

**APPENDIX C**

**"FIXED BED MODEL USER'S MANUAL/USER'S GUIDE**

## TABLE OF CONTENTS

LIST OF TABLES .....	iv
LIST OF FIGURES .....	v
 PART ONE: MODEL FORMULATION AND SOLUTION	
CHAPTER 1 INTRODUCTION .....	1-1
1.1 Code Description .....	1-1
1.2 Code Development .....	1-2
1.3 Limitations .....	1-2
1.4 Document Format .....	1-2
 CHAPTER 2 TWO-ZONE, WELL-MIXED PARTIAL EQUILIBRIUM MODEL .....	 2-1
2.1 Introduction .....	2-1
2.2 Foundations and Assumptions.....	2-1
2.3 Energy Balance .....	2-2
2.4 Gas Phase Chemistry .....	27
2.5 Devolatilization .....	2-8
2.5.1 Basis.....	2-8
2.5.2 Ultimate Composition .....	2-8
2.5.3 Ultimate Yields .....	2-12
2.5.4 Potential Tar-Forming Fraction.....	2-13
2.5.5 Arrhenius Rate Constants .....	2-15
2.5.6 Adjusting Functional Group Compositions.....	2-16
2.6 Oxidation and Gasification .....	2-17
2.7 Freeboard.....	2-17
2.8 Summary .....	2-18
 CHAPTER 3 ONE-DIMENSIONAL FIXED-BED MODEL .....	 3-1
3.1 Introduction .....	3-1
3.2 Foundations, Assumptions and Justification.....	3-1
3.3 Conservation Equations .....	3-4
3.3.1 Overall Gas and Solid Continuity Equations.....	3-8
3.3.2 Gas and Solid Energy Equations.....	3-8
3.3.3 Solid Species Continuity Equations.....	3-10
3.3.4 Gas Phase Elemental Continuity Equations.....	3-12
3.3.5 Gas Phase Tar Species and Elemental Continuity Equations ..	3-12
3.3.6 Pressure Drop.....	3-12
3.4 Gas Phase Chemistry .....	3-13
3.5 Heat and Mass Transport Properties .....	3-13
3.5.1 Physical Properties.....	3-13
3.5.2 Heat and Mass Transport Correlations.....	3-15
3.6 Drying .....	3-18
3.7 Devolatilization .....	3-19
3.8 Oxidation and Gasification .....	3-21
3.9 Summary of Model Equations .....	3-25
3.10 Summary of Model Parameters and Options.....	3-27

CHAPTER 4 SOLUTION TECHNIQUE.....	4-1
4.1 Introduction.....	4-1
4.2 Computational Algorithm.....	4-1
PART TWO: CODE USER'S MANUAL	
CHAPTER 5 USER'S GUIDE.....	5-1
5.1 General Description.....	5-1
5.2 Description of Subroutines.....	5-1
5.3 Program Input.....	5-4
5.3.1 Main Data File, mb1in.....	5-4
5.3.2 Thermodynamic Data File, mb1thm.....	5-9
5.4 Program Output.....	5-12
5.4.1 Main Output File, mb1out.....	5-12
5.4.2 Optional Output Files, outa Through outj.....	5-17
5.4.3 Plotting Output Files.....	5-19
5.5 Code Operation.....	5-20
5.5.1 Selecting Logicals.....	5-20
5.5.2 Iteration Procedure.....	5-22
CHAPTER 6 IMPLEMENTATION GUIDE.....	6-1
6.1 Compiling, Linking, and Executing Code Files.....	6-1
6.2 FORTRAN and Machine Incompatibilities.....	6-3
CHAPTER 7 SAMPLE PROBLEMS.....	6-1
7.1 Low Pressure, Air-Fired Gasification.....	6-1
7.2 High Pressure, Oxygen-Fired Gasification.....	6-2
NOMENCLATURE.....	N-1
REFERENCES.....	R-1
APPENDIX A SAMPLE MAKEFILE FOR PROGRAM MAINTENANCE.....	A-1
APPENDIX B CODE VARIABLES.....	B-1

## PART TWO: CODE USER'S MANUAL

### CHAPTER 5

#### USER'S GUIDE

##### 5.1 General Description

MBED-1D was developed on a SUN SPARCstation 1 with the UNIX operating system. The syntax of the code should be compatible with most FORTRAN 77 compilers. Plotting or graphics routines are not distributed with the code. However, graphics are important for understanding the code's voluminous output of data, and a recommendation for graphics output is discussed in this chapter. As discussed in Chapter 4, the solution technique is based on a shooting method rather than a relaxation method. The FORTRAN code listing occupies approximately 0.5 Megabytes of disk space. The executable and object code requires an additional 1.0 Megabytes of disk space.

All input data to MBED-1D are in SI units. The input files are discussed in Section 5.3. All working variables within the program are either dimensionless or in SI units. Units associated with all variables are either given in the nomenclature or can be found in Appendix B.

CPU run time depends on the particular hardware in which the code has been implemented. Also, the degree of compiler optimization also influences CPU time. One iteration on a CONVEX C-2 requires approximately 1.8 CPU minutes. The same simulation on a SUN SPARC station IPC requires 6.6 CPU minutes.

##### 5.2 Description of Subroutines

The computational algorithm for MBED-1D was given in Figure 4.1. A tree diagram of the structure of the program showing most of the actual computer routines is given in Figure 5.1. The routines which are not shown in Figure 5.1 are the subroutines associated with the equilibrium routines. Also, only one routine associated with the differential equation solver is shown in Figure 5.1: *lsode*. *lsode* is shown as a black box in Figure 5.1.

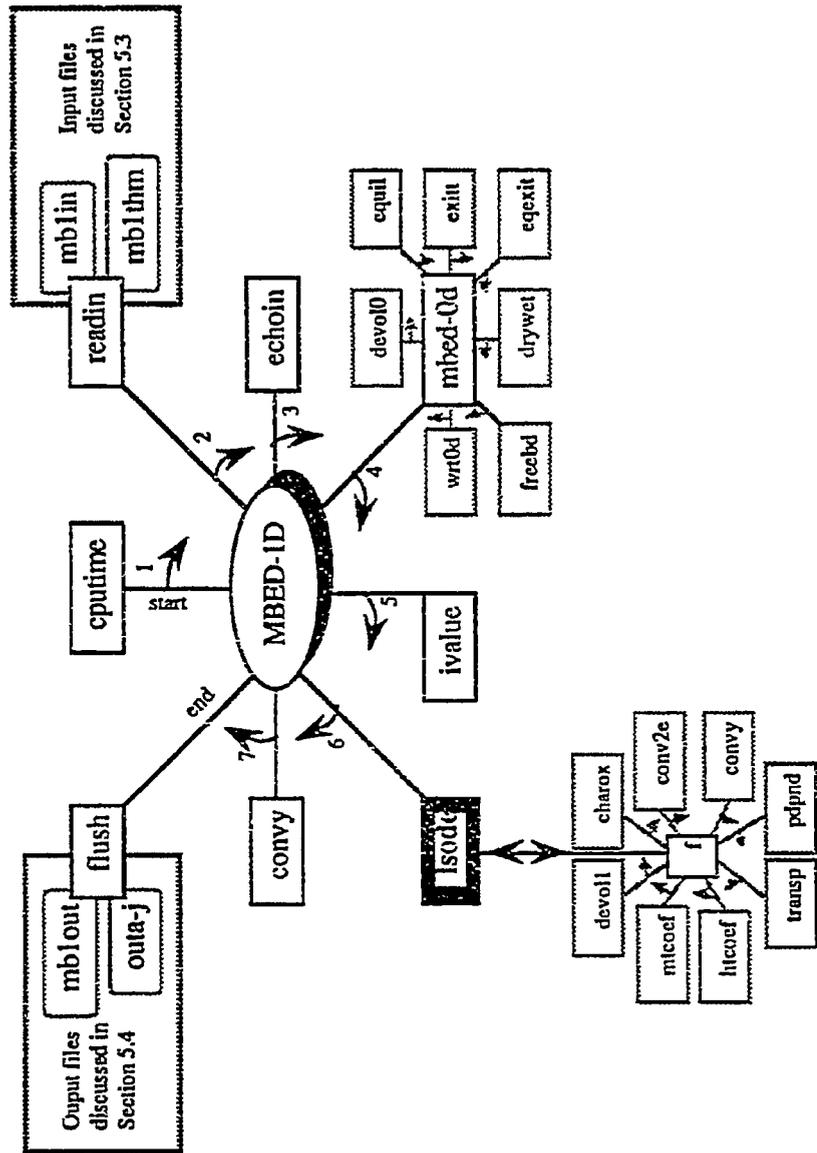


Figure 5.1 Tree diagram of the structure of MBED-1D

The main program is *mbed1d* and the routines it calls are shown in Figure 5.1. The *cputim* routine is called to track execution time and is not an integral part of the code. The *readin* routine is called to read input data from *mblin* and *mb1tim*. The input files are discussed further in Section 5.3. The *echoin* routine is used to write the input data to the output file, *mb1out*, which is discussed in more detail in Section 5.4. The *mbed0d* routine is the two-zone fixed-bed submodel which calculates the effluent gas properties. The routines associated with *mbed0d* are also shown in Figure 5.1. The *ivalue* routine is used to determine the initial values for the set of differential equations shown in Table 3.2. The differential equations are solved by repeated calls to *lsode* which requires evaluation of the right-hand-side of the set of differential equations given in Table 3.2. The *f* routine is used to calculate the right-hand-side of the differential equation set given in Table 3.2. The *convy* routine is used to obtain calculation variables from dependent variables (i. e. temperature from enthalpy). The *flush* routine causes the contents of the logical unit to be flushed to the associated file. This routine is called for writing output to the *mb1out* and *outa* through *outj* files which are discussed in more detail in Section 5.4.

