJM
00090          GO TO 23
00091      21      DO 22 M1=1,CRXN
00092      22      RVJ(M1)=0.0
00093      23      IF (TNIRP.EQ.1.0.AND.BUG.GE.1) WRITE(3,211) J,I2,RC(J)
00094      C
00095      C*****THE FOLLOWING DO LOOP IS NEEDED SINCE MANY OF THE PARAMETERS ARE
00096      C      DEPENDANT ON TOTAL REACTION RATE AND TOTAL REACTION RATE IN TURN
00097      C      IS DEPENDANT ON EACH OF THESE PARAMETERS. IN OTHER WORDS IT IS A
00098      C      TRIAL AND ERROR SOLTION FOR REACTION RATES.
00099      C
00100          DO 47 IR=1,20
00101              RHL=0.0
00102              RR0=RRJ
00103      C
00104      C*****HEAT TRANSFER BLOWING PARAMETER AND CORRECTION FACTOR
00105      C
00106          BJ=RRJ*CPG/(2.0*PI*DJ*KG*NJ)
```

```

00107      IF (TNIRP.EQ.1.0.AND.BUG.GE.2) WRITE(3,310) J,BJ
00108      FAC=1.0
00109      IF(BJ.LE.1.0E-7)GO TO 91
00110      BJJ=BJ
00111      DENOM=DEXP(BJJ)-1.0
00112      FAC=BJ/DENOM
00113  91      CONTINUE
00114  C
00115  C*****MASS TRANSFER BLOWING PARAMETER AND CORRECTION FACTOR FOR EACH OXIDIZER
00116  C
00117      DO 90 L=1,HRXN
00118      I=OXYD(L)
00119      BJM=RRJ/(2.0*PI*DIFM(I)*RHOG*DJ*NJ)
00120      IF (TNIRP.EQ.1.0.AND.BUG.GE.2)WRITE(3,309)J,BJM
00121      FACM=1.0
00122      IF(BJM.LT.1.0E-7)GO TO 65
00123      BJMJ=BJM
00124      DENOM=DEXP(BJMJ)-1.0
00125      FACM=BJM/DENOM
00126  65      CONTINUE
00127  C
00128  C*****MASS TRANSFER COEFFICIENTS
00129  C
00130      IF(X(I).NE.0.0)GO TO 69
00131      KCJ(L)=1.0
00132      GO TO 90
00133  69      KCJ(L)=2.0*DIFM(I)*FACM/DJ
00134  90      CONTINUE
00135  C
00136  C*****CONVECTIVE - CONDUCTIVE HEAT TRANSFER BETWEEN THE GAS AND PARTICLE
00137  C
00138      QZ(J)=2.0*PI*FAC*KG*DJ*NJ*(TJ-TG)
00139  C
00140  C*****WATER VAPORIZATION RATE
00141  C
00142      IF(ALPHAW(J).LE.0.0)GO TO 50
00143      IF(IVPFLG.EQ.0)PEJ=10.0**((7.9484-(1656.39/(226.86+(TJ-273.0
00144      1))))/760.0
00145      IF(IVPFLG.NE.0)PEJ=VPRCOF(1)+VPRCOF(2)*TJ+VPRCOF(3)*TJ
00146      1**2+VPRCOF(4)*TJ**3+VPRCOF(5)*TJ**4
00147      XWJ=PEJ/P
00148      IF(XWJ.GT.1.0)XWJ=1.0
00149      IF (TNIRP.EQ.1.0.AND.BUG.GE.3) WRITE(3,430) J,AJ,PEJ,XWJ
00150      BJW=RRJ/(2.0*PI*DIFMW*RHOG*DJ*NJ)
00151      FACW=1.0
00152      IF(BJW.LT.1.0E-7)GO TO 57
00153      BJWJ=BJW
00154      DENOM=DEXP(BJWJ)-1.0
00155      FACW=BJW/DENOM
00156  57      CONTINUE
00157      RWJ=2.0*PI*FACW*CG*DJ*NJ*18.01*(XWJ-XM)*DIFMW + XWJ*RRJ
00158      GO TO 44
00159  50      RWJ=0.0

```

```

00160 44 CONTINUE
00161 C
00162 C*****CHAR REACTION RATES FOR EACH OXIDIZER
00163 C
00164 DO 45 L=1,HRXN
00165 LL=OXYD(L)
00166 IF(ALPHAH(J).LE.0.0.AND.ALPHAC(J).LE.0.0)GO TO 49
00167 KL=EXP(ALOG(AL(J,L))+EMM(J,L)*ALOG(TJ)=EL(J,L)/(RGC*TJ))
00168 IF (KEQ.EQ.1.AND.NAME1(LL).EQ.02)KL=-1.68*TJ+1.32E-3*TJ*TJ
00169 IF(KL.LT.1.0E-30)GO TO 49
00170 RHJL(L)=(AJ*NJ)**2*MH*PHIL(L)*GMW*KCJ(L)*KL*XI(J)*CO(L)*CG/
00171 1(GMW*AJ*NJ*CG*(XI(J)*KL+KCJ(L))+RRJ)
00172 IF(RHJL(L).LT.0.0)GO TO 49
00173 GO TO 46
00174 RHJL(L)=0.0
00175 46 IF (TNIRP.EQ.1.0.AND.BUG.GE.3) WRITE(3,421) J,L,KL
00176 IF (TNIRP.EQ.1.0.AND.BUG.GE.2) WRITE(3,330) J,L,RHJL(L)
00177 45 RHL=RHL+RHJL(L)
00178 C
00179 C*****TOTAL REACTION RATE
00180 C
00181 RRJ=RHL+SRVJM+RWJ
00182 IF(RRJ.LT.0.0)RRJ=0.0
00183 IF(RRJ.EQ.0.0.AND.RR0.EQ.0.0)GO TO 48
00184 IF(RRJ.EQ.0.0.AND.RR0.NE.0.0)GO TO 47
00185 IF(ABS((RR0-RRJ)/RRJ).LT.DELRRJ)GO TO 48
00186 47 CONTINUE
00187 48 CONTINUE
00188 RW(J)=RWJ
00189 IF (TNIRP.EQ.1.0.AND.BUG.GE.1) WRITE(3,210) J,RW(J),QZ(J)
00190 IF(TNIRP.EQ.1.0.AND.BUG.GE.2)WRITE(3,230)RHL,SRHJM,SRVJM,SRHVJM
00191 C
00192 C*****ELEMENTAL REACTION RATES FROM STOICHIOMETRIC COEFFICIENTS
00193 C
00194 DO 11 K=1,ELEMNT
00195 RK(J,K)=RW(J)*PHIJWK(J,K)
00196 SMPHIL=0.0
00197 DO 51 L=1,HRXN
00198 51 SMPHIL=SMPHIL+PHIKL(K,L)*RHJL(L)
00199 RK(J,K)=RK(J,K)+SMPHIL
00200 SMPHIV=0.0
00201 DO 61 M3=1,CRXN
00202 61 SMPHIV=SMPHIV+PHIVK(J,K,M3)*RVJ(M3)
00203 RK(J,K)=RK(J,K)+SMPHIV
00204 IF (TNIRP.EQ.1.0.AND.BUG.GE.1) WRITE(3,220) J,K,RK(J,K)
00205 11 CONTINUE
00206 C
00207 C*****TOTAL CHAR REACTION RATE
00208 C
00209 RH(J)=SRHJM-RHL
00210 IF(ALPHAC(J).LE.0.0.AND.ALPHAH(J).LE.0.0)RH(J)=0.0
00211 C
00212 C*****ENTHALPY OF REACTION PRODUCTS FROM PARTICLE GIVEN TO GAS

```

```
00213 C
00214 IF(RRJ.EQ.0.0)HG(J)=0.0
00215 IF(RRJ.EQ.0.0)GO TO 12
00216 HG(J)=(SRHVJM+RHL*HH(J)+RW(J)*HW(J))/RRJ
00217 12 RR(J)=RRJ
00218 IF (TNIRP.EQ.1.0.AND.BUG.GE.1) WRITE(3,240) J,RR(J),RH(J),HG(J)
00219 10 CONTINUE
00220 421 FORMAT(1H ,4HJ =,I2,4X,3HL =,I2,4X,4HKL =,E12.5)
00221 311 FORMAT(1H ,3HJ =,I2,4X,3HM =,I2,4X,6HRHJM =,E12.5,4X,6HRCJM =,
00222 1E12.5)
00223 320 FORMAT(1H ,3HM =,I2,4X,6HRHCM =,E12.5)
00224 330 FORMAT(1H ,3HJ =,I2,4X,3HL =,I2,4X,6HRHJL =,E12.5)
00225 211 FORMAT(1H ,3HJ =,I2,4X,3HI =,I3,4X,7HRC(J) =,E12.5,4X)
00226 220 FORMAT(1H ,3HJ =,I2,4X,3HK =,I2,4X,9HRK(J,K) =,E12.5)
00227 230 FORMAT(1H ,4HRHL=,E12.5,7H SRHJM=,E12.5,7H SRVJM=,E12.5,7HSRVHJM=,
00228 1E12.5)
00229 240 FORMAT(1H ,3HJ =,I2,4X,7HRR(J) =,E12.5,4X,7HRH(J) =,E12.5,4X,
00230 17HHG(J) =,E12.5)
00231 200 FORMAT(1H ,4HQCB=,E12.5)
00232 420 FORMAT(1H ,19HGAS CONCENTRATION =,E12.5)
00233 430 FORMAT(1H ,3HJ =,I2,4X,6HA(J) =,E12.5,4X,5HPEJ =,E12.5,4X,5HXWJ =,
00234 1E12.5)
00235 440 FORMAT(1H ,3HJ =,I2,4X,3HM =,I2,4X,5HKMJ =,E12.5,4X,
00236 19HRV(J,M)= ,E12.5)
00237 309 FORMAT(1H ,3HJ =,I2,4X,7HBM(J) =,E12.5)
00238 310 FORMAT(1H ,3HJ =,I2,4X,6H8(J) =,E12.5)
00239 210 FORMAT(1H ,3HJ =,I2,4X,7HRW(J) =,E12.5,4X,7H0Z(J) =,E12.5)
00240 RETURN
00241 END
```

```

00001      SUBROUTINE DIFF(YT,VECFUN,DX)
00002      COMMON /APR77/DELTPJ,DELRRJ,ALEN,JFAR,HM,DIFMW,ICNVLM,
00003      1TTEST,SUMSQ,ITRSYS,GAST(255),OSPRR,NPROP,ARMAX,AMIN,SQDIF
00004      COMMON /IO/DDUCT,DYDXM,AGSTPD,CPVC(3,5,5),HFV(5,5),DELHV(5,5),
00005      1INTCPV(5,5),QRB(5)
00006      COMMON /RADI/T0(255,5),N0(5),D0(5),SIGMA,PI,E(5),IT(255),H0(5)
00007      1,NUMRDR,DEL,IRAD,TOOLD(5)
00008      COMMON /ODEVAL/XDIS,XTRMNL,VALINT(42),ODESTP
00009      COMMON /GENRAL/ALPHA(5),S(20),KG,MUG,DS,
00010      1TPJJ(5),YY(5,5),PRTCLS,SPECIE,
00011      2ELEMNT,CRXN,HRXN,HH(5),HW(5),RGC
00012      COMMON/GNRL2/NAME1(20),NAME2(20)
00013      COMMON /EDNUM/RHOG,CPG,TG,CPI(20),X(20),CO(5),HGAS,EDNAME(9),
00014      1OXYD(5),GMW,QMASS(9,20),WTM(20)
00015      COMMON /DIFEGN/OMEGAK(9),ALPHA(5),ALPHAC(5),ALPHAH(5),
00016      1ALPHAW(5),N(5),H(5),OF(5),QCB,QZ(5),P,V,HG(5),RK(5,9),
00017      2RL(5,20),RM(5,20),RC(5),RH(5),RW(5),RR(5),W(5),WG,AREA,PRESSR
00018      COMMON /CONST/OSGKM(9),OPGKM(9),SJM(3,5),PJMC(4,5),SJH(5),
00019      1PJHN(5),SGMC(3),PGMC(4),PGHN,SGHI,PGX,PJX(5)
00020      COMMON /AREA5/NPRINT,TNIRP,CHECK,BUG
00021      DIMENSION YT(42),VECFUN(42),SGKM(9),PGKM(9),SJM(5),PJM(5)
00022      1,OPGKM(9),PJH(5)
00023      REAL N
00024      INTEGER ELEMNT,PRTCLS,CRXN,BUG,EDNAME,ODESTP
00025      C
00026      C*****INITIALIZATION
00027      C
00028      KK=ELEMNT
00029      J=PRTCLS
00030      TNIRP=0.0
00031      JFAR=IFIX(XDIS*FLOAT(ODESTP)/ALEN)
00032      IF(MOD(JFAR,NPRINT).EQ.0.OR.XDIS.EQ.0.0)TNIRP=1.0
00033      SWITCH=0.0
00034      IF(TNIRP.EQ.1.0.AND.BUG.GE.1)SWITCH=1.0
00035      AZ=ARMAX
00036      C
00037      C*****REINITIALIZATION FOR BEGINING OF REACTOR
00038      C
00039      IF(XDIS.NE.0.0)GO TO 113
00040      PGHI=PGHN
00041      DO 111 L=1,KK
00042      111   OPGKM(L)=OPGKM(L)
00043      DO 112 IC=1,J
00044      112   PJH(IC)=PJHN(IC)
00045      C
00046      C*****CALCULATION OF RECIRCULATION AND SECONDARY MIXING PARAMETERS
00047      C      FIRST EVERYTHING IS ZEROED OUT.
00048      C
00049      113   SGM=0.0
00050      PGM=0.0
00051      DO 1 L=1,KK
00052      SGKM(L)=0.0
00053      1   PGKM(L)=0.0

```

```

00054      DO 2 IC=1,J
00055      SJM(IC)=0.0
00056      2    PJM(IC)=0.0
00057      C
00058      C*****THEN IF WE ARE NOT YET OUTSIDE THE SPECIFIED MIXING REGION WE
00059      C    CALCULATE THE MIXING PARAMETERS.
00060      C
00061      IF(XDIS.GE.AGSTPD)GO TO 6
00062      AZ=PI*(DDUCT/2.0+DYDXM*XDIS)**2
00063      SGM=SGMC(1)*XDIS*XDIS+SGMC(2)*XDIS+SGMC(3)
00064      PGM=PGMC(1)*XDIS**3+PGMC(2)*XDIS*XDIS+PGMC(3)*XDIS+PGMC(4)
00065      DO 3 L=1,KK
00066      SGKM(L)=OSGKM(L)*SGM
00067      3    PGKM(L)=OPGKM(L)*PGM
00068      DO 4 IC=1,J
00069      SJM(IC)=SJM(1,IC)*XDIS*XDIS+SJM(2,IC)*XDIS+SJM(3,IC)
00070      4    PJM(IC)=PJM(1,IC)*XDIS**3+PJM(2,IC)*XDIS*XDIS+PJM(3,IC)
00071      1*XDIS+PJM(4,IC)
00072      C
00073      C*****DEBUG
00074      C
00075      6    IF(SWITCH.EQ.1.0)WRITE(3,210)AZ
00076      C
00077      C*****NOW WE BEGIN THE ACTUAL FUNCTION OF THIS SUBROUTINE WHICH IS TO
00078      C    EVALUATE EACH FUNCTION AT THIS PARTICULAR LOCATION IN THE REACTOR
00079      C
00080      AREA=AZ
00081      CALL RODEVL(YT,ELEMNT,PRTCLS)
00082      CALL EDWRDS
00083      C
00084      C*****NOTE THAT VELOCITY, NUMBER PARTICLE DENSITY AND SECONDARY AND
00085      C    RECIRCULATION ENTHALPIES MUST BE HANDLED HERE INSTEAD OF
00086      C    IN RODEVL SINCE THEY REQUIRE INFORMATION WHICH MUST
00087      C    COME FROM EDWRDS.
00088      C
00089      V=WG/(RHOG*AREA)
00090      DO 5 IC=1,J
00091      IDX=IC+ELEMNT+2*PRTCLS+1
00092      5    N(IC)=YT(IDX)/(V*AZ)
00093      SGH=SGHI+HGAS-CPG*(TC-298)
00094      PGH=PHGI+HGAS-CPG*(TC-298)
00095      C
00096      C*****DEBUG
00097      C
00098      IF(SWITCH.EQ.1.0)WRITE(3,240)V,(N(JX),JX=1,PRTCLS)
00099      C
00100      C*****EVALUATING THE AUXILIARY EQUATIONS
00101      C
00102      CALL AUX1
00103      IF(MOD(JFAR,NPROP).EQ.0.OR.JFAR.EQ.1)CALL AUX2PR
00104      CALL AUX3
00105      C
00106      C*****TEST FOR THE LOCATION IN THE REACTOR TO SEE IF WE SHOULD BE SAVING

```

```

00107 C THE PROPERTIES NEEDED FOR RECIRCULATION FOR THE NEXT SYSTEM
00108 C ITERATION.
00109 C
00110 IF((XDIS.LT.(PGX-DX/2.)),OR.(XDIS.GE.(PGX+DX/2.)))GO TO 8
00111 PGHN=PGX*(IC-298) HGAS
00112 DO 7 L=1, KK
00113 7 OPGKMN(L)=OMEGAK(L)
00114 8 DO 9 IC=1, J
00115 IF((XDIS.LT.(PJX(IC)-DX/2.)),OR.(XDIS.GE.(PJX(IC)+DX/2.)))GO TO 9
00116 PJHN(IC)=H(IC)
00117 9 CONTINUE
00118 C
00119 C*****NOW UPDATE EACH OF THE DIFFERENTIAL EQUATIONS AND SAVE THEM IN VECFUN.
00120 C
00121 AB=AZ
00122 DO 10 L=1, KK
00123 SUM1=0.0
00124 DO 11 IC=1, J
00125 11 SUM1=SUM1+RK(IC, L)
00126 10 VECFUN(L)=AZ*SUM1+SGKM(L)+PGKM(L)
00127 DO 20 L=KK+1, KK+J
00128 - IDX=L-KK
00129 20 VECFUN(L)=-AZ*RR(IDX)+SJM(IDX)+PJM(IDX)
00130 SUM1=0.0
00131 SUM2=0.0
00132 L=KK+J+1
00133 DO 31 IC=1, J
00134 SUM1=SUM1+QZ(IC)
00135 31 SUM2=SUM2+RR(IC)*HG(IC)
00136 VECFUN(L)=SGH*SGM+PGH*PGM+AZ*(SUM1+SUM2)-AB*QCB
00137 DO 40 L=KK+J+2, KK+2*J+1
00138 IDX=L-(KK+J+1)
00139 40 VECFUN(L)=SJM(IDX)*SJH(IDX)+PJM(IDX)*PJH(IDX)+AZ*(QF(IDX)-
00140 1QZ(IDX)-RR(IDX)*H(IDX))-AB*QRBJ(IDX)
00141 DO 60 L=KK+2*J+2, KK+3*J+1
00142 IDX=L-(KK+2*J+1)
00143 60 VECFUN(L)=(PJM(IDX)+SJM(IDX))/ALPHA(IDX)
00144 L=KK+3*J+2
00145 SUM1=0.0
00146 DO 81 IC=1, J
00147 81 SUM1=SUM1+RR(IC)
00148 VECFUN(L)=AZ*SUM1+SGM+PGM
00149 DO 90 IDX=1, J
00150 L1=KK+3*J+2+IDX
00151 L2=L1+J
00152 L3=L2+J
00153 VECFUN(L1)=RC(IDX)/(N(IDX)*V)
00154 VECFUN(L2)=RH(IDX)/(N(IDX)*V)
00155 VECFUN(L3)=-RW(IDX)/(N(IDX)*V)
00156 90 CONTINUE
00157 210 FORMAT(5H AZ= ,E12.5)
00158 240 FORMAT(4H V= ,E12.4,7H N(J)= ,5E12.4)
00159 RETURN

```

DIFF.FOR

24-May-79 13:21

PAGE 1-3

00160

END

```

00001      SUBROUTINE EDWRDS
00002      COMMON /APR77/DELTPJ,DELRRJ,ALEN,JFAR,HM,DIFMW,ICNVLM,
00003      1TTEST,SUMSQ,ITRSYS,GAST(255),OSPRR,NRPOP,ARMAX,AMIN,SQDIF
00004      COMMON /EDWIN/QMOLWT(10),MELM(40),YINT(20)
00005      COMMON /GENRAL/ALPHA(5),S(20),KG,MUG,DS,
00006      1TPJJ(5),YY(5,5),PRTCLS,SPECIE,
00007      2ELEMNT,CRXN,HRXN,HH(5),HW(5),RGC
00008      COMMON /DIFEQN/OMEGAK(9),ALPHA(5),ALPHAC(5),ALPHAH(5),
00009      1ALPHAW(5),N(5),HZZ(5),QF(5),QCB,QZ(5),P,V,HG(5),RK(5,9),
00010      2RL(5,20),RM(5,20),RC(5),RH(5),RW(5),RR(5),W(5),WG,AREA,PRESSR
00011      COMMON /EDNUM/RHOG,CPG,TG,CPI(20),X(20),CO(5),HGAS,EDNAME(9),
00012      1OXYD(5),GMW,QMASS(9,20),WTM(20)
00013      COMMON/ODEVAL/XDIS,XTRMNL,VALINT(42),ODESTP
00014      COMMON/AZ/A(20,11),
00015      COMMON/AZ1/ANS(23),
00016      2      ATMOS
00017      COMMON/AZ2/
00018      COMMON/AZ3/B(11),
00019      5      BMIN,
00020      6      CBAR,
00021      7
00022      8      D,
00023      9
00024      COMMON/BZ/
00025      1
00026      2
00027      3      EL(23,24),
00028      4      ENTRPY,
00029      5
00030      6      H(20),
00031      7      HBAR,
00032      8      HC,
00033      9      HI,
00034      COMMON/CZ/HR(20),
00035      COMMON/CZ1/IDKIN(20),
00036      2
00037      3      IDSIN(20),
00038      4      IEV(11),
00039      COMMON/EZ/
00040      DIMENSION
00041      1
00042      2
00043      3      COI(9),
00044      4      DENS(10),
00045      5      EC(9),
00046      6      ECMAX(9),
00047      7      ECMIN(9),
00048      8      ET(9,9),
00049      9      ECONST(9),
00050      INTEGER ELEMNT,SPECIE
00051      EQUIVALENCE (QMASS(1,2),ET(1,1)),
00052      1      (QMASS(1,12),EC(1)),
00053      2      (QMASS(1,14),ECMIN(1)),

```

			RTOTO
			SCH,
	IMBALA,		SR(20)
		NCONV,	TANS(23),
		NCTXP,	
		NEQ,	
		NGIN,	
		NKIN,	TO
		NKINC,	TOL,
		NLEL,	TOLMAX,
		NM,	TOLT,
			U(20),
		NN,	Y(20),
			YBAR,
			YBC,
			YC(20),
		NSIN,	YR(20)
			Z(20,10)
		NT,	
		R,	IEVN(11)
		CBAG,	ATWT(40), WTG
			QE(10,40),
		MONTH(12),	QEI(11),
			QMDL(9),
		NAME1(10),	SPIM(9),
		NAME2(10),	
		PCT(10),	
			VOL(9),
		KU(9)	
		(QMASS(1,11),COI(1)),	
		(QMASS(1,13),ECMAX(1)),	
		(QMASS(1,15),ECONST(1)),	

