BPACK — A Computer Model Package for Boiler Reburning / Co-Firing Performance Evaluations

User's Manual, Volume I

Developed for:

U.S. DOE / PETC, AEM Italy, ENEL Italy

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AEM, Italy
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1.0 SUMMARY

This manual presents and describes a package of computer models uniquely developed for boiler thermal performance and emissions evaluations by the Energy and Environmental Research Corporation. The model package permits boiler heat transfer, fuels combustion, and pollutant emissions predictions related to a number of practical boiler operations such as fuel-switching, fuels co-firing, and reburning NO_x reductions. All computer models presented here have been applied to various process-design needs and vigorously tested against data obtained from numerous combustors ranging from bench/pilot to full-utility scales in the past several years.

Specifically, the models are adaptable to most boiler/combustor designs and can handle burner fuels in solid, liquid, gaseous, and slurried forms. The models are also capable of performing predictions for combustion applications involving gaseous-fuel reburning, and co-firing of solid/gas, liquid/gas, gas/gas, slurry/gas fuels. The outputs of the models are comprehensive and informative. Important design parameters such as heat flux distributions, attemperation flows, furnace exit temperature, unburned carbon in ash, as well as boiler thermal and NO_x reduction efficiencies are all included .

The model package is conveniently named as BPACK (Boiler Package) and consists of six computer codes, of which three of them are main computational codes and the other three are input codes. The three main codes are: (a) a two-dimensional furnace heat-transfer and combustion code; (b) a detailed chemical-kinetics code; and (c) a boiler convective passage code. The coupling of process-design information amongst the three main codes is established through input/output interfaces, and through any other available boiler data or information. The three input codes are developed to assist and guide users in preparation of model input-files, which are required to execute the three main codes.

This user's manual presents the computer model package in two volumes. Volume I describes in detail a number of topics which are of general users' interest, including the physical and chemical basis of the models, a complete description of the model applicability, options, input/output, and the default inputs. Volume II contains a detailed record of the worked examples to assist users in applying the models, and to illustrate the versatility of the codes.

The six computer codes are configured to work on IBM or IBM-compatible personal computers (PC). Each code occupies computer memory size ranging from 300 to 500 kilobytes. The execution-time of a specific code varies from several minutes to several hours for a typical case running on a 20 MHz /386 PC.

2.0 INTRODUCTION

In recent years rapidly growing concerns about the quality of the global environment have imposed a considerable pressure on industry to reduce all forms of pollutant emissions. Industrialized countries have many existing environmental regulations which set different emissions limits for fossil-fuel-fired power plants. In the U.S., future emission levels are expected to be heavily regulated by the recent legislation: Title IV of the Clean Air Act Amendments. It is foreseeable that similar trends in legislation will take place not only at the federal level, but also at State and local government levels. The same legislative trends are also prevalent in members of the European Community (EC), with a common goal to protect our environment.

To respond to the environmental concerns, engineers have been developing many new practices and processes which are aimed to reduce emissions. The development of the new boiler processes, augmented by the advance of numerical techniques and computer technology and improved understanding of fuel combustion mechanisms, has stimulated significant needs and progress in the modeling of boilers. Energy and Environmental Research Corporation (EER) has invested considerable resources in the development, validation, and application of engineering computer models over the last decade. Through continued research and understanding gained in applying them to practical situations, use of these models has been established as a reliable and cost-effective method for boiler process designs.

Background

Azienda Energetica Municipale (AEM) in Milano, Italy, was engaged in a Gas Reburning-Sorbent Injection (GR-SI) boiler process modification program to reduce emissions of NO_x and SO_2 from utility boilers. Through arrangement with the U.S. Department of Energy (DOE) in Washington, EER had conducted a process design study for the application of GR-SI technologies to a boiler located at the Cassano d'Adda Power Plant in Milan, Italy.

EER has been involved in the development and commercialization of the GR-SI technologies and is currently involved in a demonstration program on three coal-fired utility boilers in the U.S.. The GR-SI retrofit at one host unit (Illinois Power's Hennepin Station) is in operation since January 1991. Earlier test data based on short-term runs had shown that the reduction in NO_x and SO_2 emissions was in excess of the original design. EER is currently carrying out long-term load-following tests to confirm the performance under normal utility service conditions.

Recently, AEM Milano, Ente Nazionale per l'Energia Elettrica (ENEL, Italy's electricity board), and the U.S. DOE/PETC (Pittsburgh Energy Technology Center) have jointly expressed a desire to acquire a computational capability for the purpose of evaluating boiler reburning process applications and performance implications. In current reburning design and performance evaluation studies EER uses a suite of computational models, physical isothermal models, and engineering analysis techniques. The computational models have been developed primarily as in-house engineering and design tools, consequently these models are not configured for easy use by the uninitiated.

Program Objective

The overall objective of this program was to integrate EER's expertise in boiler reburning performance evaluation into a package of analytical computer tools. Specific objectives of the program were to develop a computational capability with the following features:

- can be used to predict the impact of gas reburning application on thermal conditions in the boiler radiant furnace, and on overall boiler performance.
- can estimate gas reburning NO_x reduction effectiveness based on specific reburning configurations and furnace/boiler configurations.
- can be used as an analytical tool to evaluate the impact of boiler process parameters (e.g., fuel switching and changes in boiler operating conditions) on boiler thermal performance.
- is adaptable to most boiler designs (tangential and wall fire boilers) and a variety of fuels (solid, liquid, gaseous and slurried fuels).
- is sufficiently user friendly to be exercisable by engineers with a reasonable knowledge of boilers, and with reasonable computer skills. Here, "user friendly" means that the user will be guided by computer codes during the course of setting up individual input files for the boiler performance model.

Approach

The approach to the development of the reburning boiler process model was through the modification, development, and integration of EER's current reburning system sub-models. As with any comprehensive engineering computer models, the reburning sub-models occupy a substantial amount of computer memory and usually require a list of inputs to describe the complex boiler environment. These sub-models were considered to be too unwieldy to be directly incorporated into a single generalized design/evaluation procedure. As an alternative, the approach was to package these sub-models into three main analytical tools, namely, a furnace heat transfer model, a reburning NO_x model, and a boiler performance model. The coupling of process design information amongst the three sub-models was established through input/output interfaces, and through the use of boiler design data and any available field measurements.

Computer Codes Delivered

The execution of the program has resulted in the development and delivery of six computer codes. These computer codes are packaged and conveniently named as BPACK (i.e., Boiler Package) here. As already mentioned, the six computer codes consist of three main codes, and three input codes. The three main codes and their individual roles are briefly introduced in the following:

- The 2D Furnace Heat Transfer Code (2DHT)

The purpose of the furnace heat transfer code is to provide engineers with a computational tool to model the high-temperature boiler radiant-furnaces. To achieve this objective, EER's existing 2D furnace heat transfer code was modified for most boiler designs, firing configurations, as well as different fuels. Specifically, the 2DHT code were set up for treatment of tangential and wall fired boilers, and adapted to solid, liquid, gaseous and slurried fuels. In addition, the code was incorporated with the ability to

describe gaseous reburning fuel injection, overfire air injection, flue gas recirculation, and the use of fuel-oil atomizing steams.

- The Reburning NO_x Code (RBNO_x)

The purpose of the reburning NO_x code is to provide reasonable working estimates for the expected NO_x reduction potential as a function of the major boiler process controlling parameters. The boiler process parameters include furnace gas temperature profiles and residence time distributions, local stoichiometries up- and down-stream of the reburning fuel injection zone, reburn fuel and overfire air local mixing rates, and injection locations.

The reburning NO_x code, RBNO_x, is a development of EER's detailed chemical-kinetics code. This code takes account of boiler operating conditions with the consideration of reburning zone injection temperature, stoichiometry, flue gas quench rates and residence times. The code assumes that mixing of both reburning fuel and overfire air is adequate so that bulk mixing rates of the injected jets can be represented by characteristic mixing times.

The code is coupled with the outputs of the furnace heat transfer code 2DHT, which in turn incorporates the input of boiler-specific information such as temperature gradients and gas residence times. The RBNO_x code predicts NO_x emissions for a specific set of boiler input and reburning conditions, so that the user can evaluate NO_x reduction potentials associated with the assumed operating conditions.

- The Boiler Performance Code (BPM)

The purpose of the boiler performance code, BPM, is to calculate steam- and gas-side heat balance for boiler sections that are not included in the domain of the 2DHT code, such as the backpass convective section and air preheater. To achieve this objective, EER's existing boiler code was modified in responding to any changes made in the 2DHT code to ensure mutual consistency.

The BPM code is coupled with the outputs of the furnace heat transfer code 2DHT, which in turn incorporates the input of boiler-specific information such as heat fluxes and gas temperatures. The BPM code predicts steam and gas side properties such as steam temperature, flow rates, and attemperation flows for a specific set of boiler input and reburning conditions. The user can evaluate boiler thermal efficiencies associated with the assumed operating conditions.

In conjunction with the development of the three main codes, efforts were also focus on the development of the three input codes. The three input codes are:

- The Furnace Heat-Transfer Input Code (2DINPT)
- The Reburning NO_x Input Code (RBINPT)
- The Boiler Performance Input Code (BPINPT).

Each of the three main codes requires an input file to execute. The purpose of the input codes is to help the user in the preparation of the input files. The input codes guide the user stepwise through the necessary input routines, and is provided with default values for certain key parameters. The input codes can also be used by the user to update key model inputs for cases defined.

Presentation Format

This user's manual attempts to provide self-contained information needed for the execution of the computer codes. Numerical background is not required in order to exercise the computer model package. However, due to the complexity of actual boiler environment and operations, the manual assumes the user has a modest prior knowledge of fuels combustion and practical boiler operations. The user will use this knowledge mostly in preparing the input files, so that his specific boiler configurations and operating conditions are correctly set up.

In Volume I, Chapter 3 discusses the computer hardware requirements for running the models. Chapter 4 describes the background and the execution of the three main codes in detail. Chapter 5 deals with the preparation of the input files for the three main codes. Input parameters are discussed item by item, and recommended and default values are given whenever possible. The outputs from the three main codes are described in tabulated formats in Chapter 6. Chapter 7 lists references in general, and the user may consult with the references for particular topics that he is interested in.

Volume II documents five worked examples and contains six chapters. In Chapter 1, the five example-cases are defined in terms of boiler type, fuels used, and any other specific applications such as reburning. The five worked examples are documented in Chapters 2 through 6, respectively. In each example-case, the input sessions which apply one of the three input codes are recorded step-by-step. The output files generated by the input and the main codes are also shown for each example-case.

3.0 CODE EXECUTION

The six computer codes included in the BPACK were tested and configured to work on IBM or IBM-compatible personal computers (PC). Later chapters will describe in detail procedures of executing each of the six codes. This chapter concentrates on the computer hardware needed to exercise the BAPCK.

The choice of PC for configuring the BPACK has many advantages, among which are the following :

- Computational time is essentially free, while initial capital investment is at a minimum.
- PC provides the level of numerical accuracy required by the BPACK codes. Their calculational speeds have become respectable and equivalent to many high-performance work stations, and are still being improved.
- The BPACK codes can be placed in a "laptop" or even "notebook" computers. A boiler engineers can carry this modeling package with him in the field for his special modeling purposes.

Hardware Requirement

The BAPCK needs little special-computer-hardware to execute. In these days, it may be safe to say that almost any PC can be used, or easily upgraded with a minimum cost, to carry out the boiler modeling tasks with the BPACK. The user only has to make sure that his computer has the following characteristics:

- The speed of the PC is equal or faster than IBM/AT type of machines (e.g., 286 or 386 series).
- The PC has a mathematical co-processor.
- A minimum of 5 megabytes (MB) of hard-disk space is available.
- The PC has a 5 1/4" floppy disk drive.

The six computer codes occupies a total of 2.29 MB of memory space. The following lists the memory-space requirement for each of the computer codes:

<u>Code name</u>	<u>Size (kilobytes)</u>
2DINPT	420
2DHT	472
RBINPT	242
RBNOX	496
BPINPT	282
BPM	382
Total	2.29 MB

Additional memory space is required for storage of input/output files and other necessary data such as a thermodynamic file for the execution of the RBNOX code. For a "typical" boiler reburning case, a total of 500 KB is required for the input/output file operations. Therefore, the suggested 5 MB memory would be sufficient for at least five boiler cases, deducted by the 2.29 MB memory space taken by the six computer codes. However, the user should keep in mind that the above estimates are based on default

output options. If the user selects another option for more detailed outputs, the size of the output files may increase substantially and more than 5 MB of hard disk space may be required. Of course, the user can always back up his input/output files on floppies and free the hard-disk space for new boiler cases.

The BPACK computer codes are delivered in six 5 1/4", high density floppy disks. Each floppy comprises one particular code mentioned above. The executable codes were compiled with some compiler options specifically designed for PC/AT (or newer) type of machines, therefore, earlier PC/XT machines are not recommended for use.

Execution Time

The execution time of the three main codes varies from several minutes to several hours, depending on the code used and the speed of the user's PC. For a 386/20 MHz PC, nominal code execution time is summarized as below:

<u>Code name</u>	<u>Execution time</u>
2DHT	3 hours 30 minutes
RBNOX	45 minutes
BPM	4 minutes

Again, it should be mentioned that the time estimates are based on "typical" model set-ups. For example, the time listed for the 2DHT code is based on 100 iterations of furnace energy-balance calculations. Depending on the user's selection on many other input parameters, the code execution time could be doubled or halved, compared to the time listed above.

The execution time of the three input codes (i.e., 2DINPT, RBINPT, BPINPT) depends largely on the user's proficiency levels in using the input codes, and on the completeness of his boiler data preparations. Data preparation-time using the RBINPT code is least among the three input codes. If all input data are readily available, interactive sessions using the 2DINPT and the BPINPT codes normally can be completed within a hour, for an experienced user. For an un-informed or new user, it is suggested that the user takes the time required for his own pace, such that the inputs are correctly set up. The new user usually will find that after using the input codes for two or three times, he is ready to carry out many practical boiler modeling applications.

4.0 DESCRIPTION OF MAIN CODES

This chapter describes the use of the three main computer codes: the 2DHT, the RBNOX, and the BPM codes, which have been introduced briefly up to this point. The description of their associated input codes, namely the 2DINPT, the RBINPT, and the BPINPT codes, is rendered to Chapter 5.

2DHT is a Two-Dimensional Heat Transfer code for boiler thermal performance evaluations. The code has a sophisticated submodel for radiative heat exchange calculations in boiler environment. The 2DHT code also has submodels to handle coal devolatilization, as well as char and fuels (gas, liquid, volatiles) combustion. Other unique features of the code include: (a) Direct coupling of upper-furnace radiant-heat-exchangers with the lower-furnace flame zones in the heat exchange calculations; (b) The ability to handle complicated boundary conditions as usually occur in large-scale utility boilers or combustors, such as ash deposition and wall emissivity changes. The code is decouple from the solution of the momentum conservation equations, consequently, flow field information is prescribed by the user. Section 4.1 discusses more details of the code.

RBNOX is a Reburning NO_x code for boiler reburning NO_x predictions. The code solves coupled ordinary differential equations deduced from detailed chemical kinetics mechanisms. The RBNOX code in its current form describes fuels-combustion and NO_x formation/reduction in terms of 43 chemical species and 201 elementary reactions. Boiler reburning NO_x application is modeled by four plug flow reactors connected in series. More details of the RBNOX code can be found in Section 4.2.