The *mbed0d* routine calculates effluent gas temperature and composition according to the two-zone model discussed in Chapter 2. The *mbed0d* routine calls *devol0*, *equil*, *exit*, *eqexit*, *drywet*, *freebd*, and *wrtout* as shown in Figure 5.1. The *devol0* routine calculates the ultimate volatiles yield and composition based on Equations 2.14 through 2.19. The ultimate char yield and composition are also calculated with the *devol0* routine. The *equil* routine calculates the temperature, enthalpy and composition of the gases in the oxidation and gasification zone by assuming equilibrium. The *exit* routine calculates the exit temperature by assuming the gases are nonreactive in the drying and devolatilization zone. The *eqexit* routine calculates the exit temperature by assuming all gases but tar in the drying and devolatilization zone are in equilibrium. The *drywet* routine determines the molar percentages on a dry and wet basis of the major gas species in the effluent gas stream. The *wrt0d* routine writes the raw gas composition on a dry basis, the drying and devolatilization zone temperature, the oxidation and gasification zone temperature, tar mass flow rate, and selected input data in both SI and English units.

The *f* routine determines the right-hand-side of the differential equation set given in Table 3.2. The *f* routine calls *convy*, *pdpnd*, *transp*, *htcoef*, *mtcoef*, *devoll*, *charox* and *conv2e* as shown in Figure 5.1. The *convy* routine is used to obtain calculation variables from dependent variables. For example, temperature is obtained from enthalpy. The *convy* routine calls the *ptemp* routine to calculate particle temperature. The *pdpnd* routine calculates the particle diameter and particle number density. The *transp* routine calculates the gas mixture transport properties (i. e. thermal conductivity, molecular diffusivity, and viscosity). The *htcoef* routine calculates heat transfer coefficients, and the *mtcoef* routine calculates mass transfer coefficients. The *devoll* and *charox* routines calculate the volumetric drying, devolatilization, oxidation, and gasification rates. The *conv2e* routine converts the drying, devolatilization, oxidation, and gasification rates to an elemental basis.

## 5.3 Program Input

### 5.3.1 Main Data File, *mblin*

Two input files are required by MBED-1D: the main data file (*mblin*) and the thermodynamic properties data file (*mblthm*). The main data file is given in Table 5.1.

Table 5.1 Main data file, *mblin*.

```

5,                               !nsay..(say(i),i=1,nsay) follows:
*****                          ***** MBED1D
***** BRIGHAM YOUNG UNIVERSITY SIMULATION OF *****
***** WELLMAN GALUSHA 10/30/82 TEST USING *****
***** JETSON BITUMINOUS COAL *****
***** 8/30/90 *****
-----
ESSENTIAL INPUT PARAMETERS TO RUN ZERO-DIMENSIONAL MODEL:
-----
f      * 10d      (T--> do 0-d calculation only)
t      * lgaseq  (T--> all exit gases but tar in equil., t if 10d = f)
f      * lfreeb  (T--> do FREEBoard calculation using qfreeb)
f      * ljkstm  (T--> calculate heat loss with flowjs latent heat)
f      * lashcp  (T--> use ASH composition to calculate CP)
f      * lx0     (T--> use usrx0 for x0 rather than SET model x0)
f      * lusey0  (T--> use input y0 rather than idev specified y0)
t      * lecho   (T--> echo input parameters to mblout)
1.9812 * diach   (DIAMeter of reactor CHAMber, m)
1.8288 * chlgh   (reactor CHAMber axial LenGTH, m)
101325.0 * pres   (reactor PRESSure at bed top. pa)
333.75  * twtop  (Temperature of Wall at reactor TOP, K)
287.15  * twbot  (Temperature of Wall at reactor BOTtom, K)
298.0   * tcoal  (Temperature of feed COAL, K)
-1.2e6  * qfreeb (heat loss in FREEBoard, watts)
0.3524  * flowc  (FLOW rate of feed Coal, kg/s)
0.94813 * flowo  (FLOW rate of Oxidizer in feed, air or oxygen, kg/s)
0.15624 * flows  (FLOW rate of Steam in feed, kg/s)
0.13390 * flowjs (FLOW rate of Jacket Steam, kg/s)
0.4000e6 * u     (wall heat loss, j/s)
0.0000  * trf    (Tar Recycle Fraction, only used if 10d = t)
387.6   * tmptrf (TEMPERature of Tar Recycle Fraction, K)
1.0000  * brnout (BuRNOUT or weight fraction of reacted organic matter)
elements * elem  (flag to read ELEMENT data in cree0)
thermo   * ther  (flag to read species data in cree0)
reactant * reac  (flag to read REACTant feed stream 1, steam)
300.    * tf1   (Temperature of Feed stream 1 or steam feed, K)
h2.0    01.0    0.0    0.0    h2o    1.00000m
                                           (blank Line)
reactant * reac  (flag to read REACTant feed stream 0, oxidizer)
300.    * tf0   (Temperature of Feed stream 0 or oxidizer feed, K)
o2.0    0.0    0.0    0.0    o2     0.20990m
ar1.0   0.0    0.0    0.0    ar     0.00980m
n2.0    0.0    0.0    0.0    n2     0.78030m
                                           (blank Line)
0.0426  * prxash (PRoXimate ASH fraction, dry ash-free basis)
0.4938  * prxfc  (PRoXimate Fixed Carbon fraction, dry ash-free basis)
0.0625  * prxh2o (PRoXimate moisture fraction, dry ash-free basis)
0.3994  * prxvm  (PRoXimate Volatile fraction, dry ash-free basis)

```

Table 5.1 Main data file, *mblin* (continue).

```

0.8141 * wdafc (ultimate Carbon fraction, Dry Ash-Free basis)
0.0507 * wdafh (ultimate Hydrogen fraction, Dry Ash-Free basis)
0.1015 * wdafo (ultimate Oxygen fraction, Dry Ash-Free basis)
0.0175 * wdafn (ultimate Nitrogen fraction, Dry Ash-Free basis)
0.0161 * wdafs (ultimate Sulfur fraction, Dry Ash-Free basis)
1704.0 * tmask (Melting Temperature of ASH, K)
0.4410 * asio2 (mass fraction SiO2 in Ash, see comments below)
0.0201 * acao (mass fraction CaO in Ash)
0.2310 * aal2o3 (mass fraction Al2CO3 in Ash)
0.0113 * amgo (mass fraction MgO in Ash)
0.0139 * ak2o (mass fraction K2O in Ash)
0.0013 * ana2o (mass fraction Na2O in Ash)
0.0144 * atio2 (mass fraction TiO2 in Ash)
0.0000 * amno (mass fraction MnO in Ash)
0.0416 * afeo (mass fraction FeO in Ash)
0.2125 * afe2o3 (mass fraction Fe2O3 in Ash)
0.0000 * afe (mass fraction free iron, Fe, in Ash)
0.0003 * ap2o5 (mass fraction P2O5 in Ash)
0.0000 * acaf2 (mass fraction CaF2 in Ash)
0.0126 * aso3 (mass fraction SO3 in Ash)
5 * idev (DEVolatilization FLAG, SEE COMMENTS BELOW FOR MORE)
0.1567 * usrx0 (USER supplied XC, used when lx0 is set to t)