```
00054      3      (QMASS(1,16),IDU(1)),      (QMASS(1,17),KU(1)),
00055      4      (QMASS(1,18),SPIM(1))
00056      DIMENSION NAMEM(20,4),QEM(20,4),KCHARG(20),IMPT(20)
00057      EQUIVALENCE (A(1,1),NAMEM(1,1)),(A(1,5),QEM(1,1)),
00058      1(YC(1),KCHARG(1)),(Y(1),IMPT(1))
00059      DATA R/1.98726/,NCHNG/20/,LITER/50/
00060      IF(XDIS.NE.0.0)GO TO 620
00061      C
00062      C      THIS AREA SETS UP THE PROBLEM
00063      C      WHEN NEVER DONE PREVIOUSLY...
00064      C
00065      NPROP=ELEMNT
00066      DO 1 I=1,ELEMNT
00067      DO 1 J=1,ELEMNT
00068      QE(I,J)=0.0
00069      IF(I.EQ.J)QE(I,I)=1.0
00070      1      CONTINUE
00071      DO 400 I=1,SPECIE
00072      Y(I)=YINT(I)
00073      400      IDSIN(I)=I
00074      NN=SPECIE
00075      NP=0
00076      C      NP EQUAL NUMBER OF CONDENSIBLES IN THE SYSTEM
00077      NT=NN+NP
00078      NGIN=SPECIE
00079      NSIN=NT
00080      NLEL=ELEMNT
00081      C
00082      C      EXECUTE THE PROBLEM.
00083      C
00084      C      EXHAUST SPECIES NEEDED.
00085      C
00086      510      NM=0
00087      LKDROP=3
00088      DO 530 J=1,NLEL
00089      DO 515 K=1,NPROP
00090      IF (QE(K,J)) 515,515,520
00091      515      CONTINUE
00092      GO TO 530
00093      520      NM=NM+1
00094      525      IEV(NM)=MELM(J)
00095      IEVN(NM) = J
00096      530      CONTINUE
00097      NMP1=NM+1
00098      550      CONTINUE
00099      ICALDA=0
00100      NKIN=0
00101      555      TO=3500.0
00102      ICP=1
00103      IHOT = 1
00104      ATMOS=P
00105      NFROZN=0
00106      C
```

00107 C JUGGLE A VOLUME OF MASSIVE MOLES.

00108 C

```
00109 620 SUMVOL=0.0
00110      SUMMOL=0.0
00111      SUMMAS=0.0
00112      DO 645 J=1,NPROP
00113 640 SUMMAS=SUMMAS+QMASS(J,1)
00114      VOL(J)=QMASS(J,1)
00115      SUMVOL=SUMVOL+VOL(J)
00116      QMOL(J)=QMASS(J,1)/QMOLWT(J)
00117      SUMMOL=SUMMOL+QMOL(J)
00118 645 CONTINUE
00119      DO 650 J=1,NPROP
00120      PCT(J)=(100.0*QMASS(J,1))/SUMMAS
00121 650 CONTINUE
00122      HI=HGAS*100.0
00123      NM=NMP1-1
00124      BLKDNS=SUMMAS/SUMVOL
00125      QM1=SUMMAS/SUMMOL
00126      BTOT=0.0
00127      DO 665 J=1,NM
00128      DO 655 L=1,NLEL
00129      K=L
00130      IF (IEV(J).EQ.MELM(L)) GO TO 660
00131 655 CONTINUE
00132 660 B(J)=0.0
00133      DO 665 I=1,NPROP
00134      B(J)=B(J)+QE(I,K)*PCT(I)/QMOLWT(I)
00135 665 BTOT=BTOT+B(J)
00136      BMIN=B(1)
00137      DO 670 J=1,NM
00138 670 BMIN=AMIN1(B(J),BMIN)
```

00139 C

00140 C FIND CHAMBER CONDITIONS.

00141 C

```
00142 720 NCTXP=0
00143      ANS(1)=10.0
00144      ANS(23)=10.0
00145 725 CALL EQUIL
00146 955 IF (ITE.GE.LITER) WRITE(3,1000)
00147      IF (ITE.GE.LITER) WRITE(5,1000)
00148      IF (ITE.GE.LITER) CALL TRBLE
00149 1000 FORMAT(24H EDWRDS DID NOT CONVERGE)
00150
00151      RETURN
00152      END
```

```

00001      SUBROUTINE EQUIL
00002      INTEGER ELEMNT, SPECIE, BUG, HRXN, OXYD
00003      COMMON/GENRAL/ALPHA(5), S(20), KG, MUG, DS,
00004      1TPJJ(5), YY(5,5), PRTCLS, SPECIE,
00005      2ELEMNT, CRXN, HRXN, HH(5), HW(5), RGC
00006      COMMON/GNRL2/NAME1(20), NAME2(20)
00007      COMMON /EDNUM/RHOG, CPG, TG, CPI(20), X(20), CO(5), HGAS, EDNAME(9),
00008      1OXYD(5), GMW, QMASS(9,20), WTM(20)
00009      COMMON /AREAS/NPRINT, TNIRP, CHECK, BUG
00010      COMMON /DIFEQN/OMEGAK(9), ALPHA(5), ALPHAH(5),
00011      1ALPHA(5), N(5), HZZ(5), QF(5), QCB, QZ(5), P, V, HG(5), RK(5,9),
00012      2RL(5,20), RM(5,20), RC(5), RH(5), RW(5), RR(5), W(5), WG, AREA, PRESSR
00013      COMMON/AZ/A(20,11), RTOTO
00014      COMMON/AZ1/ANS(23), SCH,
00015      2      ATMOS
00016      COMMON/AZ2/      IMBALA,      SR(20)
00017      COMMON/AZ3/B(11),      NCONV,      TANS(23),
00018      5      BMIN,      NCTXP,
00019      6      CBAR,
00020      7      NEQ,
00021      8      D,      ITE,      NGIN,
00022      9      ITER,      NKIN,      TO
00023      COMMON/BZ/      ITT,      NKINC,      TOL,
00024      1      NLEL,      NM,      TOLMAX,
00025      2      K2,      TOLT,
00026      3      EL(23,24),      K3,      U(20),
00027      4      ENTRPY,      LB,      NN,      Y(20),
00028      5      YBAR,
00029      6      H(20),      LITER,      YBC,
00030      7      HBAR,      LKDROP,      YC(20),
00031      8      HC,
00032      9      HI,      LV,      NSIN,      YR(20)
00033      COMMON/CZ/HR(20),      MAJOR,      Z(20,10)
00034      COMMON/CZ1/IDKIN(20),      NT,
00035      2      MPD,
00036      3      IDSIN(20),      MPDP,
00037      4      IEV(11),      R,      IEVN(11)
00038      COMMON/EZ/      CBAG,      ATWT(40),      WTG
00039      TOLMAX=.0001
00040      IF (BMIN.LT..001) TOLMAX=.1*BMIN
00041      TOL=TOLMAX
00042      TOLT=1.1*TOL
00043      ITER=0
00044      5      NEQ=2
00045      25      K2=NEQ-1
00046      30      NM1=NEQ+1
00047      NVL=NM+NEQ
00048      K3=NEQ
00049      NCONV=-1
00050      35      IF (ITER.GT.1.OR.NCTXP.NE.0) GO TO 50
00051      IF (ITER-1) 45,40,50
00052      40      NEQ=2
00053      K2=1

```

```

00054      ANS(K2)=50.0
00055      NM1=3
00056      NML=NM+2
00057      K3=2
00058      NCONV=-1
00059      GO TO 50
00060 45    NEQ=1
00061      K2=23
00062      ANS(K2)=50.0
00063      NM1=2
00064      NML=NM+1
00065      K3=1
00066      NCONV=-1
00067 50    LV=NML+NKIN
00068      LB=LV+1
00069      CALL SETUP1
00070      CALL SLE
00071      NCONV=0
00072      CALL TOY
00073      ITER=ITER+1
00074      IF (ITER.GT.LITER) GO TO 55
00075      IF (NCONV.EQ.0) CALL SETUP1
00076      IF (NCONV.EQ.0) GO TO 55
00077      GO TO 35
00078 55    CALL SETUP1
00079  C
00080  C      NOW WE DETERMINE IF THE SOLUTION STRADDLES A PHASE TRANSITION
00081  C      MAKING USE OF THE FACT THAT A SOLID+LIQUID PAIR HAS THE
00082  C      SAME FORMULA
00083  C
00084      MPDP=MPD
00085      MPD=0
00086      IF (NKIN.LE.0) GO TO 90
00087      IF (NKIN.LT.NM) GO TO 60
00088      MPD=1
00089      GO TO 90
00090 60    DO 80 I=1,NKIN
00091      IF (I=NKIN) 65,85,85
00092 65    IP1=I+1
00093      IDKINI=IDKIN(I)
00094      DO 75 J=IP1,NKIN
00095      IDKINJ=IDKIN(J)
00096      DO 70 K=1,NM
00097      IF (A(IDKINI,K)-A(IDKINJ,K)) 75,70,75
00098 70    CONTINUE
00099      MPD=1
00100      GO TO 85
00101 75    CONTINUE
00102 80    CONTINUE
00103 85    CONTINUE
00104  C
00105  C      CHAMBER AND TEMPERATURE SOLUTIONS.
00106  C      SAVE THE CHAMBER SOLUTION FOR INTIAL CONDITIONS ON

```

```

00107 C          THE NEXT PROBLEM.
00108 C
00109 90 CONTINUE
00110 HC=HBAR
00111 CBC=CBAR
00112 EPSLON=0.0
00113 CF=0.0
00114 PEAEM=0.0
00115 SCH=ENTRPy
00116 95 CONTINUE
00117 DO 100 I=1,NT
00118 100 YC(I)=Y(I)
00119 NKINC=NKIN
00120 IF(NKIN.LE.0) GO TO 140
00121 DO 105 I=1,NKIN
00122 105 CONTINUE
00123 140 PSI=14.696*ATMOS
00124 TG=TO
00125 HGAS=HBAR/100.0
00126 RHOG=ATMOS/(YBAR*TO*.82057)
00127 GMW = WTG/YBAR
00128 CPG=CBAG/100.0
00129 ITE=ITER
00130 C
00131 C          EXHAUST PRODUCTS STORED IN 'YOUT
00132 C
00133 DO 170 I=1,HRXN
00134 CO(I)=0.0
00135 170 CONTINUE
00136 160 DO 165 I=1,NT
00137 DO 175 IJ=1,HRXN
00138 IK=OXYD(IJ)
00139 175 CO(IJ)=Y(IK)*RHOG/100.0
00140 165 X(I)=Y(I)/YBAR
00141 IF(TNIRP.NE.1.0.OR.BUG.LT.2)GO TO 151
00142 WRITE(3,220)(CO(IXX),IXX=1,HRXN)
00143 220 FORMAT(8H CO(I)= ,5(1X,E12.5,1X))
00144 WRITE(3,230)
00145 230 FORMAT(5X,1H1,7X,4HX(I),8X,4HNAME,12X,5HMW(I),11X,5HCP(I))
00146 DO 152 IX=1,NN
00147 152 WRITE(3,240)IX,X(IX),NAME1(IX),NAME2(IX),WTM(IX),CPI(IX)
00148 240 FORMAT(2X,I3,E12.5,3X,2A6,3X,E12.5,3X,E12.5)
00149 WRITE(3,250) TG
00150 250 FORMAT(19H GAS TEMPERATURE = ,E12.5,15H DEGREES KELVIN)
00151 WRITE (3,260) HGAS
00152 260 FORMAT(16H GAS ENTHAPLY = ,E12.5,7H CAL/GM)
00153 WRITE(3,270) RHOG
00154 270 FORMAT(15H GAS DENSITY = ,E12.5,13H GM/CUBIC CM.)
00155 WRITE(3,280) GMW
00156 280 FORMAT(21H GAS MOLECULAR WT. = ,E12.5)
00157 WRITE(3,290) CPG
00158 290 FORMAT(21H GAS HEAT CAPACITY = ,E12.5,16H CAL/GM DEGREE K)
00159 151 CONTINUE

```

EQUIL.FOR

24-May-79 13:15

PAGE 1-

00160
00161

RETURN
END

```
00001 SUBROUTINE FIND (ARG,ANS,X,Y,NPTS,I)
00002 C
00003 C J. ANDERSON 6-1-65
00004 C EXTRAPOLATES FOR VALUES OUT OF TABLE RANGE
00005 C REMEMBERS LAST ARG VALUE AND BEGINS SEARCH FROM THAT VALUE
00006 C CALLING SEQUENCE IS .....
00007 C
00008 C CALL FIND (ARG,ANS,X,Y,NPTS,MEM)
00009 C
00010 C ARG IS THE ARGUMENT
00011 C ANS CONTAINS RESULT ON EXIT
00012 C X IS ONE DIMENSIONAL ARRAY OF INDEP. VARIABLE
00013 C Y IS ONE DIMENSIONAL ARRAY OF DEP. VARIABLE
00014 C NPTS IS NUMBER OF TABLE ENTRIES
00015 C MEM SHOULD BE INITIALIZED TO 1 - AFTER FIRST
00016 C CALL THE SUBROUTINE WILL PRESERVE VALUES IN IT
00017 C
00018 C DIMENSION X(50), Y(50)
00019 1 IF (X(I)-ARG) 4,2,2
00020 2 I=I-1
00021 IF (I-1) 3,3,1
00022 3 I=1
00023 GO TO 8
00024 4 IF (X(I+1)-ARG) 5,7,7
00025 5 I=I+1
00026 IF (I-NPTS) 4,6,6
00027 6 I=NPTS-1
00028 GO TO 9
00029 7 ANS=Y(I)+(Y(I+1)-Y(I))*(ARG-X(I))/(X(I+1)-X(I))
00030 RETURN
00031 8 ANS = Y(1)
00032 RETURN
00033 9 ANS = Y(NPTS)
00034 RETURN
00035 END
```

```

00001      SUBROUTINE GRPH(X,Y,NDATA,EX,EY,ASCX,NX,ASCY,NY,IP)
00002 C   X,Y:  ELEMENTS OF THE ORDERED PAIR (X,Y)
00003 C   NDATA:  NUMBER OF ORDERED PAIRS
00004 C   EX,EY:  ERROR IN THE X AND Y VALUES
00005 C   ASCX(NX), ASCY(NY):  ARRAYS CONTAINING THE LABELS OF THE AXES
00006 C   IP.LT.0:  NEW GRAPH,  IP.GT.0:  NEW CURVE, SAME GRAPH
00007 C   IP.EQ.0:  END GRAPH
00008 C   THIS ROUTINE IS SELF SCALING (IT USES ASCALE)
00009       COMMON/TRUBLE/INDX,ITRBLE
00010       DIMENSION X(NDATA),Y(NDATA),ASCX(1),ASCY(1)
00011       DATA IPLOTS/0/
00012       IF(IP.GE.0) GO TO 20
00013 C   PLOT BORDERS
00014       IF(IPLOTS.EQ.0) CALL PLOTS(KPLOTS)
00015       IPLOTS=1
00016       CALL PLOT(0.0,1.0,-3)
00017       CALL PLOT(0.0,8.5,2)
00018       CALL PLOT(11.0,8.5,1)
00019       CALL PLOT(11.0,0.0,1)
00020       CALL PLOT(0.0,0.0,1)
00021       CALL PLOT(.4,.4,-3)
00022       CALL PLOT(0.0,7.5,2)
00023       CALL PLOT(10.2,7.5,1)
00024       CALL PLOT(10.2,0.0,1)
00025       CALL PLOT(0.0,0.0,1)
00026       CALL ASCALE(X,NDATA,9.,XMIN,DX,XMAX)
00027       CALL ASCALE(Y,NDATA,6.,YMIN,DY,YMAX)
00028 C   PLOT AXES
00029       CALL PLOT(.5,.5,-3)
00030       NX=-1.0*NX
00031       IF(ITRBLE.NE.1)CALL AXIS(0.0,0.0,ASCX,NX,9.0,0.0,XMIN,DX)
00032       IF(ITRBLE.NE.1)CALL AXIS(0.0,0.0,ASCY,NY,6.0,90.0,YMIN,DY)
00033       NX=-NX
00034 C   PLOT ZERO LINES
00035       IF(XMIN.GE.0.0) GO TO 10
00036       IF(XMAX.LT.0.0) GO TO 10
00037       XZ=-1.*XMIN/DX
00038       CALL PLOT(XZ,0.,3)
00039       CALL PLOT(XZ,6.,2)
00040 10      IF(YMIN.GE.0.0) GO TO 20
00041       IF(YMAX.LT.0.0) GO TO 20
00042       YZ=-1.*YMIN/DY
00043       CALL PLOT(9.,YZ,3)
00044       CALL PLOT(0.,YZ,2)
00045 C   PLOT DATA AND ERROR
00046 20      XE=EX/DX
00047       YE=EY/DY
00048       IPEN=3
00049       DO 30 I=1,NDATA
00050       IF(X(I).LT.XMIN.OR.X(I).GT.XMAX) GO TO 30
00051       IF(Y(I).LT.YMIN.OR.Y(I).GT.YMAX) GO TO 30
00052       XT=(X(I)-XMIN)/DX
00053       YT=(Y(I)-YMIN)/DY

```

```
00054      CALL PLOT(XT,YT,IPEN)
00055      IPEN=2
00056      IF(YE,LT,0.05) GO TO 30
00057      XA=XT+XE/2.
00058      XB=XT-XE/2.0
00059      YA=YT+YE/2.0
00060      YB=YT-YE/2.0
00061      CALL PLOT(XA,YA,3)
00062      CALL PLOT(XB,YA,2)
00063      CALL PLOT(XT,YA,3)
00064      CALL PLOT(XT,YT,2)
00065      CALL PLOT(XA,YB,3)
00066      CALL PLOT(XB,YB,2)
00067      CALL PLOT(XT,YB,3)
00068      CALL PLOT(XT,YT,2)
00069      30  CONTINUE
00070      IF(IP,EQ,0) CALL PLOT(20.,-2.5,-3)
00071      101 RETURN
00072      END
```

```

00001      SUBROUTINE INPUT
00002      COMMON/AZ/A(20,11),
00003      COMMON/AZ2/
00004      COMMON/CZ/HR(20),
00005      COMMON/EZ/
00006      COMMON/CONVER/ITRMAX,DYNAMO(3),DYNTM,DYNFLG,DYNFLO
00007      COMMON/STIFF/ISASUM,ISTIFF(5),STIFVL
00008      COMMON/JAN78/V0,FUR
00009      COMMON /APR77/DELTPJ,DELRRJ,ALEN,JFAR,HM,DIFMW,ICNVLM,
00010      1TTEST,SUMSQ,ITRYS,GAST(255),OSPRR,NPROP,ARMAX,AMIN,SQDIF
00011      COMMON /EDWIN/QMOLWT(10),MELM(40),YINT(20)
00012      COMMON /LAST/GASTMN,TMIN(5),IQOJ(255,5)
00013      COMMON /IO/DDUCT,DYDXM,AGSTPD,CPVC(3,5,5),HFV(5,5),DELHV(5,5),
00014      1INTCPV(5,5),QRB(5)
00015      COMMON /H2OP/IVPFLG,VPRCOF(5)
00016      COMMON/MORE/D01(255,5),N01(255,5),ALFA0(255,5),ALFA0C(255,5),
00017      1ALFA0H(255,5),ALFA0W(255,5),ALFA0A(255,5),X0(255,20),WVG(255)
00018      COMMON /AREA13/ALFAC0(5),GAMMA,EK(20),XI(5),AMJ(5,5),
00019      1EMJ(5,5),KVD(5,5),TB,D(5),RHOC(5),RHO(5),DELTA(20),DIFM(20)
00020      2,ALFAH0(5),ALFAW0(5),ALFAA0(5)
00021      COMMON /AREA2/K(20),MU(20),SHRINK,HH0(5),HW0(5),EB,ELAM,
00022      1EUCKEN
00023      COMMON /AREA4/AL(5,5),EL(5,5),MH,PHIJWK(5,9),
00024      1PHIL(5),PHIKL(9,5),PHIVK(5,9,5),KEQ,EMM(5,5)
00025      COMMON /AREA5/NPRINT,TNIRP,CHECK,BUG
00026      COMMON /GENRAL/ALPHA(5),S(20),KG,MUG,DS,
00027      1TPJJ(5),YY(5,5),PRTCLS,SPECIE,
00028      2ELEMNT,CRXN,HRXN,HH(5),HW(5),RGC
00029      COMMON /RADI/T0(255,5),N0(5),D0(5),SIGMA,PI,E(5),IT(255),H0(5)
00030      1,NUMRDR,DEL,IRAD,TOOLD(5)
00031      COMMON /DIFEQN/OMEGAK(9),ALPHA(5),ALPHAC(5),ALPHAH(5),
00032      1ALPHAW(5),N(5),H(5),QF(5),QCB,QZ(5),P,V,HG(5),RK(5,9),
00033      2RL(5,20),RM(5,20),RC(5),RH(5),RW(5),RR(5),W(5),WG,AREA,PRESSR
00034      COMMON /EDNUM/RHOG,CPG,TG,CPI(20),X(20),CO(5),HGAS,EDNAME(9),
00035      10XYD(5),GMW,QMASS(9,20),WTM(20)
00036      COMMON /ADD/CCP(5,4,3)
00037      COMMON/GNRL2/NAME1(20),NAME2(20)
00038      COMMON /ODEVAL/XDIS,XTRMNL,VALINT(42),ODESTP
00039      COMMON /CONST/OSGKM(9),OPGKM(9),SJMC(3,5),PJMC(4,5),SJH(5),
00040      1PJH(5),SGMC(3),PGMC(4),PGH,SGH,PGX,PJX(5)
00041      INTEGER PRTCLS,SPECIE,ELEMNT,CRXN,HRXN,EUCKEN,BUG,ODESTP,
00042      1EDNAME,OSPRR,OXYD,DYNAMO,RSTRT,D3TST,DYNN3,SHRINK
00043      REAL N1,N,N0,MH,COMENT(10,20),MODH,MODS,N01
00044      REAL XBEGIN(5),TMAX(5),D1(5),XCHNG(5)
00045      DATA BLNK/5H /
00046      DATA PI/3.14159/,SIGMA/1.355E-12/,RGC/1.987/
00047      C
00048      C*****OPENING THE INPUT FILE ON DISC
00049      C
00050      CALL OPEN
00051      C
00052      C*****READING ALL INPUT INFORMATION
00053      C

```