BPM is a Boiler Performance Model for calculation of boiler steam and flue-gas properties. This code is mainly applied to the boiler backpass, which is not covered by the 2DHT code's solution domain. The BPM code predicts important boiler operational parameters such as attemperation flow rates and steam temperatures. Section 4.3 discusses the code in more detail.

The description of each of the main code in Sections 4.1 to 4.3 follows a similar presentation format. Firstly, general background of a specific code such as its capabilities/limitations and input/output file managements are presented. The description then moves on to subjects of physical model descriptions, with particular emphases on information that may facilitate the user's proficiency and comfort levels when he applies the codes.

All the main codes use a consistent way of naming the input/output files. Figure 4.1 shows an overview of the file management structure. The default output file names are termed as 2DOTcsvs.lll, RBOTcsvs.lll, and BPOTcsvs.lll, where cs is an user specified case number, vs is an user specified version number, and lll is a character string extracted from an user specified parameter describing the boiler load. For example, if cs is 01, vs is 02, and the specified boiler load is 66.0 % relative to the boiler's maximum continuous rating (MCR), the default output file name from the 2DHT code will be 2DOT0102.066. Likewise, the other two default output file names are RBOT0102.066 and BPOT0102.066. The characters "OT" denotes the "outputs" of the main codes. The user can overwrite the default output file names during the interactive input-sessions.

The default input file names are fixed, and are designated as 2DINPT.DAT, RBINPT.DAT, and BPINPT.DAT respectively for the three main codes. This means that if the user want to run a specific main code with a specific input file, for example, run the 2DHT code with an input file 2DIN0102.066, he has to copy file 2DIN0102.066 to file 2DINPT.DAT before he executes the 2DHT code. The same

Figure 4.1. File management structure for main codes.

convention applies to the main codes RBNOX and BPM. The objective of this file naming convention is to prevent accidental overwriting of the input files created by earlier user applications.

4.1 2D Furnace Heat Transfer Model (2DHT)

The Two-Dimensional Heat Transfer Code (2DHT) is a general purpose code developed for boiler and combustor thermal performance predictions. 2DHT is configured to work on IBM or IBM-compatible personal computers. The code occupies a memory size approximately at 475 kilobytes (KB).

The 2DHT code can handle gas-, liquid-, and solid- fuel fired furnaces with over- and/or under- fired air injections. The 2DHT code also has built-in submodels to simulate gaseous fuel reburning or co-firing. One unique features of the code is that direct radiative-heat-transfer coupling is performed between the lower-furnace flame zone and the upper-furnace radiant heat exchangers.

2DHT solves mass and energy conservation equations except the momentum equations. Flow field are user prescribed. The decouple flow-field prescription can be carried out based on data from isothermal physical model, past modeling experience and engineering judgement, or results from computational fluid dynamics. The prescription of the flow field includes flow components such as turbulence and flow recirculation, and is based on mass fluxes normalized by the total furnace mass input. Details of the flow field prescription are discussed in Section 5.1.

The output from the 2D furnace code is quite informative. Table 4.1 summarizes the 2DHT output information. The model provides information on boiler overall performance, as well as information on species concentrations, temperatures, and heat flux profiles in one- or two-dimensional formats.

Table 4.1. Summary of 2D Furnace Heat Transfer Code Output Information.

Overall Furnace Performance Parameters

- Furnace exit temperature
- Furnace thermal efficiency
- Heat absorption by waterwall and radiant tube banks
- Unburned carbon in ash

One Dimensional Profiles

- Furnace wall (i.e., deposit surface) temperature
- Furnace wall heat flux

Two Dimensional Profiles

- Concentrations of combustion species (CO_2 , H_2O , N_2 , O_2 , volatile, SO_2 , unburned carbon, ash)
- Combustion gas temperature
- Combustion gas radiant heat absorption/emission
- Volatile heat release rate
- Convective, radiative, and total heat absorptions by the upper furnace tube banks

In the following, the execution and the physical background of the 2DHT model components will be presented. The presentation of the model background is further divided into four sub-sections, and starts from a sub-section dealing with 2D furnace zoning. The second sub-section describes a furnace heat transfer model which constitutes the corner stone of the 2DHT code. The description then continues to a model which describes total heat balance for furnace volume and surface zones. The last sub-section describes various combustion modules used in the simulation of coal devolatilization, char oxidation, volatile and fuels combustion, and soot formation.

File Management

The default input file name for the 2DHT code is 2DINPT.DAT. The default output file name from the 2DHT code is 2DOTcsvs.lll, where cs is an user specified case number, vs is an user specified version number, and lll is a character string extracted from an user specified parameter describing the boiler load. For example, if cs is 01, vs is 02, and the specified boiler load is 95.0 % relative to the MCR, the default output file name will be 2DOT0102.095. The user can overwrite the default output file name. However, the default input file name is always fixed as 2DINPT.DAT. This means that if the user wants to execute the 2DHT code with an input file, say 2DIN0102.095, he has to copy that file to file 2DINPT.DAT first. The objective of this file structure is to prevent accidental overwriting of the input file.

The coupling among the furnace code (2DHT), the reburning NO_x code (RBNOX), and the boiler performance code (BPM), is through the output data-files BOILER.DAT and REBURN.DAT, which are generated by the 2DHT code. The file REBURN.DAT comprises furnace data required by the RBNOX

code, while the file BOILER.DAT contains furnace information required by the BPM code. These two files are over-written every time 2DHT code is executed. Therefore, the user is advised to save copies of them under different file names.

Code Execution

To execute the 2DHT code, the user has to do the following:

- Install 2DHT.EXE in the working directory
- Copy the input data file to file 2DINPT.DAT
- Type 2DHT and press "Enter".

The input data file is the one which contains the data of the boiler to be modeled. This data file should be prepared by executing the input code 2DINPT. 2DINPT.DAT is the input file name used by the 2DHT code, therefore, furnace modeling will be performed based on the contents of the file 2DINPT.DAT. The user must copy the contents of his input data file to file 2DINPT.DAT before executing the furnace code 2DHT.

2D Zoning

The 2D furnace heat transfer model is based on zone method of analysis. The furnace volume is divided into a number of volume zones, which are also referred to as gas zones or control volumes. Within each volume zone, furnace variables such as gas temperatures and compositions are assumed to be uniform. A typical 2D zone-arrangement for an axi-symmetric furnace enclosure is shown in Figure 4.2.

2DHT uses a cylindrical coordinate system as shown in Figure 4.2. The axial coordinate is denoted by X and the radial coordinate by Y. The origin of the coordinate frame is positioned on the bottom of the furnace center (or axi-symmetric) plane. The 2D zone-arrangement also creates four sides of surface (or boundary) zones, which are indicated in Figure 4.2 by symbols as M=1, 2, 3, and 4. Detailed discussions on the surface zones are presented in later sub-sections.

The volumes zones are concentrically arranged around the furnace axis, and they have rectangular cross-sections in the X-Y planes. Note that the zoning is linear and orthogonal with respect to the X-Y planes. However, the thickness of the zone-layers in both the X- and the Y- directions may vary from layer to layer. Each volume zone is identified by a pair of indices, namely, an index I in the (axial) X-direction and an index J in the (radial) Y-direction. These indices are counted from the origin of the X-Y coordinate system toward the positive X- and Y-directions, starting from I=1 and J=1. Thus, the center of the bottom zone-layer in the X-direction (Layer I=1) has indices I=1 and J=1.

The maximum numbers of volume zone layers in the X- and Y-directions are denoted by NX and NY, respectively. The current version of 2DHT limits the maximum numbers of NX to 30, and NY to 10. Note that the code can handle steps in the zoning as shown in Figure 4.2. This is useful for simulation of boiler sections which have smaller cross-sections than that of the furnace (for instance, the ash hopper and the furnace nose sections). However, for program logistic reasons, the steps in the zoning must be arranged in such a way that the furnace enclosure as seen from the inside is always concave.

The code recognizes the zoning steps through four arrays denoted by IMAX(J), IMIN(J), JMAX(I) and JMIN(I). These arrays store the maximum and the minimum I and J indices, where J ranges from 1 to NY and I ranges from 1 to NX. Note that the minimum J-Index at each I zone-layers, JMIN(I), have the value of 1. Cases in which JMIN(I) is larger than 1 have not yet been tested and should be avoided.

The furnace zones described above represent control volumes or surfaces, in which volume (e.g., gas temperatures) and surface (e.g., heat fluxes) variables are to be calculated based on mass and energy balances. The volume-zone variables are treated in a number of arrays, with I and J as indices. For instance, the volume-zone gas temperatures are represented by T(I,J). The treatment of the surface variables is more complicated. The surface (or boundary) zones are grouped into four sections, each assigned by an index M with it's value ranging from 1 to 4.

Surface zones of section M=1 are those with normals in the positive X-direction. Surface zones of section M=3 are those with normals in the negative X-direction. Similarly, surface zones with index M=2 are those with normals in the positive Y-direction, and zones with index M=4 are surface zones with normals in the negative Y-direction. Surface variables, such as the surface temperatures TW, are indexed as TW(J,M) for the M=1 and M=3 sections and as TW(I,M) for the M=2 or M=4 sections. Note that surface zones on M=2 are actually the furnace axis, and they have zero surface area under the 2D zone arrangement.

There are other variables associated with the specification of the zone arrangement. These variables are:

X(I)	→ X co-ordinate of zone layer I (m)
Y(J)	→ Y co-ordinate of zone layer J (m)
DX(I)	→ Thickness of zone layer I in the X-direction (m)
DY(J)	→ Thickness of zone layer J in the Y-direction (m)
DV(I,J)	→ Volume of zone I,J (m ³)
DF(*,M)	→ Area of surface zone * on section M (m ²)

* refers to I or J, as described above.

Furnace Heat Transfer Model

The furnace heat transfer model is a core part of the 2DHT code. The model simulates the various heat transfer processes, including thermal radiation and convection, occurred in/on each of the volume and surface zones. The description of this model includes the following topics:

- A "semi-stochastic" beam-tracking method used for radiative heat exchange calculations.
- Simulation of radiant heat exchangers.
- Total radiative heat balances for the volume and the surface zones.
- Radiative property modules to describe non-gray gas radiation, and combustion generated particulates such as char, soot, and ash.

Radiative exchange sub-model — A key part of the 2D furnace heat transfer model is the sub-model for calculating the multi-directional radiative heat exchanges among all volume and surface zones. This sub-model is derived from the conventional Monte-Carlo technique. The following sub-sections describe the essence of the radiative exchange sub-model. The description assumes that the gas is gray, although the furnace code actually considers non-gray radiation as will be explained later.

Assuming that the following volume and surface zone variables are known, either from initial guesses or from a previous iteration:

- volume zone temperatures $T(I,J)$ (K)
- gray gas absorption coefficient $AK(I,J)$ (1/m)
- surface zone temperatures $TW(*,M)$ (K)
- surface zone emissivities $EW(*,M)$ (-)

Total emission from a volume zone can be expressed as:

$$EM(I,J) = 4 \cdot AK(I,J) \cdot DV(I,J) \cdot SIGMA \cdot T(I,J)^4 \quad (4.1)$$

where $SIGMA$ is the Stefan-Boltzmann constant ($5.67E-11$ kW/m² K⁴). Part of this emitted radiation is re-absorbed by the emitting volume zone itself. The magnitude of this self-absorption is initially unknown, but is calculated by the radiative exchange model.

The emission of a surface or boundary zone is expressed by:

$$EM(*,M) = EW(*,M) \cdot F(*,M) \cdot SIGMA \cdot TW(*,M)^4 \quad (4.2)$$

The objective of the radiative exchange submodel is to determine how much of the radiation emitted, as shown in equations (4.1) and (4.2), is re-absorbed by the various volume and surface zones. For this purpose, the emissive power of each of the furnace zones are distributed in the model by a discrete number of beams. Each beam is tracked till it's intensity is smaller than a very small tolerance. Absorption of the beams is calculated according to the Beer's law and also to the geometry of zone-beam interceptions. This subject will be described in detail later on. Simulation of isotropic volume-zone emissions using a discrete number of energy beams is described below.

The first step is to decide how many beams are emitted by each of the volume zones. For this purpose, a volume zone is further subdivided into "cells" as shown in Figure 4.3. The extension (or thickness) of a cell in the X-direction is denoted by $DDX(I)$, and in the Y-direction by $DDY(J)$. The number of cells in the X-direction is given by $NNX(I)$ and in the Y-direction by $NNY(J)$. The extensions and numbers of the cells are automatically calculated by the 2DHT code based on an input parameter, $NMAX$. $NMAX$ is the number of subdivisions on the largest extension of a volume zone either in the X- or the Y-direction:

$$NMAX = [DX(I)]_{max} / DDX(I) \text{ or } NMAX = [DY(J)]_{max} / DDY(J) \quad (4.3)$$

$DDX(I)$ and $DDY(J)$ are determined in a way that they are as uniform as possible for a given zone arrangement and $NMAX$.

Based on the above definition, the radiative energy emitted from each volume cell per unit solid angle is:

$$EO = (1. / (4\pi)) \cdot (YS0 / Y(J)) \cdot EM(I,J) / (NNX(I) \cdot NNY(J)) \quad (4.4)$$

where YS0 is the center Y co-ordinate of the cell. The 2D code actually uses a division of 2π in equation (4.4) instead of 4π . Therefore, only beams emerging into one half of the furnace are tracked.

The second step of the discretization procedure is to determine the direction and the energy flux of each beam emerging from each volume cell. The direction of a beam is determined with the help of two angles: the polar angle PHIS, and the azimuthal angle PSIS. The orientation of these angles with respect to the volume zone coordinate system is shown in Figure 4.4. Since the volume emission is isotropic, the energy flux through the surface of an imaginary sphere surrounding the emitting volume element should be as uniform as possible. This is achieved by discretization of the solid angle 4π using the following technique.

The polar angle PHIS which ranges from zero to π , is evenly subdivided into NPHI sections resulting in arc lengths of DPHI. NPHI is an user input parameter and should always be an even, positive number (e.g. 2, or 4, etc.). The sub-division of the azimuthal angle PSIS is automatically performed by the code, resulting in NPSI(L) sections with arc lengths DPSI(L), where L starts from 1 and ends at NPHI. The discretization of the solid angle is then expressed by equation (4.5):

$$DRW(L) = 2\pi * (\cos(PHIS - DPHIH) - \cos(PHIS + DPHIH)) / NPSI(L) \quad (4.5)$$

where DWR(L) is a solid-angle element (i.e. a surface element of the imaginary sphere with radius 1) and DPHIH stands for DPHIS/2.

Figure 4.5 shows an example for the sub-division of the imaginary sphere into solid angle elements of NPHI=4. The view presented in Figure 4.5 is towards the "north pole" of the sphere. Note that the dots in the center of the elements represent beam directions starting from the center of the sphere. The number of beams starting from the center of the sphere is a unique function of a given NPHI. The relationship between NPHI, NPSI(L) and the number of beams emitting from a volume cell is tabulated in Table 4.2.

Table 4.2. Relationship Among NPHI, NPSI(L), and Volume-Zone Beam Numbers.

NPHI	Value of NPSI(L) where L = 1 to NPHI/2	Number of Beams Starting From a Volume Cell
2	4	8
4	4,8	24
6	4,12,12	56
8	4,12,16,16	96
10	4,12,16,20,20	144
12	4,12,16,20,24,24	200
14	4,12,16,20,24,28,28	264
16	4,12,16,14,18,32,32,32	360
18	4,12,16,24,28,32,36,36,36	448
20	4,12,16,24,28,32,36,40,40,40	544

Figure 4.4. Definition of angles $PHIS$ and $PSIS$ with respect to volume-zone-orientated coordinate-frame X^* , Y^* , and θ^* .