```

-----  
ADDITIONAL INPUT PARAMETERS TO RUN ONE-DIMENSIONAL MODEL:  
-----

```

t * lsp (T--> Shell Progressive rather than ash segregation)
f * ltareq (T--> let TAR go to equilibrium in the gas phase)
f * lstiff (T--> use STIFF LSODE solver)
t * lstop (T--> STOP calculation when bottom of reactor reached)
t * louta (T--> print gas/solid flow rate, energy rates, etc.)
t * loutb (T--> print gas/solid transport properties)
t * loutc (T--> print sherwood numbers and mass transport coef.)
t * loutd (T--> print film, ash and total resistances)
t * loute (T--> print chemical, bulk and total resistance)
t * loutf (T--> print diameters,  $\rho$  density, consumption rates)
t * loutg (T--> print enthalpies, reynolds and prandtl numbers)
t * louth (T--> print heat transfer rates)
t * louti (T--> print first fifteen gas mole percents)
t * loutj (T--> print residence times, heating rates,  $\rho$  vel.)
1 * itask (LSODE parameter used to specify output, see comments)
0.020 * deltax (step size for output, m)
1.0e-15 * abstol (ABSolute TOLerance)
1.0e-8 * reltol (RELative TOLerance)
0.02032 * pd0 (initial Particle Diameter, m)
0.25 * gamma (swelling parameter, fraction)
1.0 * zi (heat of rxn partition, if zi = 1, rxn heat to solid)
0.64 * vflash (Void Fraction in ASH zone, volume void/total volume)
0.33 * vfcoal (Void Fraction in COAL zone at reactor solid feed)
1192.0 * rhosm (apparent coal density, kg/m3)
0.1359 * poros (POROSity of coal)
1092.4 * rhotar (TAR density, kg/m3)
391.0 * tbtar (Boiling point for TAR, K)
4.4 * ffco2 (Frequency Factor for CO2 gasification, m/K_s)
4.4 * ffh2 (Frequency Factor for H2 gasification, m/K_s) <--GUESS
1.33 * ffh2o (Frequency Factor for H2O gasification, m/K_s)
2.5 * ffo2 (Frequency Factor for O2 oxidation, m/K_s)
1.62e8 * eco0 (activation Energy for CO2 gasification, j/kmol)

```

Table 5.1 Main data file, *mblin* (continue).

```

1.62e8 * eh2 (activation Energy for H2 gasification, j/kmol)<--GUESS
1.47e8 * eh2o (activation Energy for H2O gasification, j/kmol)
9.29e7 * eo2 (activation Energy for O2 oxidation, j/kmol)
1.0 * zeta (particle area factor to account for internal burning)
0.5 * apdivt (developing Ash Porosity DIVided by Tortuosity)
0.05 * fdgsg (FuDGe factor for Solid to Gas heat transfer coef.)
1.0 * fdgdev (DEVolatilization FuDGe factor)
1.0 * fdgco2 (co2 gasification FuDGe factor)
1.0 * fdgh2 (h2 gasification FuDGe factor)
1.0 * fdgh2o (h2o gasification FuDGe factor)
1.0 * fdgo2 (o2 oxidation FuDGe factor)
1.0 * fhwg (Fudge factor for Gas-to-Wall Heat transfer coef.)
1.0 * fhws (Fudge factor for Solid-to-Wall Heat transfer coef.)
-----
ADDITIONAL COMMENTS
-----
idev = 1 n. d. zap lignite (y0's adjusted to match ultimate)
idev = 2 gillette subbit. (y0's adjusted to match ultimate)
idev = 3 montana rosebud subbit. (y0's adjusted to match ultimate)
idev = 4 illinois #6 bituminous (y0's adjusted to match ultimate)
idev = 5 kentucky #9 bituminous (y0's adjusted to match ultimate)
idev = 6 pittsburg #8 bituminous (y0's adjusted to match ultimate)
idev = 7 utah blind canyon bituminous (y0's adjusted)
idev = 8 wyodak subbituminous (y0's adjusted to match ultimate)
itask = 1 overshoot and interpolate to get z at tout
itask = 2 take one step only and return
itask = 3 stop at first internal mesh point at or beyond tout

```

When setting up a new problem for simulation, it is easiest to start by editing input files from a previous simulation, since much of the information will remain unchanged. The *mblin* input file is divided into two major sections. The first section contains the required data to run the two-zone, zero-dimensional model. The last section contains the the additional parameters required to run the one-dimensional model.

Most of the input data in *mblin* are single line, format free entries. After the format free data entries, an extensive comment statement is given describing the input parameter. The code variable is given in lower case followed by the description of the code variable in parenthesis. Units are also given in parenthesis if required. Upper case is used in the code variable description indicating the reason for choosing the code variable name (e. g. diach DIAMeter of reactor CHamber, m).

The *mblin* file starts by reading the integer *nsay* which indicates the number of comment statements that are printed out at the top of the main output file *mblout*. Any number of comment statements may be included in the header. In the example file shown in Table 5.1, five comment lines are used to describe the simulation. Following the five comment lines, three more lines are used to differentiate the zero-dimensional input parameters from the one-dimensional input parameters. These three lines are required in the input file.

Eight lines of logical input lines follow the three comment lines that describe the zero-dimensional input parameters. These parameters are *l0d*, *lgaseq*, *lfreeb*, *ljkstm*, *lashcp*, *lx0*, *lusey0*, and *lecho*. The logical parameters require an L5 format. The model options are discussed in more detail in Section 5.5. The fifteen lines following the logical inputs are format free and describe the reactor geometry (*diach* and *chlgh*), reactor pressure (*pres*), temperature of the wall at the top of the reactor (*twtop*), temperature of

the wall at the bottom of the reactor (*twbot*), the feed coal temperature (*tcoal*), the freeboard heat loss (*qfreeb*), the flow rate of the feed coal (*flowc*), the flow rate of the oxidizer in the feed (*flowo*), the flow rate of the steam in the feed (*flows*), the flow rate of jacket steam (*flowjs*), the 0-D overall wall heat loss (*u*), the tar recycle fraction (*trf*), the temperature of the tar recycle fraction (*tmprf*), and the burnout (*brnout*). Not all of these fifteen parameters are used in the zero-dimensional calculation. For example, the jacket steam flow rate is used to calculate the wall heat loss based on the vaporization enthalpy of steam provided the logical *ljkstn* is set to "true". When the wall heat loss is calculated based on the jacket steam flow rate, the estimated wall heat loss is not used. Code operation is discussed in more detail in Section 5.5.

The keywords "elem" and "ther" are used to invoke reading of data from the thermodynamic input file *mblthm*. The keyword "reac" invokes reading of stream temperature and composition. Only two gaseous reactant streams are allowed. The first reactant stream is for steam, and the second reactant stream is for the oxidizer which is usually oxygen or air. A blank line signifies the end of defining a reactant stream. Following the keyword "reac", the temperature of the stream is input as a format free code variable. Following the stream temperature, the stream species composition is input. A separate line is used for each species. The atomic composition of each species is described by formatted code variables, 4(a2,f7.5). The character string, formatted by a2, describes the element. For example, "h" is used for hydrogen as shown in Table 5.1. Note the blank before the "h" is required for the a2 formatted input. The real number following the element character string describes the number of atoms formatted as f4.5. For example, in Table 5.1, "h2.0" indicates two hydrogen atoms per water molecule. The four blanks following the 2.0 are consistent with the f7.5 format specification. Following the description of the atomic composition of the species, the species name is described by the 2a4 format specification. Next, the composition of the species in the reactant stream is input with a format specification of (1x,f7.5,1a). For example, pure water is specified as "1.00000m" in Table 5.1. There is a blank in front of the concentration fraction. The letter following the concentration fraction, "m", specifies the fraction as a mole fraction. Weight fractions can be specified by using a "w" instead of an "m" after the species concentration fraction. The complete formatted specification for the species definition is (4(a2,f7.5),2a4,1x,f7.5,a1).

The format free proximate analysis of the feed coal on a dry, ash-free basis is specified as *prxash*, *prxfc*, *prxh2o*, and *prxvm*. The dry, ash-free ultimate analysis is specified as *wdafc*, *wdafh*, *wdafo*, *wdafn*, and *wdafs*. Next, the melting point of the ash followed by the ash composition is specified. The last two parameters essential to run the zero-dimensional portion of the code are related to devolatilization. The variable, *idev*, is an integer which describes the base coal used in the functional group composition calculation. The variable, *usrx0*, is used to specify the potential tar-forming fraction when the flag *lx0* is set to "true".

The second half of the input file *mblin* is used to describe the additional input parameters that are necessary to run the one-dimensional fixed-bed model which is described in Chapter 3. The additional one-dimensional parameters are separated from the essential zero-dimensional input parameters by three comment lines which are followed by fifteen lines of logical input parameters: *lsp*, *ltareq*, *lstiff*, *lstop*, *louta*, *loutb*, *loutc*, *loutd*, *loute*, *loutf*, *loutg*, *louth*, *louti*, and *loutj*. Parameters essential to the differential equation solver follow the fifteen logical input parameters. The differential equation solver, *lsode*, requires *itask* and *deltaz* to specify output. Tolerances are specified with *abstol* and *reltol*. For more information on *LSODE* see Hindmarsh (1983).