```

00054      READ(1,5)NCARD
00055      IF(NCARD .EQ.0)GO TO 11
00056      DO 10 I=1,NCARD
00057 10      READ(1,15)(COMENT(I,J),J=1,20)
00058 11      READ(1,5)ODESTP,OSPRR,DYNAMO(1),DYNAMO(2),DYNAMO(3),NPRINT
00059      READ(1,5)ELEMNT,SPECIE,PRTCLS,CRXN,HRXN,ICNVLM,ITRMAX,NPROP,
00060      1BUG,ISASUM,EUCKEN,KEQ,SHRINK,IRAD
00061      READ(1,25)DYNTM,SQDIF,DELTPJ,DELRRJ,TTEST,STIFVL,FUR
00062      READ(1,25)GMW,HGAS,RHOG,WG,P
00063      READ(1,25)SGH,(SGMC(I),I=1,3)
00064      READ(1,25)PGX,PGH,(PGMC(I),I=1,4)
00065      DO 40 J=1,PRTCLS
00066      READ(1,25)D1(J),E(J),H(J),XI(J),W(J)
00067      READ(1,25)ALPHA(J),ALPHAC(J),ALPHAH(J),ALPHAW(J),HHO(J),HWO(J)
00068      READ(1,25)TMIN(J),XBEGIN(J),TMAX(J),XCHNG(J)
00069      READ(1,25)SJH(J),(SJMCI(J),I=1,3)
00070      READ(1,25)PJX(J),PJH(J),(PJMCI(J),I=1,4)
00071      DO 30 M=1,CRXN
00072      READ(1,25)AMJ(J,M),EMJ(J,M),YY(J,M)
00073 30      READ(1,25)(CPVC(I,J,M),I=1,3),HFV(J,M)
00074      DO 32 L=1,HRXN
00075 32      READ(1,25)AL(J,L),EL(J,L),EMM(J,L)
00076      READ(1,25)(PHIJWK(J,KI),KI=1,ELEMNT)
00077      DO 35 KI=1,ELEMNT
00078 35      READ(1,25)(PHIVK(J,KI,M),M=1,CRXN)
00079      READ(1,27)((CCP(J,NI1,NI2),NI2=1,3),NI1=1,4)
00080 40      CONTINUE
00081      DO 50 KI=1,ELEMNT
00082      READ(1,55)EDNAME(KI),ATWT(KI),OMEGAK(KI),OSGKM(KI),OPGKM(KI)
00083      READ(1,25)(PHIKL(KI,L),L=1,HRXN)
00084 50      CONTINUE
00085      DO 60 I=1,SPECIE
00086      READ(1,65)NAME1(I),NAME2(I),S(I),EK(I),DELTA(I),YINT(I)
00087      READ(1,25)(A(I,IX),IX=1,ELEMNT)
00088      READ(1,25)HR(I),SR(I)
00089      READ(1,25)(Z(I,IX),IX=1,5)
00090      READ(1,25)(Z(I,IX),IX=6,10)
00091 60      CONTINUE
00092      READ(1,25)DDUCT,DS,ALEN,AGANGL,EB,TB
00093      READ(1,25)ELAM,GAMMA,MH
00094      READ(1,5)(OXYD(L),L=1,HRXN)
00095      READ(1,25)(PHIL(L),L=1,HRXN)
00096      READ(1,26)IVPFLG,(VPRCOF(I),I=1,5)
00097      READ(1,5)RSTRT
00098      C
00099      C*****SETTING UP ALL DEFAULT VALUES
00100      C      AND CALCULATING INITIAL VALUES FROM INPUT CONDITIONS
00101      C
00102      IF (NPRINT.LE.0) NPRINT=15
00103      IF (SQDIF.LE.0.0) SQDIF=0.01
00104      IF (STIFVL.LE.0.0) STIFVL=0.001
00105      IF (EUCKEN.NE.1) EUCKEN=0
00106      IF (SHRINK.NE.1) SHRINK=0

```

```
00107      IF (IRAD.NE.1) IRAD=0
00108      IF ((FUR.LE.0.0).OR.(FUR.GT.1.0)) FUR=1.0
00109      NUMRDR=ODESTP/OSPRR
00110      ODESTP=NUMRDR*OSPRR
00111      IF(DYNAMO(3).GT.OSPRR)DYNAMO(3)=OSPRR
00112      D3TST=OSPRR/DYNAMO(3)
00113      IF(MOD(OSPRR,D3TST).EQ.0)GO TO 61
00114      DYNM3=1
00115      IF(FLOAT(DYNAMO(3))/FLOAT(OSPRR).GT.0.5)DYNM3=OSPRR
00116      DYNAMO(3)=DYNM3
00117      GO TO 62
00118 61      DYNAMO(3)=OSPRR/D3TST
00119 62      CONTINUE
00120      DEL=ALEN/FLOAT(NUMRDR)
00121      AMIN=PI*(DDUCT/2.0)**2
00122      ANGLE=AGANGL
00123      AGANGL=AGANGL*PI/180.0
00124      ARMAX=PI*(DS/2.0)**2
00125      PRESSR=P
00126      DYDXM=SIN(AGANGL)/COS(AGANGL)
00127      IF(ANGLE.EQ.0.0) AGSTPD=0.0
00128      IF(ANGLE.EQ.0.0)GO TO 74
00129      AGSTPD=(DS-DDUCT)/(2.0*DYDXM)
00130 74      IF(ODESTP.LT.NUMRDR)ODESTP=NUMRDR
00131      V=WG/(RHOG*AMIN)
00132      V0=V
00133      DO 1021 J1=1,PRTCLS
00134      ALPHA(J1)=ALPHAA(J1)+ALPHAC(J1)+ALPHAH(J1)+ALPHAW(J1)
00135      N(J1)=W(J1)*RHOG/(WG*ALPHA(J1))
00136      ALFACO(J1)=ALPHAC(J1)
00137      ALFAHO(J1)=ALPHAH(J1)
00138      ALFAWO(J1)=ALPHAW(J1)
00139      ALFAAO(J1)=ALPHAA(J1)
00140      X5=E(J1)
00141      IF(X5.EQ.0.0)E(J1)=1.0
00142      CONN=N(J1)*TMIN(J1)
00143      SLOPET=(TMAX(J1)-TMIN(J1))/(XCHNG(J1)-XBEGIN(J1))
00144      DO 68 INCI=1,NUMRDR
00145      INCIZ7=INCI
00146      CONT=(FLOAT(INCIZ7-1)+.5)*DEL
00147      IF(CONT.GE.XCHNG(J1))GO TO 66
00148      IF(CONT.LT.XBEGIN(J1))GO TO 63
00149      T0(INCI,J1)=TMIN(J1)+SLOPET*(CONT-XBEGIN(J1))
00150      GO TO 67
00151 63      T0(INCI,J1)=TMIN(J1)
00152      GO TO 67
00153 66      T0(INCI,J1)=TMAX(J1)
00154 67      N01(INCI,J1)=CONN/T0(INCI,J1)
00155 68      D01(INCI,J1)=D1(J1)
00156      N0(J1)=N(J1)
00157      D0(J1)=D1(J1)
00158      H0(J1)=H(J1)
00159 1021 CONTINUE
```

```
00160      DO 75 KI=1,ELEMNT
00161      QMOLWT(KI)=ATWT(KI)
00162      MELM(KI)=EDNAME(KI)
00163 75      CONTINUE
00164 C
00165 C*****WRITING OUT ALL INPUT VALUES IN SAME ORDER AS READ IN
00166 C
00167      WRITE(3,399)
00168      DO 201 I=1,NCARD
00169 201      WRITE(3,400)(COMENT(I,KI),KI=1,20)
00170      WRITE(3,403)
00171      WRITE(3,405)ODESTP,OSPRR,DYNAMO(1),DYNAMO(2),DYNAMO(3),NPRINT,
00172 1ELEMNT,SPECIE,PRTCLS,CRXN,HRXN,ICNVLM,ITRMAX,NPROP
00173      WRITE(3,406)BUG
00174      IF(ISASUM.GT.0)WRITE(3,409)ISASUM
00175      IF(EUCKEN.EQ.1)WRITE(3,407)
00176      IF(EUCKEN.NE.1)WRITE(3,408)
00177      IF(KEQ.EQ.1)WRITE(3,459)
00178      IF(SHRINK.EQ.1)WRITE(3,410)
00179      IF(IRAD.EQ.1)WRITE(3,414)
00180      WRITE(3,411)DYNTM,SQDIF,DELTPJ,DELRRJ,TTEST
00181      IF(ISASUM.GT.0)WRITE(3,412)STIFVL
00182      IF(FUR.NE.1.0)WRITE(3,413)FUR
00183      WRITE(3,415)
00184      WRITE(3,420)GMW,HGAS,RHOG,WG,P
00185      WRITE(3,423)
00186      WRITE(3,425)SGH,(SGMC(I),I=1,3)
00187      WRITE(3,424)
00188      WRITE(3,426)PGX,PGH,(PGMC(I),I=1,4)
00189      DO 430 J=1,PRTCLS
00190      WRITE(3,433)J
00191      WRITE(3,435)D1(J),E(J),H(J),XI(J),W(J)
00192      WRITE(3,440)ALPHA(J),ALPHAC(J),ALPHAH(J),ALPHAW(J),HHO(J),HWO(J)
00193      WRITE(3,445)TMIN(J),XBEGIN(J),TMAX(J),XCHNG(J)
00194      WRITE(3,423)
00195      WRITE(3,425)SJH(J),(SJM(I,J),I=1,3)
00196      WRITE(3,424)
00197      WRITE(3,426)PJX(J),PJH(J),(PJM(I,J),I=1,4)
00198      WRITE(3,451)
00199      DO 453 M=1,CRXN
00200 453      WRITE(3,455)M,AMJ(J,M),EMJ(J,M),YY(J,M)
00201      DO 454 M=1,CRXN
00202 454      WRITE(3,458)(CPVC(I,J,M),I=1,3),HFV(J,M)
00203      WRITE(3,456)
00204      DO 457 L=1,HRXN
00205 457      WRITE(3,460)L,AL(J,L),EL(J,L),EMM(J,L)
00206      IF(KEQ.EQ.1)WRITE(3,459)
00207      WRITE(3,464)
00208      WRITE(3,465)(EDNAME(KI),PHIJWK(J,KI),KI=1,ELEMNT)
00209      WRITE(3,467)
00210      WRITE(3,470)((EDNAME(KI),M,PHIVK(J,KI,M),KI=1,ELEMNT),M=1,CRXN)
00211 430      WRITE(3,475)((CCP(J,NI1,NI2),NI2=1,3),NI1=1,4)
00212      WRITE(3,477)(L,L=1,HRXN)
```

```

00213      WRITE(3,478)
00214      DO 431 KI=1,ELEMNT
00215 431      WRITE(3,480) EDNAME(KI),ATWT(KI),OMEGAK(KI),OSGKM(KI),OPGKM(KI),
00216      1(PHIKL(KI,L),L=1,HRXN)
00217      WRITE(3,482)(EDNAME(IX),IX=1,ELEMNT)
00218      DO 432 I=1,SPECIE
00219 432      WRITE(3,485)NAME1(I),NAME2(I),S(I),EK(I),DELTA(I),YINT(I),
00220      1(A(I,IX),IX=1,ELEMNT)
00221      WRITE(3,487)
00222      DO 436 I=1,SPECIE
00223 436      WRITE(3,490)NAME1(I),NAME2(I),HR(I),SR(I),(Z(I,IX),IX=1,10)
00224      WRITE(3,399)
00225      WRITE(3,495)DDUCT,DS,ALEN,ANGLE,EB,TB
00226      WRITE(3,500)ELAM,GAMMA,MH
00227      WRITE(3,509)
00228      DO 505 L=1,HRXN
00229      LL=OXYD(L)
00230 505      WRITE(3,510)L,NAME1(LL),NAME2(LL),PHIL(L)
00231      IF(IVPFLG.EQ.0)GO TO 520
00232      WRITE(3,515)(VPRCOF(I),I=1,5)
00233 520      CONTINUE
00234      IF(RSTRT.EQ.1)CALL RSTRT(RSTRT)
00235      RETURN
00236 5      FORMAT(16I5)
00237 15      FORMAT(20A4)
00238 25      FORMAT(8E10,3)
00239 26      FORMAT(15,5X,7E10,3)
00240 27      FORMAT(3E10,4)
00241 55      FORMAT(A2,8X,7E10,3)
00242 65      FORMAT(2A4,2X,7E10,3)
00243 399      FORMAT(1H1)
00244 400      FORMAT(1H ,20A4)
00245 403      FORMAT(1H-,32HRUN PARAMETERS*****))
00246 405      FORMAT(1H0,10X,30HINITIAL NUMBER OF O.D.E. STEPS,20X,15/11X,44HNUM
00247      1BER OF INITIAL STEPS PER RADIATION REGION,6X,15/11X,36HDYNAMIC REG
00248      2ION MULTIPLICATION FACTOR,14X,15/11X,44HMULTIPLICATION FACTOR AFTE
00249      3R DEVOLATILIZATION,6X,15/11X,34HDIVISION FACTOR AFTER CHAR BURNOUT
00250      4,16X,15/11X,25HNUMBER OF STEPS PER PRINT,25X,15/11X,18HNUMBER OF E
00251      5LEMENTS,32X,15/11X,17HNUMBER OF SPECIES,33X,15/11X,30HNUMBER OF PA
00252      6RTICLE TYPES/SIZES,20X,15/11X,24HNUMBER OF COAL REACTIONS,26X,15/1
00253      71X,24HNUMBER OF CHAR REACTIONS,26X,15/11X,28HMAXIMUM NUMBER OF COR
00254      8RECTORS,22X,15/11X,35HMAXIMUM NUMBER OF SYSTEM ITERATIONS,15X,15/1
00255      91X,42HNUMBER OF STEPS PER PHY. PROP. CALCULATION,8X,15)
00256 406      FORMAT(11X,11HDEBUG LEVEL,39X,15)
00257 407      FORMAT(11X,55HTHERMAL CONDUCTIVITY CALCULATIONS USE
00258      1 EUCKEN CORRECTION)
00259 408      FORMAT(11X,62HTHERMAL CONDUCTIVITY CALCULATIONS USE
00260      1 SAGE-GALLOWAY CORRECTION)
00261 409      FORMAI(11X,46HSTIFF PARTICLE ENERGY EQUATION ASSUMPTION USED,4X,
00262      1I5)
00263 410      FORMAT(11X,49HSHRINKING PARTICLE ASSUMPTION DURING CHAR BURNOUT)
00264 411      FORMAT(11X,42HDYNAMIC REGION INITIATION TEMP.(DEGREES K),8X,F11.2/
00265      111X,46HMAXIMUM ACCEPTABLE ROOT MEAN SQUARE(DEGREES K),4X,F11.2/11X

```

```

00266      2,33HTEMP. CHANGE TOLERANCE(DEGREES K),17X,F11.8/11X,45HTOTAL PARTI
00267      3CLE REACTION RATE CHANGE TOLERANCE,5X,F11.8/11X,37HCCORRECTOR CONVE
00268      4RGENCE SLOPE TOLERANCE,13X,F11.8)
00269      412      FORMAT(11X,42HTOLERANCE FOR STIFF ASSUMPTION APPLICATION,8X,F11.8)
00270      413      FORMAT(11X,23HUNDER RELAXATION FACTOR,27X,F11.8)
00271      414      FORMAT(11X,45HDIFFUSION APPROXIMATION FOR RADIATION IS USED)
00272      415      FORMAT(1H-,31HGAS PARAMETERS*****/1H0,14X,
00273      113HGAS MOLECULAR,2X,19HENTHALPY OF THE GAS2X,18HDENSITY OF THE GAS
00274      2,4X,14HMASS FLOW RATE,9X,8HPRESSURE/19X,6HWEIGHT/17X,9H(G/GMOLE),
00275      3 9X,7H(CAL/G),12X,9H(G/CM**3),13X,7H(G/SEC),14X,5H(ATM))
00276      420      FORMAT(1H ,14X,F10.4,F17.4,9X,E12.5, 2(10X,F10.4))
00277      423      FORMAT(1H0,34X,11HENTHALPY OF,27X,17HMASS ADDITION RATE/34X,13HTHE
00278      1 SECONDARY,27X,14HFROM SECONDARY/37X,7H(CAL/G),32X,10H(G/CM-SEC))
00279      424      FORMAT(1H0,14X,12HDISTANCE FOR,8X,11HENTHALPY OF,27X,18HMASS ADD
00280      1ITION RATE/14X,13HRECIRCULATION,7X,13HRECIRCULATION,25X,18HFROM
00281      2 RECIRCULATION/13X,15HPROPERTIES (CM),9X,7H(CAL/G),32X,10H(G/
00282      3CM-SEC))
00283      425      FORMAT(1H ,22X,F20.4,20X,F10.4,7HX**2 + ,F8.4,5HX + ,F8.4)
00284      426      FORMAT(1H ,2X,2(F20.4),10X,F10.4,7HX**3 + ,F8.4,7HX**2 + ,F8.4
00285      1,4HX + ,F8.4)
00286      433      FORMAT(26H1PARAMETERS FOR THE NUMBER,12,21H PARTICLE PHASE*****
00287      435      FORMAT(1H-,14X,8HDIAMETER,7X,10HEMISSIVITY,7X,8HENTHALPY,5X,
00288      112HSURFACE AREA,3X,14HMASS FLOW RATE/17X,4H(CM),27X,7H(CAL/G),8X,6
00289      2HFACTOR,10X,7H(G/SEC)/12X,2(F10.4,6X),F10.4,5X,E12.5,3X,F10.4)
00290      440      FORMAT(1H-,13X,8HASH MASS,6X,9HCOAL MASS,4X,9HCHAR MASS,5X,10HWATE
00291      1R MASS,4X,9HCHAR REF.,3X,10HWATER REF./70X,8HENTHALPY,4X,
00292      28HENTHALPY/17X,3H(G),11X,3H(G),11X,3H(G),11X,3H(G),
00293      39X,7H(CAL/G),6X,7H(CAL/G)/11X,3(E12.5,2X),E12.5,4X,2(F10.4,5X))
00294      445      FORMAT(1H-,10X,20HSTARTING TEMPERATURE,6X,13HDISTANCE TEMP,6X,15HI
00295      1NITAL MAXIMUM,4X,20HDISTANCE INITIAL MAX,/38X,11HRISE BEGINS,
00296      27X,15HTEMP IS REACHED/20X,3H(K),17X,4H(CM),15X,3H(K),18X,4H(CM)/
00297      316X,4(F10.4,10X))
00298      450      FORMAT(1H-,11X,18HMASS ADDITION RATE,3X,18HMASS ADDITION RATE,7X,
00299      11HENTHALPY IN,10X,11HENTHALPY IN/14X,14HFROM SECONDARY,5X,
00300      218HFROM RECIRCULATION,8X,9HSECONDARY,10X,13HRECIRCULATION,/13X,
00301      310H(G/CM-SEC),14X,10H(G/CM-SEC),13X,7H(CAL/G),14X,7H(CAL/G)/13X,
00302      44(E12.5,10X))
00303      451      FORMAT(1H-,10X,46HPARAMETERS FOR EACH COAL REACTION AND PARTICLE//
00304      1/12X,8HREACTION,5X,14HPYROLYSIS PRE-,6X,17HACTIVATION ENERGY,6X,
00305      213HMASS FRACTION/23X,18HEXPOENTIAL FACTOR
00306      3,8X,11HIN REACTION/27X,7H(1/SEC),15X,13H(CAL/GMOLE-K))
00307      455      FORMAT(12X,14,8X,E12.5,15X,F10.4, 5X,F10.4,11X,E12.5)
00308      456      FORMAT(1H-,10X,46HPARAMETERS FOR EACH CHAR REACTION AND PARTICLE///
00309      112X,8HREACTION,2X,21HSURFACE REACTION PRE-,5X,17HACTIVATION ENERGY
00310      2,7X,1HM/24X,18HEXPOENTIAL FACTOR/24X,13H(CM/SEC-K**M),12X,11H(CAL
00311      3/GMOLE))
00312      458      FORMAT(1H0,45X,15HCP COEFFICIENTS,25X,1HH/87X,3HFVJ/51X,7H(CAL/G)/
00313      130X,3(E10.3,5X),8X,F10.3)
00314      459      FORMAT(11X,66HTHE K EQUATION OF FIELD ET. AL. IS USED FOR CHAR
00315      1 OXIDATION WITH O2)
00316      460      FORMAT(13X,13,7X,E12.5,15X,F10.4,10X,F5.2)
00317      464      FORMAT(1H1,10X,82HSTOICHIOMETRIC COEFFICIENT FOR JTH PARTICLE TO K
00318      1TH ELEMENT IN MOISTURE EVAPORATION/1H0,12X,7HELEMENT,5X,11HCOEFFIC

```

```

00319      2IENT)
00320      465      FORMAT(14X,A2,5X,F10.4)
00321      467      FORMAT(1H-,10X,9HSTOICHIOMETRIC COEFFICIENT FOR JTH PARTICLE TO K
00322      1TH ELEMENT IN MTH REACTION (DEVOLATILIZATION)/1H0,12X,7HELEMENT,3X
00323      2,8HREACTION,8X,11HCOEFFICIENT)
00324      470      FORMAT(14X,A2,9X,I2,9X,F10.4)
00325      475      FORMAT(1H-,10X,52HCOEFFICIENTS FOR QUADRATIC EQUATION OF HEAT CAPA
00326      1CITY/1H-,11X,9HCOAL PART,10X,1H1,19X,1H2,19X,1H3/14X,4HCOAL,8X,3AS
00327      23(E10.3,10X)/14X,4HCHAR,8X,3(E10.3,10X)/14X,5HWATER,7X,13HMOLES,
00328      33(E10.3,10X)/15X,3HASH,8X,3(E10.3,10X))
00329      477      FORMAT(35HELEMENT PARAMETERS*****//12X,7HELEMENT,3X,
00330      110HATOMIC WT.,3X,12HINITIAL MASS,1X,13HMASS FRACTION,2X,13HMASS FR
00331      2ACTION,12X,45HSTOICHIOMETRIC COEFFECIENTS FROM LTH REACTION/36X,8H
00332      3FRACTION,7X,7HIN SEC.,6X,10HIN RECIRC.,3X,5(6X,I1,7X))
00333      478      FORMAT(50X,10H(G/CM-SEC),4X,10H(G/CM-SEC))
00334      480      FORMAT(1H ,14X,A2,1X,9(1X,F12.5,1X))
00335      482      FORMAT(34H-SPECIES PARAMETERS*****//13X,7HSPECIES,4X,
00336      19HCOLLISION,5X,9HEPSILON/K7X,5HDELTA,7X,11HMOL FRAC IN,14X,31HNUMB
00337      2ER OF ELEMENTS IN A SPECIES/24X,8HDIAMETER,46X,10(1X,A2,2X)/40X,3H
00338      3(A),11X,3H(K))
00339      485      FORMAT(1H ,12X,2A4,4(2X,F10.5,2X),10(1X,F2.0,2X))
00340      487      FORMAT(1H0,11X,7HSPECIES,10X,8HENTHALPY,5X,
00341      17HENTROPY,25X,32HHEAT CAPACITY COEFF. FOR EDWARDS/)
00342      490      FORMAT(15X,2A4,1X,2(1X,F12.5,1X)/2(66X,5(F10.4,2X)/).
00343      495      FORMAT(33H-PHYSICAL PARAMETERS*****/1H0,10X,
00344      116HDIAMETER OF DUCT,3X,19HDIAMETER OF CHAMBER,2X,14HREACTOR LENGTH
00345      2,2X,17HGROWTH AREA ANGLE,2X,17HEMISSIVITY OF THE,3X,
00346      318HTEMPERATURE OF THE/17X,4H(CM),16X,4H(CM),
00347      415X,4H(CM),12X,9H(DEGREES),8X,4HWALL,15X,8HWALL (K)/
00348      51H ,6X,3(5X,F10.4,5X),1X,F10.4,2X,2(5X,F10.4,5X))
00349      500      FORMAT(1H-,T40,12X,10HABSORBTION,5X,8HPARTICLE,7X,9HMOLECULAR/T40,
00350      112X,10HEFFICIENCY,5X,8HSWELLING,5X,14HWEIGHT OF CHAR/T40,
00351      242X,9H(G/GMOLE)/T40,10X,F10.4,5X,3(F10.4,5X))
00352      509      FORMAT(32H-CHAR REACTION DATA*****/1H0,11X,8HREACTION,
00353      14X,8HOXYDIZER,8X,14HSTOICHIOMETRIC/41X,11HCOEFFICIENT)
00354      510      FORMAT(1H0,14X,I1,8X,2A4,7X,F10.4)
00355      515      FORMAT(34H-VAPOR PRESSURE CURVE COEFFICIENTS/,10X,
00356      123H A+BX+CX**2+DX**3+EX**4/1H0,10X,5(2X,F10.4,2X))
00357      END

```