Figure 4.5. Sub-division of unit-sphere into solid angle elements $DRW(L)$ when $N\Phi=4$ (Dots indicate centers of the elements).

Equation (4.5) generates the most uniform beam distribution for a given NPHI. It also ensures conservation of the energy flux from a volume cell, when the energy fluxes from all beams are added up over the polar angle between zero and π , and over the azimuthal angle between zero and 2π . The initial energy flux (in KW) of a beam from a volume cell is calculated according to Equation (4.6):

$$ES0 = E0 * DRW(L) \quad (4.6)$$

where E0 is the energy flux per solid angle expressed by equation (4.4).

Although the volume cells are ring-shaped, the starting points of all beams from a cell fall into the plane spanned by the X-Y coordinate frame. The code blurs the starting points and the directions of a beam with the use of random numbers.

The distribution of the surface radiative-energy follows the same principles. The surface zones are assumed to follow the ideal Lambert's rule, i.e., the energy fluxes are distributed over a hemisphere of solid angle 2π according to the Cosine Law. Surface zones are sub-divided into surface cells with their geometric parameters (NNY(J), DDY(J) or NNX(I), DDX(I)) determined from the adjacent volume zones. Equations (4.7a) and (4.7b) express the radiative energy fluxes per unit solid angle from surface cells of M=1 to M=4:

$$E0 = (\cos(\text{PHIS}) / \pi) * EM(I, M) * (YS0 / Y(J)) / NNY(J) \quad \text{for } M=1 \text{ or } 3 \quad (4.7a)$$

$$E0 = (\cos(\text{PHIS}) / \pi) * EM(J, M) * YS0 / NNX(I) \quad \text{for } M=2 \text{ or } 4 \quad (4.7b)$$

where PHI is the polar angle with respect to a surface orientated coordinate frame and YS0 is the radial coordinate of the center of the surface cell.

The beams emitting from a surface cell are again distributed in a way that, the highest uniformity over a hemisphere of solid angle 2π is achieved for a given NPHI. The direction of the beams are determined in terms of the polar (PHIS) and the azimuthal (PSIS) angles, with respect to the surface-orientated coordinate frames as shown in Figure 4.6, for sections M=1, M=3 and M=4. The M=2 section was omitted because the surface areas of this section are zero in 2D applications.

The discretization of the solid angle is expressed by:

$$\begin{aligned} CDRW(L) / \cos(\text{PHIS}) = & (\pi / \cos(\text{PHIS})) * ((\sin(\text{PHIS} + \text{DPHIH}))^2 \\ & - (\sin(\text{PHIS} - \text{DPHIH}))^2) / \text{NPSI}(L) \end{aligned} \quad (4.8)$$

where CDRW(L) represents the solid-angle element times $\cos(\text{PHI})$, and DPHIH stands for $\text{DPHIS} / 2$. Thus, the initial energy flux for beams emerging from surface cells is:

$$ES0 = E0 * CDRW(L) / \cos(\text{PHIS}) \quad (4.9)$$

where E0 is the energy flux associated with an unit of solid-angle given by equations (4.7a) or (4.7b).

Although the surface cells are ring-shaped, the starting points of all beams from a surface cell fall into the plane spanned by the X-Y coordinate frame. As it was the case for emissions from volume cells, the starting points and beam directions are blurred by the use of random numbers. The blurring is carried out

to reduce systematical errors when radiative heat fluxes are calculated from coarse zone arrangements, and to reduce the number of beam numbers used. Although this blurring increases the statistical variations of local heat flux distributions, it has been shown that a gain in overall numerical accuracy can be achieved.

The blurring is achieved by the following means. For radiation from volume cells, the reference coordinate frame, in which the beam directions (PHIS and PSIS) are originally determined, is randomly rotated around the theta axis (see Figure 4.4) of the furnace coordinate system. The angle of rotation, PHIR, is calculated according to:

$$PHIR = RUDRAN(0., 2\pi) \quad (4.10)$$

where RUDRAN is a random number generator which produces normalized random numbers within the range of 0. and 2π . The blurring of the beam directions, within an increment DPSI(L) of the azimuthal angle, is achieved by setting:

$$PSIS = PSIS + RUDRAN(-DPSIH, +DPSIH) \quad (4.11)$$

where RUDRAN produces normalized random numbers within the range of $-DPSI(L)/2$ and $+DPSI(L)/2$. Equation (4.11) applies to beams from both the volume and surface cells.

The blurring of beam directions starting from surface cells, over an increment DPHI of the polar angle, is carried out by the following means:

$$PHIS = PHIS + RUDRAN(-DPHIH, +DPHIH) \quad (4.12)$$

where RUDRAN produces normalized random numbers within the range $-DPHI/2$. and $+DPHI/2$.

The random displacement of beam-starting-points in the X-direction, is described by:

$$XS = RUDRAN(XS0-DDX(I)/2., XS0+DDX(I)/2.) \quad (4.13)$$

where XS0 is the center of the cell in the axial direction. The equation applies to beams from volume cells and surface cells on sections M=2 and M=4. The random displacement of beam-starting-points in the Y-direction is expressed by:

$$YS = \text{SQRT}(YSN^2 + RUDRAN(0., 1.) * (YSP^2 - YSN^2)) \quad (4.14)$$

where YSN represents $(YS0-DDY(J)/2.)$ and YSP equals to $YS0+DDY(J)/2.$ YS0 is the center of the cell in the radial direction. RUDRAN(0.,1.) produces normalized random numbers between zero and 1. Equation (4.14) takes into account the fact that the probabilities for beams to start from the outer radii are higher. The equation applies to beams from volume cells and surface cells on sections M=1 and M=3.

Beam tracking — The directions of beams calculated in terms of PHIS and PSIS are initially related to a coordinate system which is orientated at the cells (or zones). The actual beam tracking and directional calculations are carried out under the spatially-fixed furnace-orientated X-Y coordinate frame. To

determine the beam directions (PHI and PSI) in the furnace coordinate system, coordinate transformations are performed according to:

$$PHI = ACOS (COS (PHIR) *COS (PHIS) -SIN (PHIR) *SIN (PHIS) *SIN (PSIS)) \quad (4.15a)$$

$$PSI = PSIR+ATAN2 [(COS (PHIR) *SIN (PHIS) *SIN (PSIS) +SIN (PHIR) *COS (PHIS)) / (SIN (PHIS) *COS (PSIS))] \quad (4.15b)$$

Although already mentioned briefly, the meanings of the various angles are repeated here (see also Figures 4.4 and 4.6) :

PHI		Polar angle in furnace-orientated coordinate frame
PSI		Azimuthal angle in furnace-orientated coordinate frame
PHIS		Polar angle in cell-orientated coordinate frame
PSIS		Azimuthal angle in cell-orientated coordinate frame
PHIR		Rotation of cell-orientated coordinate frame around Theta axis of furnace-orientated coordinate frame
PSIR		Rotation of cell-orientated coordinate frame around Y-axis of furnace-orientated coordinate frame

In brief, the radiative energy emitted by every volume or surface zone is distributed into a discrete and well-defined number of beams. The initial energy flux associated with a beam, ES_0 , is calculated by equations (4.6) or (4.9). All beams start from the plane formed by the X- and the Y- axes of the furnace orientated coordinate frame. The starting coordinates in this plane are XS and YS . The initial directions of the beams are described by the angles PHI and PSI . Due to symmetry considerations, only beams with azimuthal angle $\pi/2 < PSI < (3/2)\pi$ are actually tracked.

Neglecting scattering, a beam will follow a straight path from the starting point until it encounters a surface zone. Contrary to pure Monte-Carlo methods, the gradual attenuation of the beam's initial energy flux ES_0 is calculated deterministically. It is assumed that the attenuation of a beam along its path follows the Beer's Law. The attenuated flux E across a volume zone boundary is calculated according to:

$$E = ES_0 * EXP (-\sum ABK * DS) \quad (4.16)$$

The summation in equation (4.16) is carried out over all volume zones traversed by the beam, including the emitting zone. ABK (or $AK(I,J)$) is the absorption coefficient of a volume zone I,J . DS is the path length of the beam across the volume zone which is being traversed. The cumulative energy flux absorbed by a volume zone ISA,JSA is:

$$QG (ISA, JSA) = QG (ISA, JSA) + EA - E \quad (4.17)$$

where EA and E are the energy fluxes of a beam entering and leaving the volume zone ISA,JSA , respectively. EA and E are calculated according to equation (4.16).

The path lengths DS spent by a beam in the various volume zones I,J are in principle calculated with the following formula (see also Figure 4.7):

$$\sin \psi > 0: \Delta s_x = \frac{x_p - x_o}{\sin \phi \sin \psi} \quad (4.18a)$$

$$\sin \psi < 0: \Delta s_x = \frac{x_n - x_o}{\sin \phi \sin \psi} \quad (4.18b)$$

$$\cos \phi > 0: \Delta s_y = \frac{-y_o \cos \phi + \sqrt{y_o^2 \cos^2 \phi + (1 - \sin^2 \phi \sin^2 \psi) (y_p^2 - y_o^2)}}{1 - \sin^2 \phi \sin^2 \psi} \quad (4.18c)$$

$$\cos \phi < 0: \Delta s_y = \frac{-y_o \cos \phi - \sqrt{y_o^2 \cos^2 \phi + (1 - \sin^2 \phi \sin^2 \psi) (y_p^2 - y_o^2)}}{1 - \sin^2 \phi \sin^2 \psi} \quad (4.18d)$$

where z_o and r_o are the coordinates of the starting point within an emitting zone or, alternatively, the coordinates of the beam entering the zone in consideration. z_p and z_n are the radial boundaries of the zone in the positive and negative Z-directions; similarly, r_p and r_n are the upper and lower cylindrical boundaries.

At any time in the history of a beam, the zone indices (ISA, JSA) of the volume zone that a beam is leaving, and the indices (IS, JS) of the volume zone that the beam is entering, are known. Also known are the path length (DS), and the angles PHI and PSI. This allows calculation of the current beam coordinates XS and YS possible.

Absorption and Reflection at Surface Zones—An inspection is made every time a beam leaves a volume zone to determine whether the boundaries of that zone coincide with a surface zone. If this occurs, the beam will be attenuated according to:

$$E = EA*(1.-EW(*,MS)) \quad (4.19)$$

where EW(*,MS) represents the emissivity of a surface zone, ISA,MS or JSA,MS, depending on the section number MS. The accumulated energy flux absorbed by a surface zone *,MS, is:

$$QW(*,MS) = QW(*,MS) + EA - E \quad (4.20)$$

If the emissivity EW(*,MS) of the absorbing surface zone is 1 (i.e the surface zone is black), the tracking of the current beam is terminated. The calculation is then resumed for a new beam, starting from the same or a new cell but pointing to a different direction. In case the emissivity EW(*,MS) of the absorbing surface zone is less than 1, the energy flux reflected is given by equation (4.19). The model assumes that all surface zones behave like ideal diffuse reflectors. The energy flux reflected from the incident beam is distributed over a solid angle of 2π according to the Cosine Law.

The reflected energy flux given by equation (4.19) is assigned to one single beam starting from the interception point (XS,YS) on the *,MS surface. The angles of direction, PHISR and PSISR, of the

reflected beam with respect to the surface-orientated coordinate frame, are determined with the help of weighted random numbers according to:

$$\text{PHISR} = \text{ASIN}(\text{SQRT}(\text{RUDRAN}(0., 1.))) \quad (4.21)$$

$$\text{PSISR} = \text{RUDRAN}(0., 2\pi) \quad \text{for MS=1 or MS=3} \quad (4.22a)$$

$$\text{PSISR} = \text{RUDRAN}(\pi/2., 3\pi/2.) \quad \text{for MS=2 or MS=4} \quad (4.22b)$$

The function RUDRAN(A,B) generates random numbers normalized between A and B. It can be shown that, when the procedure outlined above is applied to a large assembly of reflected beams, the distribution will statistically obey the Cosine Law of ideal diffuse reflection.

Prior to resuming the tracking of the reflected beam, the angles PHISR and PSISR are transformed into the furnace-oriented coordinate system using a system of equations similar to equations (4.15a) and (4.15b). Note that for symmetry reasons, only beams with azimuthal angles between $\pi/2$ and $3\pi/2$ are tracked. Beams reflected in other directions are in-active and abandoned by the model. The tracking of active beams follows the same algorithm as described earlier for beams emitted from surface cells.

Termination of Beam Tracking — A beam is no longer traced when:

- The beam encounters a black-body surface zone.
- The energy flux of a beam has been attenuated to a value (EXACT) smaller than the fraction of a reference energy flux EAMAX.

In the latter case, the remaining energy of the beam is added to the absorbed fluxes of the zone where the last beam attenuation had occurred. This provides a fully conservative formulation of the radiative heat exchange.

The minimum beam energy for continuing the beam tracing, EXACT, is an user input and is expressed as the fraction of the reference energy flux EAMAX. The reference flux is calculated by the code in the following way.

In order to select EAMAX, distinctions are made among the furnace volume and the surface zones which are expressed by M=1 to M=4. An average cell intensity EAYER(M) is calculated as:

$$\text{EAYER}(5) = (1./4\pi) * \sum \text{EM}(I,J) / \text{NSS} \quad \text{for volume zones} \quad (4.23a)$$

$$\text{EAYER}(M) = (1./\pi) * \sum \text{EM}(*,M) / \text{NSS} \quad \text{for M=1 through M=4} \quad (4.23b)$$

where NSS represents the total number of volume-zone cells, or of a surface section from M=1 to M=4. The actual coding uses $(1./2\pi)$ and $(4./\pi)$ as multiplying factors in equations (4.23a) and (4.23b), respectively, to account for symmetry.

During the scanning of the various sections, the largest value of EAYER(M) is always stored in a variable EAMAXA. EAMAXA is then used to determine the reference energy fluxes EAMAX for termination of beam tracking. The reference energy fluxes are determined by:

$$\text{EAMAX} = \text{EAMAXA} * \text{DRW}(L) \quad \text{for volume zones} \quad (4.24a)$$

$$\text{EAMAX} = \text{EAMAXA} * \text{CDRW}(L) \quad \text{for M=1 through M=4} \quad (4.24b)$$

where DRW(L) is the solid-angle element and CDRW(L) is the solid-angle element multiplied by COS(PHIS). Calculation of both of these quantities has been described already.

Beam tracking is terminated if E/EAMAX is smaller than EXACT where E is the actual energy flux contained in a beam. EXACT is referred to as the beam "cut-off" factor, and has a recommended value between 0.01 and 0.001.

Handling of Radiant Heat Exchangers— The radiative heat exchange sub-model has an option to include the radiant heat-exchanger surfaces usually placed in boiler upper furnaces.

The radiant heat exchanger surfaces are simulated in the 2D model as concentric ring- surfaces embedded in any of the selected I zone-layers. A typical configuration of such radiant heat exchanger surfaces is shown in Figure 4.8. Note that the radial spacing of the ring surfaces can vary between I zone-layers. The ring elements are assumed to have zero thickness in the radial direction.

To activate the heat exchanger option, The user has to set model input parameters NHSINK and NCOOL to 1 and 0, respectively. It is also necessary to specify parameters ISHL and ISHU, which indicate the lowest and the uppermost I zone-layers in which radiant heat exchanges exist.

The code recognizes volume zones where radiant heat exchanger surfaces are embedded, when the variable DASINK(I,J) has values larger than 0. DASINK(I,J) is the actual heat sink surface area within a volume zone I,J divided by the volume V(I,J) of that zone. For volume zones with DASINK(I,J)=0.0, the emission and beam tracking procedures are identical with those described previously.