The diameter of the feed coal is specified as *pd0*. Multiple particle sizes in the feed coal are not treated. Particle swelling is assumed to be proportional to devolatilization. The proportionality factor is input as *gamma*. The heat of reaction partition, *zi*, is not active and is ignored. The partition between the heat of reaction is not arbitrarily partitioned as discussed in Chapter 3. The void fractions at the top and bottom of the bed are represented by *vfcoal* and *vflash*, respectively. The format free apparent coal density, coal porosity, tar density, and tar boiling point are represented by *rho<sub>sm</sub>*, *poros*, *rhotar*, and *tbtar*, respectively. The gasification and oxidation kinetics are also format free. The frequency factors are entered first followed by the activation energies: *ffco<sub>2</sub>*, *ffh<sub>2</sub>*, *ffh<sub>2o</sub>*, *ffo<sub>2</sub>*, *eco<sub>2</sub>*, *eh<sub>2</sub>*, *eh<sub>2o</sub>*, and *eo<sub>2</sub>*. The remaining parameters required to run MBED-1D are used to look at sensitivities of various parameters. Some of these values represent observed physical phenomena. The remaining format free parameters are the particle area factor which is used to account for internal particle burning (*zeta*), the developing ash porosity divided by tortuosity (*apdivt*), the solid-to-gas heat transfer correction factor (*fdgsg*), the devolatilization mass transfer correction factor (*fdgdev*), the CO<sub>2</sub> gasification correction factor (*fdgco<sub>2</sub>*), the H<sub>2</sub> gasification correction factor (*fdgh<sub>2</sub>*), the H<sub>2</sub>O gasification correction factor (*fdgh<sub>2o</sub>*), the gas-to-wall heat transfer correction factor (*fhwg*), and the solid-to-wall heat transfer correction factor (*fhw<sub>s</sub>*). Additional comments at the end of the *mblin* input file are used to define different options using the integer flags *idev* and *itask*. These final comment lines are not read by MBED-1D.

### 5.3.2 Thermodynamic Data File, *mblthm*

The thermodynamic properties data file, *mblthm*, is given in Table 5.2. Typically, this file does not change unless a new species or element is needed. The thermodynamic properties data file is called from the *cree0* routine. The keywords "elem" and "ther" are used to invoke reading of data from the thermodynamic input file *mblthm*.

The input file *mblthm* is divided into three major sections: element data, species thermodynamic data, and species transport data. The elemental data is read in initially by specifying the species name, molecular weight, and valence. The elemental data uses the following format specification: a2,8x,2f10.6. The order in which the elements are listed is the order in which they are treated in the program calculations. A blank line is required between the elemental data and the species thermodynamic data as shown in Table 5.2.

The thermodynamic data for each species are entered on three separate lines. The first line is used to specify the species name and elemental composition. The second and third lines are used to specify heat capacity coefficients for the species. The format for specifying the species name and elemental composition is as follows: 3a4,12x,4(a2,f3.0). The source and date of the thermodynamic data are also shown in Table 5.2 following the species name (e. g. j 9/65). The "j" indicates the source of the data as being the JANNAF thermochemical tables (Stull and Prophet, 1971). Also, the "g 300.000 5000.000" entry indicates that the species is a gas over the temperature range from 300 to 5000 K. MBED-1D does not use the literature source and date, species physical state, and valid temperature range. However, this information is available in Table 5.2 for reference.

A blank line is required between the species thermodynamic data and the species transport data. The format free species transport data is read by the *readin* routine. The species transport data includes the Stockmeyer collision diameter (*s*), Lennard-Jones temperature parameter (*ek*), and the nonpolar correction factor for the Lennard-Jones parameter (*delta*).

Table 5.2 Thermodynamic Data File, *mb1.thm*.

```

c      12.01115      4.0
h      1.00797      1.0
n      14.0067      0.0
s      32.06        4.0
o      15.9994     -2.0
ar     39.9480      0.0

ar      1 5/66ar 1.00 0.00 0.00 0.g 300.000 5000.000
0.25000000e 01 0.0 0.0 0.0 0.0 0.0
-0.74537500e 03 0.43660002e 01 0.25000000e 01 0.0 0.0
0.0 0.0 -0.74537476e 03 0.43660002e 01
co      j 9/65c 1.0 1.00 0.00 0.g 300.000 5000.000
0.29840689e 01 0.14891387e-02-0.57899678e-06 0.10364576e-09-0.69353499e-14
-0.14245227e 05 0.63479147e 01 0.37100916e 01-0.16190964e-02 0.36923584e-05
-0.20319673e-08 0.23953344e-12-0.14356309e 05 0.29555340e 01
co2     j 9/65c 1.0 2.00 0.00 0.g 300.000 5000.000
0.44608040e 01 0.30981717e-02-0.12392566e-05 0.22741323e-09-0.15525948e-13
-0.48961438e 05-0.98635978e 00 0.24007788e 01 0.87350905e-02-0.66070861e-05
0.20021860e-08 0.63274039e-15-0.48377520e 05 0.96951447e 01
ch4     j 3/61c 1.h 4.00 0.00 0.g 300.000 5000.000
0.15027056e 01 0.10416795e-01-0.39181514e-05 0.6777872e-09-0.44283706e-13
-0.99787031e 04 0.10707143e 02 0.38261929e 01-0.39794557e-02 0.24558321e-04
-0.22732920e-07 0.69626952e-11-0.10144945e 05 0.86690062e 00
c2h6    cr2178c 2h 60 00 0g 300.000 5000.000
1.67107058e+00 1.88078150e-02-6.98943156e-06 1.16385735e-09-7.17707692e-14
-1.14683543e+04 1.26317347e+01 1.92453270e+00 1.68224303e-02-2.24906498e-06
-3.40875417e-09 1.49239675e-12-1.14789269e+04 1.16292438e+01
h2      j 3/61h 2.0 0.0 0.0 0.g 300.000 5000.000
0.31001883e 01 0.51119458e-03 0.52444204e-07-0.34909964e-10 0.36945341e-14
-0.87738013e 03-0.19629412e 01 0.30574446e 01 0.26765198e-02-0.58099149e-05
0.55210343e-08-0.18122726e-11-0.98890430e 03-0.22997046e 01
hcn     000000h 1.c 1.n 1.0 0.g 300.000 5000.000
0.37068110e 01 0.33362799e-02-0.11913307e-05 0.19992916e-09-0.12826451e-13
0.14962633e 05 0.20794888e 01 0.24513550e 01 0.87208301e-02-0.10094202e-04
0.67255677e-08-0.17626959e-11 0.15213000e 05 0.80830069e 01
h2o     j 3/61h 2.0 1.00 0.00 0.g 300.000 5000.000
0.27167616e 01 0.29451370e-02-0.80224368e-06 0.10226681e-09-0.48472104e-14
-0.29905820e 05 0.66305666e 01 0.40701275e 01-0.11084499e-02 0.41521180e-05
-0.29637404e-08 0.80702101e-12-0.30279719e 05-0.32270038e 00
h2s     j12/65h 2.s 1.00 0.00 0.g 300.000 5000.000
0.28479090e 01 0.38415990e-02-0.14099360e-05 0.24278735e-09-0.15783280e-13
-0.34469788e 04 0.74781399e 01 0.38811293e 01-0.13211856e-03 0.36517713e-05
-0.21820441e-08 0.28783779e-12-0.36350916e 04 0.25161505e 01
n2      j 9/65n 2.0 0.0 0.0 0.g 300.000 5000.000
0.28963194e 01 0.15154863e-02-0.57235275e-06 0.99807385e-10-0.65223536e-14
-0.90586182e 03 0.61615143e 01 0.36748257e 01-0.12081496e-02 0.23240100e-05
-0.63217520e-09-0.22577253e-12-0.10611587e 04 0.23580418e 01
nh3     j 9/65n 1.h 3.00 0.00 0.g 300.000 5000.000
0.24165173e 01 0.61871186e-02-0.21785136e-05 0.37599057e-09-0.24448854e-13
-0.64747109e 04 0.77043467e 01 0.35912762e 01 0.49388665e-03 0.83449304e-05
-0.83833385e-08 0.27299092e-11-0.66717070e 04 0.22520962e 01
no      j 6/63n 1.0 1.00 0.00 0.g 300.000 5000.000
0.31889992e 01 0.13382279e-02-0.52899316e-06 0.95919314e-10-0.64847928e-14
0.98283242e 04 0.67458115e 01 0.40459509e 01-0.34181783e-02 0.79219174e-05

```

Table 5.2 Thermodynamic Data File, *mblthm* (continue).

```

-0.61139254e-08 0.15919072e-11 0.97453867e 04 0.29974976e 01
o2      j 9/65o 2.0 0.0 0.0 0.g 300.000 5000.000
0.36219521e 01 0.73618256e-03-0.19652219e-06 0.36201556e-10-0.28945623e-14
-0.12019822e 04 0.36150942e 01 0.36255980e 01-0.18782183e-02 0.70554543e-05
-0.67635071e-08 0.21555977e-11-0.10475225e 04 0.43052769e 01
oh      j 3/66o 1.h 1.00 0.00 0.g 300.000 5000.000
0.29106417e 01 0.95931627e-03-0.19441700e-06 0.13756646e-10 0.14224542e-15
0.39353811e 04 0.54423428e 01 0.38375931e 01-0.10778855e-02 0.96830354e-06
0.18713971e-09-0.22571089e-12 0.36412820e 04 0.49370009e 00
so2     j 6/61s 1.o 2.00 0.00 0.g 300.000 5000.000
0.52451363e 01 0.19704204e-02-0.80375759e-06 0.15149969e-09-0.10557998e-13
-0.37556227e 05-0.10873518e 01 0.32665329e 01 0.53237863e-02 0.68437544e-06
-0.52809987e-08 0.25590450e-11-0.36908145e 05 0.96513472e 01