```
00001      SUBROUTINE LGND (ASTRG,NA,NL)
00002 C   ASTRG(NA):  ARRAY OF CHARS TO BE PRINTED (44 CHARS MAX)
00003 C               CHARACTER SIZE:  3/16 X 9/64 IN.
00004 C   NA:  NUMBER OF CHARS AND SPACES IN ASTRG
00005 C   NA.LT.0,RETURN:  ASTRG HAD MORE THAN 44 CHARS
00006 C   NL:  LINE NUMBER (1: 1ST LINE, 2: 2ND, ETC.)
00007 C               LINES ARE PRINTED IN 1/4 IN. STEPS
00008 C   NL.LT.0:  END GRAPH AFTER THIS LINE
00009      DIMENSION ASTRG(1)
00010      IF(NA.LE.44) GO TO 10
00011      NA=-NA
00012      RETURN
00013 10      NLT=ABS(NL)
00014      X=4.5-(NA*.1875)/2.0
00015      Y=6.8125-NLT*.25
00016      CALL SYMBOL(X,Y,0.1875,ASTRG,0.0,NA)
00017      IF(NL.LT.0) CALL PLOT(12.,-2.5,-3)
00018      RETURN
00019      END
```

```
00001      SUBROUTINE OPEN
00002      C
00003      C*****OPENING THE DATA FILE ON DISC ON THE DEC-10
00004      C
00005          DOUBLE PRECISION DATFIL
00006          TYPE 5
00007      5      FORMAT(25H0ENTER INPUT FILE NAME: 5)
00008          READ(5,10)DATFIL
00009      10      FORMAT(A10)
00010          OPEN(UNIT=1,FILE=DATFIL,ACCESS='SEQIN')
00011          RETURN
00012          END
```

```

00001      SUBROUTINE OUTPUT
00002      COMMON/IO/DDUCT,DYDXM,AGSTPD,CPVC(3,5,5),HFV(5,5),DELHV(5,5),
00003      1INTCPV(5,5),QRB(5)
00004      COMMON/GNRL2/NAME1(20),NAME2(20)
00005      COMMON/MORE/D01(255,5),N01(255,5),ALFA0(255,5),ALFA0C(255,5),
00006      1ALFA0H(255,5),ALFA0W(255,5),ALFA0A(255,5),X0(255,20),WVG(255)
00007      COMMON /AREA13/ALFAC0(5),GAMMA,EK(20),XI(5),AMJ(5,5),
00008      1EMJ(5,5),KVD(5,5),TB,D(5),RHOC(5),RHO(5),DELTA(20),DIFM(20)
00009      2,ALFAH0(5),ALFAW0(5),ALFAA0(5)
00010      COMMON /RADI/T0(255,5),N0(5),D0(5),SIGMA,PI,E(5),IT(255),H0(5)
00011      1,NUMRDR,DEL,IRAD,TOOLD(5)
00012      COMMON /GENRL/ALPHA0(5),S(20),KG,MUG,DS,
00013      1TPJJ(5),YY(5,5),PRTCLS,SPECIE,
00014      2ELEMNT,CRXN,HRXN,HH(5),HW(5),RGC
00015      COMMON /LAST/GASTMN,TMIN(5),IQ0J(255,5)
00016      COMMON /APR77/DELTPJ,DELRRJ,ALEN,JFAR,HM,DIFMW,ICNVLM,
00017      1TTEST,SUMSQ,ITRYS,GAST(255),OSPRR,NPROP,ARMAX,AMIN,SQDIF
00018      COMMON/JAN78/V0,FUR
00019      DIMENSION X(255),Y(255),ASCX(5),ASCY1(9),ASTRG1(8),NORM(5)
00020      1,ASCY2(9),ASTRG2(4),SPAXX(3),SPAXY(3),ASCY3(4),ASTRG3(7),
00021      2ASTRG4(10),ASTRG5(6),ASTRG6(6),ASTRG7(6),ASTRG8(6),ASTRG9(6),
00022      3ASTRG10(5),TODAY(2)
00023      INTEGER PRTCLS,SPECIE,P
00024      REAL NO,N01,NORM
00025      DATA ASCX/20HAXIAL LOCATION (CM,)/,NX/20/
00026      DATA ASCY1/33HTEMPERATURE (DEGREES KELVIN X100)/,NY1/33/
00027      DATA ASTRG1/29HPARTICLE AND GAS TEMPERATURES/,NA1/29/
00028      DATA ASCY2/36HCOMPONENT MASS/INITIAL PARTICLE MASS/,NY2/36/
00029      DATA ASTRG2/13HPARTICLE MASS/,NA2/13/
00030      DATA ASCY3/13HMOLE FRACTION/,NY3/13/
00031      DATA ASTRG3/26HGAS SPECIES MOLE FRACTIONS/,NA3/26/
00032      DATA ASTRG4/37Hnote: scaling(if X>0.6 then X=X-0.4)/,NA4/37/
00033      DATA ASTRG5/24HMASS OF PARTICLE TYPE #1/,NA5/24/
00034      DATA ASTRG6/24HMASS OF PARTICLE TYPE #2/,NA6/24/
00035      DATA ASTRG7/24HMASS OF PARTICLE TYPE #3/,NA7/24/
00036      DATA ASTRG8/24HMASS OF PARTICLE TYPE #4/,NA8/24/
00037      DATA ASTRG9/24HMASS OF PARTICLE TYPE #5/,NA9/24/
00038      DATA ASTR10/19HTOTAL PARTICLE MASS/,N10/19/
00039      C
00040      C*****THIS SUBROUTINE PRINTS AND PLOTS ALL OUTPUT INFORMATION
00041      C
00042      C
00043      C*****FINDING TODAY'S DATE
00044      C
00045      CALL DATE(TODAY)
00046      C
00047      C*****FINDING THE NORMALIZED X-POSITION DOWN THE REACTOR
00048      C
00049      XX=0.0
00050      X(1)=XX
00051      DELX=ALEN/FLOAT(NUMRDR)
00052      DO 10 IO=2,NUMRDR+1
00053      XX=XX+DELX

```

```

00054 10      X(IO)=XX
00055 C
00056 C*****INITIALIZING AND WRITING OUT PARTICLE SPECS
00057 C
00058      TNORM=0.0
00059      TC0=0.0
00060      TH0=0.0
00061      TW0=0.0
00062      TA0=0.0
00063      DO 30 J=1, PRTCLS
00064      NORM(J)=ALFAC0(J)+ALFAH0(J)+ALFAW0(J)+ALFAA0(J)
00065      TC0=TC0+ALFAC0(J)*N01(1,J)*WVG(1)
00066      TH0=TH0+ALFAH0(J)*N01(1,J)*WVG(1)
00067      TW0=TW0+ALFAW0(J)*N01(1,J)*WVG(1)
00068      TA0=TA0+ALFAA0(J)*N01(1,J)*WVG(1)
00069      WRITE(3,100)
00070      WRITE(3,101)J
00071      WRITE(3,105)(TODAY(ID),ID=1,2)
00072      WRITE(3,110)
00073      WRITE(3,120)
00074      WRITE(3,110)
00075      WRITE(3,140)X(1),GASTMN,TMIN(J),V0,N0(J),D0(J),ALFAC0(J)
00076      1,ALFAH0(J),ALFAW0(J),ALFAA0(J),NORM(J)
00077      DO 20 IO=1,NUMRDR
00078      A=ARMAX
00079      IF(X(IO+1).LT,AGSTPD)A=PI*(DDUCT/2.0+DYDXM*X(IO+1))*2
00080      V=WVG(IO)/A
00081      WRITE(3,140)X(IO+1),GAST(IO),T0(IO,J),V,N01(IO,J),D01(IO,J),
00082      1ALFA0C(IO,J),ALFA0H(IO,J),ALFA0W(IO,J),ALFA0A(IO,J),ALFA0(IO,J)
00083 20      CONTINUE
00084 30      CONTINUE
00085      TNORM=TC0+TH0+TW0+TA0
00086 C*****TOTAL
00087      WRITE(3,100)
00088      WRITE(3,103)
00089      WRITE(3,105) (TODAY(ID),ID=1,2)
00090      WRITE(3,110)
00091      WRITE(3,125)
00092      WRITE(3,110)
00093      TC=TC0/TNORM
00094      TH=TH0/TNORM
00095      TW=TW0/TNORM
00096      TA=TA0/TNORM
00097      TP=1.0
00098      WRITE(3,160) X(1),TC,TH,TW,TA,TP
00099      DO 36 IO=1,NUMRDR
00100      TC=0.0
00101      TH=0.0
00102      TW=0.0
00103      TP=0.0
00104      DO 35 J=1,PRTCLS
00105      TC=TC+ALFA0C(IO,J)*N01(IO,J)
00106      TH=TH+ALFA0H(IO,J)*N01(IO,J)

```

```

00107      35 TW=TW+ALFAOW(IO,J)*N01(IO,J)
00108          TC=TC*WVG(IO)/TNORM
00109          TH=TH*WVG(IO)/TNORM
00110          TW=TW*WVG(IO)/TNORM
00111          TP=TC+TH+TW+TA
00112          WRITE(3,160)X(IO+1),TC,TH,TW,TA,TP
00113      36 CONTINUE
00114  C
00115  C*****WRITING OUT GAS PHASE SPECS
00116  C
00117          I=1
00118      40  CONTINUE
00119          NS=10
00120          IF(SPECIE.LE.10)NS=SPECIE
00121          IF(I.EQ.2)NS=SPECIE
00122          WRITE(3,100)
00123          WRITE(3,102)
00124          WRITE(3,105)(TODAY(ID),ID=1,2)
00125          WRITE(3,110)
00126          IF(I.EQ.1)WRITE(3,130)(NAME1(IS),NAME2(IS),IS=1,NS)
00127          IF(I.EQ.2)WRITE(3,130)(NAME1(IS),NAME2(IS),IS=11,NS)
00128          WRITE(3,135)
00129          WRITE(3,110)
00130          DO 50 IO=1,NUMRDR
00131              IF(I.EQ.1)WRITE(3,150)X(IO+1),WVG(IO),(X0(IO,IS),IS=1,NS)
00132              IF(I.EQ.2)WRITE(3,150)X(IO+1),WVG(IO),(X0(IO,IS),IS=11,NS)
00133      50  CONTINUE
00134          IF(SPECIE.GT.10)I=I+1
00135          IF(I.EQ.2)GO TO 40
00136  C
00137  C*****PLOTING OUT TEMPERATURE PROFILES
00138  C
00139          Y(1)=GASTMN/100.0
00140          DO 55 IO=1,NUMRDR
00141              IOO=IO+1
00142      55  Y(IOO)=GAST(IO)/100.0
00143          CALL GRPH(X,Y,NUMRDR+1,0.,0.,ASCX,NX,ASCY1,NY1,-1)
00144          DO 65 J=1,PRCLSL
00145              Y(1)=TMIN(J)/100.0
00146          DO 60 IO=1,NUMRDR
00147              IOO=IO+1
00148      60  Y(IOO)=T0(IO,J)/100.0
00149      65  CALL GRPH(X,Y,NUMRDR+1,0.,0.,ASCX,NX,ASCY1,NY1,1)
00150          CALL LGND(STRG1,NA1,-1)
00151  C
00152  C*****PLOTING PARTICLE MASS FOR EACH PARTICLE
00153  C
00154          P=PRCLSL+1
00155          L=P
00156          IF(PRCLSL.EQ.1)L=1
00157          DO 95 J=1,L
00158  C
00159  C*****SCALING FOR PARTICLE MASS

```

```
00160 C
00161 67 SPAXX(1)=0.0
00162 SPAXX(2)=0.0
00163 SPAXX(3)=ALEN
00164 SPAXY(1)=0.98
00165 SPAXY(2)=0.0
00166 SPAXY(3)=0.0
00167 CALL GRPH(SPAXX,SPAXY,3,0.,0.,ASCX,NX,ASCY2,NY2,-1)
00168 Y(1)=1.0
00169 DO 70 IO=1,NUMRDR
00170 IOO=IO+1
00171 IF(J.NE.P)Y(IOO)=ALFA0(IO,J)/NORM(J)
00172 IF(J.NE.P)GO TO 70
00173 Y(IOO)=0.0
00174 DO 69 K=1,PRTCLS
00175 69 Y(IOO)=Y(IOO)+ALFA0(IO,K)*N01(IO,K)*WVG(IO)/TNORM
00176 70 CONTINUE
00177 CALL GRPH(X,Y,NUMRDR+1,0.,0.,ASCX,NX,ASCY2,NY2,1)
00178 IF(J.NE.P)Y(1)=ALFA0(J)/NORM(J)
00179 IF(J.EQ.P)Y(1)=TC0/TNORM
00180 DO 75 IO=1,NUMRDR
00181 IOO=IO+1
00182 IF(J.NE.P)Y(IOO)=ALFA0C(IO,J)/NORM(J)
00183 IF(J.NE.P)GO TO 75
00184 Y(IOO)=0.0
00185 DO 74 K=1,PRTCLS
00186 74 Y(IOO)=Y(IOO)+ALFA0C(IO,K)*N01(IO,K)*WVG(IO)/TNORM
00187 75 CONTINUE
00188 CALL GRPH(X,Y,NUMRDR+1,0.,0.,ASCX,NX,ASCY2,NY2,1)
00189 IF(J.NE.P)Y(1)=ALFA0(J)/NORM(J)
00190 IF(J.EQ.P)Y(1)=TH0/TNORM
00191 DO 80 IO=1,NUMRDR
00192 IOO=IO+1
00193 IF(J.NE.P)Y(IOO)=ALFA0H(IO,J)/NORM(J)
00194 IF(J.NE.P)GO TO 80
00195 Y(IOO)=0.0
00196 DO 79 K=1,PRTCLS
00197 79 Y(IOO)=Y(IOO)+ALFA0H(IO,K)*N01(IO,K)*WVG(IO)/TNORM
00198 80 CONTINUE
00199 CALL GRPH(X,Y,NUMRDR+1,0.,0.,ASCX,NX,ASCY2,NY2,1)
00200 IF(J.NE.P)Y(1)=ALFA0W(J)/NORM(J)
00201 IF(J.EQ.P)Y(1)=TW0/TNORM
00202 DO 85 IO=1,NUMRDR
00203 IOO=IO+1
00204 IF(J.NE.P)Y(IOO)=ALFA0W(IO,J)/NORM(J)
00205 IF(J.NE.P)GO TO 85
00206 Y(IOO)=0.0
00207 DO 84 K=1,PRTCLS
00208 84 Y(IOO)=Y(IOO)+ALFA0W(IO,K)*N01(IO,K)*WVG(IO)/TNORM
00209 85 CONTINUE
00210 CALL GRPH(X,Y,NUMRDR+1,0.,0.,ASCX,NX,ASCY2,NY2,1)
00211 IF(J.NE.P)Y(1)=ALFAA0(J)/NORM(J)
00212 IF(J.EQ.P)Y(1)=TA0/TNORM
```

```

00213      DO 90 IO=1,NUMRDR
00214      IOO=IO+1
00215      IF(J.NE.P)Y(IOO)=ALFA0A(IO,J)/NORM(J)
00216      IF(J.NE.P)GO TO 90
00217      Y(IOO)=0.0
00218      DO 89 K=1,PRTCLS
00219 89      Y(IOO)=Y(IOO)+ALFA0A(IO,K)*N01(IO,K)*WVG(IO)/TNORM
00220 90      CONTINUE
00221      CALL GRPH(X,Y,NUMRDR+1,0.,0.,ASCX,NX,ASCY2,NY2,1)
00222      IF(J.EQ.P)CALL LGND(ASTR10,N10,-1)
00223      IF(J.EQ.P) GO TO 95
00224      IF(PRTCLS.EQ.1)CALL LGND(ASTRG2,NA2,-1)
00225      IF(PRTCLS.EQ.1)GO TO 95
00226      IF(J.EQ.1)CALL LGND(ASTRG5,NA5,-1)
00227      IF(J.EQ.2)CALL LGND(ASTRG6,NA6,-1)
00228      IF(J.EQ.3)CALL LGND(ASTRG7,NA7,-1)
00229      IF(J.EQ.4)CALL LGND(ASTRG8,NA8,-1)
00230      IF(J.EQ.5)CALL LGND(ASTRG9,NA9,-1)
00231 95      CONTINUE
00232      C
00233      C*****SCALING FOR GAS PHASE MOLE FRACTIONS
00234      C
00235      SPAXX(1)=0.0
00236      SPAXX(2)=0.0
00237      SPAXX(3)=ALEN
00238      SPAXY(1)=0.58
00239      SPAXY(2)=0.0
00240      SPAXY(3)=0.0
00241      CALL GRPH(SPAXX,SPAXY,3,0.,0.,ASCX,NX,ASCY3,NY3,-1)
00242      C
00243      C*****PLOTting GAS PHASE MOLE FRACTIONS
00244      C
00245      DO 96 IO=1,NUMRDR
00246 96      X(IO)=X(IO+1)
00247      DO 98 IS=1,SPECIE
00248      DO 97 IO=1,NUMRDR
00249      Y(IO)=X0(IO,IS)
00250 97      IF(X0(IO,IS).GT.0.6)Y(IO)=X0(IO,IS)-0.4
00251      CALL GRPH(X,Y,NUMRDR,0.,0.,ASCX,NX,ASCY3,NY3,1)
00252 98      CONTINUE
00253      CALL LGND(ASTRG3,NA3,1)
00254      CALL LGND(ASTRG4,NA4,-2)
00255      RETURN
00256 100     FORMAT(1H1)
00257 101     FORMAT(1H0,23X,83HBYU -- ONE Dimensional Combustion Or Gasificatio
00258         1n model (1=DICOG): particle number ,11)
00259 102     FORMAT(1H0,20X,91HBYU -- ONE Dimensional Combustion Or Gasificatio
00260         1n model (1=DICOG): gas phase mole fractions)
00261 103     FORMAT(1H0,20X,87HBYU -- ONE Dimensional Combustion Or Gasificatio
00262         1n model (1=DICOG): total particle phase)
00263 105     FORMAT(1H0,62X,2A5)
00264 110     FORMAT(1H0,129(1H*))
00265 120     FORMAT(1H0,11X,8HDISTANCE,5X,3HGAS,4X,8HPARTICLE,2X,8HVELOCITY,

```

```
00266      12X,8HPARTICLE,2X,8HPARTICLE,4X,4HCOAL,6X,4HCHAR,7X,3HH2O,7X,
00267      23HASH,6X,4HPART/24X,4HTEMP,6X,4HTEMP,14X,8HNO, DENS,4X,4HDIA,,
00268      35(6X,4HMASS)/14X,4H(cm),4X,8H(kelvin),2X,8H(kelvin),2X,8H(cm/sec)
00269      43X,6H(#/cc),5X,4H(cm),5(6X,4H(gr)))
00270  125    FORMAT(1H0,29X,8HDISTANCE,6X,4HCOAL,8X,4HCHAR,8X,3HH2O,9X,3HASH,
00271      17X,5HTOTAL/31X,4H(cm),14X,38H(component mass/initial particle mass
00272      1))
00273  130    FORMAT(1H0,7X,8HDISTANCE,3X,10HFLOW RATE,3X,10(1X,2A4,1X))
00274  135    FORMAT(10X,4H(cm),6X,8H(cc/sec))
00275  140    FORMAT(13X,F6.2,4X,F6.1,4X,F6.1,2X,1PE9.2,7(1X,1PE9.2))
00276  150    FORMAT(9X,F6.2,4X,1PE9.2,2X,10(2X,0PF6.5,2X))
00277  160    FORMAT(30X,F6.2,5X,5(F7.5,5X))
00278      END
```

```

00001      SUBROUTINE PROFIL(J,IDISP)
00002      COMMON /TRUBLE/INDX,ITRBLE
00003      COMMON /EDNUM/RHOG,CPG,TG,CPI(20),X(20),CO(5),HGAS,EDNAME(9),
00004      10XYD(5),GMW,QMASS(9,20),WTM(20)
00005      COMMON /AREA13/ALFAC0(5),GAMMA,EK(20),XI(5),AMJ(5,5),
00006      1EMJ(5,5),KVD(5,5),TB,D(5),RHOC(5),RHO(5),DELTA(20),DIFM(20)
00007      2,ALFAH0(5),ALFAW0(5),ALFAA0(5)
00008      COMMON /DIFEQN/OMEGAK(9),ALPHA(5),ALPHAC(5),ALPHAH(5),
00009      1ALPHAH(5),NN(5),H(5),QF(5),QCB,QZ(5),P,V,HG(5),RK(5,9),
00010      2RL(5,20),RM(5,20),RC(5),RH(5),RW(5),RR(5),W(5),WG,AREA,PRESSR
00011      COMMON/MORE/D01(255,5),N01(255,5),ALFA0(255,5),ALFA0C(255,5),
00012      1ALFA0H(255,5),ALFA0W(255,5),ALFA0A(255,5),X0(255,20),WVG(255)
00013      COMMON /RADI/T0(255,5),N0(5),D0(5),SIGMA,PI,E(5),IT(255),H0(5)
00014      1,NUMRDR,DEL,IRAD,T0OLD(5)
00015      COMMON /GENRAL/ALPHAA(5),S(20),KG,MUG,D3,
00016      1TPJJ(5),YY(5,5),PRTCLS,SPECIE,
00017      2ELEMNT,CRXN,HRXN,HH(5),HW(5),RGC
00018      COMMON /ODEVAL/XDIS,XTRMNL,VALINT(42),ODESTP
00019      COMMON /APR77/DELTPJ,DELRRJ,ALEN,JFAR,HM,DIFMW,ICNVLM,
00020      1TTEST,SUMSQ,ITRSYS,GAST(255),OSPRR,NPROP,ARMAX,AMIN,SQDIF
00021      REAL NN,N01
00022      INTEGER PRTCLS,OSPRR,SPECIE,ODESTP
00023      C
00024      C*****THIS SUBROUTINE SAVES ALL THE PROFILES WHICH WILL BE OUTPUT IN
00025      C      THEIR APPROPRIATE ARRAYS IN PREPERATION FOR PRINTOUT AND PLOTTING.
00026      C      IN ADDITION SOME OF THE PROFILES PREPARED HERE ARE USED FOR THE
00027      C      NEXT PASS THROUGH THE REACTOR IN CALCULATING INITIAL PROFILES FOR
00028      C      RINTS. IT SHOULD BE NOTED THAT VALUES ARE ONLY STORED FOR THE
00029      C      RADIATIONL REGIONS. THIS MEANS THAT THE VALUES CALCULATED AT EACH
00030      C      O.D.E. STEP ARE AVERAGED(LINEARLY) TO OBTAIN VALUES FOR THE
00031      C      RADIATION REGION IN QUESTION.
00032      C
00033      IF(XDIS,NE,0.0)GO TO 30
00034      C
00035      C*****INITIALIZATIONL AT THE BEGINING OF THE REACTOR
00036      C      I.E.-- ZEROING OUT THE INITIAL RADIATION REGION
00037      C      NOTE: THE PAST VALUES OF THE ARRAYS ARE NEEDED LATER IN THIS
00038      C      SUBROUTINE FOR CALCULATING THE ROOT MEAN SQUARE.
00039      C
00040      SUMSQ=0.0
00041      GAST(1)=0.0
00042      WVG(1)=0.0
00043      DO 5 IJ=1,PRTCLS
00044      T0OLD(IJ)=T0(1,IJ)
00045      N01(1,IJ)=0.0
00046      D01(1,IJ)=0.0
00047      T0(1,IJ)=0.0
00048      ALFA0(1,IJ)=0.0
00049      ALFA0C(1,IJ)=0.0
00050      ALFA0H(1,IJ)=0.0
00051      ALFA0W(1,IJ)=0.0
00052      ALFA0A(1,IJ)=0.0
00053      5  CONTINUE

```