The distribution of radiant energy emitted by the radiant heat sink surfaces follows the same principles as explained earlier for surface zones on sections M=2 and M=4. However, the code uses different variable names. The following lists the most important variables:

NSH	→	Current index of ring surface counting from the furnace axis.
YSH	→	Radius of the NSH ring-surface.
DEL(I)	→	Equidistant spacing of ring surfaces within volume zone layer I. The spacing between the outermost element and the furnace wall may differ from DEL(I).
NSHS(I)	→	Total number of ring surfaces within the volume zone layer I.
PROB(I)	→	Ratio of intercepting ring-surface-area (one side) to area $2\pi \cdot YSH \cdot DX(I)$ in volume zone layer I.
TWSINK(I,J)	→	Temperature of heat sink surface within volume zone I,J.
EWSINK(I,J)	→	Emissivity of heat sink surface within volume zone I,J.

Based on the above definitions, the radiating surface area, FSH, of a ring element NSH within layer I is:

$$FSH = 2\pi \cdot NSH \cdot DEL(I) \cdot DX(I) \cdot PROB(I) \quad (4.25)$$

where FSH represents either the inner or the outer radiating surfaces of the ring element. In analogy to the wall surface sections, inner ring surfaces are identified by a section index MSS=4, and outer ring surfaces by an index MSS=2.

Figure 4.8. 2D simulation of a tangentially-fired boiler furnace.

The emission of the inner and outer ring surfaces is calculated in analogy to equation (4.2). Distribution of the emissive powers into cells and energy beams is carried out with formulas similar to equations (4.7b), (4.8) and (4.9). Directions and starting coordinates of the beams emitted by the heat exchanger surface cells are expressed by equations (4.11), (4.12) and (4.13).

After transformation from the surface-oriented coordinate frame into the spatially-fixed furnace-orientated coordinate frame, beams starting from the heat exchanger surfaces are tracked in exactly the same way as beams of other origin. When the radiant heat exchanger option is exercised, all beams entering volume zones with $DASINK(I,J)$ greater than 0.0 are evaluated for the possibility of being intercepted by a radiant heat exchanger surface.

At any radial beam position YSH, whether a beam is intercepted is determined by comparing the random number generated against the effective intercepting area of the radiant heat exchanger at that position, i.e., :

$$IF (RUDRAN(0.,1.) .GT. PROB(I)) \rightarrow \text{No Interception} \quad (4.26)$$

$RUDRAN(0.,1.)$ generates random numbers normalized between 0 and 1.

If interception occurs, beam attenuation is calculated according to:

$$E = EA * (1. - EWSINK(ISA, JSA)) \quad (4.27)$$

where ISA and JSA are the indices of the volume zone in which the intercepting heat exchanger surface area is embedded. The accumulated energy fluxes absorbed by the heat exchanger surfaces are:

$$QWSINK(ISA, JSA) = QWSINK(ISA, JSA) + EA - E \quad (4.28a)$$

Order of Scanning—The radiative heat exchange calculation is carried out iteratively during the solution of the total heat balance for the furnace zones. During one radiative exchange calculation, the furnace zones are scanned in the following order:

- 1) Volume zones (M=5)
- 2) Surface or boundary zones on section M=1
- 3) Surface or boundary zones on section M=2
- 4) If the heat exchanger option is exercised, heat exchanger surface zones with normals in the positive Y-direction (i.e., MSS=2).
- 5) Surface or boundary zones on section M=3
- 6) Surface or boundary zones on section M=4
- 7) If the heat exchanger option is exercised, heat exchanger surface zones with normals in the negative Y-direction (i.e., MSS=4).

The volume zones are scanned first in the Y-direction and then in the X-direction. For the volume cells, the same order applies.

The beam directions, with respect to the cell-orientated coordinate frame, are scanned first by increasing the azimuthal angle PSIS from 0 to 2π and then by increasing the polar angle PHIS. The latter is scanned for volume zones from 0 to π , and for surface zones from 0 to $\pi/2$.

The total number of beams (NSTR) which are actually tracked during one radiative exchange calculation (or during all iterations of the "Averaging Process" discussed later on) is recorded in the final printout.

Total Radiative Balance — At the end of each radiative heat exchange calculation, radiative heat fluxes are checked for energy conservation at each zone. The total flux absorbed (QRADIN) is subtracted from the total flux emitted (QRADEX) to obtain the net radiative flux (QRADNT) out of that zone:

$$QRADNT = QRADEX - QRADIN \quad (4.28)$$

For a volume zone I,J, QRADEX is represented by:

$$QRADEX = EM(I, J) \quad (4.29)$$

where EM(I,J) is calculated according to equation (4.1). QRADIN is represented by

$$QRADIN = QG(I, J) \quad (4.30)$$

where QG(I,J) is the total radiative energy absorbed as shown by equation (4.17).

Similarly, for surface zones of sections M=1 to M=4, the radiative fluxes are given by:

$$QRADEX = EM(*, M) \quad \text{and} \quad (4.31)$$

$$QRADIN = QW(*, M) \quad (4.32)$$

with EM(*,M) and QW(*,M) are computed according to equations (4.2) and (4.20), respectively.

The net radiative heat flux from the heat exchanger surface zones is calculated in a similar way as the furnace wall surfaces have. The emitted flux is expressed according to:

$$-QRSINK = DASINK(I, J) * V(I, J) * EWSINK(I, J) * SIGMA * 2. * FAKPR(I) / \pi * TWSINK(I, J)^4 \quad (4.33)$$

where FAKPR(I) represents the ratio of the effective radiating surface area to the geometrically projected surface area. This factor is related to the earlier defined quantity PROB(I) by:

$$FAKPR(I) = PROB(I) * 2\pi * YSH * DX(I) / A_{proj} \quad (4.34)$$

where A_{proj} is the (one-sided) geometrically projected area positioned at radius YSH. A_{proj} can be calculated from input specifications of the heat exchanger surfaces. The accumulated heat flux absorbed by all heat exchanger surfaces in a volume zone I,J is represented as QWSINK(I,J).

The net radiative fluxes computed as described above form an important input to the total energy balance calculations solved later for each of the furnace zones.

The radiative exchange model is self-conservative provided that the model input parameters are appropriately set-up. The code automatically checks conservation of the radiative heat fluxes at the last iteration of the total heat balance, or during the Monte-Carlo Averaging Process. It also prints total residue of the radiative balance near the end of the program output.

In the conservation check, the initial heat fluxes of all emitted beams at the last iteration (or during the iterations of the "Averaging Process") are accumulated in a variable array ESUM(M), where M denotes the beam origin (i.e., M=5 for volume zones and M=1 to 4 for surface zones). The heat fluxes absorbed by all zones are accumulated in another variable array ASUM(M).

When the radiant heat exchanger option is exercised, the initial energy fluxes emitted by the heat exchanger surfaces are accumulated in ESUM(2) and ESUM(4), depending on whether the beams start from MSS=2 or MSS=4. The energy fluxes absorbed by the heat exchangers are added to ASUM(5).

The residue of the radiative heat balance is calculated as:

$$\text{PERCNT} = ((\sum \text{ESUM}(M) - \sum \text{ASUM}(M)) / \sum \text{ESUM}(M)) * 100 \quad (4.34a)$$

and is printed out as "Error of the Radiative Heat Balance" in percent. If the model is correctly set-up, the only factors contributing to the PERCNT are computer round-off errors. Typical absolute values of PERCNT stay between 1.0E-04 and 1.0E-05 when the code is executed on IBM AT or compatible personal computers.

When absolute errors of the radiative heat balance are larger than 1.0E-01, it is very likely that model inputs, especially *geometric data*, are not correctly specified. In this case, all results obtained from the 2DHT code may subject to errors. The user is strongly recommended to identify the source of the problem before performing extensive modeling studies.

Modeling of Non-Gray Radiation — The description in the preceding sub-sections assumed that radiation emitted by the volume zones was gray and could be characterized by a single absorption coefficient, AK(I,J), representative of each zone I,J. This simplified description was chosen for ease of explanation. The code is actually more sophisticated, and it simulates more realistic non-gray radiation among volume-zone heat-exchange calculations.

The radiating species considered are the gas species: H₂O and CO₂; and the particle species: soot, char and ash. The overlapping of gas and particle radiation is simulated with a three weighted-gray-gas approach suggested by Johnson and Beer. Based on studies of large gas-fired boiler furnaces, Smith, et. al. replaces the three weighted-gray-gas approach by a four weighted-gray-gas approach. The original Smith model was only developed for gaseous radiation. The constants used in the current model are obtained from data fitting using Edward's exponential wide band model.

The 2DHT code uses the four weighted-gray-gase model of Smith modified to account for particle radiation. Radiation from soot particles is assumed to be non-gray, whereas the radiation from char and ash particles is treated as gray.

The four-weighted-gray-gas approach represents non-gray volume radiation by the sum of weighted contributions in $NK=4$ gray ranges, each with different absorption coefficients AK . The temperature dependent weighing factors of these ranges are denoted by $B(TT,N)$, in which TT is the temperature $T(I,J)$ of the emitting volume zone and N is the current gray range. The temperature dependance of the weighing factor is expressed in polynomial form:

$$B(TT, N) = BN(4, N) * TT^3 + BN(3, N) * TT^2 + BN(2, N) * TT + BN(1, N) \quad (4.35)$$

$BN(*,N)$ are model constants and Table 4.3 documents the values of $B(*,N)$ used in the code. These were determined such that the condition:

$$\sum B(TT, N) = 1 \quad (4.36)$$

is fulfilled for any temperature TT .

The absorption coefficients, $AK(I,J)$, of the four gray ranges depend on species concentrations at volume zone I,J . The overall absorption coefficient AKK for the N th gray range is calculated according to:

$$AKK = CKN(N, 1) * PG(1) + CKN(N, 2) * PG(2) + CKN(N, 6) * PG(6) + CKN(N, 7) * PC(7) + CKN(N, 8) * PC(8) + CKN(N, 9) * PC(9) \quad (4.38)$$

where $PG(*)$ are concentrations of the gaseous species, $PC(*)$ are particle-phase concentrations. $CKN(N,*)$ are specific absorption coefficients of the various species for the N th gray range. The following lists the variable nomenclatures used in equation (4.38):

$PG(1)$	→	H_2O concentration	(bar)
$PG(2)$	→	CO_2 concentration	(bar)
$PG(6)$	→	SO_2 concentration	(bar)
$PC(7)$	→	Ash particle concentration	(kg/m ³)
$PC(8)$	→	Char particle concentration	(kg/m ³)
$PC(9)$	→	Soot particle concentration	(kg/m ³)
$CKN(N,1)$	→	Specific absorption coefficient of H_2O	(1/bar m)
$CKN(N,2)$	→	Specific absorption coefficient of CO_2	(1/bar m)
$CKN(N,6)$	→	Specific absorption coefficient of SO_2	(1/bar m)
$CKN(N,7)$	→	Specific absorption coefficient of ash	(1/(kg/m ³) m)
$CKN(N,8)$	→	Specific absorption coefficient of char	(1/(kg/m ³) m)
$CKN(N,9)$	→	Specific absorption coefficient of soot	(1/(kg/m ³) m)

The species concentrations within the volume zone I,J are calculated by the combustion model described later. The specific absorption coefficients for the gaseous species and soot are listed in Table 4.3. The coefficients for the gaseous species are those reported by Smith et al. for H_2O/CO_2 mixtures with a total pressure of 1 bar and with partial pressures $p_{H_2O} = 0.1$ bar and $p_{CO_2} = 0.1$ bar. The values listed for soot were chosen in analogy to those published by Johnson and Beer. The specific absorption coefficients of the ash are identical for the four weighted-ranges due to the assumption of gray radiation, and are user input. Guidelines to assess a specific absorption coefficient of the ash clouds are given in Section 5.1.

Table 4.3. Constants of "Four-Weighted-Gray-Gase" Radiative Property Module.

n	$b_{n,1} \cdot 10^1$	$b_{n,2} \cdot 10^4$	$b_{n,3} \cdot 10^7$	$b_{n,4} \cdot 10^{11}$	$k_{n,gas}$	$k_{n,soot}$	$k_{n,char}$	$k_{n,ash}$
	—	1/K	1/K ²	1/K ³	1/m·atm	1/(m·Kg/m ³)	1/(m·Kg/m ³)	1/(m·Kg/m ³)
PH ₂ O/PCO ₂ = 1								
1	2.1681	0.7280	0.7583	-1.7638	0.0000	3460	Xa,char·Schar/4	Xa,ash·Sash/4
2	5.1500	-2.3303	0.9779	-1.4940	0.4303	960	"	"
3	0.7749	3.6990	-2.2970	3.7700	7.0550	960	"	"
4	1.9070	-1.8240	0.5608	-0.5122	178.1000	960	"	"
PH ₂ O/PCO ₂ = 1								
1	1.0244	2.5570	-0.3680	0.4370	0.0000	3460	"	"
2	6.5080	-5.5510	3.0290	-5.3530	0.4201	960	"	"
3	-0.2504	6.1120	-3.8820	6.5280	6.5160	960	"	"
4	2.7180	-3.1180	1.2210	-1.6120	131.9000	960	"	"

$$P_t = 1\text{atm}, \text{PCO}_2 = 0.1\text{atm}, 0.001 \leq (\text{PCO}_2 + \text{PH}_2\text{O}) \leq 10\text{atm.m}$$

$$600\text{K} \leq T \leq 2400\text{K}$$

The specific absorption coefficients of the char particles are also identical for the four ranges, due to the assumption of gray particles, and are calculated by:

$$\text{CKN}(N, 8) = 0.85 \cdot \text{SPECSU} / 4.0 \quad (4.39)$$

where SPECSU is specific surface area (m²/kg) of the char particle cloud within the volume zone I,J. SPECSU is determined from the zonal mass concentration of char particles, AA(I,J,L), in 10 size classes:

$$\text{SPECSU} = 6 \cdot \sum (\text{AA}(I, J, L) / \text{XAV}) / (\sum \text{AA}(I, J, L) \cdot \text{RHOP}) \quad (4.40)$$

where XAV is the average diameter (m) of the char particles within the Lth size class, $\sum \text{AA}(I, J, L)$ represents the total mass concentration of char particles in volume zone I,J, and RHOP is the density (kg/m³) of the char particles. The average diameter XAV of the Lth size class is calculated by:

$$\text{XAV} = \text{XAV0} \cdot (\text{AA}(I, J, L) / \text{AA0}(L))^{(1./3.)} \quad (4.41)$$

where XAV0 is the initial char (also coal) particle diameter of the Lth size class, and AA0(L) is the mass concentration of the Lth-class char particles at the furnace inlets.

Calculation of radiative transfer using the four weighted-gray-gas model does not differ very much from the procedures outlined in the previous sections. Instead of scanning the zones once, the emission and beam tracking process is now carried out for the four gray ranges.

The emission of volume zones within the Nth range is calculated by multiplying equation (4.1) with the weighing factor B(TT,N):

$$\text{EM}(I, J) = B(\text{TT}, N) \cdot 4 \cdot \text{AK}(I, J) \cdot V(I, J) \cdot \text{SIGMA} \cdot \text{TT}^4 \quad (4.42)$$

Equation (4.42) replaces equation (4.1) in the actual coding. $AK(I,J)$ now represents the absorption coefficient of the N th gray range. If $AK(I,J)$ had the same value for all four gray ranges, equation (4.42) would be identical to equation (4.1). The emission of surface (or boundary) zones on sections $M=1$ to $M=4$ is modified in a similar way:

$$EM(*,M) = B(TT,N) * F(*,M) * SIGMA * TW(*,M)^4 \quad (4.43)$$

The emission of heat exchanger surfaces is calculated in analogy to equation (4.43).