```

```

3.418,124.,0., * ar s(i), ek(i), delta(i)
3.590,110.,0., * co most data from rps except as noted
3.996,190.,0., * co2
3.758,148.6,0.0, * ch4
4.418,230.0,0.0, * c2h6
2.915,38.,0., * h2
3.0,300.0,0.0 * hcn blind guess (after rdb above)
2.641,809.1,1., * h2o
3.49,343.0,0.0, * h2s
3.681,91.5,0., * n2
3.15,358.0,0.7, * nh3
3.47,119.0,0., ! no bsl
3.433,113.,0., * o2
3.0,300.0,0.0, ! oh obtained from rdb
4.04,347.0,0.42, ! so2

```

```

!this file should always contain the following species:
! ar, co, co2, ch4, c2h6, h2, hcn, h2o, h2s, n2, nh3, and o2
! other species may be added if desired. the subroutines wrtout and addgas
! should be modified to obtain printout of any added species. if these
! files are not modified, the added species will be part of "others"
! in the output file.

```

## 5.4 Program Output

### 5.4.1 Main Output File, *mblout*

Eleven output files are available from MBED-1D: the main output file (*mblout*) and ten optional output file (*outa* through *outj*). The main output file is given in Table 5.3. The output file in Table 5.3 corresponds to the input data given in Table 5.1 and Table 5.2.

Table 5.3 Main Output File, *mblout*.

```

..... MBED1D
***** BRIGHAM YOUNG UNIVERSITY SIMULATION OF *****
***** WELLMAN GALUSHA 10/30/82 TEST USING *****
***** JETSON BITUMINOUS COAL *****
..... 8/30/90
-----
Zero-dimensional input parameters:
-----
F      T--> do 0-d calculation only
T      T--> all exit gases in equil., t if 10d = f
F      T--> do FREEBoard calculation using qfreeb
F      T--> calculate heat loss with flowjs latent heat
F      T--> use ASH composition to calculate CP
F      T--> use usrxC for x0 rather than SET model x0
F      T--> use input y0 rather than idev
T      T--> echo input parameters to mblout
0.198E+01 DIAMeter of reactor CHAMber, m
0.183E+01 reactor CHAMber axial LenGth, m
0.101E+06 reactor PRESSure at bed top, ps
0.334E+03 Temperature of Wall at reactor TOP, K
0.287E+03 Temperature of Wall at reactor BOTtom, K
0.298E+03 Temperature of feed COAL, K
-0.120E+07 heat loss in FREEBoard, watts
0.352E+00 FLOW rate of feed Coal, kg/s
0.948E+00 FLOW rate of Oxidizer in feed, kg/s
0.156E+00 FLOW rate of Steam in feed, kg/s
0.134E+00 FLOW rate of Jacket Steam, kg/s
0.400E+06 Overall wall ht coefficient, j/sm^2K
0.000E+00 Tar Recycle Fraction, only used if 10d = t
0.388E+03 Tar Recycle Temperature, K
0.100E+01 BuRNOU, wt fract of reacted organic matter
0.426E-01 PRoXimate ASH fraction, dry ash-free basis
0.494E+00 PRoXimate Fixed Carbon fraction, daf basis
0.625E-01 PRoXimate moisture fraction, daf basis
0.399E+00 PRoXimate Volatile fraction, daf basis
0.814E+00 Dry, Ash-Free ultimate mass fraction C
0.507E-01 Dry, Ash-Free ultimate mass fraction H
0.102E+00 Dry, Ash-Free ultimate mass fraction O
0.175E-01 Dry, Ash-Free ultimate mass fraction N
0.161E-01 Dry, Ash-Free ultimate mass fraction S
0.170E+04 melting temperature of ash, K
0.441E+00 SiO2 weight fraction in ash
0.201E-01 CaO weight fraction in ash
0.231E+00 Al2O3 weight fraction in ash
0.113E-01 MgO weight fraction in ash
0.139E-01 K2O weight fraction in ash
0.130E-02 Na2O weight fraction in ash
0.144E-01 TiO2 weight fraction in ash
0.000E+00 MnO weight fraction in ash
0.416E-01 FeO weight fraction in ash
0.213E+00 Fe2O3 weight fraction in ash
0.000E+00 Fe (free iron) weight fraction in ash
0.300E-03 P2O5 weight fraction in ash
0.000E+00 CaF2 weight fraction in ash
0.126E-01 SO3 weight fraction in ash
S      1-zap, 2-gill, 3-rose, 4-ill16, 5-kty9, 6-pit8
0.157E+00 USer supplied X0, used when 1x0 is set to t

```

Table 5.3 Main Output File, *mb1out* (continue).

---

One-dimensional input parameters:

---

T	T--> Shell Progressive rather than AS model
F	T--> let TAR go to equilibrium
F	T--> use STIFF LSODE solver
T	T--> T--> STOP when bottom of reactor reached
T	T--> print gas/solid flow rate, energy rates
T	T--> print gas/solid transport properties
T	T--> print sherwood numbers and mt coef.
T	T--> print film, ash and total resistances
T	T--> print chemical, bulk and total resistance
T	T--> print diameters, $\rho$ density, c rates
T	T--> print enthalpies, re and pr numbers
T	T--> print heat transfer rates
T	T--> print first fifteen gas mole percents
T	T--> print res. times, heating rates, $\rho$ vel.
1	LSODE parameter used to specify output
0.200E-01	step size for output, m
0.100E-14	ABSolute TOLerance used in LSODE
0.100E-07	RELative TOLerance used in LSODE
0.203E-01	initial Particle Diameter, m
0.250E+00	swelling parameter, fraction
0.100E+01	heat of rxn partition
0.640E+00	Void Fraction in ASE zone
0.330E+00	Void Fraction in COAL zone
0.119E+04	apparent coal density, kg/m <sup>3</sup>
0.136E+00	POROSity of coal
0.109E+04	TAR density, kg/m <sup>3</sup>
0.391E+03	Boiling point for TAR, K
0.440E+01	Frequency Factor for CO2 gasification, m/K_s
0.440E+01	Frequency Factor for H2 gasification, m/K_s
0.133E+01	Frequency Factor for H2O gasification, m/K_s
0.230E+01	Frequency Factor for O2 oxidation, /K_s
0.162E+09	activation Energy for CO2 gasification, j/kmol
0.162E+09	activation Energy for H2 gasification, j/kmol
0.147E+09	activation Energy for H2O gasification, j/kmol
0.929E+08	activation Energy for O2 oxidation, j/kmol
0.100E+01	particle area factor for internal burning
0.500E+00	developing Ash Porosity DIVided by Tortuosity
0.500E-01	FuDGe factor for Solid to Gas ht coef.
0.100E+01	DEVolatilization FuDGe factor
0.100E+01	co2 gasification FuDGe factor
0.100E+01	h2 gasification FuDGe factor
0.100E+01	h2o gasification FuDGe factor
0.100E+01	o2 oxidation FuDGe factor
0.100E+01	Fudge factor for Gas-to-Wall HT coefficient
0.100E+01	Fudge factor for Solid-to-Wall HT coefficient

---

Calculated input parameters:

---

0.310E+03	Temperature of WALL used in 0-d calc, K
0.373E+03	SATurated water Temp. at reactor pressure, K
0.154E+07	VAPorization enthalpy of water at TW, j/kg
0.206E+06	heat loss through reactor walls, j/s or watts
0.792E+01	AVeraGe Atomic Weight of coal, kg/kmol
0.332E+08	Higher Heating Value of coal, j/kg

Table 5.3 Main Output File, *mb1out* (continue).