```

00054      DO 10 IS=1, SPECIE
00055 10      X0(1, IS)=0.0
00056      GO TO 1000
00057 30      CONTINUE
00058 C
00059 C*****ZEROING OUT THE PRESENT STORAGE LOCATION IN THE ARRAY WHEN WE
00060 C ARE THROUGH WITH IT IN CALCULATION THE ROOT MEAN SQUARE AND ARE
00061 C READY TO START FILLING IT UP AGAIN WITH PRESENT VALUES.
00062 C TIMET IS ALSO CALLED AT THIS POINT TO SEE IF THE TIME OF DAY IS
00063 C ACCEPTABLE TO CONTINUE EXECUTION.
00064 C
00065 C
00066      JM=J-1+IDISP
00067      INDX=JM/OSPRR+1
00068      IF (MOD(JM, OSPRR).NE.0.OR, JM.EQ.0) GO TO 80
00069      GAST(INDX)=0.0
00070      WVG(INDX)=0.0
00071      DO 70 IJ=1, PRTCLS
00072      SUMSQ=SUMSQ+(T0OLD(IJ)-T0(INDX-1, IJ))**2
00073      T0OLD(IJ)=T0(INDX, IJ)
00074      N01(INDX, IJ)=0.0
00075      D01(INDX, IJ)=0.0
00076      T0(INDX, IJ)=0.0
00077      ALFA0(INDX, IJ)=0.0
00078      ALFA0C(INDX, IJ)=0.0
00079      ALFA0H(INDX, IJ)=0.0
00080      ALFA0W(INDX, IJ)=0.0
00081      ALFA0A(INDX, IJ)=0.0
00082 70      CONTINUE
00083      DO 75 IS=1, SPECIE
00084 75      X0(INDX, IS)=0.0
00085      CALL TIMET
00086 80      CONTINUE
00087 C
00088 C*****AVERAGING THE O.D.E. STEP VALUES AND STORING THEM IN THE ARRAYS
00089 C
00090      GAST(INDX)=GAST(INDX)+TG/FLOAT(OSPRR)
00091      WVG(INDX)=WVG(INDX)+(WG/RHOG)/FLOAT(OSPRR)
00092      DO 90 IJ=1, PRTCLS
00093      N01(INDX, IJ)=N01(INDX, IJ)+NN(IJ)/FLOAT(OSPRR)
00094      D01(INDX, IJ)=D01(INDX, IJ)+D(IJ)/FLOAT(OSPRR)
00095      T0(INDX, IJ)=T0(INDX, IJ)+TPJJ(IJ)/FLOAT(OSPRR)
00096      ALFA0(INDX, IJ)=ALFA0(INDX, IJ)+ALPHA(IJ)/FLOAT(OSPRR)
00097      ALFA0C(INDX, IJ)=ALFA0C(INDX, IJ)+ALPHAC(IJ)/FLOAT(OSPRR)
00098      ALFA0H(INDX, IJ)=ALFA0H(INDX, IJ)+ALPHAH(IJ)/FLOAT(OSPRR)
00099      ALFA0W(INDX, IJ)=ALFA0W(INDX, IJ)+ALPHAW(IJ)/FLOAT(OSPRR)
00100      ALFA0A(INDX, IJ)=ALFA0A(INDX, IJ)+ALPHA A(IJ)/FLOAT(OSPRR)
00101 90      CONTINUE
00102      DO 100 IS=1, SPECIE
00103      IF (X(IS).LT.1.0E-30) GO TO 100
00104      X0(INDX, IS)=X0(INDX, IS)+X(IS)/FLOAT(OSPRR)
00105 100     CONTINUE
00106 C

```

```
00107 C*****PICKING UP THE LAST VALUE FOR ROOT MEAN SQUARE CALCULATIONS
00108 C
00109     IF(J.NE.(ODESTP-IDISP))GO TO 1000
00110     DO 999 IJ=1,PRCL5
00111 999   SUMSQ=SUMSQ+(T0OLD(IJ)-T0(INDX,IJ))**2
00112 1000  RETURN
00113     END
```

```

00001      SUBROUTINE RESTRT(RSTRT)
00002      COMMON/GENRAL/ALPHA(5),S(20),KG,MUG,DS,
00003      1TPJJ(5),YY(5,5),PRTCLS,SPECIE,
00004      2ELEMNT,CRXN,HRXN,HH(5),HW(5),RGC
00005      COMMON/RADI/T0(255,5),N0(5),D0(5),SIGMA,PI,E(5),IT(255),H0(5)
00006      1,NUMRDR,DEL,IRAD,T0OLD(5)
00007      COMMON/MORE/D01(255,5),N01(255,5),ALFA0(255,5),ALFA0C(255,5),
00008      1ALFA0H(255,5),ALFA0W(255,5),ALFA0A(255,5),X0(255,20),WVG(255)
00009      COMMON/CONST/OSGKM(9),OPGKM(9),SJMC(3,5),PJMC(4,5),SJH(5),
00010      1PJH(5),SGMC(3),PGMC(4),PGH,SGH,PGX,PJX(5)
00011      INTEGER RADCHK,ELEMNT,PRTCLS
00012      C
00013      C*****THIS SUBROUTINE DOES ALL THE WORK NECESSARY FOR READING AND WRITING
00014      C      INFORMATION NECESSARY FOR A RESTART.
00015      C
00016      IF(RSTRT.EQ.0)GO TO 100
00017      C
00018      C*****IF RESTART DATA IS GOING TO BE USED IN INPUT AND RINTS FOR AN
00019      C      INITIAL PROFILE THIS AREA DOES THE WORK.
00020      C
00021      OPEN(UNIT=21,FILE='RESTRT',ACCESS='SEGIN')
00022      READ(21)RADCHK
00023      IF(RADCHK.NE.NUMRDR)CLOSE(UNIT=21)
00024      IF(RADCHK.NE.NUMRDR)RETURN
00025      WRITE(3,200)
00026      READ(21)PGH,(OPGKM(I),I=1,ELEMNT),(PJH(I),I=1,PRTCLS)
00027      DO 10 L=1,PRTCLS
00028      READ(21)(T0(I,L),I=1,NUMRDR)
00029      READ(21)(N01(I,L),I=1,NUMRDR)
00030      10 READ(21)(D01(I,L),I=1,NUMRDR)
00031      CLOSE(UNIT=21)
00032      RETURN
00033      C
00034      C*****THIS AREA WRITES OUT ALL THE INFORMATION NECESSARY FOR A RESTART
00035      C      AFTER ONE OR MORE PASSES THROUGH THE REACTOR.
00036      C
00037      100 OPEN(UNIT=21,FILE='RESTRT',ACCESS='SEOUT')
00038      WRITE(21)NUMRDR
00039      WRITE(21)PGH,(OPGKM(I),I=1,ELEMNT),(PJH(I),I=1,PRTCLS)
00040      DO 110 L=1,PRTCLS
00041      WRITE(21)(T0(I,L),I=1,NUMRDR)
00042      WRITE(21)(N01(I,L),I=1,NUMRDR)
00043      110 WRITE(21)(D01(I,L),I=1,NUMRDR)
00044      CLOSE(UNIT=21)
00045      RETURN
00046      200 FORMAT(1H0/1H0/1H0/1H0,102H*****THIS RUN WILL USE RESTART
00047      1T DATA FOR INITIAL PROFILES*****')
00048      END

```

```

00001      SUBROUTINE RINTS
00002      COMMON /LAST/GASTMN,TMIN(5),IQ0J(255,5)
00003      COMMON/MORE/D01(255,5),N01(255,5),ALFA0(255,5),ALFA0C(255,5),
00004      1ALFA0H(255,5),ALFA0W(255,5),ALFA0A(255,5),X0(255,20),WVG(255)
00005      COMMON /RADI/T0(255,5),N0(5),D0(5),SIGMA,PI,E(5),IT(255),H0(5)
00006      1,NUMRDR,DEL,IRAD,TOOLD(5)
00007      COMMON /AREAS/NPRINT,TNIRP,CHECK,BUG
00008      COMMON /GENRAL/ALPHA(5),S(20),KG,MUG,DS,
00009      1TPJJ(5),YY(5,5),PRTCLS,SPECIE,
00010      2ELEMNT,CRXN,HRXN,HH(5),HW(5),RGC
00011      COMMON /APR77/DELTPJ,DELRRJ,ALEN,JFAR,HM,DIFMW,ICNVLM,
00012      1TTEST,SUMSQ,ITRSYS,GAST(255),OSPRR,NPROP,ARMAX,AMIN,SGDIF
00013      INTEGER RADREM,Q,P,BUG,PRTCLS
00014      REAL NO,IT,SUMA(255),IQ0J,SUMIOP(255),N01
00015      C
00016      C*****THIS SUBROUTINE IS A COMPACT CALCULATION OF INTENSITIES ETC.
00017      C      WHICH ARE NEEDED FOR THE RADIATION CALCULATIONS WITHIN THE
00018      C      REACTOR. IT IS FOR THIS SUBROUTINE ALONE THAT AN INITIAL OR
00019      C      A PAST TEMPERATURE PROFILE, NUMBER PARTICLE DENSITY PROFILE
00020      C      AND DIAMETER PROFILE OF THE PARTICLES IS NEEDED BEFORE CAL-
00021      C      CULATIONS CAN BEGIN. THESE INTIAL PROFILES COME FROM INPUT
00022      C      OR FROM RESTRT, OR OF COURSE FROM THE IMMEDIATLY PAST CALCU-
00023      C      LATION. THESE VALUES ARE USED IN AUX1 AND AUX3.
00024      C
00025      PI4=PI/4.0
00026      DELX=ALEN/FLOAT(NUMRDR)
00027      DO 10 P=1,NUMRDR
00028      SUMA(P)=0.0
00029      SUMIOP(P)=0.0
00030      DO 20 J=1,PRTCLS
00031      AJ=PI4*E(J)*N01(P,J)*D01(P,J)**2
00032      AJT=AJ*T0(P,J)**4
00033      IF (BUG.GE.5) WRITE(3,410) P,J,AJ,AJT
00034      SUMA(P)=SUMA(P)+AJ
00035      IQ0J(P,J)=AJT*SIGMA*DELX
00036      20 SUMIOP(P)=SUMIOP(P)+IQ0J(P,J)
00037      10 IF (BUG.GE.2) WRITE(3,310) P,SUMIOP(P)
00038      DO 40 Q=1,NUMRDR
00039      SUMIPQ=0.0
00040      SUMPQR=0.0
00041      SUMPQL=0.0
00042      IF (Q.EQ.1) GO TO 42
00043      M3=Q-1
00044      DO 41 I=1,M3
00045      41 SUMPQL=SUMPQL+SUMA(I)*DELX
00046      42 CONTINUE
00047      DO 50 P=1,NUMRDR
00048      IF (P=0) 45,50,55
00049      45 IF(P.EQ.1)GO TO 44
00050      SUMPQL=SUMPQL-SUMA(P-1)*DELX
00051      44 SUMPQ=SUMPQL
00052      GO TO 70
00053      55 SUMPQR=SUMPQR+SUMA(P)*DELX

```

```
00054      SUMPQ=SUMPQR
00055  70    IF(SUMPQ.GT.85.0)SUMPQ=85.0
00056      SUMIPQ=SUMIPQ+SUMIOP(P)*EXP(-SUMPQ)
00057      IF (BUG.GE.5) WRITE(3,320) P,Q,SUMIPQ
00058  50    CONTINUE
00059      IT(Q)=SUMIPQ
00060  40    IF (BUG.GE.2) WRITE(3,330) Q,IT(Q)
00061  410   FORMAT(1H ,3HP =,I4,4X,3HK =,I4,4X,3HJ =,I4,4X,4HAJ =,E12.5,
00062        15X,5HAJT= ,E12.5)
00063  310   FORMAT(1H ,3HP =,I4,4X,11HSUMIOP(P) =,E12.5)
00064  320   FORMAT(1H ,3HP =,I4,4X,3HQ =,I4,4X,8HSUMIPQ =,E12.5)
00065  330   FORMAT(1H ,3HQ =,I4,4X,7HIT(Q) =,E12.5)
00066      IF(BUG.GE.6)STOP
00067      RETURN
00068      END
```

```

00001      SUBROUTINE RODEVL(YZ, KK, J)
00002      COMMON /LAST/GASTMN, TMIN(5), IQ0J(255, 5)
00003      COMMON /ODEVAL/XDIS, XTRMNL, VALINT(42), ODESTP
00004      COMMON /DIFEQN/OMEGAK(9), ALPHA(5), ALPHAC(5), ALPHAH(5),
00005      1ALPHAW(5), N(5), H(5), QF(5), QCB, QZ(5), P, V, HG(5), RK(5, 9),
00006      2RL(5, 20), RM(5, 20), RC(5), RH(5), RW(5), RR(5), W(5), WG, AREA, PRESSR
00007      COMMON /EDNUM/RHOG, CPG, TG, CPI(20), X(20), CO(5), HGAS, EDNAME(9),
00008      10XYD(5), GMW, QMASS(9, 20), WTM(20)
00009      COMMON /AREAS/NPRINT, TNIRP, CHECK, BUG
00010      REAL YZ(42)
00011      INTEGER BUG, EDNAME
00012  C
00013  C*****RODEVL(RETURN O.D.E. VALUES) TAKES THE DIFFERENTIAL EQUATION FUNCTIONS
00014  C      WHICH ARE PREDICTED IN SOLVE IN EITHER A PREDICTOR OR CORRECTOR
00015  C      OR A RUNGE-KUTTA METHOD AND EXTRACTS THE INDIVIDUAL VALUES OF
00016  C      THE MODEL PARAMETERS. THIS IS TRUE OF ALL PARAMETERS APPEARING
00017  C      IN THE DIFFERENTIAL EQUATIONS EXCEPT FOR VELOCITY AND NUMBER
00018  C      PARTICLE DENSITY. THESE TWO SPECIAL CASES REQUIRE INFORMATION
00019  C      FROM EDWRDS BEFORE THEY CAN BE UPDATED SO THEY ARE HANDLED
00020  C      SEPERATELY IN DIFF.
00021  C
00022      IA=KK+3*J+2
00023      WG=YZ(IA)
00024      DO 10 IC=1, KK
00025 10      OMEGAK(IC)=YZ(IC)/WG
00026      IBIG=1
00027      SUBT=0.0
00028      AMFRAC=0.0
00029      DO 80 IK=1, KK
00030      IF(OMEGAK(IK).LE, AMFRAC)GO TO 81
00031      IBIG=IK
00032      AMFRAC=OMEGAK(IK)
00033 81      QMASS(IK, 1)=OMEGAK(IK)
00034      IF(OMEGAK(IK).GT.0.000001)GO TO 80
00035      QMASS(IK, 1)=.000001
00036      SUBT=SUBT+.000001
00037 80      CONTINUE
00038      QMASS(IBIG, 1)=QMASS(IBIG, 1)-SUBT
00039      DO 20 IC=1, J
00040      IDX=IC+KK
00041 20      W(IC)=YZ(IDX)
00042      IB=KK+J+1
00043      HGAS=YZ(IB)/WG
00044      DO 30 IC=1, J
00045      IDX=IC+KK+J+1
00046 30      H(IC)=YZ(IDX)/W(IC)
00047      DO 60 IC=1, J
00048      IDX1=IC+KK+3*J+2
00049      IDX2=IDX1+J
00050      IDX3=IDX2+J
00051      ALPHAC(IC)=YZ(IDX1)
00052      ALPHAH(IC)=YZ(IDX2)
00053      ALPHAW(IC)=YZ(IDX3)

```

```
00054      IF(ALPHAC(IC).LT.1.0E-30)ALPHAC(IC)=0.0
00055      IF(ALPHAH(IC).LT.1.0E-30.AND.ALPHAC(IC).EQ.0.0)ALPHAH(IC)=0.0
00056  60      IF(ALPHAW(IC).LT.1.0E-30)ALPHAW(IC)=0.0
00057      IF(TNIRP.NE.1.0.OR.BUG.LT.1)GO TO 70
00058      WRITE(3,100)WG,P,AREA,HGAS
00059  100      FORMAT(5H WG= ,E12.5,4H P= ,E12.5,7H AREA= ,
00060  1E12.5,7H HGAS= ,E12.5)
00061      WRITE(3,110)(OMEGAK(IX),IX=1,KK)
00062  110      FORMAT(12H OMEGAK(K)= ,8(1X,E12.5,1X))
00063      WRITE(3,130)
00064  130      FORMAT(6X,1HJ,8X,4HW(J),10X,4HH(J),10X,9HALPHAC(J),
00065  15X,23HAPPHAH(J)      ALPHAW(J))
00066      DO 90 IX=1,J
00067  90      WRITE(3,140)IX,W(IX),H(IX),ALPHAC(IX),ALPHAH(IX),ALPHAW(IX)
00068  140      FORMAT(6X,I1,5(1X,E12.5,1X))
00069  70      RETURN
00070      END
```

```

00001      SUBROUTINE SETUP1
00002      INTEGER ELEMNT, SPECIE
00003      COMMON /EDNUM/RHOG,CPG,TG,CPI(20),X(20),CO(5),HGAS,EDNAME(9),
00004      10XYD(5),GMW,QMASS(9,20),WTM(20)
00005      COMMON /DIFEQN/OMEGAK(9),ALPHA(5),ALPHAC(5),ALPHAH(5),
00006      1ALPHAW(5),NX(5),HZZ(5),QF(5),QCB,QZ(5),P,V,HG(5),RK(5,9),
00007      2RL(5,20),RM(5,20),RC(5),RH(5),RW(5),RR(5),W(5),WG,AREA,PRESSR
00008      COMMON/AZ/A(20,11),
00009      COMMON/AZ1/ANS(23),
00010      2      ATMOS
00011      COMMON/AZ2/
00012      COMMON/AZ3/B(11),
00013      5      BMIN,
00014      6      CBAR,
00015      7      NEQ,
00016      8      D,
00017      9      ITE,
00018      COMMON/BZ/
00019      1      ITT,
00020      2      K2,
00021      3      EL(23,24),
00022      4      ENTRPY,
00023      5      LB,
00024      6      H(20),
00025      7      HBAR,
00026      8      HC,
00027      9      HI,
00028      COMMON/CZ/HR(20),
00029      COMMON/CZ1/IDKIN(20),
00030      2      MPD,
00031      3      IDSIN(20),
00032      4      IEV(11),
00033      COMMON/EZ/
00034      DIMENSION C(20),
00035      1      S(20),
00036      DATA NCOUNT/0/
00037      IERR=0
00038      IF (NCONV.EQ.0.AND.NCOUNT.LE.1) GO TO 370
00039      5 NM1=NEQ+1
00040      NML=NEQ+NM
00041      NC1=NML+1
00042      IF (TO,LT.50.0) TO=50.0
00043      RTO=TO*1.98726
00044      RTOTO=TO*RTO
00045      CBAR=0.0
00046      HBAR=0.0
00047      LKDROP=LKDROP+1
00048      IMPL=1
00049      TTO=TO/1000.0
00050      IF (ABS(ANS(K2)).GT.(.001*TO)) MAJOR=0
00051      IF (TO,LE.6000.0) GO TO 10
00052      IERR=1
00053      IMPL=2

```

```

00054 10 IF (MAJOR.EQ.1) GO TO 15
00055 IF (ABS(TO-TCEN).GT.(0.1*TCEN)) IMPL=2
00056 IF (ABS(TO-TPREV).GT.(.001*TCEN)) GO TO 15
00057 IF (IMBALA.EQ.1) GO TO 15
00058 IMPL=3
00059 MAJOR=1
00060 TOL=0.1*TOLMAX
00061 15 IF (ITER.GT.1) GO TO 20
00062 IF (NCTXP.EQ.0.OR.NCTXP.EQ.4) IMPL=3
00063 20 IF (LKDROP.EQ.8) IMPL=3
00064 IF (NCONV.EQ.(-1)) GO TO 25
00065 IF (NCOUNT.LE.1) GO TO 25
00066 NCONV=-1
00067 IMPL=3
00068 25 IF (IMPL.EQ.3) LKDROP=0
00069 GO TO (30,35,35), IMPL
00070 30 C1=TO-TPREV
00071 C2=ALOG(TO/TPREV)
00072 GO TO 50
00073 35 IF (TO-1200.0) 40,45,45
00074 C
00075 C START SETUP OF COEFF. FOR UNDER 1200.0
00076 C
00077 40 TSWTCH=-1.0
00078 C0=TO/1000.0
00079 C1=C0*C0
00080 C2=C0*C1
00081 C3=C0*C2
00082 C4=ALOG(C0)-0.18232
00083 C5=C0-1.2
00084 C6=0.5*(C1-1.44)
00085 C7=0.33333333*(C2-1.728)
00086 C8=0.25*(C3-2.0736)
00087 C9=.2*(C0*C3-2.48832)
00088 GO TO 50
00089 C
00090 C END UNDER 1200.0 COEFF. SETUP START OF OVER 1200.0 COEFF. SETUP
00091 C
00092 45 TSWTCH=1.0
00093 IF (TO.GT.6000.) TO=6000.
00094 C0=1000.0/TO
00095 C1=C0*C0
00096 C2=C0*C1
00097 C3=C0*C2
00098 C4=(TO/1000.0)-1.2
00099 C5=ALOG(TO/1000.0)-0.18232
00100 C6=0.83333333-1000.0/TC
00101 C7=0.5*(0.69444444-C1)
00102 C8=0.33333333*(0.57870370-C2)
00103 C9=0.25*(0.48225308-C3)
00104 C
00105 C END OVER 1200.0 COEFFICIENT SETUP
00106 C

```

```
00107      50 IRE=0
00108      GO TO(125,125,55)IMPLE
00109      C
00110      C          FULL BLOWN SOLUTION FOR TOTAL NUMBER OF SPECIES
00111      C          CONSIDERED.  IMPL=3.
00112      C
00113      55 ISTOP=NT
00114      GO TO 155
00115      60 IF (ITER,LT,1) GO TO 85
00116      BLOGAT=ALOG(ATMOS)
00117      C
00118      C          TEST FOR ADDING GASES TO THE SOLUTION.
00119      C
00120      DO 70 I=1,NN
00121      IF (Y(I),GE,TOLT) GO TO 70
00122      SUMAPI=0.0
00123      DO 65 J=1,NM
00124      J1=J+NEQP
00125      65 SUMAPI=SUMAPI+ANS(J1)*A(I,J)
00126      EXPP=SUMAPI-BLOGAT-HS(I)
00127      IF( ABS(EXPP) ,LT. 85.0 ) GO TO 64
00128      IF( EXPP ) 61,61, 62
00129      61 EXPP = -85.0
00130      GO TO 64
00131      62 EXPP = 85.0
00132      64 CONTINUE
00133      Y(I)=YBAR*EXP(EXPP)
00134      63 CONTINUE
00135      IF (Y(I),LT,TOL) GO TO 70
00136      Y(I)=TOL
00137      IRE=1
00138      70 CONTINUE
00139      85 NKIN=0
00140      100 IF (IRE,NE,0) GO TO 105
00141      IF (NCONV) 185,370,370
00142      C
00143      C          COUNT THE NUMBER OF GASES IN THE SYSTEM.
00144      C
00145      105 NCONV=-1
00146      110 NGIN=0
00147      DO 120 I=1,NN
00148      IF (Y(I),LT,TOL) GO TO 120
00149      115 NGIN=NGIN+1
00150      IDSIN(NGIN)=I
00151      120 CONTINUE
00152      C
00153      C          COUNT THE NUMBER OF SPECIES IN FOR ALL IMPL VALUES
00154      C
00155      125 NSIN=NGIN
00156      135 LV=NML+NKIN
00157      LB=LV+1
00158      GO TO (140,150,185), IMPL
00159      C
```