The distribution of the emitted energy fluxes into cells and beams, and the beam tracking procedures are identical with the methods described earlier. Here, the absorbed energy fluxes are not only accumulated during the scanning of all zones, but also during the scanning of the four gray ranges.

Total Heat Transfer Model

The computation of radiative heat exchange described in the preceding sections is based upon known temperatures and absorption coefficients of every volume zone I,J . It was also assumed that temperatures of the surface zones were known. However, these quantities are initially unknown and must be obtained from an iterative solution on total heat balances.

Total Heat Balance for Volume Zones — Total heat balance is carried out for all volume zones. In the balance, the net flux of sensible heat ($QCONNT$), the net convective fluxes to boundary zones ($QDIFNT$), and the net radiative fluxes ($QRADNT$) are equated to the release of the chemical heat ($-QCHENT$) in that zone as:

$$QCONNT + QDIFNT + QRADNT + QCHENT = 0 \quad (4.44)$$

Equation (4.44) is referred to as the total heat balance equation. All heat fluxes have units of kW. The net heat fluxes are further divided into out- and in-fluxes. For instance, the sensible heat fluxes, which flow into and out of a volume zone, can be shown as $QCONIN$ and $QCONOT$ respectively. These energy fluxes are based on the prescribed mass flow field, and the mass flow field is normalized with the total mass flow rate, $DMTOT$, of the furnace.

Figure 4.9 shows the orientation of the mass fluxes with respect to an annular volume zone I,J . $DM1(I,J)$ is the relative mass flux in the positive X -direction, entering the lower boundary of the volume zone I,J . $DM3(I,J)$ is the mass flux across the same boundary but in the negative X -direction. The mass flux leaving the upper zone-boundary in the positive X -direction is denoted by $DM1(I+1,J)$, and the mass flux entering at the same boundary is $DM3(I+1,J)$. The coding of the radial mass fluxes in the Y -direction, $DM2(I,J)$ and $DM4(I,J)$, is similar to the specifications in the X -direction. All mass fluxes have positive signs.

Figure 4.9. Definition of zonal mass fluxes.

The prescription of the relative mass flux distribution is supported by the interactive input program 2DINPT (see Section 5.1). Mass fluxes at the same boundary can simultaneously have values larger than zero in both the negative and the positive directions. This feature allows simulation of turbulent exchange or small scale recirculation over the zone boundary.

After the relative mass fluxes have been defined, the sensible heat fluxes leaving and entering a volume zone I,J are expressed in the following way :

$$QCONEX = (DM1(I+1,J) + DM2(I,J+1) + DM3(I,J) + DM4(I,J)) * DMTOT * CPP(I,J) * (T(I,J) - 298.15) \quad (4.45)$$

$$QCONIN = (DM1(I,J) * DMTOT * CPP(I-1,J) * (T(I-1,J) - 298.15) + \\ DM2(I,J) * DMTOT * CPP(I,J-1) * (T(I,J-1) - 298.15) + \\ DM3(I+1,J) * DMTOT * CPP(I+1,J) * (T(I+1,J) - 298.15) + \\ DM4(I,J+1) * DMTOT * CPP(I,J+1) * (T(I,J+1) - 298.15)) \quad (4.46)$$

CPP is the species mean specific heat at constant pressure between 298.15 K and the zonal gas temperature. The temperature dependency of CPP for the gaseous species is formulated with polynomials, using coefficients taken from Gordon and McBride. The coefficients for the solid species were determined from various sources, and they must be considered as approximate values. However, uncertainties in specific heats of the solids do not affect the overall heat balance very much.

QDIFNT is split into two terms: QDIFEX and QDIFIN. QDIFEX represents the convective heat flux from a volume zone nearby the furnace wall to a surface zone. This heat flux is expressed as:

$$QDIFEX = DA * ALPH1 * (T(I,J) - TW(*,M)) \quad (4.47)$$

where DA (m²) is the area of the surface zone, ALPH1 is the convective heat transfer coefficient of the furnace wall (kW/m²K), and TW(*,M) is the surface temperature. ALPHA is an user input. Convective heat transfer to furnace walls is usually small.

Convective heat transfer to the upper furnace heat exchangers is calculated in the same way as shown by equation (4.47), and is lumped into the term QDIFEX. The convective heat transfer coefficients of the radiant heat exchangers play a somewhat larger role in heat exchange calculations, but may be assessed using an option provided by the input code of the Boiler Performance Model, BPINPT.

The third and also the most important term in the total heat balance equation is the contribution of radiative heat transfer: QRADNT = QRADEX - QRADIN. This term is obtained from the radiative exchange model as described in the previous sections.

The fourth term in the total heat balance equation is the chemical heat release term, QCHNT. QCHNT is expressed as:

$$QCHNT = QCHEX - QCHEIN + QCHREX - QCHRIN - SOURCE \quad (4.48)$$

The most important contributions are heat release due to char combustion (QCHRIN-QCHREX), and the release due to combustion of volatiles and any co-firing/reburning gaseous fuel. Both contributions are calculated by the combustion model described later. The chemical source term includes heat required to evaporate fuel moisture.

Special attentions are given to the formulation of the total heat balance equation at the furnace boundary zones. The boundary zones need additional treatment to include heat fluxes associated with the various fuel and air jets.

Solution of Volume Zone Temperatures — The total heat balance equation (eq. 4.44) is solved for the zonal gas temperature T(I,J), using a Newton Raphson Gauss-Seidel solution scheme.

During the solution of the volume zone heat balances, participating volume zones are scanned in order of increasing I first, and then of increasing J. Temperatures are updated according to:

$$TNEW = TOLD - QTOTNT/DFUNC \quad (4.49)$$

QTOTNT represents the net heat energy accumulated in the zone I,J, and DFUNC is its derivative with respect to the old zonal temperature, TOLD. T(I,J) is over-written as soon as the new zonal temperature TNEW becomes available. The above algorithm has been shown to be very robust, and seldom divergence occur.

Total Heat Balance for Surface Zones — 2DHT can keep surface zone temperatures of the furnace wall sections constant, or, alternatively, the wall surface temperatures can be calculated based on deposit thermal/physical properties. Surface temperatures of radiant heat exchangers are always calculated. However, if extremely high deposit conductivities are chosen, the model effectively simulates the condition that surface temperatures of the heat exchangers are constant.

The heat balance equation for wall surface zones is formulated in analogy to the volume zone heat balances:

$$Q_{CONNT} + Q_{DIFNT} + Q_{RADNT} = 0 \quad (4.50)$$

where Q_{CONNT} (kW) is the heat conducted through the deposit layer covering the wall surface zone and is given by:

$$Q_{CONNT} = CLDS * DA * (TW(*,M) - TOUT) \quad (4.51)$$

$CLDS$ is the deposit thickness to conductivity ratio, and has dimensions in kW/m² K. $CLDS$ is an user input and may vary from one surface to another. DA is the projected gas-side surface area of a surface zone (*,M). $TW(*,M)$ is the gas-side surface temperature and $TOUT$ is the metal-side surface temperature of the deposit surface layer. $TOUT$ is also an user input and can be assessed from the saturation temperature of the water in the water-wall tubes. The variable - Q_{DIFNT} is the convective flux transported from an adjacent volume zone to the surface. - Q_{RADNT} is the net radiative heat flux received by the surface.

Heat balance equation for radiant heat-exchanger surfaces is formulated similar to equation (4.50). Here, all surfaces embedded in one volume zone are assumed to have uniform temperatures regardless of the orientation of the surfaces. Deposit thickness in one volume zone is also assumed to be uniform. The heat balance equation of the surface zones are solved by the Newton-Raphson iterative solution scheme for surface temperatures.

Combustion Model

The total heat balance of volume zones requires the source terms to be defined to account for combustion of various fuel components. These source terms are calculated in the combustion model. The combustion model has the following modules:

- Module for calculation of species concentrations
- Coal devolatilization module
- Volatile combustion module
- Char burn-out module
- Combustion module for gaseous and liquid fuels
- Calculation of soot concentrations.

The combustion model involves the solution of a considerable number of zonal variables. These variables are stored in a staggered two-dimensional array, $AA(I,J+(NRV-1)*NY)$, where NRV is the variable index, and I and J are volume zone indices. In order to clarify the model descriptions, variable names in the following sub-sections are abbreviated as $AA(NRV)$ whenever appropriate.

Species Mass Balance — Excluding the volatile combustion module, the combustion model is based on Eulerian formulation of conservation equations. The zonal species mass balance equation may be written as:

$$\text{CONEX} - \text{CONIN} + \text{SOUNT} = 0 \quad (4.52)$$

CONEX represents the total mass flux (kg/s) leaving a volume zone I,J. CONIN represents the total mass flux (kg/s) entering the control volume. Furthermore, CONEX and CONIN may be shown as:

$$\text{CONEX} = (\text{DM1}(\text{I}+1, \text{J}) + \text{DM2}(\text{I}, \text{J}+1) + \text{DM3}(\text{I}, \text{J}) + \text{DM4}(\text{I}, \text{J})) * \text{DMTOT} * \text{AA}(\text{I}, \text{J} + (\text{NRV}-1) * \text{NY}) \quad (4.53)$$

$$\begin{aligned} \text{CONIN} = & (\text{DM1}(\text{I}, \text{J}) * \text{DMTOT} * \text{AA}(\text{I}-1, \text{J} + (\text{NRV}-1) * \text{NY})) + \\ & (\text{DM2}(\text{I}, \text{J}) * \text{DMTOT} * \text{AA}(\text{I}, \text{J}-1 + (\text{NRV}-1) * \text{NY})) + \\ & (\text{DM3}(\text{I}+1, \text{J}) * \text{DMTOT} * \text{AA}(\text{I}+1, \text{J} + (\text{NRV}-1) * \text{NY})) + \\ & (\text{DM4}(\text{I}, \text{J}+1) * \text{DMTOT} * \text{AA}(\text{I}, \text{J}+1 + (\text{NRV}-1) * \text{NY})) \end{aligned} \quad (4.54)$$

AA(NRV) is the species mass concentration in kg/kg-mixture, and DM*(*,*) are the relative mass fluxes across the volume zone boundaries. DMTOT is the total mass fed into the furnace in kg/s. Note that the mass balance equations, eq. (4.52) to (4.54), include the contribution of the turbulence on the mass fluxes. SOUNT in equation (4.52) represents a sink term, in kg/s, for the species mass balance equations. If a species is "generated" in the volume zone I,J, SOUNT has a negative sign.

Solution of Species Mass Balance Equations — The species mass balance equations are solved iteratively according to a Newton-Raphson Gauss-Seidel solution scheme.

During one sub-iteration of the combustion model, participating volume zones are scanned in the order of increasing I, and then in order of increasing J. Variable values are updated according to:

$$\text{AANEW} = \text{AAOLD} - (\text{CONEX} - \text{CONIN} + \text{SOUNT}) / (\text{SOUNEN} + \text{DCONEX}) \quad (4.55)$$

where (SOUNEN+DCONEX) represents the derivative of the species mass balance equation with respect to the species concentration AA(NRV), in the volume zone I,J. SOUNEN is the contribution of the sink term to this derivation. DCONEX is the contribution of the convective term, i.e., CONEX-CONIN, to the derivation.

AAOLD is the existing (or old) value of AA(NRV) in the volume zone I,J before the variable is scanned. AANEW is the updated value of AA(NRV). The iteration scheme overwrites the old value as soon as the updated value becomes available.

Devolitilization Module — The devolatilization module yields information regarding mass concentrations of volatile matter and total char, at each volume zone I,J. As an approximation, the module uses a first order rate equation to describe coal devolatilization.

A species mass balance equation is solved for mass concentrations of non-devolatilized coal. The sink term, SOUNT, for this equation is calculated according to an Arrhenius formulation:

$$\text{SOUNT} = \text{V}(\text{I}, \text{J}) * \text{RHOM} * \text{AAOLD} * 114000. * \text{EXP}(-8800./\text{T}(\text{I}, \text{J})) \quad (4.56)$$

where V(I,J) is the volume of zone I,J, and RHOM is the mixture density in that zone.

The solution of the species equation for non-devolatilized coal leads to volatile matter (in kg/s) released into the volume zone I,J. The amount of the volatile released is represented by a variable array, AA(17). Following coal devolatilization, the combustion of volatile matter and char is simulated by two different methods.

Volatile Combustion Module — The volatile combustion module is based on a statistical approach. The model solves two variables: AA(15), for volatile heat release rate; and AA(16), for concentration of unburnt volatiles. The essence of the statistical approach is described in the following.

The total amount of volatiles are divided into NVLTOT number of volatile lumps. The number of volatile lumps (NWLMP) associated with each volume zone I,J, can be calculated from AA(17), which is a variable calculated by the devolatilization module discussed above.

Each of the volatile lumps released into a volume zone is then tracked under the user prescribed flow field. The tracking process uses random numbers weighted with an empirical burnout equation, to describe volatile lifetime distributions. The tracking procedure also requires information on the distribution of zonal residence times. The values of the zonal residence times are calculated and stored in another variable array, AA(14).

When the lifetime of a volatile lump is expired, the lump is considered to be burned. The total amount of volatile fuel contained in the lump is added to AA(15) of that volume zone I,J. After all volatile lumps have been tracked for one iterative cycle of the total heat balance, AA(15) contains the volatile heat release rates for each volume zones. These values are also transferred to the total heat transfer model.

The decision as to whether a volatile lump expires its life is based on a volatile life time, TLIFE, calculated as:

$$TLIFE = TLFMAX * \sqrt{-CLIFE * \text{ALOG}(RNR)} \quad (4.57)$$

where RNR is a random number normalized between 0 and 1, and TLFMAX is an user specified input. If the accumulated volatile residence time (TIMEP) is larger than the life time TLIFE, the volatile lump is burned and the tracking procedure is terminated for that lump. Otherwise, the tracking is continued. If the volatile lump enters a volume zone where oxygen concentration is zero, then the volatile can not expire it's life time in that zone. The tracking process will be continued and the time spent in the oxygen-depleted zone is not counted.

Equation (4.57) represents an exponential burnout function. TLFMAX and CLIFE are empirical constants. Due to the setting of the constant CLIFE, TLFMAX represents the time required to burn 99.9 percent of the initial volatile heat content. In practice, TLFMAX represents the characteristic mixing time of the burner. The user can change it's value in order to match boiler flame locations if visual observation of the flame has been conducted.

Char Combustion Module — The char combustion model assumes that char can burn regardless of whether the volatile matter is released or not. The initial mass of the char particle is sub-divided into ten size classes, each with diameter XMNO(L) and mass fraction CMFR(L). The initial char sizes are the same as the sizes of the initial coal, which are inputs by the user.

Mass balances for the char particles are solved according to equation (4.52). Char combustion considers boundary layer diffusion and the global rate equation. Thus, the sink term SOUNT for a size class $NRV=L$ is expressed as the following:

$$SOUNT = V(I,J) * RHOM * AAOLD * (6. / RHOP * XAV) * PO2 / (DKS + DKD) \quad (4.58)$$

Every variable in equation (4.58) is related to volume zone I,J. The terms in this equation have the following meaning:

V(I,J)		Volume of zone I,J	(m ³)
RHOM		Mixture density	(kg/m ³)
AAOLD		Mass concentration of char in Lth size class	(kg/kg-mix)
RHOP		Density of char particle	(kg/m ³)
XAV		Average diameter of char particle	(m)
PO2		Partial pressure of O ₂	(bar)
DKS		Inverse of chemical rate coefficient	(m ² s bar)/kg
DKD		Inverse of diffusion rate coefficient	(m ² s bar)/kg

The chemical rate coefficient is expressed as:

$$1. / DKS = FREQFC * EXP (-ACENER / (RR * T(I, J))) \quad (4.59)$$

where

FREQFC		Frequency factor	(kg/m ² s bar)
ACENER		Activation energy	(kJ/kmole)
RR		Universal gas constant	(kJ/kmole K).