-0.857E+06	Heat of Formation of Coal, j/kg				
-0.165E+03	SENSible enthalpy of Coal, j/kg				
0.594E+03	a in Cp(ash) = a + bT - ct <sup>-2</sup>				
0.586E+00	b in Cp(ash) = a + bT - ct <sup>-2</sup>				
0.000E+00	c in Cp(ash) = a + bT - ct <sup>-2</sup>				
0.159E+04	liquid ash heat capacity, j/kg_K				
0.230E+06	heat of melting for ash, j/kg				
INPUT ECHO (idev =	5)				
-----					
ifreeb, 1jxstm, 1x0			F	F	F
burnout			1.0000		
-----					
u, watts/m <sup>2</sup> K	*****		(*****	btu/hrft <sup>2</sup> F)	
Blast Steam Temp., K	300.00		(	80.33 F)	
Blast Oxidizer Temp., K	300.00		(	80.33 F)	
-----					
HHV OF DAF COAL, j/kg	0.331798E+08		(14264.7	btu/lb)	
Freeboard heat loss, watts	-.120000E+07		(-.1138E+04	btu/s)	
-----					
Chamber diameter, m	1.9812		(	6.4999 ft)	
Chamber length, m	1.8289		(	5.9999 ft)	
Wall temp., K	310.45		(	99.14 F)	
Chamber Pressure, KPa	.10133E+03		(	1.0 atm)	
Inlet coal temp., K	298.00		(	76.7 F)	
-----					
Coal mass flow, kg/s	0.3524		(	1.3984 t/hr)	
Oxidizer mass flow, kg/s	0.94813		(	3.7624 t/hr)	
Steam mass flow, kg/s	0.15624		(	0.6200 t/hr)	
Jacket steam flow, kg/s	0.13390		(	0.5314 t/hr)	
Tar recycle wt. fraction	0.0000				
-----					
UA, w/K	0.400000E+06		(0.25E+07	btu/hr.F)	
Tsat, K	373.14		(211.99	F)	
Enthalpy of Vap., j/kg	0.1540E+07		(0.6623E+03	btu/lb)	
Wall heat loss, watts	0.4000E+06		(0.3794E+03	btu/s)	
-----					
Proximate (ash, fc, H2O, VM)	0.0426	0.4938	0.0625	0.3994	
Ultimate anal. (input-CHNSO)	0.8112	0.0507	0.0175	0.0161	0.1015
Ultimate anal. (devol-CHNSO)	0.8142	0.0508	0.0175	0.0161	0.1015
-----					

Table 5.3 Main Output File, *mb1out* (continue).

OUTPUT RESULTS:  $V^* = 0.547878048311968$   $x0 = 0.221957148909373$

-----  
 Exit temp., K 921.33 (1198.72 F)  
 Equilibrium temp., K 1471.39 (2188.83 F)  
 Product tar flow, kg/s 0.0648 ( 0.2572 t/hr)

Recycle tar flow, kg/s 0.0000 ( 0.0000 t/hr)  
 Total tar flow, kg/s 0.0648 ( 0.2572 t/hr)

RAW GAS COMPOSITION (DRY)--->

COMPONENT	(DRY) MOLE %
CO	18.89
CO2	10.83
H2	21.32
CH4	1.09
C2H6	0.00
H2S	0.23
INERTS (AR = 0.59% & N2 = 47.05%)	47.64
OTHERS	0.01
(CHX = 0.00%, HCN = 0.00%, NH3 = 0.01%, etc. = 0.00%)	

ZERO-D CPU TIME: 0 hours, 0 minutes, 0.189 seconds!

Distance from top	ts (K)	tg (K)	mol% H2	mol% CO2	KPa	Inches H2O
0.1828800000E+01	297.6	921.3	20.13	10.23	0.000E+00	0.000E+00
0.1808800000E+01	444.7	940.9	20.38	9.34	0.278E-01	0.112E+00
0.1788800000E+01	544.5	960.5	20.40	8.56	0.547E-01	0.220E+00
0.1768800000E+01	604.0	980.3	20.35	7.98	0.800E-01	0.322E+00
0.1748800000E+01	617.5	1002.7	20.33	7.57	0.105E+00	0.424E+00
0.1728800000E+01	666.3	1032.0	20.18	7.23	0.130E+00	0.522E+00
0.1708800000E+01	972.9	1366.9	9.25	9.79	0.155E+00	0.624E+00
0.1688800000E+01	988.9	1400.2	9.01	9.63	0.181E+00	0.727E+00
0.1668800000E+01	1047.8	1432.2	8.81	9.48	0.206E+00	0.830E+00
0.1648800000E+01	1165.9	1459.0	8.66	9.38	0.231E+00	0.929E+00
0.1628800000E+01	1225.1	1480.7	8.54	9.29	0.256E+00	0.103E+01
0.1608800000E+01	1238.4	1382.5	11.12	8.14	0.280E+00	0.112E+01
0.1588800000E+01	1256.6	1394.6	11.04	8.10	0.302E+00	0.121E+01
0.1568800000E+01	1285.0	1406.1	10.95	8.06	0.323E+00	0.130E+01
0.1548800000E+01	1314.1	1416.5	10.85	8.05	0.344E+00	0.138E+01
0.1528800000E+01	1336.1	1426.1	10.75	8.05	0.364E+00	0.146E+01
0.1508800000E+01	1351.6	1435.3	10.64	8.06	0.385E+00	0.155E+01
0.1488800000E+01	1363.0	1444.4	10.52	8.09	0.406E+00	0.163E+01
0.1468800000E+01	1371.9	1453.6	10.39	8.12	0.427E+00	0.172E+01
0.1448800000E+01	1379.3	1463.0	10.26	8.15	0.442E+00	0.178E+01
0.1428800000E+01	1385.8	1472.6	10.12	8.19	0.463E+00	0.186E+01
0.1408800000E+01	1391.9	1462.6	9.97	8.24	0.476E+00	0.191E+01
0.1388800000E+01	1397.7	1492.8	9.81	8.29	0.496E+00	0.199E+01
0.1368800000E+01	1403.5	1503.5	9.65	8.34	0.509E+00	0.205E+01
0.1348800000E+01	1409.2	1514.6	9.48	8.39	0.525E+00	0.211E+01
0.1328800000E+01	1415.0	1526.1	9.30	8.45	0.544E+00	0.219E+01
0.1308800000E+01	1420.8	1538.1	9.11	8.52	0.560E+00	0.225E+01
0.1288800000E+01	1426.7	1550.6	8.91	8.58	0.577E+00	0.232E+01
0.1268800000E+01	1432.8	1563.5	8.71	8.66	0.587E+00	0.236E+01
0.1248800000E+01	1438.9	1577.0	8.49	8.74	0.603E+00	0.242E+01
0.1228800000E+01	1445.2	1591.1	8.27	8.82	0.617E+00	0.248E+01
0.1208800000E+01	1451.5	1605.7	8.03	8.91	0.631E+00	0.254E+01

Table 5.3 Main Output File, *mb/out* (continue).

0.1188800000E+01	1458.0	1620.9	7.79	9.00	0.647E+00	0.260E+01
0.1168800000E+01	1464.7	1636.8	7.53	9.11	0.657E+00	0.264E+01
0.1148800000E+01	1471.4	1653.3	7.27	9.21	0.672E+00	0.270E+01
0.1128800000E+01	1478.3	1670.4	6.99	9.33	0.686E+00	0.276E+01
0.1108800000E+01	1485.3	1688.2	6.70	9.45	0.696E+00	0.280E+01
0.1098800000E+01	1492.5	1706.8	6.40	9.58	0.708E+00	0.285E+01
0.1068800000E+01	1499.9	1726.2	6.08	9.72	0.721E+00	0.290E+01
0.1048800000E+01	1507.4	1746.6	5.75	9.87	0.732E+00	0.294E+01
0.1028800000E+01	1515.2	1768.2	5.40	10.04	0.747E+00	0.300E+01
0.1008800000E+01	1523.4	1791.2	5.02	10.23	0.757E+00	0.304E+01
0.9888000000E+00	1531.9	1815.9	4.61	10.45	0.767E+00	0.309E+01
0.9688000000E+00	1540.8	1842.4	4.17	10.70	0.780E+00	0.314E+01
0.9488000000E+00	1550.3	1870.9	3.70	10.99	0.791E+00	0.318E+01
0.9288000000E+00	1560.3	1901.5	3.20	11.33	0.801E+00	0.322E+01
0.9088000000E+00	1570.9	1924.3	2.67	11.71	0.814E+00	0.327E+01
0.8888000000E+00	1582.2	1969.4	2.10	12.15	0.824E+00	0.331E+01
0.8688000000E+00	1594.2	2006.7	1.51	12.65	0.836E+00	0.336E+01
0.8488000000E+00	1606.6	2044.8	0.89	13.22	0.846E+00	0.340E+01
0.8288000000E+00	1617.6	2067.3	0.32	13.68	0.858E+00	0.345E+01
0.8088000000E+00	1615.7	2005.4	0.08	13.12	0.868E+00	0.349E+01
0.7888000000E+00	1597.6	1889.8	0.02	11.89	0.878E+00	0.353E+01
0.7688000000E+00	1571.6	1754.6	0.00	10.46	0.888E+00	0.357E+01
0.7488000000E+00	1540.2	1606.6	0.00	8.95	0.896E+00	0.360E+01
0.7288000000E+00	1504.0	1447.2	0.00	7.40	0.904E+00	0.364E+01
0.7088000000E+00	1462.7	1276.7	0.00	5.80	0.911E+00	0.366E+01
0.6888000000E+00	1416.4	1100.9	0.00	4.22	0.917E+00	0.369E+01
0.6688000000E+00	1363.5	917.6	0.00	2.67	0.922E+00	0.371E+01
0.6488000000E+00	1302.8	731.8	0.00	1.17	0.926E+00	0.372E+01
0.6288000000E+00	1233.8	573.8	0.00	0.00	0.929E+00	0.374E+01
0.6088000000E+00	1220.6	548.9	0.00	0.00	0.932E+00	0.375E+01
0.5888000000E+00	542.2	528.1	0.00	0.00	0.935E+00	0.376E+01
0.5688000000E+00	528.2	528.3	0.00	0.00	0.938E+00	0.377E+01
0.5488000000E+00	528.5	528.6	0.00	0.00	0.941E+00	0.378E+01
0.5288000000E+00	528.8	528.9	0.00	0.00	0.944E+00	0.379E+01
0.5088000000E+00	529.2	529.2	0.00	0.00	0.947E+00	0.381E+01
0.4888000000E+00	529.5	529.5	0.00	0.00	0.949E+00	0.382E+01
0.4688000000E+00	529.8	529.9	0.00	0.00	0.951E+00	0.383E+01
0.4488000000E+00	530.1	530.2	0.00	0.00	0.954E+00	0.384E+01
0.4288000000E+00	530.4	530.5	0.00	0.00	0.956E+00	0.385E+01
0.4088000000E+00	530.7	530.8	0.00	0.00	0.959E+00	0.386E+01
0.3888000000E+00	531.1	531.1	0.00	0.00	0.961E+00	0.386E+01
0.3688000000E+00	531.4	531.5	0.00	0.00	0.963E+00	0.387E+01
0.3488000000E+00	531.7	531.8	0.00	0.00	0.966E+00	0.388E+01
0.3288000000E+00	532.0	532.1	0.00	0.00	0.968E+00	0.389E+01
0.3088000000E+00	532.3	532.4	0.00	0.00	0.970E+00	0.390E+01
0.2888000000E+00	532.7	532.8	0.00	0.00	0.972E+00	0.391E+01
0.2688000000E+00	533.0	533.1	0.00	0.00	0.974E+00	0.392E+01
0.2488000000E+00	533.3	533.4	0.00	0.00	0.976E+00	0.392E+01
0.2288000000E+00	533.7	533.7	0.00	0.00	0.978E+00	0.393E+01
0.2088000000E+00	534.0	534.1	0.00	0.00	0.979E+00	0.394E+01
0.1888000000E+00	534.3	534.4	0.00	0.00	0.981E+00	0.394E+01
0.1688000000E+00	534.6	534.7	0.00	0.00	0.983E+00	0.395E+01
0.1488000000E+00	535.0	535.1	0.00	0.00	0.984E+00	0.396E+01
0.1288000000E+00	535.3	535.4	0.00	0.00	0.986E+00	0.397E+01
0.1088000000E+00	535.7	535.8	0.00	0.00	0.988E+00	0.397E+01
0.8880000000E-01	536.0	536.1	0.00	0.00	0.989E+00	0.398E+01