```

00160 C          QUICK CALCULATIONS OF H AND S FOR IMPL=1.
00161 C
00162 140 DO 145 J=1, NSIN
00163     I=IDSIN(J)
00164     H(I)=H(I)+C(I)*C1
00165     S(I)=S(I)+C(I)*C2
00166 145 HS(I)=(H(I)/RTO)-(S(I)/R)
00167     GO TO 185
00168 C
00169 C          CALCULATE H AND S FOR ONLY THE SPECIES IN THE
00170 C          SOLUTION AT THE PRESENT TIME.  IMPL=2.
00171 C
00172 150 ISTOP=NSIN
00173 C
00174 C          CALCULATE H AND S FOR IMPL=2 OR IMPL=3.
00175 C
00176 155 IF (TSWCH) 160,170,170
00177 160 DO 165 J=1, ISTOP
00178     I=J
00179     IF (IMPL.EQ.2) I=IDSIN(J)
00180     C(I)=Z(I,6)+Z(I,7)*C0+Z(I,8)*C1+Z(I,9)*C2+Z(I,10)*C3
00181     S(I)=SR(I)+Z(I,6)*C4+Z(I,7)*C5+Z(I,8)*C6+Z(I,9)*C7+Z(I,10)*C8
00182     H(I)=HR(I)+Z(I,6)*C5+Z(I,7)*C6+Z(I,8)*C7+Z(I,9)*C8+Z(I,10)*C9
00183     H(I)=1000.0*H(I)
00184     HS(I)=(H(I)/RTO)-(S(I)/R)
00185 165 CONTINUE
00186     GO TO 180
00187 170 DO 175 J=1, ISTOP
00188     I=J
00189     IF (IMPL.EQ.2) I=IDSIN(J)
00190     C(I)=Z(I,1)+Z(I,2)*C0+Z(I,3)*C1+Z(I,4)*C2+Z(I,5)*C3
00191     S(I)=SR(I)+Z(I,1)*C5+Z(I,2)*C6+Z(I,3)*C7+Z(I,4)*C8+Z(I,5)*C9
00192     H(I)=HR(I)+Z(I,1)*C4+Z(I,2)*C5+Z(I,3)*C6+Z(I,4)*C7+Z(I,5)*C8
00193     H(I)=1000.0*H(I)
00194     HS(I)=(H(I)/RTO)-(S(I)/R)
00195     IF (IERR.EQ.0) GO TO 175
00196     H(I)=H(I)+C(I)*(TTO-6.)*1000.
00197     S(I)=S(I)+C(I)*ALOG(TTO/6.)
00198     HS(I)=(H(I)/RTO)-(S(I)/R)
00199 175 CONTINUE
00200 180 CONTINUE
00201 C
00202 C          BRANCH BACK FOR IMPL=3.
00203 C
00204 C          IF (IMPL.EQ.3) GO TO 60
00205 C
00206 C          ALL IMPL'S WIND UP HERE SO CALCULATE THE REST
00207 C          OF THE GARBAGE FOR EACH ITERATION.
00208 C
00209 185 NEQP=NEQ
00210     TCEN=TO
00211 190 YBAR=0.0
00212     WTG = 0.0

```

```

00213      NMM = NM
00214      DO 195 J=1,NGIN
00215        I=IDSIN(J)
00216        WM = 0.0
00217        DO 192 K = 1,NMM
00218          M = IEVN(K)
00219 192      WM = WM + A(I,K)*ATWT(M)
00220          WTM(I)=WM
00221          CPI(I)=C(I)/WM
00222          WTG = WTG + Y(I)*WM
00223 195      YBAR=YBAR+Y(I)
00224          PYLN=ALOG(ATMOS/YBAR)
00225          TOLT=TOL
00226          TO=TTO*1000.0
00227          SUMYU=0.0
00228          DO 200 J=1,NGIN
00229            I=IDSIN(J)
00230            CBAR=CBAR+C(I)*Y(I)
00231            YH(I)=Y(I)*H(I)
00232            HBAR=HBAR+YH(I)
00233            IF( Y(I) ) 196, 196, 197
00234 196      YLN(I) = -1.0E-37
00235            GO TO 198
00236 197      YLN(I)=ALOG(Y(I))
00237 198      U(I)=HS(I)+PYLN+YLN(I)
00238 200      SUMYU=SUMYU+Y(I)*U(I)
00239            SUMYH=HBAR
00240            CBAG = CBAR
00241            IF (NKIN,LT,1) GO TO 210
00242            N=NGIN+1
00243            DO 205 J=N,NSIN
00244              I=IDSIN(J)
00245              CBAR=CBAR+C(I)*Y(I)
00246 205      HBAR=HBAR+H(I)*Y(I)
00247 210      IMBAL=0
00248      C
00249      C          START SETTING UP THE ELEMENTS OF THE 'EL' ARRAY.
00250      C
00251 225      DO 275 M=NM1,NML
00252          MT=M-NEQ
00253          SUMAY=0.0
00254          SUMAYH=0.0
00255          SUMAYU=0.0
00256          DO 230 K=1,MT
00257 230      SUMAAY(K)=0.0
00258          DO 240 J=1,NGIN
00259            I=IDSIN(J)
00260            AY=A(I,MT)*Y(I)
00261            IF (AY,EQ,0.0) GO TO 240
00262            SUMAY=SUMAY+AY
00263            SUMAYH=SUMAYH+AY*H(I)
00264            SUMAYU=SUMAYU+AY*U(I)
00265            DO 235 K=1,MT

```

```
00266 235 SUMAAY(K)=SUMAAY(K)+A(I,K)*AY
00267 240 CONTINUE
00268 TSMAY=SUMAY
00269 DEN = TSMAY
00270 IF( ABS(DEN) .LT. 1.0E-37) DEN = 1.0
00271 BRAY = B(MT)/DEN
00272 250 IF ((TSMAY-B(MT)).LT.(.2*B(MT))) GO TO 265
00273 IMBAL=1
00274 255 DO 260 J=1,NSIN
00275 I=IDSIN(J)
00276 IF (A(I,MT).EQ.(0.0)) GO TO 260
00277 Y(I)=BRAY*Y(I)
00278 260 CONTINUE
00279 GO TO 275
00280 265 EL(M,K3)=SUMAY
00281 EL(M,K2)=SUMAYH/RTOTO
00282 EL(M,LB)=B(MT)+SUMAYU
00283 DO 270 M1=NM1,M
00284 K=M1-NEQ
00285 270 EL(M,M1)=SUMAAY(K)
00286 275 CONTINUE
00287 C
00288 C BRANCH BACK FOR ANY IMBALANCES.
00289 C
00290 IF (IMBAL.EQ.1) GO TO 190
00291 EL(K3,K3)=0.0
00292 EL(K3,K2)=SUMYH/RTOTO
00293 EL(K3,LB)=SUMYU
00294 C
00295 C FLIP THE SMALL ARRAY.
00296 C
00297 310 LVM1=LV-1
00298 DO 315 I=K3,LVM1
00299 DO 315 J=I,LVM1
00300 315 EL(I,J+1)=EL(J+1,I)
00301 C
00302 C CHAMBER AND AREA RATIO SOLUTIONS.
00303 C
00304 335 SUMYHH=0.0
00305 SUMYHU=0.0
00306 DO 340 J=1,NGIN
00307 I=IDSIN(J)
00308 SUMYHH=SUMYHH+YH(I)*H(I)
00309 340 SUMYHU=SUMYHU+YH(I)*U(I)
00310 C
00311 C CHAMBER SOLUTION ONLY.
00312 C
00313 DO 345 I=K3,LV
00314 345 EL(K2,I)=EL(I,K2)*RTOTO
00315 EL(K2,LB)=HI+SUMYHU
00316 EL(K2,K2)=CBAR+SUMYHH/RTOTO
00317 EL(K2,K3)=SUMYH
00318 GO TO 405
```

```

00319 C
00320 C          AREA RATIO SOLUTION ONLY.
00321 C
00322 C
00323 C          GET ENTROPY SEEING AS WE HAVE REACHED CONVERGANCE
00324 C
00325 370 ENTRPY=YBAR*R*ALOG(YBAR/ATMOS)
00326     YRYLNS=0.0
00327     DO 375 J=1,NGIN
00328     I=IDSIN(J)
00329     YRYLN=Y(I)*R*YLN(I)
00330     YRYLNS=YRYLNS+YRYLN
00331 375 ENTRPY=ENTRPY+Y(I)*S(I)-YRYLN
00332     IF (NCTXP.EQ.0) YRYLNC=YRYLNS
00333     IF (NKIN) 390,390,380
00334 380 DO 385 J=1,NKIN
00335     K=IDKIN(J)
00336 385 ENTRPY=ENTRPY+Y(K)*S(K)
00337 390 IF (NCTXP.EQ.0.OR.NCTXP.EQ.4) GO TO 405
00338     IF (ABS(ENTRPY-SCH).GT.0.002) NCONV=-1
00339     GO TO 405
00340 405 TPREV=TO
00341 415 RETURN
00342 C
00343 C
00344     END

```

```
00001  FUNCTION SIGMAD(TEK)
00002  DIMENSION ABC(3,3)
00003  DATA (ABC(I,1),I=1,3)/0.36934,-0.48595,0.02574/
00004  DATA (ABC(I,2),I=1,3)/0.343,-0.44203,0.07549/
00005  DATA (ABC(I,3),I=1,3)/0.09454,-0.17612,0.00272/
00006  IF (TEK.LT.0.3) TEK=0.3
00007  IF (TEK.GT.100.0) TEK=100.0
00008  M=1
00009  IF (1.55.LE.TEK.AND.TEK.LT.7.0) M=2
00010  IF (TEK.GT.7.0) M=3
00011  ALOGT=ALOG(TEK)
00012  SIGMAD=EXP(ABC(1,M)+ALOGT*(ABC(2,M)+ALOGT*ABC(3,M)))
00013  RETURN
00014  END
```

```
00001  FUNCTION SIGMAM(TEK,DEL)
00002  DIMENSION DELTA(8),AM(8,3),BM(8,3),CM(8,3)
00003  DATA (DELTA(I),I=1,8)/0.0,0.25,0.5,0.75,1.0,1.5,2.0,2.5/
00004  DATA (AM(I,1),I=1,8)/0.47395,0.47808,0.50119,0.54668,0.60910,
00005  10.45351,0.89016,1.01037/
00006  DATA (AM(I,2),I=1,8)/0.43969,0.44882,0.48192,0.53732,0.60815,
00007  10.76710,0.91660,1.04383/
00008  DATA (AM(I,3),I=1,8)/0.16152,0.16285,0.17807,0.20258,0.23287,
00009  10.31112,0.41063,0.52600/
00010  DATA (BM(I,1),I=1,8)/-0.53203,-0.51551,-0.49752,-0.49670,-0.51945,
00011  1-0.57471,-0.60747,-0.62594/
00012  DATA (BM(I,2),I=1,8)/-0.44832,-0.45212,-0.47283,-0.50951,-0.55388,
00013  1-0.64309,-0.70603,-0.73772/
00014  DATA (BM(I,3),I=1,8)/-0.15835,-0.15840,-0.16626,-0.17878,-0.16314,
00015  1-0.23119,-0.27807,-0.33159/
00016  DATA (CM(I,1),I=1,8)/-0.05410,-0.04057,-0.01404,0.01,0.01832,
00017  10.01467,0.00901,0.00461/
00018  DATA (CM(I,2),I=1,8)/0.07758,0.07756,0.08067,0.08685,0.09367,
00019  10.10489,0.10718,0.10078/
00020  DATA (CM(I,3),I=1,8)/0.00186,0.00178,0.00281,0.00442,0.00627,
00021  10.01075,0.01625,0.02242/
00022  DATA IDEL/1/
00023  IF (DEL.GT.2.5) DEL=2.5
00024  IF (TEK.LT.0.1) TEK=0.1
00025  IF (TEK.GT.100.0) TEK=100.0
00026  M=1
00027  IF (TEK.LT.9.0.AND.1.4.LE.TEK) M=2
00028  IF (TEK.GE.9.0) M=3
00029  ALOGT=ALOG(TEK)
00030  CALL FIND (DEL,A,DELTA,AM(1,M),8,IDEI)
00031  CALL FIND (DEL,B,DELTA,BM(1,M),8,IDEI)
00032  CALL FIND (DEL,C,DELTA,CM(1,M),8,IDEI)
00033  SIGMAM=EXP(A+ALOGT*(B+C*ALOGT))
00034  RETURN
00035  END
```

```

00001      SUBROUTINE SLE
00002      COMMON/XZ/P,HGAS,GMW,ELEMNT,SPECIE
00003      INTEGER ELEMNT,SPECIE
00004      COMMON/AZ/A(20,11),
00005      COMMON/AZ1/ANS(23),
00006      2      ATMOS
00007      COMMON/AZ2/
00008      COMMON/AZ3/B(11),
00009      5      BMIN,
00010      6      CBAR,
00011      7
00012      8      D,
00013      9
00014      COMMON/BZ/
00015      1
00016      2
00017      3      EL(23,24),
00018      4      ENTRPY,
00019      5
00020      6      H(20),
00021      7      HBAR,
00022      8      HC,
00023      9      HI,
00024      COMMON/CZ/HR(20),
00025      COMMON/CZ1/IDKIN(20),
00026      2
00027      3      IDSIN(20),
00028      4      IEV(11),
00029      DIMENSION NORDER(23),MORDER(24)
00030      DO 5 I=1,LB
00031      NORDER(I)=I
00032      5 MORDER(I)=I
00033      DO 50 L=1,LV
00034      DIVB=0.0
00035      DO 10 I=L,LV
00036      IN=NORDER(I)
00037      DO 10 J=L,LV
00038      JN=MORDER(J)
00039      IF(ABS(DIVB).GT.ABS(EL(IN,JN))) GO TO 10
00040      DIVB=EL(IN,JN)
00041      IT=IN
00042      JT=JN
00043      IFROM=I
00044      JFROM=J
00045      10 CONTINUE
00046      NORDER(IFROM)=NORDER(L)
00047      NORDER(L)=IT
00048      MORDER(JFROM)=MORDER(L)
00049      MORDER(L)=JT
00050      35 DO 40 J=L,LB
00051      JN=MORDER(J)
00052      40 EL(IT,JN)=EL(IT,JN)/DIVB
00053      IF(L.GE.LV)GO TO 55

```

RTOTO
SCH,

SR(20)
TANS(23),

NCONV,
NCTXP,

NEQ,
NGIN,

TO
TOL,
TOLMAX,
TOLT,
U(20),
Y(20),
YBAR,
YBC,
YC(20),

NSIN,
NT,

YR(20)
Z(20,10)

R, IEVN(11)

```
00054      MN=L+1
00055      DO 50 I=MN,LV
00056      IN=NORDER(I)
00057      FMULT=EL(IN,JT)
00058      DO 50 J=MN,LB
00059      JN=MORDER(J)
00060 50 EL(IN,JN)=EL(IN,JN)-EL(IT,JN)*FMULT
00061 55 I=LV
00062      SIGMA=0.0
00063 60 IN=NORDER(I)
00064      JN=MORDER(I)
00065      ANS(JN)=EL(IN,LB)-SIGMA
00066      IF(I,LE.1) GO TO 70
00067      IN=NORDER(I-1)
00068      SIGMA=0.0
00069      DO 65 J=I,LV
00070      JN=MORDER(J)
00071 65 SIGMA=SIGMA+EL(IN,JN)*ANS(JN)
00072      I=I-1
00073      GO TO 60
00074 70 CONTINUE
00075      RETURN
00076      END
```

```

00001      SUBROUTINE SOLVE(IDISP,J)
00002      COMMON/CONVER/ITRMAX,DYNAMO(3),DYNTM,DYNFLG,DYNFLO
00003      COMMON/STIFF/ISASUM,ISTIFF(5),STIFVL
00004      COMMON/IO/ODUCT,OYDXM,AGSTPD,CPVC(3,5,5),HFV(5,5),DELHV(5,5),
00005      1INTCPV(5,5),ORBJ(5)
00006      COMMON /LAST/GASTMN,TMIN(5),IQOJ(255,5)
00007      COMMON /DIFEGN/OMEGAK(9),ALPHA(5),ALPHAC(5),ALPHAH(5),
00008      1ALPHAH(5),NN(5),HXZ(5),QF(5),QCB,QZ(5),P,V,HG(5),RK(5,9),
00009      2RL(5,20),RM(5,20),RC(5),RH(5),RW(5),RR(5),W(5),WG,AREA,PRESSR
00010      COMMON /AREA13/ALFACO(5),GAMMA,EK(20),XI(5),AMJ(5,5),
00011      1EMJ(5,5),KVD(5,5),TB,D(5),RHOC(5),RHO(5),DELTA(20),DIFM(20)
00012      2,ALFAH(5),ALFAW(5),ALFAA(5)
00013      COMMON/MORE/DO1(255,5),NO1(255,5),ALFA0(255,5),ALFA0C(255,5),
00014      1ALFA0H(255,5),ALFA0W(255,5),ALFA0A(255,5),X0(255,20),WVG(255)
00015      COMMON /RAOI/TO(255,5),NO(5),DO(5),SIGMA,PI,E(5),IT(255),HO(5)
00016      1,NUMRDR,DEL,IRAD,TOOLD(5)
00017      COMMON /ODEVAL/X,XTRMNL,VALINT(42),ODESTP
00018      COMMON /AREA5/NPRINT,TNIRP,CHECK,BUG
00019      COMMON /GENRAL/ALPHAA(5),S(20),KG,MUG,D8,
00020      1TPJJ(5),YY(5,5),PRCLS,SPECIE,
00021      2ELEMNT,CRXN,HRXN,HH(5),HW(5),RGC
00022      COMMON /EDNUM/RHOG,CPG,TG,CPI(20),XX(20),CO(5),HGAS,EDNAME(9),
00023      1OXYD(5),GMW,QMASS(9,20),WTM(20)
00024      COMMON /APR77/DELTPJ,DELRRJ,ALEN,JFAR,HM,DIFMW,ICNVLM,
00025      1TTEST,SUMSQ,ITRSYS,GAST(255),OSPRR,NPROP,ARMAX,AMIN,SQDIF
00026      COMMON /JAN78/YO,FUR
00027      C NUMERICAL TREATMENT OF A SYSTEM OF FIRST ORDER DIFFERENTIAL EQUATIONS.
00028      C RUNGE-KUTTA FOURTH ORDER IS USED FOR STARTING THE NUMERICAL SOLUTION.
00029      C ADAMS-MOULTON PREDICTOR CORRECTOR IS USED TO CONTINUE THE SOLUTION.
00030      C
00031      C THE REQUIRED VECTOR FUNCTION IS INPUT BY THE SUBROUTINE DIFF(YT,VECFUN,H).
00032      C
00033      C
00034      C INPUT VARIABLES
00035      C      N= THE NUMBER OF EQUATIONS IN THE SYSTEM
00036      C      X = THE INITIAL VALUE OF INDEPENDENT VARIABLE
00037      C      X1= THE TERMINAL VALUE F INDEPENDENT VARIABLE
00038      C      VALINT(I),I=1,N = THE INITIAL VALUES OF THE DEPENDENT VARIABLES.
00039      C      ODESTEP = THE TOTAL NUMBER OF STEPS IN THE NUMERICAL TREATMENT
00040      C      NOTE: TO HELP SPEED CALCULATIONS SOLVE ALLOWS FOR
00041      C      CHANGING STEP SIZE (ODESTEP) IN DIFFERENT REGIONS OF THE
00042      C      REACTOR:
00043      C          1) UP TO BEGINNING OF DYNAMIC REGION AT A SPECIFIED
00044      C              TEMPERATURE.
00045      C          2) UP TO COMPLETION OF PYROLYSIS,
00046      C          3) UP TO INITIATION OF STIFF ASSUMPTION IF LEVEL 2
00047      C          4) UP TO CHAR BURNOUT
00048      C      IT IS IMPORTANT TO REALIZE THAT CHANGING STEP SIZE CAN ONLY
00049      C      TAKE PLACE AT THE BEGINNING OF A RADIATION REGION -- REGARDLESS
00050      C      OF THE STEP SIZE OF THE DIFFERENTIAL EQUATIONS STEPS (ODESTEP).
00051      C
00052      C
00053      C

```

```
00054 C
00055     REAL YT(42),K(42,4),F(42,4),YZ(42),VECFUN(42),AWOLD(5),AHOLD(5)
00056     1,XCORR(12),ACOLD(5),YTO(42)
00057     INTEGER BUG,ODESTP,PRTCLS,OSPRR,ELEMNT,NCORR(12),CPOINT,OSTIFF(5)
00058     1,DYNAMO,DYNFLG,DYNFLO
00059 C
00060 C*****PRINT SWITCH AND INITIALIZATION
00061 C
00062     NRUTER=0
00063     SWITCH=0.0
00064     IF(BUG.GE.1)SWITCH=1.0
00065     N=ELEMNT+6*PRTCLS+2
00066     DO 4 IJ=1,PRTCLS
00067         AWOLD(IJ)=0.0
00068         ACOLD(IJ)=0.0
00069         AHOLD(IJ)=0.0
00070         IF(X.EQ.0.0.AND.ALPHAW(IJ).NE.0.0)AWOLD(IJ)=1.0
00071         IF(X.EQ.0.0.AND.ALPHAC(IJ).NE.0.0)ACOLD(IJ)=1.0
00072 4      IF(X.EQ.0.0.AND.ALPHAH(IJ).NE.0.0)AHOLD(IJ)=1.0
00073         X1=ALEN
00074 C
00075 C*****INITIALIZATION WHEN WE'RE AT THE BEGINING OF THE REACTOR
00076 C
00077     IF (X.NE.0.0) GO TO 7
00078     NCORCT=1
00079     CPOINT=0
00080     ICDYN=0
00081     IHDYN=0
00082     DO 3 IJ=1,PRTCLS
00083         IF(ALFAC(IJ).EQ.0.0)ICDYN=ICDYN+1
00084 3      ISTIFF(IJ)=0
00085         IF(BUG.EQ.0)WRITE(3,270)
00086         DO 10 I=1,N
00087             YZ(I)=VALINT(I)
00088 10     YT(I) = YZ(I)
00089         H = (X1-X)/FLOAT(ODESTP)
00090         H1=H
00091         CALL PROFIL(J,IDISP)
00092 C
00093 C*****INITIALIZATION WHEN RESTARTING INTEGRATION.
00094 C     EXPLANATION: WHEN THERE ARE SHARP DISCONTINUITIES IN THE
00095 C     DIFFERENTIAL EQUATIONS THE NUMERICAL SOLUTION WOULD HAVE
00096 C     DIFFICULTIES WITH ITS FOUR BACK POINTS AND TRYING TO PREDICT
00097 C     THE NEXT VALUE. THE WAY WE HANDLE THIS PROBLEM IS TO RESTART
00098 C     THE DIFFERENTIAL EQUATION SOLUTION AS IF WE WERE STARTING THE
00099 C     INTEGRATION WITH A NEW INTEGRAL. THIS RESTART OCCURS WHEN
00100 C     1) MOISTURE IS COMPLETELY EVAPORATED FROM PARTICLE
00101 C     2) MIXING IS COMPLETE
00102 C     3) PYROLYSIS IS COMPLETE
00103 C     4) CHAR COMBUSTION IS COMPLETE
00104 C
00105 7      IF(X.EQ.0.0) GO TO 5
00106     DO 9 I=1,N
```