FREQFC and ACENER are user inputs. The diffusion rate coefficient is expressed as:

$$1. / DKD = 4. * AMJ(QC) * DO2N2 / (XAV * 100. * RR * T(I, J)) \quad (4.60)$$

where

AMJ(QC)		Atomic weight of carbon	(kg/kmole)
DO2N2		Binary Diffusion coefficient of O ₂ and N ₂	(m ² /s).

DO2N2 is calculated as a function of gas temperature. The mean particle diameter XAV of the Lth class char in volume zone I,J is:

$$XAV = XMN0(L) * (AAOLD / AA0(L))^{1/3} \quad (4.61)$$

in which AA0(L) represents the average mass concentration of char particles, in size class L, at the coal inlet zones.

The oxygen concentration needed in equation (4.58) is obtained by solving an oxygen mass balance equation. The solution of oxygen mass balance is carried out in terms of a composite variable AA(12):

$$AA(12) = AA(11) - 'm_{O_2}' / STOICH \quad (4.62)$$

where AA(11) is the mass concentration of the total char, " m_{O_2} " is the mass concentration of the oxygen (kg/kg-mixture), and STOICH is the stoichiometric ratio, i.e., the mass of O_2 required to burn 1 kg of char.

The mass balance for A(12) includes a sink term for oxygen consumption due to volatile combustion. The char combustion module is performed as sub-iterations within each cycle of the total furnace heat balance. The number of sub-iterations, NIMX1, is an user input.

Combustion Module for Gaseous and Liquid Fuels — The combustion module used to treat gaseous and liquid fuel combustion is the same one as the volatile combustion module of coal. Both fuels are treated as "pseudo" solid fuels with very high percentages of "volatiles" to simulate the fuel's compositions.

For a gaseous fuel, the coal devolatilization module is deactivated, and the gaseous "volatiles" are tracked immediately starting from the burner inlet zones. The "volatile" burnout time, TLFMAX, in this case should simulate the characteristic mixing time of the gas burner.

Similar procedures are adopted for simulation of liquid fuel combustion. Again, the coal devolatilization module is deactivated if fuel oil is fired. The code does not calculate ballistic droplet trajectories, due to the coarse zoning used and the decouple nature of the flow fields. The "volatile" burnout time, TLFMAX, in this case should include the time required for droplet evaporation, and the characteristic mixing time of the oil burner. The fuel evaporation time, for a properly atomized liquid fuel, usually is small compared to the burner mixing time.

If the option of gaseous fuel reburning is exercised, the combustion module will be called twice during each iteration. The first call is for tracking the "volatiles" from the burner fuel and the later one is for tracking the reburn fuel. In this application, oxygen concentrations are recorded for each volume zones and the volatiles will not burn in oxygen-depleted zones. The tracking and recording of the zonal oxygen concentrations will increase the code execution time somewhat.

Calculation of Soot Concentrations — Soot concentration is calculated by a simple but powerful approach. In this approach, the amount of soot released into a volume zone is assumed to be in direct proportion to the carbon content of the volatiles. The proportional constant is called CMCVLS, and is an user input. The burnout of soot is assumed to be proportional to the burnout of the volatiles.

4.2 Reburning NO_x Model (RBNOX)

The objective of the Reburning NO_x Model is to calculate reasonable working estimates for the expected NO_x reduction potential as a function of the major boiler process controlling parameters. The boiler process parameters include furnace gas temperature profiles and residence time distributions, local stoichiometries up- and down-stream of the reburning fuel injection zone, reburn fuel and overfire air local mixing rates, and injection locations.

The RBNOX code uses a series of plug-flow reactors (PFR) to simulate NO_x formation and destruction in boiler environment. The code is configured to work on IBM or IBM-compatible personal computers, and occupies a memory size approximately at 500 kilobytes (KB).

A basic part of the Reburning NO_x Model is based on a package of detailed fuel/air chemistry modules up to C₂, which includes 43 species and 201 elementary reaction steps. The kinetics model simulates bulk mixing rates of the reburn and overfire air (OFA) jets by characteristic mixing times, which may be derived from isothermal flow modeling measurements. NO_x reduction effectiveness is obtained by comparing predictions of the inlet and outlet NO_x concentrations at the exit of the burnout (or over-fire air) zone.

The following sub-sections present the execution and the physical background of the Reburning NO_x Model.

File Management

The default input file name for the RBNOX code is RBINPT.DAT. The default output file name from the RBNOX code is RBOTcsvs.lll, where cs is an user specified case number, vs is an user specified version number, and lll is a character string extracted from a user specified parameter describing the boiler load. For example, if cs is 01, vs is 02, and the specified boiler load is 95.0 % relative to the MCR, the default output file name will be RBOT0102.095. The user can overwrite the default output file name. However, the default input file name is always fixed as RBINPT.DAT. This means that if the user wants to execute the RBNOX code with an input file, say RBIN0102.095, he has to copy that file to file RBINPT.DAT first. The objective of this file structure is to prevent accidental overwriting of the input file.

The coupling between the furnace code (2DHT) and the reburning NO_x code is through the output data file REBURN.DAT generated by the 2DHT code. This file contains furnace information required by the RBNOX code. The furnace data transferred by the REBURN.DAT file are:

- Mean furnace gas temperatures
- Mean furnace gas residence times
- Burner-fuel ultimate analysis
- Burner, reburn gas, and overfire air injection-locations.

Code Execution

To execute the RBNOX code, the user has to do the following:

- Install RBNOX.EXE in the working directory.
- Copy the input data file to file RBINPT.DAT.
- Have file REBURN.DAT ready in the same working directory.
- Include file THERMO.DAT in the same working directory.
- Type RBNOX and press "Enter".

The input data file is the one which contains the boiler reburning information. This data file should be prepared by executing the input code RBINPT. RBINPT.DAT is the input file- name used by the RBNOX code, therefore, reburning NO_x calculations will be performed based on the contents of the file RBINPT.DAT. The user must copy the contents of his input data file to file RBINPT.DAT before executing the Reburning NO_x Model.

File THERMO.DAT contains species thermodynamic data as a function of temperature. The data include heat capacity, enthalpy, and entropy, which are needed for the execution of the RBNOX code. The thermodynamic data file is included in the model package delivered, and the user should not change the contents of this file. The user is also strongly suggested to make a backup copy of the THERMO.DAT file.

Reburn Chemistry

Gas reburning applied to boiler furnaces can be viewed as a NO_x reduction technique which combines fuel and air staging practices. Figure 4.10 shows a schematic application of the reburning process and the reburn chemistry involved.

Figure 4.10. Boiler gas reburning and reburn NO_x reduction schematics.

The process may be considered to occur in a series of zones, each of which is characterized by a local stoichiometric ratio (SR, or air ratio), defined as the total air supplied divided by the theoretical air required for complete combustion. In reburning, burners in the main combustion zone are typically operated at reduced excess air levels, for example at $\text{SR}_1 = 1.1$ (i.e., 10 % excess air). Reburning fuel, such as natural gas (NG), is injected externally into a plane above the burner zone so that a fuel rich zone is created ($\text{SR}_2 < 1.0$). The exact chemistry which occurs in the reburn zone is still not clear, however, the main NO reduction and formation pathways have been constructed from previous experimental investigations. In the reburn zone, fuel fragments such as CH species react with NO to form nitrogen species XN which consist of NH_3 , NO , and HCN . The XN species subsequently react with NO to form N_2 . Above the reburn zone the injection of overfire air takes place to complete combustion. This zone is generally referred to as the "burnout zone". Some XN species may be further reduced to N_2 or NO in the burnout zone.

The RBNOX model has a kinetics package which consists of elementary reaction mechanisms up to C_2 chemistry. The package in its current form considers 43 species (see Table 4.4) and 201 reactions. Gas phase species important for NO_x formation and destruction, such as NH_3 , HCN , NO_x , and N_2O , are all included. This kinetics package will be imbedded in the input file when the user executes the model's input code, RBINPT. The user may not change the contents of the kinetics package.

Table 4.4. Chemical Species Considered by the RBNOX Model.

	0	1	2	3	4
1	H ₂	CH ₄	C ₂ H	NH ₂	SO ₂
2	O ₂	CH ₃	CH ₂ O	NH	SO ₃
3	HO	CH ₂	CH ₃ O	HN ₂	HSO ₃
4	O	CH	CHO	N ₂ H ₂	
5	H	C ₂ H ₄	N	HNO	
6	H ₂ O	C ₂ H ₆	NO	CN	
7	CO ₂	C ₂ H ₅	N ₂	NCO	
8	HO ₂	C ₂ H ₃	NO ₂	CHN	
9	H ₂ O ₂	C	N ₂ O	HNCO	
10	CO	C ₂ H ₂	NH ₃	HOCN	

For many situations, a detailed chemical kinetics model is not absolutely essential for boiler NO_x modeling. For gas reburning, however, detailed chemistry models become essential for one main reason: NO reduction in the reburn zone is accomplished by fuel fragments such as CH (see Figure 4.10). Simpler models which do not consider such chemistry can not be applied and must be excluded.

NO_x Modeling

Success in the practical application of NO_x controls does not appear to have stimulated corresponding progress in the development of NO_x prediction models for engineering design purposes. This may be attributed to the nature and complexity of modeling NO_x formation in large enclosures. The prediction of NO_x generation in boilers is difficult because it generally involves all aspects of the computational arena: turbulence, chemistry, and radiation modeling. This complexity is compounded by various boiler practices such as soot blowing, unknown operating conditions, and burner design specifics, which make model validation difficult.

In order to predict NO_x formation, a mathematical model requires submodels which describe both turbulent mixing and fuel chemistry. One immediate difficulty here is the incompatibility of the mathematical zones with actual turbulent mixing scales. This results in the use of approximations of turbulent models in describing transport phenomena of mass and momentum. Also, the fuel chemistry has to be simplified, since reliable techniques for solving turbulence-chemistry interactions are still

under development. In most instances, chemistry packages which describe fuel combustion and NO_x formation/destruction kinetics are reduced to a manageable set of mechanisms. Radiation modeling is important because it can contribute up to 90 % of the heat absorbed by waterwalls in boiler radiant furnaces. It affects flame temperature, and therefore has an impact on NO_x formation and destruction. Radiation complicates model set-up and calculations because its transport is governed by integral rather than by differential equations.

The difficulties recounted above have however not discouraged scientists and engineers from NO_x modeling. The literature shows that engineers have approached NO_x modeling in boilers by two means: semi-empirical correlations, and predictive modeling. In the first approach, NO_x emissions are correlated with fuel properties, boiler design and operation, and specific burner scaling laws. This approach has generated NO_x correlation equations which are most useful if gross changes, such as switching coal or coal burners, are made. One major disadvantage of the empirical approach is that it requires extensive boiler data to establish reliable correlations, and often the appropriate data are not available or are simply not obtainable in full scale boilers. The second approach is typically based on solving three-dimensional (3D) coupled mass, energy, and momentum equations. These models are comprehensive in nature and require substantial computer resources in terms of man-power, computational budget, and hardware to apply. Current effort in predictive modeling is on the detailed validation of 3D model predictions.

Process considerations that are essential to the design and practical application of the reburning system are: the reburn zone stoichiometry SR_2 , the temperature (or location) at which the NG is injected, the OFA injection location, and any impacts on boiler thermal performance. The reburn zone air ratio has strong impact on overall NO_x reduction levels. More fuel rich reburn zone conditions tend to increase NO_x reduction at the expense of increased use of NG. When specifying injection locations for the NG and the OFA, adequate residence times should be provided in the reburn and the burnout zones.

The current approach used for the modeling of NO_x formation is a compromise between semi-empirical and fully predictive models. In this approach, the 2D furnace heat transfer model and the Reburning NO_x Model are coupled for reburning NO_x predictions. The heat transfer model is used to calculate mean time-temperature profiles for the boiler, based on actual operating conditions. Information on flue gas temperature and residence time is then used in the Reburning NO_x Model for kinetics calculations.

In setting up the Reburning NO_x Model, distinctive zones in the boiler are identified and represented by a series of Plug Flow Reactors (PFR). The PFR allows for the injection of side streams, so that the reburn fuel and the OFA injection can be simulated. Figure 4.11 illustrates the model set-up for boiler reburning NO_x predictions. The sequence comprises four PFR reactors, with each reactor accompanied by a specified residence time and temperature profiles obtained from the 2DHT code.

In Figure 4.11, the first PFR (reactor #1) is used to simulate chemical interactions between the flue gas from the burners and the reburning jets. Likewise, reactor #3 simulates NO_x formation/destruction and residual fuel burnout in the overfire air (or burnout) zone. Reactor #2 represents the available furnace volume between the point that the reburn-gas achieves complete mixing, and the introduction of the lower OFA jets. Sufficient residence time must be provided to this volume zone (or reactor) for adequate NO_x reductions. Reactor #4 simulates the steam generation zone where the flue gas experiences a steep temperature decay. This reactor represents the furnace volume starting from the point that the OFA jets achieve complete mixing with the flue gas, to the end of the boiler upper furnace defined by the furnace code 2DHT.

Figure 4.11. Model setup for reburn NO_x modeling.

The 45-degree arrows in Figure 4.11 indicate that temperatures within the PFR's are decreasing. For example, reactor #4 simulates the temperature drop of the flue-gas from 1634 K to 1101 K in 1.929 seconds in the boiler upper furnace. The input code (RBINPT) can extract these temperature profiles from the 2D furnace results and offer them as default values.

The user has to specify mixing times for the reburn and the OFA jets, as required by reactors #1 and #2, respectively. These mixing time information must be evaluated separately based on physical isothermal modeling, or other engineering calculations. The RBINPT input-code calculates residence times of the other two reactors (i.e., reactors #2 and #4), and offers them as default values.

Conservation equations

Conservation equations which describe the plug-flow reactors are formulated from consideration of an one-dimensional stream-tube. The equations include total mass continuity, species mass conservation, and momentum conservation equations. Gas phase energy conservation equation is also included, but is deactivated from the solution scheme as the gas-phase temperatures are established by the more accurate furnace heat transfer code (2DHT).

The momentum equation can be solved by specifying any one of the following: (a) constant reactor pressure, (b) reactor pressure gradient, or (c) the stream tube cross-sectional area. The RBNOX model chooses the option of constant reactor pressure at 1 atmosphere. To conserve total mass continuity, the cross-sectional area of the stream-tube may expand or contract, depending on the imposed reactor temperature-profiles and the changes of total molar numbers in the reactor.

Solution algorithm

The governing differential equations mentioned above are integrated to obtain time-resolved solutions. An implicit solution scheme is incorporated in the RBNOX code to solve the ordinary differential equation sets. Non-linear terms in the equations are linearized via Taylor series expansion and are truncated after the first-order term. A Gauss-Jordan reduction algorithm is used to solve the resulting matrix set.

The numerical procedure is basically non-iterative. In order to control the truncation error due to the linearization of the non-linear terms, the integration steps are regulated in a careful manner. The method used is to limit the step size so that no variable solutions may vary by more than a small fraction (EPS1) of their values at the last step. The value of EPS1 is set to 0.05 based on extensive numerical experience. The integration step size will be cut-back automatically, to half of its original value, if this criterion is violated. In this case, the integration procedures will be repeated.