The *outa* output file contains the gas and solid mass flow rates ( $W_g$  and  $W_s$ ), gas and solid energy rates ( $W_{ghg}$  and  $W_{shs}$ ), and the right hand side of the gas and solid continuity and energy equations ( $y_{dot}$ ), gas mass flow rate ( $gasflo$ ), and the char mass flow rate ( $floch_r$ ).

The *outb* output file contains the gas and solid temperature ( $t_g$  and  $t_s$ ), the gas heat capacity ( $c_{pg}$ ), the gas mixture conductivity ( $gk$ ), the gas mixture molecular weight ( $gmw$ ), the gas mixture viscosity ( $gvisc$ ), the solid conductivity ( $sk$ ), the diffusivity of  $CO_2$  ( $difco_2$ ), the diffusivity of  $H_2$  ( $difh_2$ ), the diffusivity of  $H_2O$  ( $difn_2o$ ), and the diffusivity of  $O_2$  ( $difo_2$ ).

The *outc* output file contains the number of calls to the  $f$  routine ( $ncalls$ ), the fraction of carbon remaining in the char particle ( $cfrac$ ), the surface area of the particle ( $areap$ ), the Schmidt number for  $CO_2$ ,  $H_2$ ,  $H_2O$ , and  $O_2$  ( $sco_2$ ,  $sh_2$ ,  $sh_2o$ , and  $so_2$ ), the Reynolds number ( $re$ ), and the volumetric heterogeneous elemental reaction rate for carbon, hydrogen, nitrogen, oxygen, and sulfur ( $rc$ ,  $rh$ ,  $rn$ ,  $ro$ , and  $rs$ ).

The *outd* output file contains the film resistances for gasification and oxidation ( $frc_2$ ,  $frh_2$ ,  $frh_2o$ , and  $fro_2$ ), the ash resistances for gasification and oxidation ( $arco_2$ ,  $arh_2$ ,  $arh_2o$ , and  $aro_2$ ), and the total resistances for the  $CO_2$  and  $H_2$  gasification reactions ( $trco_2$  and  $trh_2$ ).

The *oute* output file contains the chemical resistances to gasification and oxidation ( $crco_2$ ,  $crh_2$ ,  $crh_2o$ , and  $cro_2$ ), the energy term associated with mass exchange between solid and gas phases ( $zirihi$ ), the volumetric drying rate ( $rw$ ), and the total resistance to gasification and oxidation ( $trco_2$ ,  $trh_2$ ,  $trh_2o$ , and  $tro_2$ ).

The *ouf* output file contains the overall particle diameter ( $pd$ ), the unreacted core diameter ( $pdu$ ), the dry ash-free particle burnout ( $brnout$ ), the volumetric  $H_2$  and  $H_2O$  gasification rates ( $rh_2$  and  $rh_2o$ ), the volumetric oxidation rate ( $ro_2$ ), and the total volumetric gasification and oxidation rate ( $risum$ ).

The *outg* output file contains the total enthalpy production rate for the gasification and oxidation reactions ( $CO_2$  is  $hrxn1$ ,  $H_2$  is  $hrxn2$ ,  $H_2O$  is  $hrxn3$ , and  $O_2$  is  $hrxn4$ ), the overall volumetric energy production from gasification and oxidation ( $smrhi$ ), Reynolds number ( $re$ ), Prandtl number ( $pr$ ), ratio of the solid conductivity to the gas conductivity ( $rskgk$ ), and the bed packing parameter ( $phi$ ).

The *outh* output file contains the bed-to-wall heat transfer coefficient ( $hw$ ), the gas-to-wall heat transfer coefficient ( $hwg$ ), the solid-to-wall heat transfer coefficient ( $hws$ ), the solid-to-gas heat transfer coefficient ( $hsg$ ), the solid radiation coefficient ( $hrs$ ), the void-to-void radiation coefficient ( $hrv$ ), the solid thermal conductivity ( $sk$ ), the gas mixture thermal conductivity ( $gk$ ), the effective radial gas conductivity ( $ergk$ ), the effective radial solid conductivity ( $ersk$ ), the volumetric heat transfer from the gas to the wall ( $qwg$ ), the volumetric heat transfer from the solid to the wall ( $qws$ ), and the volumetric heat transfer from the solid to the gas ( $qpg$ ).

The *outi* output file gives the concentration in mole percent of the gas phase. Only the mole percentages for the first 15 gas species in the *mb1thm* file are printed. For the example in Table 5.4, the mole percentages are for AR, CO,  $CO_2$ ,  $CH_4$ ,  $C_2H_6$ ,  $H_2$ , HCN,  $H_2O$ ,  $H_2S$ ,  $N_2$ ,  $NH_3$ , NO,  $O_2$ , OH, and  $SO_2$ .

The *outj* output file gives the solid residence time ( $stime$ ), the gas residence time ( $gtime$ ), the gas heating rate ( $gashr$ ), the solid heating rate ( $solhr$ ), the  $k$  factor ( $s2gk$ ) used in calculating the correction factor for solid-to-gas heat transfer in a reacting bed following Dzhapbyev et al. (1986), the calculated correction factor for solid-to-gas heat transfer in a reacting bed ( $fdgsg$ ) following Dzhapbyev et al. (1986), the gas velocity ( $gvel$ ), and the solid velocity ( $svel$ ).

### 5.4.3 Plotting Output Files

As discussed at the beginning of this chapter, plotting or graphics routines are not distributed with the code. However, graphics are important for understanding the code's voluminous output of data, and a recommendation for graphics output is discussed in this section.

Simple graphics can be viewed using inexpensive software available on personal computers. During development of MBED-1D, data was transferred between the SUN™ workstation and an Apple Macintosh™ by logging into the workstation with an Apple Macintosh™ using the terminal emulator VersaTerm Pro™. Output files were transferred to the Macintosh™ by using the UNIX command "cat". The output file to be plotted was concatenated to the screen and placed into the Macintosh™ clipboard by using the "• copy table" command which is located in the "Edit" menu of VersaTerm Pro™. This command is also available with other terminal emulators. The copy table command copies the columns of output with a "tab character" as the delimiter between data columns. With tabs placed between data columns, the data in the clipboard is formatted correctly to be pasted into either a spreadsheet (e. g. Excel™) or a graphics program (e. g. Cricket Graph™). The data can then be viewed with the graphics software. Data can also be plotted using packages available for the workstation. However, the choice of graphics software is left to the discretion of the user.