```
00107 9      YT(I)=YZ(I)
00108 5      CONTINUE
00109      IF(SWITCH.EQ.0.0)GO TO 8
00110      WRITE(3,211)
00111      WRITE(3,212)(YT(IX),IX=1,N)
00112 C
00113 C*****RUNGE-KUTTA FOURTH ORDER
00114 C
00115 8      DO 1000 J=1,3
00116 C
00117 C*****COMPUTE K1 = H*F(X,Y)
00118 C
00119      CALL DIFF(YT,VECFUN,H)
00120      IF(X.EQ.0.0)GASTMN=TG
00121      DO 15 I=1,N
00122 15 K(I,1) = H*VECFUN(I)
00123 C
00124 C*****COMPUTE X+H/2 AND Y+K1/2
00125 C
00126      X = X + H/2.
00127      DO 20 I=1,N
00128 20 YT(I) = YZ(I) + K(I,1)/2.
00129 C
00130 C*****COMPUTE K2 = H*F(X+H/2,Y+K1/2)
00131 C
00132      CALL DIFF(YT,VECFUN,H)
00133      DO 25 I=1,N
00134 25 K(I,2) = H*VECFUN(I)
00135 C
00136 C*****COMPUTE Y+K2/2
00137 C
00138      DO 30 I=1,N
00139 30 YT(I) = YZ(I) + K(I,2)/2.
00140 C
00141 C*****COMPUTE K3 = H*F(X+H/2,Y+K2/2)
00142 C
00143      CALL DIFF(YT,VECFUN,H)
00144      DO 35 I=1,N
00145 35 K(I,3) = H*VECFUN(I)
00146 C
00147 C*****COMPUTE X+H AND Y+K3
00148 C
00149      X = X + H/2.
00150      DO 40 I=1,N
00151 40 YT(I) = YZ(I) + K(I,3)
00152 C
00153 C*****COMPUTE K4 = H*F(X+H,Y+K3)
00154 C
00155      CALL DIFF(YT,VECFUN,H)
00156      DO 50 I=1,N
00157 50 K(I,4) = H*VECFUN(I)
00158 C
00159 C*****COMPUTE Y(X+H)= Y(X) + (K1+2K2+2K3+K4)/6
```

```
00160 C
00161 DO 60 I=1,N
00162 YT(I) = YZ(I) + (K(I,1)+2.*K(I,2)+2.*K(I,3)+K(I,4))/6.
00163 60 YZ(I) = YT(I)
00164 C
00165 C*****SAVE FUNCTION EVALUATIONS FOR USE IN PREDICTOR CORRECTOR
00166 C
00167 DO 70 I=1,N
00168 70 F(I,J) = K(I,1)
00169 JJ=J
00170 C
00171 C*****PROFIL PREPARES INFORMATION FOR OUTPUT
00172 C
00173 CALL PROFIL(JJ,IDISP)
00174 C
00175 C*****DEBUG
00176 C
00177 IF(SWITCH.EQ.0.0)GO TO 999
00178 WRITE(3,219)
00179 WRITE(3,220)(YT(IX),(K(IX,JX),JX=1,4),IX=1,N)
00180 WRITE(3,250)X,TG,(TPJJ(IJ),IJ=1,PRCL9)
00181 C
00182 C*****TEST FOR RESTART AT COMPLETION OF MIXING
00183 C
00184 999 IF(X.LT.AGSTPD.OR.CPOINT.EQ.1) GO TO 138
00185 CPOINT=1
00186 NRUTER=1
00187 138 DO 145 IJ=1,PRCL9
00188 IW=IJ+ELEMNT+2+5*PRCL9
00189 IC=IJ+ELEMNT+2+3*PRCL9
00190 IH=IJ+ELEMNT+2+4*PRCL9
00191 C
00192 C*****TEST FOR RESTART DUE TO DISAPPEARANCE OF MOISTURE FROM THE PARTICLE
00193 C
00194 IF(YT(IW).GT.0.0.OR.AWOLD(IJ).LE.0.0)GO TO 140
00195 YZ(IW)=0.0
00196 RW(IJ)=0.0
00197 NRUTER=1
00198 C
00199 C*****TEST FOR RESTART DUE TO COMPLETION OF PYROLYSIS
00200 C
00201 140 IF(YT(IC).GT.0.0.OR.ACOLD(IJ).LE.0.0)GO TO 142
00202 YZ(IC)=0.0
00203 RC(IJ)=0.0
00204 ICDYN=ICDYN+1
00205 NRUTER=1
00206 C
00207 C*****TEST FOR RESTART DUE TO COMPLETION OF CHAR OXIDATION (CHAR BURNOUT)
00208 C
00209 142 IF(YT(IH).GT.0.0.OR.AHOLD(IJ).LE.0.0)GO TO 144
00210 YZ(IH)=0.0
00211 RH(IJ)=0.0
00212 IF(ISASUM.LT.2)IHDYN=IHDYN+1
```

```
00213      NRUTER=1
00214      C
00215      C*****RESETTING OLD ALPHA VALUES
00216      C
00217      144      AWOLD(IJ)=ALPHAW(IJ)
00218              ACOLD(IJ)=ALPHAC(IJ)
00219              AHOLD(IJ)=ALPHAH(IJ)
00220      C
00221      C*****TEST FOR CHANGE IN STEP SIZE DUE TO INITIATION OF DYNAMIC REGION
00222      C
00223              IF((TPJJ(IJ).LT.DYNTEM.OR.DYNFLG.GE.1).OR.MOD((J+IDISP),OSPRR)
00224              1,NE.0)GO TO 145
00225              DYNFLG=1
00226              IF(DYNAMO(1).LE.1)DYNFLO=DYNFLG
00227              IF(DYNAMO(1).LE.1)GO TO 145
00228              H=H1/FLOAT(DYNAMO(1))
00229              RETURN
00230      145      CONTINUE
00231      C
00232      C*****TEST FOR CHANGE IN STEP SIZE DUE TO COMPLETION OF PYROLYSIS
00233      C
00234              IF((ICDYN.NE.PRTCLS.OR.DYNFLG.NE.1).OR.MOD((J+IDISP),
00235              1OSPRR).NE.0)GO TO 146
00236              DYNFLG=2
00237              IF(DYNAMO(1).EQ.DYNAMO(2))DYNFLO=DYNFLG
00238              IF(DYNAMO(1).EQ.DYNAMO(2))GO TO 146
00239              H=H1/FLOAT(DYNAMO(2))
00240              RETURN
00241      C
00242      C*****TEST FOR CHANGE IN STEP SIZE DUE TO COMPLETIN OF CHAR OXYDATION
00243      C
00244      146      IF((IHDYN.NE.PRTCLS.OR.DYNFLG.NE.2).OR.MOD((J+IDISP),
00245              1OSPRR).NE.0)GO TO 147
00246              DYNFLG=3
00247              IF((DYNAMO(2).EQ.DYNAMO(3)).AND.DYNAMO(3).LE.1)DYNFLO=DYNFLG
00248              IF((DYNAMO(2).EQ.DYNAMO(3)).AND.DYNAMO(3).LE.1)GO TO 147
00249              H=H1*FLOAT(DYNAMO(3))
00250              RETURN
00251      147      CONTINUE
00252              IF(NRUTER.EQ.1)RETURN
00253      1000 CONTINUE
00254      C
00255      C*****DEBUG
00256      C
00257              IF(SWITCH.EQ.0.0)GO TO 75
00258              WRITE(3,229)
00259              WRITE(3,230)((F(IX,JX),JX=1,3),IX=1,N)
00260      C
00261      C*****EVALUATE FUNCTION AT (XN,YN)
00262      C
00263      75      CALL DIFF(YT,VECFUN,H)
00264              DO      80 I=1,N
00265              80 F(I,4) = H*VECFUN(I)
```

```
00266 C
00267 C*****PREDICTOR CORRECTOR PACKAGE
00268 C
00269 DO 2000 J=4,(ODESTP-IDISP)
00270 C
00271 C*****ADAMS-BASHFORTH PREDICTOR
00272 C
00273 DO 90 I=1,N
00274 90 YT(I) = YZ(I)+(55.*F(I,4)-59.*F(I,3)+37.*F(I,2)-9.*F(I,1))/24.
00275 C
00276 C*****THE FOLLOWING SET OF TESTS FOR RESTART AND STEP SIZE CHANGE ARE
00277 C SIMILAIR TO THE PRECEDING SET IN THE RUNGE-KUTTA SECTION.
00278 C NOTE THAT THIS SET OF TESTS IS APPLIED IMMEDIATELY AFTER THE
00279 C PREDICTOR BUT BEFORE AN EVALUATION. IN A WAY THIS ALLOWS THE
00280 C PROGRAM TO LOOK AHEAD AND TRY TO DETERMINE IF THE NEXT STEP WILL
00281 C CAUSE ANY PROBLEMS AND IF IT MIGHT THE TESTS ARE INITIATED TO
00282 C RETURN TO THE MAIN PROGRAM AND RESTART OR MAKE APPROPRIATE STEP
00283 C SIZE CHANGES BEFORE TAKING THE STEP.
00284 C
00285 C
00286 C*****TEST FOR COMPLETION OF MIXING.
00287 C
00288 IF((X+H).LT.AGSTPD.OR.CPOINT,EQ,1)GO TO 148
00289 CPOINT=1
00290 NRUTER=1
00291 148 DO 155 IJ=1,PRCL3
00292 IW=IJ+ELEMNT+2+5*PRCL3
00293 IC=IJ+ELEMNT+2+3*PRCL3
00294 IH=IJ+ELEMNT+2+4*PRCL3
00295 C
00296 C*****TEST FOR COMPLETION OF MOISTURE EVAPORATION.
00297 C
00298 IF(ALPHAH(IJ).LE.0.0.AND.AHOLD(IJ).GT.0.0)YT(IW)=0.0
00299 IF(YT(IW).GT.0.0.OR.AHOLD(IJ).LE.0.0)GO TO 150
00300 YZ(IW)=0.0
00301 RW(IJ)=0.0
00302 NRUTER=1
00303 C
00304 C*****TEST FOR COMPLETION OF PYROLYSIS.
00305 C
00306 150 IF(ALPHAC(IJ).LE.0.0.AND.ACOLD(IJ).GT.0.0)YT(IC)=0.0
00307 IF(YT(IC).GT.0.0.OR.ACOLD(IJ).LE.0.0)GO TO 152
00308 YZ(IC)=0.0
00309 RC(IJ)=0.0
00310 ICDYN=ICDYN+1
00311 NRUTER=1
00312 C
00313 C*****TEST FOR COMPLETION OF CHAR BURNOUT.
00314 C
00315 152 IF(ALPHAH(IJ).LE.0.0.AND.AHOLD(IJ).GT.0.0)YT(IH)=0.0
00316 IF(YT(IH).GT.0.0.OR.AHOLD(IJ).LE.0.0)GO TO 154
00317 YZ(IH)=0.0
00318 RH(IJ)=0.0
```

```
00319      IF(ISASUM.LT.2)IHDYN=IHDYN+1
00320      NRUTER=1
00321      C
00322      C*****UPDATING OLD ALPHA VALUES.
00323      C
00324      154      AWOLD(IJ)=ALPHAW(IJ)
00325              ACOLD(IJ)=ALPHAC(IJ)
00326              AHOLD(IJ)=ALPHAH(IJ)
00327      C
00328      C*****TEST FOR STEP SIZE CHANGE DUE TO INITIATION OF DYNAMIC REGION.
00329      C
00330              IF((TPJJ(IJ).LT.DYNTEM.OR.DYNFLG.GE.1).OR.MOD((J+IDISP-1),
00331      10SPRR).NE.0)GO TO 155
00332              DYNFLG=1
00333              IF(DYNAMO(1).LE.1)DYNFLO=DYNFLG
00334              IF(DYNAMO(1).LE.1)GO TO 155
00335              H=H1/FLOAT(DYNAMO(1))
00336              RETURN
00337      155      CONTINUE
00338      C
00339      C*****TEST FOR STEP SIZE CHANGE INITIATION DUE TO COMPLETION OF PYROLYSIS.
00340      C
00341              IF((ICDYN.NE.PRTCLS.OR.DYNFLG.NE.1).OR.MOD((J+IDISP-1),
00342      10SPRR).NE.0)GO TO 156
00343              DYNFLG=2
00344              IF(DYNAMO(1).EQ.DYNAMO(2))DYNFLO=DYNFLG
00345              IF(DYNAMO(1).EQ.DYNAMO(2))GO TO 156
00346              H=H1/FLOAT(DYNAMO(2))
00347              RETURN
00348      C
00349      C*****TEST FOR STEP SIZE CHANGE INITIATION DUE TO CHAR BURNOUT.
00350      C
00351      156      IF((IHDYN.NE.PRTCLS.OR.DYNFLG.NE.2).OR.MOD((J+IDISP-1),
00352      10SPRR).NE.0)GO TO 157
00353              DYNFLG=3
00354              IF((DYNAMO(2).EQ.DYNAMO(3)).AND.DYNAMO(3).LE.1)DYNFLO=DYNFLG
00355              IF((DYNAMO(2).EQ.DYNAMO(3)).AND.DYNAMO(3).LE.1)GO TO 157
00356              H=H1*FLOAT(DYNAMO(3))
00357              RETURN
00358      157      CONTINUE
00359      C
00360      C*****RETURN IF ANY OF THE ABOVE CRITERION ARE MEET
00361      C
00362              IF(NRUTER.EQ.1)RETURN
00363      C
00364      C*****MOVE DOWN THE REACTOR.
00365      C
00366              X = X + H
00367      C
00368      C*****SAVE PREVIOUSLY COMPUTED FUNCTION EVALUATIONS
00369      C
00370              DO 100 I=1,N
00371              F(I,1) = F(I,2)
```

```
00372      F(I,2) = F(I,3)
00373      100 F(I,3) = F(I,4)
00374      C
00375      C*****EVALUATE FUNCTION AT (XN+1,YN+1(0))
00376      C
00377          CALL DIFF(YT,VECFUN,H)
00378          DO 110 I=1,N
00379      110 F(I,4) = H*VECFUN(I)
00380      C
00381      C*****GET THE SUM OF THE SLOPES OF THE PARTICLE ENERGIES FOR USE LATTER ON.
00382      C
00383          IPE=ELEMNT+PRTCLS+1
00384          SUMT=0.0
00385          DO 116 IJ=1,PRTCLS
00386          IJPE=IJ+IPE
00387      116 SUMT=SUMT+F(IJPE,4)
00388          SUMT=SUMT/FLOAT(PRTCLS)
00389      C
00390      C*****ADAMS-MOULTON CORRECTOR WITH UNDER RELAXATION WHEN REPEATING CORRECTOR
00391      C
00392          ICONV=ICNVLM
00393      115 IFLAG=0
00394          SUMTO=SUMT
00395          DO 120 I=1,N
00396          YTO(I)=YT(I)
00397          YT(I) = YZ(I)+(9.*F(I,4)+19.*F(I,3)-5.*F(I,2)+F(I,1))/24.
00398          IF(ICONV.LT.ICNVLM)YT(I)=FUR*YT(I)+(1.0-FUR)*YTO(I)
00399      120 CONTINUE
00400      C
00401      C*****EVALUATE FUNCTION AT (XN+1,YN+1(1))
00402      C
00403          CALL DIFF(YT,VECFUN,H)
00404          DO 130 I=1,N
00405      130 F(I,4) = H*VECFUN(I)
00406      C
00407      C*****DEBUG
00408      C
00409          IF(SWITCH.EQ.0.0)GO TO 135
00410          IF(BUG.LE.2.AND.TNIRP.EQ.0.0)GO TO 134
00411          WRITE(3,239)
00412          WRITE(3,2395)X
00413          WRITE(3,240)(F(IX,4),YT(IX),IX=1,N)
00414      134 WRITE(3,250)X,TG,(TPJJ(IJ),IJ=1,PRTCLS)
00415      C
00416      C*****TEST: IS SLOPE OF THE PARCTICLE ENERGY CHANGING?
00417      C      TEST: DO WE WANT TO APPLY THE STIFF EQUATION ASSUMPTION AND IF
00418      C      SO, AT WHAT LEVEL?
00419      C      THIS ALL AMOUNTS TO SUM NUMERICAL GIMMICKRY WHICH IS VERY IMPORTANT.
00420      C      IN THIS SYSTEM IT IS FOUND THAT THE PARTICLE ENERGY IS A VERY SENSITIVE
00421      C      MEASURE OF THE STABILITY OF THE SYSTEM OF DIFFERENTIAL EQUATIONS.
00422      C      THUS IF THE SLOPE OF THE PARTICLE ENERGY IS CHANGING DRASTICALLY FROM
00423      C      PREDICTOR TO CORRECTOR THEN WE APPLY ANOTHER CORRECTOR AND ANOTHER
00424      C      EVALUATION. THEN WE TEST TO SEE IF IT STILL CHANGED DRASTICALLY OR NOT
```

```

00425 C   TO DETERMINE WHETHER STILL ANOTHER CORRECT, EVALUATE STEP SHOULD BE
00426 C   APPLIED. THIS CONTINUES UNTIL AN EXTERNALLY SPECIFIED MAXIMUM NUMBER
00427 C   OF CORRECTORS IS REACHED. THE STIFF EQUATION ASSUMPTION IS A NEAT ,
00428 C   WAY OF SIDE STEPPING NUMERICAL STIFFNESS. IN THIS SYSTEM STIFFNESS
00429 C   IS ONLY REACHED WHEN THE PARTICLE ENERGY STOPS CHANGING SIGNIFICANTLY.
00430 C   AT THAT POINT THE DIFFERENCE BETWEEN THE PARTICLE AND THE GAS TEMPERATURE
00431 C   IS MADE CONSTANT AND WE STOP USING THE NOW STIFF PARTICLE ENERGY
00432 C   EQUATION. WHEN A LEVEL 2 STIFF PARTICLE ENERGY ASSUMPTION IS USED
00433 C   WE ALSO CHANGE STEP SIZE WHEN STIFFNESS OCCURS JUST AS IF CHAR
00434 C   BURNOUT HAD BEEN REACHED.
00435 C
00436 C
00437 135  SUMT=0.0
00438      DO 117 IJ=1, PRTCLS
00439      IJPE=IJ+IPE
00440      IF (ISASUM.GT.0.AND.ISTIFF(IJ).EQ.1.AND.ICONV.EQ.ICONVLM)
00441 1    SUMTO=SUMTO-F(IJPE,3)/FLOAT(PRTCLS)
00442      IF (ISASUM.GT.0.AND.ISTIFF(IJ).EQ.1) GO TO 117
00443      SUMT=SUMT+F(IJPE,4)
00444 117  CONTINUE
00445      SUMT=SUMT/FLOAT(PRTCLS)
00446      IF (SUMT.EQ.0.0) GO TO 118
00447      IF (ABS((SUMT-SUMTO)/SUMT).GT.TTEST) IFLAG=1
00448 118  ICONV=ICONV-1
00449      IF (IFLAG.EQ.1.AND.ICONV.GE.0) GO TO 115
00450      DO 136 I=1,N
00451 136  YZ(I)=YT(I)
00452      JJ=J
00453      CALL PROFIL(JJ, IDISP)
00454      NCORR(NCORCT)=ICONVLM-ICONV
00455      XCORR(NCORCT)=X
00456      IF (BUG.EQ.0.AND.(NCORCT.EQ.12.OR.J.EQ.(ODESTP-IDISP)))
00457 1    WRITE(3,260)(XCORR(IX),NCORR(IX),IX=1,NCORCT)
00458      NCORCT=1+NCORCT
00459      IF (NCORCT.EQ.13) NCORCT=1
00460      IF (ISASUM.LT.1) GO TO 131
00461      DO 137 IJ=1, PRTCLS
00462      OSTIFF(IJ)=ISTIFF(IJ)
00463      IF (ISTIFF(IJ).EQ.1.OR.(ABS(QF(IJ)-QRB(IJ)-QZ(IJ))).LT.STIFVL)
00464 1    GO TO 210
00465      GO TO 137
00466 210  IF (X.LE.AGSTPD) GO TO 137
00467      ISTIFF(IJ)=1
00468      IF (OSTIFF(IJ).NE.0.OR.ISTIFF(IJ).NE.1) GO TO 137
00469      WRITE(3,280) IJ,X
00470      IF (ISASUM.GT.1) IHDPN=IHDPN+1
00471 137  CONTINUE
00472 131  CONTINUE
00473 2000 CONTINUE
00474      RETURN
00475 211  FORMAT(21X,6HY(I)=.)
00476 212  FORMAT(1H,9(1X,E12.5,1X)/)
00477 219  FORMAT(SX,5HYT(I),9X,6HK(I,1),8X,6HK(I,2),8X,6HK(I,3),8X,

```

```

00478      16HK(I,4))
00479      220      FORMAT(1H ,5(1X,E12.5,1X))
00480      229      FORMAT(5X,6HF(I,1),8X,6HF(I,2),8X,6HF(I,3))
00481      230      FORMAT(1H ,3(1X,E12.5,1X)/)
00482      239      FORMAT(7X,1HX,11X,6HF(1,4),8X,5HYT(1),9X,6HF(2,4),8X,
00483      15HYT(2),9X,42HETC.....)
00484      2395     FORMAT(1H ,E12.5)
00485      240      FORMAT(11(13X,8(1X,E12.5,1X)/))
00486      250      FORMAT(20X,7HAT X = ,F6.2,3HCM,,5X,12HGAS TEMP. = ,F10.2,
00487      11HK,5X,19HPARTICLE TEMPS (K);,5F10.2)
00488      260      FORMAT(1H ,12(1H(,F6.2,1H,,12,1H)))
00489      270      FORMAT(77H1THE ORDERED PAIR OF (X,# OF CORRECTORS APPLIED) FOLLOWS
00490      1 FOR EACH O.D.E. STEP,/,75H *****
00491      2*****
00492      280      FORMAT(77H THE STIFF PARTICLE ENERGY EQUATION ASSUMPTION IS INITIA
00493      1TED FOR PARTICLE NO. ,I1,4H AT ,F6.2,21H CM, DOWN THE REACTOR)
00494      END

```

```
00001      SUBROUTINE TIMET
00002 C---THIS SUBROUTINE WILL ACCEPT A TIME OF DAY AND IF THE CURRENT TIME
00003 C   OF DAY AT RUN TIME IS BEYOND THE ACCEPTED AMOUNT THEN THE PROGRAM
00004 C   WILL TERMINATE.
00005 C
00006       INTEGER H,HT
00007       IF(IN.EQ.1)GO TO 12
00008       TYPE 5
00009 5      FORMAT(54H ENTER LATEST ACCEPTABLE TIME (24 HR CLOCK)--HH:MM --S)
00010       READ(5,10)H,M
00011 10     FORMAT(I2,1X,I2)
00012       IN=1
00013 12     CALL TIME(T)
00014       DECODE(5,10,T)HT,MT
00015       IF(HT.LT.H)GO TO 25
00016       IF(MT.LT.M)GO TO 25
00017       WRITE(5,20)T
00018 20     FORMAT(47H EXECUTION TERMINATED SINCE THE TIME OF DAY IS ,A5)
00019       CALL TRBLE
00020 25     RETURN
00021       END
```

```

00001      SUBROUTINE TOY
00002      COMMON/AZ/A(20,11),
00003      COMMON/AZ1/ ANS(23),
00004      2      ATMOS
00005      COMMON/AZ2/
00006      COMMON/AZ3/B(11),
00007      5      BMIN,
00008      6      CBAR,
00009      7
00010      8      D,
00011      9
00012      COMMON/BZ/
00013      1
00014      2
00015      3      EL(23,24),
00016      4      ENTRPY,
00017      5
00018      6      H(20),
00019      7      HBAR,
00020      8      HC,
00021      9      HI,
00022      COMMON/CZ/HR(20),
00023      COMMON/CZ1/IDKIN(20),
00024      2
00025      3      IDSIN(20),
00026      4      IEV(11),
00027      DATA DELPO/.01/,DELTO/.01/,DELXY/.0001/,DELPI/.001/
00028      SLIMIT=1.0E-30
00029      NKINT=NKIN
00030      KINSM=-1
00031      SMLRA=1.0
00032      AK=ANS(K2)/RTOTO
00033      PMPD=0.0
00034      RPMPA=0.0
00035      IF(NEQ,EQ.1)ANS(K2)=0.0
00036      25 RAT=ANS(K2)/TO
00037      IF (ABS(RAT).LT.(0.09)) GO TO 40
00038      IF (RAT) 30,40,35
00039      30 ANS(K2)=TO*(-0.09)
00040      GO TO 40
00041      35 ANS(K2)=0.09*TO
00042      C
00043      C
00044      C
00045      40 DO 50 KK=1,NGIN
00046      I=IDSIN(KK)
00047      SUMAPI=0.0
00048      DO 45 J=1,NM
00049      J1=J+NEQ
00050      45 SUMAPI=SUMAPI+ANS(J1)*A(I,J)
00051      YR(I)=ANS(K3)-U(I)+SUMAPI+AK*H(I)-RPMPA
00052      IF( YR(I) .GT. 0.0 .OR. Y(I) .LE. SLIMIT) GO TO 50
00053      IMBALA=1

```

RTOTO
SCH,

SR(20)
TANS(23),

TO
TOL,
TOLMAX,
TOLT,
U(20),
Y(20),
YBAR,
YBC,
YC(20),

YR(20)
Z(20,10)

IEVN(11)

FIND THE LARGEST SMALL RATIO FOR GASES.