On the other hand, a lower fractional limit (EPS2) is also set in the RBNOX code so that the step size can be doubled. The value of EPS2 is set to 0.02. Therefore, if the maximum variation of a variable solution is smaller than 2% of its value at the last time step, the step size will be doubled automatically for the next time step.

4.3 Boiler Performance Model (BPM)

The objective of the Boiler Performance Model, BPM, is to calculate boiler steam side heat balance for all heat exchanger surfaces in the flue gas pass of the boiler. For boiler sections not handled by the furnace code (2DHT), such as the backpass convective tube-banks and the air heater, the BPM code calculates a heat balance for both the steam and the gas sides. For sections that are included in the domain of the 2DHT code, it is not necessary for the BPM code to re-calculate the gas side heat balance as this has been done in the furnace code.

The BPM code is basically a one-dimensional heat transfer model which solves the coupled energy balance equations of the boiler steam and gas sides. The code is configured to work on IBM or IBM-compatible personal computers, and occupies a memory size approximately at 385 kilobytes (KB).

The user must define a boiler cross-section, referred here as "the inlet plan", for the BPM code to start its steam/gas calculations. The inlet plan can be the lower boundary of the first heat exchanger section following the lower furnace exit. The user may also define this inlet plane further downstream from the upper furnace, depending on his 2DHT model set-up. It is essential that the mean gas temperature of the inlet plane is known. BPM performs the coupled heat balance calculations only for boiler sections downstream of the user-defined inlet plane.

For all of the sections upstream of the inlet plan, heat fluxes to steam/water are transferred from the furnace code predictions. The BPM also displays the calculated gas temperatures for these sections. However, these temperatures in general are not the same as the furnace code (2DHT) predictions. The temperatures displayed are simply back-calculated without the consideration of radiative heat exchanges, and should not be used for boiler design purposes. Instead, the user should use the predictions of the 2DHT code when gas temperatures are needed for the upstream radiant-sections.

The output generated by the BPM code is quite informative. Table 4.5 summarizes the output information. The model provides information on boiler steam- and gas- side performance, as well as information on boiler gross and net efficiencies. The following sub-sections present the execution and the physical background of the Boiler Performance Model.

Table 4.5. Summary of Boiler Performance Code Output Information.

Steam Side

- Superheated steam properties (temperature, flow rate)
- Reheat steam properties (temperature, flow rate)
- Heat absorption along boiler convective passage
- Superheat and reheat attemperation flow rates

Gas Side

- Gas temperature drop across each convective unit
- Wall (i.e., deposit surface) temperature of each convective unit

General Information

- Boiler gross and net thermal efficiency
- Heat transfer coefficients for each convective unit

File Management

The default input file name for the BPM code is BPINPT.DAT. The default output file name from the BPM is BPOTcsvs.lll, where cs is an user specified case number, vs is an user specified version number, and lll is a character string extracted from a user specified parameter describing the boiler load. For example, if cs is 01, vs is 02, and the specified boiler load is 95.0 % relative to the MCR, the default output file name will be BPOT0102.095. The user can overwrite the default output file name. However, the default input file name is always fixed as BPINPT.DAT. This means that if the user wants to execute the BPM code with an input file, say BPIN0102.095, he has to copy that file to file BPINPT.DAT first. The objective of this file structure is to prevent accidental overwriting of the input file.

The coupling between the furnace code (2DHT) and the boiler code (BPM) is through the output data file BOILER.DAT generated by the 2DHT code. This file contains furnace information required by the BPM code. The information transferred by the BOILER.DAT file includes:

- Mean furnace gas temperatures
- Heat fluxes to furnace walls and to radiant heat exchangers in the upper furnace
- Flue gas mass flow rates
- Flue gas composition
- Furnace operational and fuel parameters.

Code Execution

To execute the BPM code, the user has to do the following:

- Install BPM.EXE in the working directory.
- Copy the input data file to file BPINPT.DAT.
- Have file BOILER.DAT ready in the same working directory.
- Type BPM and press "Enter".

The input data file is the one which contains the data of the boiler backpass to be modeled. This data file should be prepared by executing the input code BPINPT. BPINPT.DAT is the input file name used by the BPM code, therefore, steam/gas side calculations will be performed based on the contents of the file BPINPT.DAT. The user must copy the contents of his input data file to file BPINPT.DAT before executing the Boiler Performance Model.

Computerized Steam/water Tables

BPM uses a computerized steam/water tables for all thermodynamic calculations. The properties of saturated and superheated steams are calculated from interpolation formulae published by Irvine and Liley. These authors claim, that predicted enthalpies of superheated steam have a maximum error of less than 1 percent, over a wide range of pressures and temperatures.

The formulae have been tested by comparing the predictions with data in conventional steam tables. It was found that the saturation properties are predicted accurately, as are the superheated steam properties which reside in regions away from the saturation curve. However, errors somewhat larger than 1 percent were obtained for just superheated conditions at normal boiler operating pressures. Therefore, a special interpolation approach is included in BPM for this region. The user is advised to check predicted enthalpies and other properties occasionally with his own steam tables. This can be done easily, since BPM prints out enthalpies, temperatures, etc., at all important boiler steam/water locations. Calculations on the properties of pressurized water rely on the Maxwell relations. Again, an occasional check with the steam/water tables is useful, especially when the pressure approaches the critical pressure.

The interpolation formula used by the steam table, in principle, can be used to calculate steam properties when pressures are above the critical pressure. However, it should be noted that the current version of BPM can only be applied to boilers operated at sub-critical pressures. The reason for this restriction is, that the steam flow rate is currently controlled by the heat needed for evaporation of waters supplied to the furnace water walls and the economizer.

Boiler Type Considered

The BPM code considers two general types of boiler configurations. Figures 4.12 and 4.13 shows the outlines of the two boiler configurations (see also Figures 5.5 through 5.7).

The first type of boiler (ITYPE=1) is a so-called "tower" boiler, which has only one passage up to the economizer outlet. The second type of boiler (ITYPE=2) has a separate convective passage connected to the furnace by a horizontal transition section. These distinctions were made because the two types of boilers have different steam/water flow patterns. For both types of the boilers, the user can switch-off sections that he does not want to model.

Two particular heat exchangers of the Type 1 boiler can be treated by the "Triflux" mode (ITRIX=1) defined here. In this triflux mode, the tubes of a superheater and a reheater are intermingled in one volume section from the flue gas point of view. If the Triflux mode is not chosen (ITRIX=0), the two heat exchangers are treated separately like any other independent sections. Type 2 boiler can include a heat exchanger section and treat it as a boiler drum (IDRUM=1), i.e. as a water-cooled convective heat exchanger. If the option IDRUM=0 is used, this particular section is treated as walls cooled by the steam.

Figure 4.12. Outline of a tower boiler.

Figure 4.13. Outline of a two-pass boiler.

The BPM code considers steam/flue gas contacting patterns in terms of parallel and counter flows. Only single reheat is allowed for both types of boilers. However, the model can handle boilers which are operated without reheat.

Calculation of Heat Transfer

Solution of a coupled gas and steam/water side heat balance is carried out only for sections downstream of the user defined inlet plane. These sections are treated as heat exchangers with counter or parallel flows, depending on the particular boiler. Heat transfer calculations are based on the mean logarithmic-temperature differences. For example, heat flux absorbed by the steam/water side of a heat exchanger, in parallel flow pattern, is determined by:

$$Q = A h \frac{(T_{g,in} - T_{s,in}) - (T_{g,out} - T_{s,out})}{\ln \frac{T_{g,in} - T_{s,in}}{T_{g,out} - T_{s,out}}} \quad (4.76)$$

Index g in equation (4.76) refers to the gas side, and index s to the steam/water side. For heat exchanger sections in counter flow patterns, a formula similar to equation (4.76) is used. The symbol h denotes the overall heat transfer coefficient (kW/m² K) with respect to the tube outer diameter, including any ash deposits. A is the outer surface area (m²) of the heat exchanger exposed to the flue gas, including the contribution of the ash deposits.

Overall Heat Transfer Coefficient

Overall heat transfer coefficient (h) is one of the most important model parameters of the BPM code. It includes convective and also the radiative effects when tube temperatures are high. The impact of tube fouling and any other thermal resistance should also be considered in formulating this coefficient.

BPM neglects thermal resistance imposed by the metal conductivity and the steam/water streams. The overall coefficient is expressed as:

$$h = \frac{1}{\frac{1}{h_g} + \frac{ds}{k}} \quad (4.77)$$

where h_g is the overall gas side heat transfer coefficient, ds is the deposit thickness, and k is the deposit thermal conductivity. The formulation of h in the BPM code includes, however, the impact of tube curvatures.

The user can prescribe values of h_g for each heat exchanger section by setting ICALUS=0 and ITC=0 (details see Section 5.3). This option has the advantage that any radiative influence can be incorporated into h_g manually. As an alternative (ICALUS=1), the BPM code offers an option for automatic calculation of the heat transfer coefficient h_g . It should be noted that this option does not include any radiative heat transfer effect.

If performance data are available for certain boiler conditions, h can be determined indirectly for each convective sections, by matching the flue gas temperature distributions. The overall heat transfer coefficient so obtained can be used as basis to evaluate the coefficients at other operating conditions. For example, a Reynolds- and Prandtl Number correlation may be used to correct the impact of boiler load (i.e., the effect of flue gas volume).

Automatic calculation of the convective heat transfer coefficient, h_g , is based on formulas and guidelines developed by major boiler manufacturers. The calculation needs additional inputs as shown below:

- Outer tube diameter
- Flue Gas velocity
- Flue gas composition
- Mean gas temperature in tube boundary layers
- Tube arrangement factor, which depends on longitudinal and lateral pitches.

It should be mentioned that current version of the BPM code calculates h_g for in-line tube arrangements only. The equations used for the in-line arrangements may also be applied to staggered arrangements as an approximation. This should not affect model performance considering all other simplifications made. The BPM code also provides an option to automatically calculate the thermal conductivities of a generic ash-deposits. The conductivities calculated depend on mean deposit-temperatures of each heat exchanger section. This option can be activated by setting the switch ITC to 1.

Pressure Distribution

The BPM code does not solve the steam/water pressure distributions in the various boiler sections. The pressure distributions are user inputs. The interactive input program, BPINPT, may be used as a tool in setting up the pressure distributions. Only a few input/output pressures are required by the input code. A rough pressure assessment should be sufficient for boiler performance predictions.

Solution Algorithm

Heat balance equations such as eq. (4.76) are set-up for every heat exchanger section downstream of the user-defined inlet plane. The equations can also include the amount of heat transferred to wall sections surrounding the heat exchangers, and can take into account user-defined wall losses. Heat fluxes received by sections upstream of the inlet plane are provided by the 2DHT code or by the user, and are used in the overall steam/water heat balances. Parallel to the gas-side heat balances, steam/water mass balances are also set-up for steam-side calculations. The steam-side balances considers any steam attemperations. The gas-side balance equations are coupled through the heat exchanger inlet and outlet gas temperatures. The steam/water side heat balances are coupled through the steam inlet and outlet temperatures.

Boundary conditions required to solve the equations include:

- Heat fluxes absorbed by sections upstream of the user-defined inlet plane. For instance, heat fluxes absorbed by the furnace walls.
- Gas temperature at the user-defined inlet plane

- Attemperator control temperatures
- Economizer water inlet temperature
- Cold reheat inlet temperature
- Ratio of cold reheat flow to final superheated steam flow
- Attemperation spray water temperatures.

The system of balance equations is non-linear, due to the non-linear dependence of gas and steam properties on temperature, and due to the logarithmic expression as shown in equation (4.76). Further non-linearities are introduced if the user choose the option of automatic calculation of h_g (ICALUS=1), and/or the option of automatic calculation of deposit conductivities (ITC=1).

The non-linear equations are solved iteratively with the use of a Newton- Raphson/Gauss-Seidel method. In this method, initial guesses of the flue gas and the steam/water temperatures are upgraded when the heat balance equations are "swept". Each sweep is carried out from the user-defined inlet plane to the economizer outlet plane. At the beginning of the sweep, initial feedwater inlet flow is used, and attemperation sprays are added if required. In the next step, the initial feedwater flow is updated to match total heat absorption of the furnace walls and the economizer. Then the sweep is repeated, until solutions of all gas and steam/water temperatures and the steam/water mass flow rates are converged.

Air Preheater Module

BPM includes a simple module for air preheater energy balance calculations. The module does not take air leakages into account. The air preheater module will not affect the boiler efficiency predictions made by the BPM code, since the efficiency calculations are based on steam/water heat absorptions and the prescribed air temperature used by the 2DHT code.

Chapter 5

5.0 DESCRIPTION OF INPUT CODES

Each of the three main computer models (2DHT, RBNOX, BPM) discussed in the last chapter is accompanied by an interactive input-code for ease of input-data preparations. The three input codes are the 2DINPT, the RBINPT, and the BPINPT codes. This chapter describes the use of these three input codes and the required input-data in detail. The descriptions are presented in three major sections, with Section 5.1 devoted to the 2DINPT code and Sections 5.2 and 5.3 to the RBINPT and the BPINPT codes.

2DINPT is an input code for preparing a data file to run the Two-Dimensional Heat Transfer code 2DHT. Likewise, RBINPT is an input code for the Reburning NO_x model (RBNOX); and BPINPT is an input code for the Boiler Performance Model (BPM). The input codes 2DINPT and BPINPT can be used either to create a new input data file, or to update (i.e., modify) an existing data file. The input code RBINPT was designed to be used for updating an existing data file only. The user should consult Sections 5.1 to 5.3 for more information concerning the operation of the three input codes.

The description of each input code in Sections 5.1 to 5.3 follows a similar presentation format. Firstly, general background of a specific input code such as its capabilities/limitations and input/output file managements are presented. The description moves on to subjects of input requirement and the general input structure. Finally, the input-data required are discussed item- by-item, with particular emphases on parameters that need special attention from the user.

All the input codes use a consistent way of naming the input/output files. Figure 5.1 shows an overview of the file management structure.

Figure 5.1. File management structure for input codes.

The default output file names are termed as 2DINcsvs.III, RBINcsvs.III, and BPINcsvs.III, where cs is an user specified case number, vs is an user specified version number, and III is a character string extracted from an user specified parameter describing the boiler load. For example, if cs is 01, vs is 02, and the specified boiler load is 66.0 % relative to the MCR, the default output file name from the 2DINPT

will be 2DIN0102.066. Likewise, the other two default output file names are RBIN0102.066 and BPIN0102.066. The characters "IN" are referred to the main codes, since the outputs from the input codes are the inputs of the main codes. The user can overwrite the default output file names during the interactive input-sessions.

The default input file names are fixed, and are designated as INPUT.DAT, RINPUT.DAT, and BINPUT.DAT respectively for the three input codes. This means that if the user wants to modify an existing input data file, for example 2DIN0102.066, he has to copy that file to file INPUT.DAT before he executes the input code 2DINPT. The same convention applies to the input codes RBINPT and BPINPT. The objective of this file naming structure is to prevent accidental overwriting of the input files created by earlier user applications.

5.1 2D-Heat-Transfer Input Code (2DINPT)

2DINPT (Two Dimensional Input) is an interactive computer code which can be used to prepare an input data file needed to execute the two-dimensional heat transfer code 2DHT. The input code can operate in two modes: file creation and file updating (or modification). When the code is in the updating mode, a data file must exist so that it can be updated.