## 5.5 Code Operation

MBED-1D is a "user-specialist" code that requires familiarity with the theory and structure of the code in order to be used correctly and efficiently. This section gives several hints for new users. A thorough understanding of the problem physics and numerical assumptions is essential. Several iterations are required to obtain a converged solution. Presently, these iterations are done by hand to gain insight into the solution method. The iteration procedure is also discussed in this section.

### 5.5.1 Selecting Logicals

Several logical parameters can be set to run different code options. The "l0d" flag is available to let the user run either the complete one-dimensional model (see Chapter 3) or just the two-zone model (see Chapter 2). Only efficient properties are calculated when the "l0d" flag is set to "true."

The "lgaseq" flag is used to control the gas phase submodel. Two model assumptions can be made: 1) all gases in the drying and devolatilization zone are nonreactive ("lgaseq" is set to "false"), and 2) all gases in the drying and devolatilization zone, except tar, are in chemical equilibrium ("lgaseq" is set to "true"). Both these options are specifically for the two-zone model calculation. When the one-dimensional model is executed (i. e. "l0d" is set to "false"), "lgaseq" is automatically set to "true" since there is no allowance to keep all gases nonreactive in the one-dimensional portion of MBED-1D. One additional flag related to the gas phase chemistry is available when running MBED-1D, "ltareq." Setting "ltareq" to "true" causes the tar in the gas phase to react to equilibrium. If "ltareq" is set to "false," tar is assumed to be nonreactive in the gas phase.

The "lfreeb" flag is used to calculate the freeboard temperature using the freeboard heat loss which is input as "qfreeb". Heat loss is input as a negative quantity. If "lfreeb" is set to "false," the freeboard temperature is not calculated. Typical temperature drop

from the top of the coal bed to the top of the freeboard in a Wellman-Galusha reactor may be 10-20 K (Hobbs, 1990).

The "ljkstrn" flag is used to calculate the reactor heat loss based on the jacket steam flow rate which can be specified using the variable "flowjs." The heat of vaporization is calculated using the Pitzer-Chen equation (Reid and Sherwood, 1966). This equation gives acceptable results at high pressures but should be used with caution at atmospheric conditions.

The "lashcp" flag is used to specify the method of calculating the heat capacity of the ash. The complete ash composition is used if "lashcp" is set to "true." Otherwise, the correlation given by Merrick (1983) is used for the ash heat capacity.

The "lx0" flag is used to specify the potential tar-forming fraction. The potential tar-forming fraction is calculated with a semi-empirical model (Ko, et al., 1988) if "lx0" is set to "false". Otherwise, the potential tar-forming fraction is specified with the variable "usrx0."

The "lusey0" flag is used to specify the dry, ash-free functional group fractions. Actual functional group data can be used for calculations if "lusey0" is set to "true." The dry, ash-free functional group data should be entered after the "usrx0" variable. Otherwise, the functional group compositions are calculated based on a base set of eight coals. The base coal is specified with the integer flag "idev" as shown in Table 5.1.

The "lecho" flag is used to print input data to the "mblout" file. Input data are printed to the "mblout" file for verification if "lecho" is set to "true".

The "lsp" flag is used to specify the shell progressive or ash segregation char oxidation and gasification model. The shell progressive model is used if "lsp" is set to "true". Otherwise, the ash segregation model is used.

The "lstiff" flag is used to control the type of algorithm used to solve the set of first order differential equations. A stiff solver is used if "lstiff" is set to "true." Otherwise, a non-stiff solver is used to solve the differential equations. Both methods give the same results. However, the non-stiff solver is faster.

The "lstop" flag is used to terminate the integration of the differential equations when the bottom of the reactor has been reached. For example, the integrator stops at the bottom of the reactor if "lstop" is set to "true." Otherwise, the integrator continues to march past the bottom of the reactor. Either a ^C or the UNIX command KILL must be used to terminate the program when "lstop" is set to "true".

The "lout" flags control printing of output variables. Printing is enabled when the flags are set to "true". The various output files were discussed in Section 5.4.

### 5.5.2 Iteration Procedure

The two-zone, well-mixed model discussed in Chapter 2 is used to convert the split boundary value problem into an initial value problem by providing an initial estimate of the effluent gas composition and temperature. However, the gas exit temperature predicted by the two-zone model is always high due to the assumption that the devolatilization zone is at a single temperature. Likewise, the exit solid temperature is high due to the well-mixed assumption. Thus after integrating from the top to the bottom of the reactor, the calculated feed gas temperature will be higher than the input feed gas temperature. Therefore, a new exit gas temperature must be estimated which is smaller than the temperature predicted by the two-zone model discussed in Chapter 3. This procedure can be repeated in an iterative manner until the calculated feed gas temperature is equal to the input feed gas temperature. Detail on this iteration technique is given in this section.

To start a calculation, the heat loss from the reactor must be estimated. The heat loss can be estimated using the jacket steam flow rate. Using this estimate of heat loss, the effluent gas temperature and composition can be determined using the two-zone model discussed in Chapter 2. The differential equations listed in Table 3.2 are integrated from the top of the reactor to the bottom of the reactor. At the bottom of the reactor, the calculated gas temperature can be compared to the known gas temperature. If the calculated feed gas temperature is equal to the known feed gas temperature, convergence is obtained. However, the initial calculated effluent temperature using the two-zone model is expected to be high since the exit temperature is calculated by assuming the drying and devolatilization zone to be one temperature.

After the initial guess, the zero-dimensional wall heat loss can be adjusted to regress the effluent gas temperature. For these subsequent iterations, "ljkstm" is set to "true" and the overall 0-D heat loss is used as an iteration variable. Increasing the overall 0-D heat loss causes the exit temperature to decrease. An example iteration scheme is shown in Table 5.5. After the initial temperature is guessed using the two-zone model, the exit temperature is lowered by estimating the 0-D heat loss. Four iterations were required to match the calculated feed gas temperature with the "known" feed gas temperature using this method as shown in Table 5.5. The 0-D heat loss represents the heat loss necessary to lower the exit gas temperature and is significantly different than the calculated 1-D heat loss as shown in Table 5.5. The 0-D heat loss is only used as a method to iterate exit gas temperature. Measured heat loss values should be compared to the calculated 1-D heat loss values.

Table 5.5 Iteration of MBED-1D using feed gas temperature as an iteration variable

Iteration #	0-D Heat Loss, MW <sup>§</sup>	$T_{exit}^g$ , K	$T_{feed}^g$ , K <sup>‡</sup>
1	Jacket steam flow <sup>+</sup>	1030	791
2	0.80	892	403
3	0.70	906	453
4	0.69 <sup>§</sup>	907	459

<sup>§</sup> The 1-D heat loss for iteration #4 was 0.23 MW. The one-dimensional heat loss should be compared to measurements since the 0-D heat loss is used for iteration purposes only.

<sup>‡</sup> The known feed gas temperature is 460 K for this case.

<sup>+</sup> The jacket steam flow rate was used to estimate the overall heat loss which was 0.21 MW.

## **SATISFACTION GUARANTEED**

**NTIS strives to provide quality products, reliable service, and fast delivery. Please contact us for a replacement within 30 days if the item you receive is defective or if we have made an error in filling your order.**

- ▶ **E-mail: [info@ntis.gov](mailto:info@ntis.gov)**
- ▶ **Phone: 1-888-584-8332 or (703)605-6050**

# **Reproduced by NTIS**

National Technical Information Service  
Springfield, VA 22161

***This report was printed specifically for your order from nearly 3 million titles available in our collection.***

For economy and efficiency, NTIS does not maintain stock of its vast collection of technical reports. Rather, most documents are custom reproduced for each order. Documents that are not in electronic format are reproduced from master archival copies and are the best possible reproductions available.

Occasionally, older master materials may reproduce portions of documents that are not fully legible. If you have questions concerning this document or any order you have placed with NTIS, please call our Customer Service Department at (703) 605-6050.

## **About NTIS**

NTIS collects scientific, technical, engineering, and related business information – then organizes, maintains, and disseminates that information in a variety of formats – including electronic download, online access, CD-ROM, magnetic tape, diskette, multimedia, microfiche and paper.

The NTIS collection of nearly 3 million titles includes reports describing research conducted or sponsored by federal agencies and their contractors; statistical and business information; U.S. military publications; multimedia training products; computer software and electronic databases developed by federal agencies; and technical reports prepared by research organizations worldwide.

For more information about NTIS, visit our Web site at <http://www.ntis.gov>.

# **NTIS**

**Ensuring Permanent, Easy Access to  
U.S. Government Information Assets**



U.S. DEPARTMENT OF COMMERCE  
Technology Administration  
National Technical Information Service  
Springfield, VA 22161 (703) 605-6000

---