```
00054      SMLRAT=.99/(1.0-YR(I))
00055      IF (SMLRAT.GE.SMLRA) GO TO 50
00056      SMLRA=SMLRAT
00057 50 CONTINUE
00058 C
00059 C      RATIO NEW MOLES FOR GASES.
00060 C
00061 60 JJ=0
00062      DO 70 KK=1,NGIN
00063      I=IDSIN(KK)
00064      Y(I)=Y(I)*(1.0+SMLRA*(YR(I)-1.0))
00065      IF (Y(I).GE.TOL) GO TO 65
00066 C
00067 C      DROP THE GAS SPECIE FROM SOLUTION.
00068 C
00069      Y(I)=0.0
00070      GO TO 70
00071 65 JJ=JJ+1
00072      IDSIN(JJ)=I
00073 70 CONTINUE
00074      NGIN=JJ
00075      IF (JJ.EQ.0) NGIN=1
00076 80 I1=NEG+1
00077      I2=I1+NM-1+NKIN
00078 85 DO 100 I=I1,I2
00079      IF (ABS(TANS(I)-ANS(I))-DFLPI) 95,90,90
00080 90 NCONV=-1
00081 95 CONTINUE
00082 100 TANS(I)=ANS(I)
00083 C
00084 C      CONVERGENCE CRITERIA TESTS.
00085 C
00086      IF (MAJOR.EQ.0) GO TO 105
00087      IF (ABS(ANS(K2)).GE.DELTO) GO TO 105
00088      IF (ABS(ANS(K3)-1.0).GE.DELXY) GO TO 105
00089      IF (NEG.NE.3) GO TO 110
00090      IF (ABS(ANS(1))-DELPO) 110,105,105
00091 105 NCONV=-1
00092 110 TO=TO+ANS(K2)
00093      ATMOS=ATMOS+PMPO
00094      IMBALA=0
00095      IF (TO.LT.0.0) TO=0.002
00096      IF (ATMOS.LT.0.0) ATMOS=0.02
00097 115 RETURN
00098 C
00099 C
00100 120 FORMAT (10X,3HTOY)
00101 125 FORMAT (8(1X,A6,1H=,F8.5))
00102      END
```

```
00001      SUBROUTINE TRBLE
00002      C
00003      C      A SUBROUTINE TO GET OUTPUT AND KILL THE PROGRAM WHEN IT GETS IN TROUBLE
00004      C
00005      COMMON/ODEVAL/XDIS,XTRMNL,VALINT(42),ODESTP
00006      COMMON/TRUBLE/INDX,ITRBLE
00007      COMMON/RADI/T0(255,5),N0(5),D0(5),SIGMA,PI,E(5),IT(255),H0(5)
00008      1,NUMRDR,DEL,IRAD,T0OLD(5)
00009      COMMON/ APR77/DELTPJ,DELRRJ,ALEN
00010      ITRBLE=1
00011      TYPE 100,XDIS
00012      WRITE(3,100)XDIS
00013      NUMRDR=INDX-1
00014      ALEN=NUMRDR*DEL
00015      CALL OUTPUT
00016      100  FORMAT(12H-TROUBLE AT ,F6.2,21H CM. DOWN THE REACTOR)
00017      STOP
00018      END
```

```
00001      SUBROUTINE VALUE
00002      COMMON /APR77/DELTPJ,DELRRJ,ALEN,JFAR,HM,DIFMW,ICNVLM,
00003      1TTEST,SUMSQ,ITRSYS,GAST(255),OSPRR,NPROP,ARMAX,AMIN,SQDIF
00004      COMMON /ODEVAL/XDIS,XTRMNL,VALINT(42),ODESTP
00005      COMMON /GNRAL/ALPHA(5),S(20),KG,MUG,DS,
00006      1TPJJ(5),YY(5,5),PRTCLS,SPECIE,
00007      2ELEMNT,CRXN,HRXN,HH(5),HW(5),RGC
00008      COMMON/GNRAL2/NAME1(20),NAME2(20)
00009      COMMON /DIFCON/OMEGAK(9),ALPHA(5),ALPHAC(5),ALPHAH(5),
00010      1ALPHAW(5),N(5),H(5),QF(5),QCB,QZ(5),P,V,HG(5),RK(5,9),
00011      2RL(5,20),RM(5,20),RC(5),RH(5),RW(5),RR(5),W(5),WG,AREA,PRESSR
00012      COMMON /EDNUM/RHOG,CPG,TG,CPI(20),X(20),CO(5),HGAS,EDNAME(9),
00013      1OXYD(5),GMW,QMASS(9,20),WTM(20)
00014      INTEGER PRTCLS,ELEMNT,SPECIE,CRXN,EDNAME
00015      REAL N
00016      C
00017      C*****THIS SUBROUTINE SETS UP ALL THE INITIAL VALUES NEEDED FOR
00018      C      THE PREDICTOR-CORRECTOR DIFFERENTIAL EQUATION SOLUTION.
00019      C      THESE VALUES ARE THEN STORED IN VALINT(42).
00020      C
00021      DO 10 K1=1,ELEMNT
00022      10  VALINT(K1)=WG*OMEGAK(K1)
00023      M2=ELEMNT+1
00024      M3=ELEMNT+PRTCLS
00025      DO 11 J1=M2,M3
00026      J=J1-ELEMNT
00027      11  VALINT(J1)=W(J)
00028      IA=ELEMNT+PRTCLS+1
00029      VALINT(IA)=WG*HGAS
00030      M2=ELEMNT+PRTCLS+2
00031      M3=ELEMNT+2*PRTCLS+1
00032      DO 12 J1=M2,M3
00033      J=J1-(ELEMNT+PRTCLS+1)
00034      12  VALINT(J1)=W(J)*H(J)
00035      M2=ELEMNT+2*PRTCLS+2
00036      M3=ELEMNT+3*PRTCLS+1
00037      DO 13 J1=M2,M3
00038      J=J1-(ELEMNT+2*PRTCLS+1)
00039      13  VALINT(J1)=V*N(J)*AMIN
00040      IA=ELEMNT+3*PRTCLS+2
00041      VALINT(IA)=WG
00042      M2=ELEMNT+3*PRTCLS+3
00043      M3=ELEMNT+4*PRTCLS+2
00044      DO 15 J1=M2,M3
00045      J=J1-(ELEMNT+3*PRTCLS+2)
00046      VALINT(J1)=ALPHAC(J)
00047      J2=J1+PRTCLS
00048      VALINT(J2)=ALPHAH(J)
00049      J3=J2+PRTCLS
00050      15  VALINT(J3)=ALPHAW(J)
00051      RETURN
00052      END
```

APPENDIX C

Thermochemical data for a wide variety of chemical species are required input for 1-DICOG. These data include reference enthalpy, reference entropy and heat capacity coefficients. For 1-DICOG computations performed at Brigham Young University, these parameters have generally been obtained from the data compilation of the EDWARDS thermochemical program (39). In turn, these data were generally obtained from the JANAF thermochemical tables. In order to assist the user, data from Reference 39 for several of the more relevant chemical species for propagating flames are summarized in this appendix. Data for 51 species are included. Most are hydrocarbons, while O, H, N, S and Si-containing species are also reported. Table C-1 provides a definition of the various data columns, while Table C-2 summarizes these thermochemical data.

TABLE C-1

DEFINITION OF ENTRIES IN THERMOCHEMICAL DATA TABLE

Enthalpy at 1200 K (Kcal/gmole) $H_{1200} = H_{298} + \int_{298}^{1200} C_p dT$

Entropy at 1200 K $S_{1200} = S_{298} + \int_{298}^{1200} \frac{C_p}{T} dT$
(cal/gmole · K)

Elemental composition of the species	Number of elements in species	Importance code	Ionic charge	Enthalpy at 1200 K (Kcal/gmole)	Entropy at 1200 K (cal/gmole · K)	Species name	Species order number	Date last updated
C 1. H 1.	2	20	-0.	148.6820	53.8529	CH	126	12 67
			-0.	-49.4959	27.2901			
			-0.	1.4885	-.8919			

Z_1, Z_2, Z_3, Z_4, Z_5 for $C_p \approx f(T)$ $T \geq 1200$ K,
 C_p is in (cal/gmole · K), $C_p = \sum_{i=0}^4 Z_{i+1} (1000/T)^i$

Z_1, Z_2, Z_3, Z_4, Z_5 for $C_p = f(t)$ $T < 1200$ K,
 C_p is in (cal/gmole · K), $C_p = \sum_{i=0}^4 Z_{i+1} (T/1000)^i$

Importance Code

00 = Very important gas	75 = Ordinary solid species
10 = Somewhat important gas	76 = Ordinary liquid species
20 = Ordinary gas species	80 = Important solid species
30 = Minor gas species	81 = Important liquid species

TABLE C-2

THERMOCHEMICAL DATA FOR SELECTED CHEMICAL SPECIES (Ref. 39)

C 1.	H 1.	-0.	-0.	-0	20	2	148.6820	53.8529	CH	
	11.0963	-8.7294	28.6231	-49.4959	27.2901					126
	7.1769	-1.1289	1.1386	1.4885	-0.8919				12	67
C 1.	H 1.	N 1.	-0.	-0	20	3	42.1828	62.8468	CHN	
	15.2434	1.8755	-16.8188	19.5803	-8.0666					132
	4.6340	18.9621	-23.9757	17.2927	-4.9071				12	69
C 1.	H 1.	O 1.	-0.	0	30	3	19.7540	67.4750	CHO	
	15.1173	-6.7024	10.4998	-12.9785	5.6361					134
	8.2363	-4.9887	22.9333	-20.9570	6.2576				12	70
C 1.	H 2.	-0.	-0.	-0	30	2	101.3120	59.6360	CH2	
	14.2815	1.2507	-13.2541	13.7633	-5.3053					135
	7.9753	-1.4636	10.7907	-8.9782	2.5554				12	72
C 1.	H 2.	O 1.	-0.	-0	20	3	-16.3003	68.6165	CH2O	
	19.8380	.4866	-10.7249	5.8798	-0.6320					139
	7.4712	-4.3840	34.5523	-32.5894	9.7654				3	61
C 1.	H 3.	-0.	-0.	-0	20	2	46.0347	62.7556	CH3	
	19.8198	.8401	-16.2918	12.3426	-2.5675					140
	6.6837	9.1229	-1.8892	.4556	-2.838				6	69
C 1.	H 4.	-0.	-0.	-0	20	2	-5.1606	62.4344	CH4	
	25.7473	1.2222	-22.0015	15.0340	-2.7867					145
	7.4307	-6.3982	44.3471	-39.8204	11.5976				3	61
C 1.	N 1.	-0.	-0.	-0	20	2	110.8413	58.7514	CN	
	9.4169	25.4727	-120.0550	178.1924	-87.5608					147
	7.6308	-5.2858	13.0671	-10.1486	2.7333				6	69
C 1.	O 1.	-0.	-0.	-0	10	2	-19.6215	57.4999	CO	
	9.6744	-4.2373	9.0746	-12.0826	5.6376					153
	7.5994	-4.8661	11.5395	-8.5080	2.1666				3	61
C 1.	O 1.	S 1.	-0.	-0	20	3	-21.7061	72.2478	COS	
	17.1359	-11.6948	26.3510	-31.7470	13.8840					154
	4.5713	25.9918	-32.8967	21.6287	-5.6733				3	61
C 1.	O 2.	-0.	-0.	-0	10	2	-83.4226	66.7552	CO2	
	16.9476	-12.9426	31.5939	-40.9050	18.7665					155
	4.4269	19.8206	-19.3181	10.4840	-2.4332				3	61
C 2.	H 1.	-0.	-0.	-0	30	2	124.0789	64.5162	C2H	
	14.1456	28.7952	-124.1832	173.9470	-82.7927					952
	5.0723	18.1857	-22.5959	16.0230	-4.5081				12	66
C 2.	H 2.	-0.	-0.	-0	20	2	67.3992	67.3772	C2H2	
	25.3511	-22.9443	42.8352	-52.8723	24.5897					165
	2.2156	42.0345	-59.0289	43.1920	-12.0946				3	61
C 2.	H 4.	-0.	-0.	-0	20	2	29.3345	76.0505	C2H4	
	31.7065	1.2707	-23.4483	16.0964	-3.1221					166
	1.6350	31.5873	-7.5583	-6.7478	3.5218				9	65
C 2.	H 4.	O 1.	-0.	-0	30	3	7.8430	86.6526	C2H4O	
	37.6688	1.2606	-24.2979	15.8614	-2.9578					167
	-1.8289	51.5980	-23.6962	-2.1593	3.5566				9	65
CO 1.	-0.	-0.	-0.	-0	20	1	107.0557	51.3473	CO	
	13.7502	-63.5756	192.0777	-243.6459	110.4042					997
	2.9773	13.5238	-20.9454	14.3872	-3.6537				9	67
H 1.	-0.	-0.	0.	0	20	1	56.5830	34.3090	H	
	4.9680	-0.0000	0.0000	-0.0000	0.0000					288
	4.9680	-0.0000	0.0000	-0.0000	0.0000				07	75
H 1.	O 1.	-0.	-0.	0	20	2	15.9830	53.8470	HO	
	10.4006	-7.8575	13.6006	-16.7214	8.1607					300
	8.3779	-7.2606	13.7350	-10.8105	3.2783				12	70
H 2.	-0.	-0.	-0.	0	0	1	6.4048	41.0349	H2	
	12.8548	-23.8674	52.9484	-61.0990	27.0132					304
	6.1563	4.6572	-9.6723	8.7834	-2.7044				3	61
H 2.	O 1.	-0.	-0.	0	0	2	-49.5570	57.4463	H2O	
	15.5208	-6.7693	.7168	-2.1223	2.6974					309



	8.0455	-1.8538	7.2725	-4.7628	1.1489				3 61
H 2.	0 2.	-0. -0.	-0 30	2 -20.1375	73.9745		H2O2		
	17.4433	-5.7557	24.7797	-41.6068	20.3816				310
	3.8051	30.5698	-35.1344	20.2595	-4.4805				12 60
H 2.	S 1.	-0. -0.	-0 20	2 4.0633	62.3988		H2S		
	16.1636	-11.5781	21.5242	-28.1551	13.3205				313
	7.8488	-1.2480	9.7461	-6.9585	1.5540				12 65
H 3.	N 1.	-0. -0.	-0 20	2 -3.763	61.4113		H3N		
	28.6650	-57.9455	128.1207	-147.0536	62.9049				314
	6.9777	2.2529	13.0714	-12.6480	3.8128				9 65
N 1.	O 1.	-0. -0.	-0 20	2 28.5411	60.8811		NO		
	9.6120	-3.4797	7.1128	-9.1987	4.1679				351
	8.1959	-7.8995	18.6061	-14.9907	4.2114				6 63
N 1.	O 2.	-0. -0.	-0 20	2 18.1762	72.5308		NO2		
	13.9064	.0495	-1.9801	.3637	.1327				352
	6.4906	6.9902	5.6850	-10.6396	3.9407				9 64
N 2.	-0.	-0. -0.	-0 0	1 6.7187	55.9578		N2		
	9.7325	-4.9604	11.2348	-15.2917	7.2885				360
	7.5309	-4.0828	8.9494	-5.9095	1.3277				2 61
N 2.	O 1.	-0. -0.	-0 20	2 30.4321	68.5678		N2O		
	14.8993	.0745	-2.8842	.9113	.1206				361
	4.8717	19.5613	-19.5098	10.6848	-2.4944				12 64
O 1.	-0.	-0. 0.	0 20	1 64.1030	45.5270		O		
	6.5063	-11.2484	30.3127	-35.3996	15.1363				381
	6.0377	-4.3190	7.0253	-5.1596	1.4154				07 75
O 2.	-0.	-0. -0.	-0 10	1 7.1149	59.7320		O2		
	10.7994	-1.0300	-16.8890	32.3940	-17.5193				389
	7.1663	-3.3897	12.9769	-12.1542	3.7360				2 61
O 2.	S 1.	-0. -0.	-0 10	2 -60.0788	75.4643		O2S		
	16.0201	-11.0806	25.7165	-30.4358	13.0862				391
	5.9938	14.2911	-8.3110	.0191	1.0272				6 61
S 1.	-0.	-0. -0.	-0 20	1 71.0570	47.5460		S		
	5.5345	2.0554	-16.2242	27.7989	-14.4921				424
	4.3786	10.0034	-26.2304	25.5022	-8.4940				6 71
C 1.	-0.	-0. -0.	-0 75	1 3.8831	6.8097		C (GRAPHITE)		
	8.3590	-16.9179	46.1293	-57.0516	25.2313				111
	-1.3182	13.8272	-8.9229	.6866	.8785				3 61
C 1.	SI 1.	-0. -0.	-0 75	2 -8.1943	17.4991		CSI(C)		
	13.3313	5.9169	-28.1704	37.5808	-17.5698				967
	-3.7576	52.3970	-75.5179	52.4643	-14.0109				3 67
C 1.	SI 1.	-0. -0.	-0 75	2 -7.8100	17.4482		CSI(C)		
	13.8546	7.2903	-40.5070	58.6620	-28.6105				159
	-4.0167	54.0007	-78.9907	55.4776	-14.9196				3 67
C 1.	SI 1.	-0. -0.	-0 76	2 1.7387	22.1706		CSI(L)		
	20.4721	-65.4217	265.8848	-431.2995	230.2591				732
	-6.9888	73.7410	-121.0145	91.4087	-25.7120				12 62
CA 1.	O 1.	-0. -0.	0 80	2 -140.7730	25.7160		CAO(C)		
	21.9378	-164.8799	751.8131	-1227.7795	659.7266				1125
	-2.6477	77.1953	-151.4812	130.8390	-40.9659				6 73
CA 1.	O 1.	-0. -0.	-0 76	2 -122.1890	31.4780		CAO(L)		
	-14.3162	232.4233	-643.5790	737.6251	-303.0620				1126
	2.9855	38.5998	-62.2836	46.5261	-12.9822				6 73
CA 1.	S 1.	-0. -0.	0 75	2 -102.2360	30.6260		CAS(C)		
	11.2024	62.7453	-215.3163	268.3116	-115.8028				1138
	1.0493	67.0475	-145.8728	135.1104	-44.2035				12 71
CS 1.	-0.	-0. -0.	-0 75	1 8.0085	32.5830		CS(C)		
	9.0000	0.0000	0.0000	0.0000	-0.0000				1036
	.1903	44.3756	-81.5957	64.8712	-18.8362				6 68
CS 1.	-0.	-0. -0.	-0 76	1 7.2119	32.4099		CS(L)		
	7.5965	-6.132	2.6331	-4.4440	2.2691				1037

TABLE C-2, (Continued)

	9.4088	-9.4134	16.2393	-12.2846	3.4580		6 68
0 2. SI 1.	-0.	-0.	-0 80	2 -203.0249	31.1969	02SI(C)	
	17.4194	10.6043	-38.9722	49.3371	-22.1372		991
	-28.8169	196.5277	-330.4013	249.6179	-70.1979		6 67
0 2. SI 1.	-0.	-0.	-0 76	2 -201.9826	31.6643	02SI(L)	
	27.3920	-76.7732	292.8746	-447.7383	227.0980		393
	-.5593	55.7166	-75.4259	50.0228	-12.9394		6 67
S 1.	-0.	-0.	-0 75	1 7.6890	18.5335	S(C)	
	17.4444	12.5422	-5.7026	-76.9714	67.0189		422
	3.0531	8.7177	-3.6585	3.0558	-.9205		12 65
S 1.	-0.	-0.	-0 76	1 7.4932	19.5903	S(L)	
	7.6940	-0.0000	0.0000	-0.0000	0.0000		423
	-3.7030	69.4416	-139.1975	114.7737	-33.6687		12 65
S 2. SI 1.	-0.	-0.	0 75	2 -33.1830	46.3320	S2SI(C)	
	24.8711	-22.9432	99.9160	-169.0095	90.5579		427
	17.4255	3.8655	-.6445	-.9953	.7459		6 72
S 2. SI 1.	-0.	-0.	0 76	2 -31.2780	47.7250	S2SI(L)	
	21.7500	0.0000	-0.0000	0.0000	-0.0000		428
	13.4714	36.0502	-91.2332	102.1707	-38.7092		6 72
SI 1.	-0.	-0.	-0 75	1 5.3294	12.4773	SI(C)	
	6.2791	19.5157	-64.8911	75.0192	-29.8269		431
	1.5307	17.5413	-27.9681	21.1647	-5.9722		12 66
SI 1.	-0.	-0.	-0 76	1 17.4480	19.6804	SI(L)	
	6.5000	0.0000	0.0000	0.0000	-0.0000		432
	6.5000	0.0000	0.0000	0.0000	-0.0000		3 67