This section describes the use of the 2DINPT code in detail. The description begins with some background information relating to the code structure. The user is suggested to familiarize himself with the background information provided, before concerning too much about the model details. Model inputs are addressed item by item in later sub-sections.

2DINPT is designed to work on IBM or IBM-compatible personal computers. The code occupies a memory size approximately at 420 kilobytes (KB). The code accepts inputs in upper case only. Consequently, the user is advised to set his keyboard accordingly (i.e., Caps Lock).

During the course of an interactive session, 2DINPT communicates with the user through a number of statements in the form of "data-blocks". These data-blocks usually contain:

- Name, current value(s), and dimension(s) of the input variable(s) associated with a particular data-block
- Recommended default value(s)
- Available options and key strokes used to select the options.

Numerical input data can be supplied in any format provided that the number of significant digits is sufficient for the input variable under concern.

File Management

The default input file name is INPUT.DAT. The default output file name is 2DINcsvs.lll, where cs is an user specified case number, vs is an user specified version number, and lll is a character string extracted from a user specified parameter describing the boiler load. For example, if cs is 01, vs is 02, and the specified boiler load is 95.0 % relative to the MCR, the default output file name will be 2DIN0102.095. The user can overwrite the default output file name. However, the default input file name is always fixed as INPUT.DAT. This means that if the user wants to modify an existing file, say 2DIN0102.095, he has

to copy that file to file INPUT.DAT first. The objective of this file structure is to prevent accidental overwriting of the input files created earlier.

Input Requirement

Inputs required by the 2DINPT code may be grouped into two major categories: "essential" and "desirable" boiler data. The essential data represents data which are minimum requirement for the commencement of the furnace modeling work. Table 5.1 describes the contents of the essential data. In general this kind of data are easy to retrieve from the original boiler design sheets or blue prints. It is expected that provision of the essential information should not become a problem.

Table 5.1. Essential Boiler Data for the 2DHT Furnace Heat Transfer Model

Boiler Geometry

- Boiler height,width, and depth
- Boiler dimensions at the nose plane
- Locations and dimensions of the burner assemblies
- Firing configuration (tangential, wall)
- Boiler radiant tube bank locations
- Tube bank heat transfer surface areas (or alternatively, tube diameters, number of tubes)

Fuel Properties

- Proximate analysis
- Ultimate analysis
- Fuel heating value

Boiler operating parameters

- Fuel flow rates
- Total air flow rates (or excess oxygen %)
- Primary air flow rates
- Air temperatures (primary, secondary, underfire, overfire airs)
- Burners in operation
- Burner tilt
- Reburning fuel flow rates (or reburning zone stoichiometry) and injection locations
- Overfire air flow rates (or burnout zone stoichiometry) and injection locations

Table 5.2 lists the desirable data suggested for the 2DHT code. The desirable data means data which are useful and helpful both to the calibration of the model, and to the characterization of the boiler behavior itself. Lack of the desirable data will not disrupt the basic boiler thermal modeling work, since some data can be assumed based on engineering and previous modeling experiences. However, the desirable data as its name stands, is desirable in order to accelerate the model calibration process for the boiler of interest. The importance of the desirable data increases with the level of details that a boiler thermal performance evaluation should provide. Therefore, provision of the desirable data is highly recommended whenever possible.

Table 5.2. Desirable Boiler Data for the 2DHT Furnace Heat Transfer Model

Fuel Properties

- Coal particle size distributions
- Fuel moisture vaporized in the mill (or supporting data)
- Ash analysis (size distribution, softening temperature)

Boiler Operating Parameters

- Fuel distribution to individual burners
- Air distributions (i.e., to individual burners, over- and under- fire air ports)

Boiler Field Observations and Data

- Documents describing boiler slagging characteristics (e.g., visual observation of slagging patterns, slag thickness, and its distribution)
- Carbon in ash data
- Any observations relating to boiler flame pattern and length
- Data from field temperature measurements

Boiler Geometry

- Dimensions of the boiler radiant tube banks
- Radiant tube-bank geometries (tube diameter, spacing, number of tubes, arrangement)

Input Structure

2DINPT organizes the input requirement listed in Tables 5.1 and 5.2 into blocks of data and labels them in the form of chapters. The code advances through each of these chapters but allows the user to skip chapters where no changes are to be made. At any chapter, the user can also exit the program by entering a designated key stroke. 2DINPT will save changes that had been made in an user specified output-data-file.

Typical information displayed for each input data includes: the variable name, current value, a brief explanation of the variable's meaning, any default or recommended values, and a list of options for selection. The user may then select one of these options. The options will generally include: leaving the current value unchanged; changing to a value specified by the user; or assigning a default value to the variable.

The following paragraphs describe the sequence of the input chapters. The chapter numbers shown may not be consecutive because reservations have been made for future code expansion.

Chapter 1: Input/Output Specifications and Parameters Which Control the Extent of Numerical Calculations.

In this chapter, the user can specify or modify names of various input and output files, the user's comments, and the level of output details he prefers. The user can also specify some numerical parameters to control the extent of the model calculations.

CHAPTER 2: BOILER FURNACE OPERATING DATA.

This chapter specifies furnace operating data such as fuel type, fuel/air mass flows and temperatures, and the fuel analysis. Waterwall heat transfer coefficient and the furnace cool-side- temperature are also specified here.

CHAPTER 3: INITIAL PARTICLE SIZE DISTRIBUTION.

This chapter specifies initial coal or droplet size distribution if the furnaces are coal or oil fired. For a gas-fired furnace, no input is necessary.

CHAPTER 4: PARAMETERS FOR CHAR AND VOLATILE BURN-OUT.

This chapter specifies some physical and chemical kinetics parameters associated with fuels combustion (including char, soot, and volatiles).

CHAPTER 5: PARAMETERS FOR ASH REACTIVITIES.

This chapter specifies only one input parameter which describes the fraction of total sulfur retained in the ash. This sulfur is also called "pyritic sulfur" by the code.

CHAPTER 7: SPECIFICATION OF FURNACE MODEL GEOMETRY.

This chapter sets the 2D furnace model geometry. The user can modify or specify geometry parameters such as the number of volume zones in the axial and radial directions, the grid locations, and the shape of the model furnace.

CHAPTER 8: PARAMETERS FOR REBURNING OR CO-FIRING.

If gas reburning (or co-firing) option is selected, the user can input parameters related to the reburning applications, e.g., reburn fuel mass flow and compositions, injection locations, flue gas recirculation (FGR) mass flow, and the reburn fuel and the FGR temperatures.

CHAPTER 9: SPECIFICATION OF HEAT EXCHANGERS.

If the user exercises the heat exchanger option, he will be requested to provide data relating to the heat exchangers. The data includes the location, surface area, and the tube diameter of each heat exchanger. The user also have to specify heat exchanger boundary conditions, including steam side metal temperatures, the initial heat-exchanger surface temperature, as well as surface emissivities.

CHAPTER 11: RELATIVE MASS FLOW RATE DISTRIBUTION.

This chapter prescribes the relative inlet and outlet mass flow rates at boundary zones. Following the prescription, mass fluxes across each internal grid lines can be generated by a computer-aided option. The user may also select direct prescription to input these mass fluxes zone-by-zone. The computer aided option is carried out in two parts. In the first part, the user can use a default plug flow or create a flow

field to describe the boiler forward flow field. He then can superimpose a recirculation flow field on the forward flow, to establish a complete boiler flow field.

CHAPTER 12: PRESCRIPTION OF RECIRCULATING FLOW FIELD.

The user can establish a recirculation flow field in this chapter. This flow field can be prescribed at each grid lines in the furnace axial direction. The user has to provide recirculation mass percentages, and describe recirculation profiles at each location where flow recirculation occurs.

CHAPTER 13: PRESCRIPTION OF TURBULENT MASS FLUX VECTORS.

This chapter can be used to establish a turbulence flow field so that it can be superimposed to the mean flow field as explained in Chapters 11 and 12. Mass flows and velocities are reported throughout the flow field and turbulence specification chapters. Residuals of the mass balances at each volume zones are also shown. If mass continuity is satisfied, all of the residuals should be zero.

CHAPTER 14: FUEL INLET FLOWS.

In this chapter, the fuel mass flows through each burner are specified as fractions of total fuel inlet flow.

CHAPTER 15: DATA FOR INITIAL VOLUME AND SURFACE ZONE TEMPERATURES.

This chapter specifies initial values of gas and surface zone temperatures.

CHAPTER 16: DATA FOR EMISSIVITIES AND DEPOSIT CONDUCTIVITIES.

This chapter specifies the emissivity and the deposit thermal conductivity to thickness ratios for all surfaces, including the furnace walls and the heat exchanger surfaces.

After completion of the input chapters, a message will be displayed to show the name of the output file where 2DINPT writes the input data.

2D Grids

Figure 5.2 is a diagram which shows the transformation of a typical 3D boiler configuration into a 2D zone arrangement. The general rule of thumb in the transformation is to keep the furnace volume the same. By keeping the grid to represent the same volume as in the actual furnace, residence times which is an important furnace parameter, can be preserved.

The surface areas of the furnace walls may not be preserved as the design when the residence times are preserved. This will in general have some slight impact on the predicted waterwall heat absorptions. This concern in general can be excused. Past modeling experience has shown that the assumed deposit conductivity/thickness ratios have greater impact on the predicted heat absorptions. The user can lump his surface area considerations together with the specification of the deposit conductivity/thickness ratios. More detailed discussions on the deposit ratios are presented in later sub-sections.

Figure 5.2. 2D representation of a 3D boiler configuration.

For the hopper, the calculation of dimensions based on volume and surface area requires further attention because layers with different radii are involved. However, it is less critical to exactly match surface area in the hopper as this section usually does not contribute as much to the total wall heat transfer as the lower and upper furnace. A minimum of two radial layers in the bottom hopper layer is suggested. This allows a better specification of recirculation in this zone.

Special Key Functions

There are some frequently used keys by the 2DINPT code. These keys are: C, D, P, Y, N, R, and the Return (or Enter). In general, key C designates that the user prefers a "Change" on model inputs, or to "Create" a new input data file. Key D is used for selecting "Default" values. Key P is used to "by-Pass" a chapter or a block of input data. Key Y represents "Yes" and is used only to answer few input prompts. Key N has opposite meaning as compared to key Y discussed here. Key R is used to exit the program and automatically saves the input file created by the 2DINPT. The Return key is used to advance the interactive input session without changing the value of any existing data item.

File Creation Using 2DINPT

If 2DINPT is being used for the first time, the user should be familiar with the type of input data required. The user must also understand notations used to describe the 2D zone arrangement, the mass fluxes, and the four surface sections ranging from M=1 to M=4.

The following two steps must be exercised to begin a file creation session:

- Install 2DINPT.EXE in the user's working directory.
- Type 2DINPT and press "Enter".

2DINPT then asks the user whether a file creation or file update session will follow. At that moment, enter C and press Return. After all the above steps are completed, the user is in the file creation mode.

In the creation session, 2DINPT will create a blank version of the input data file INPUT.DAT. The data in this file will be filled-in with zeros as initial settings. Later, the blank data will be replaced by the user's inputs as the input session continues.

Entering wrong data can occur. There are several ways that 2DINPT responses to the wrong inputs:

- The format of the input data is wrong. For example, a character is mistakenly entered and 2DINPT expects to read-in a numerical number. Under this circumstance, 2DINPT will display a warning message then return to an earlier input section. The user can press Return and advance to the input item where the error had occurred. Subsequently, the user can press C and enter the correct value.
- 2DINPT detects an un-acceptable input data. In this case 2DINPT will not proceed until an acceptable input is given.

- The user entered an input data that he does not intend to do so. In this case, he is recommended to continue the session as if no error had occurred (but takes notes). After the file creation session is completed, he can re-run 2DINPT under the update mode (see next section) to correct the errors made. Entering "Return" frequently in order to proceed to the end of a file creation session is not recommended.

Updating Input Data File Using 2DINPT

The following procedures are required to update an input data file needed to run the heat transfer code (2DHT):

- Install 2DINPT.EXE in the user's working directory.
- Copy the file to be updated to file INPUT.DAT in the same directory.
- Type 2DINPT and press Return. The interactive code will start prompting the user to enter the required inputs.
- When 2DINPT shows "STATUS OF INPUT FILE", press Return to choose the updating mode.

After these procedures are completed, the system is in the proper updating mode. The user can proceed to the chapter he wishes to make changes by pressing P. After reaching the chapter, he can press Return and proceed to the specific input blocks and make changes.

The updating mode can also be used simply for checking existing input data. If no data are changed, the output file from an updating session may not be exactly the same as the input file (INPUT.DAT). This is due to some small truncation errors in the flow field set-up. However, this by no means can affect model performance predictions.

2DINPT allows the user to change grid numbers (NX and NY) during an updating run. The user has to be extremely careful to make sure input data are modified accordingly with the new grid dimensions.

2DINPT writes the updated file to file 2DINcsvs.lll, where cs is the user specified case number, vs is the version number, and lll is the boiler load. If this file already exists in the same directory, the code will ask the user whether he wants to over-write the file contents. The user can specify any other file name, with a maximum of 12 characters, if he prefers not to over-write the existing file. If an user does not specify the case and version numbers, the updated file will have a name exactly as "2DINcsvs.lll".

Description of Specific Input Items

This subsection discusses the 2DINPT inputs item by item. Since a large part of the inputs are self-explanatory, the discussion will focus on items which need special user attention.

Input/Output Parameters—The first input section addressed by the 2DINPT code concerns specification of input/output file names, user's comments, and numerical controlling parameters. Some of the character inputs such as boiler name, case and version numbers, as well as load percentage are needed only for the completeness of the output. This information helps the user to organize and quickly identify files he may wish to work on later.

The name of the output-data-file generated by 2DINPT is 2DINcsvs.lll by default, where cs is the case number, vs is the version number, and lll is the load percentage specified by the user. This default name is recommended to use.

File name for the input arrays, which supply variable solutions obtained from a previous run, is not required when 2DHT is executed from scratch (i.e. with NREAD=0). The user may supply an arbitrary name just for the sake of proceeding through the 2DINPT code. For a continuation (or restarting) run, the name of the file containing previous solutions should be specified correctly as "the name of the input array file".

2DHT writes output information to a disk file with a default name 2DOTcsvs.lll. If the user prefers the output be directed to his screen monitor, he has to specify the output file name as characters "CON". In this case, output information will not be saved as disk files.

The amount of output information is controlled by a parameter LOUTPUT. Lower output level, for example LOUTPUT=1, yields the most concise output. The highest output level, LOUTPUT=4, yields the most comprehensive output. In general, output level 4 should be used only for debugging purposes, and output level 1 is recommended when extensive parametric studies are planned. 2DINPT recommends the user to use a default-output-option by pressing D. The default option generates detailed furnace performance information after an user specified iteration number has been reached.

Numerical Parameters — These parameters include: the maximum number of iterations allowed, NIMAX; and the iteration number (NITACC) at which an averaging process is activated to smooth out Monte-Carlo fluctuations.

NIMAX and NITACC should be determined such that after 2DHT runs, the overall heat balance is converged and the Monte-Carlo fluctuations are sufficiently smoothed out. In most model applications, the total heat balance is considered as converged when each of the following three conditions are met:

- (1) The absolute value of the "actual error" is less than 1 % at the last iteration.
- (2) The absolute value of the last "20 iteration error" is also less than 1 %.
- (3) The averaging process had been started when the "20 iteration error" was below 1 % and does not fluctuate very much.

The number of iterations required to meet these conditions also depends upon parameters NMAX and NPHI, which determine the number of beams to be tracked, and also on the beam cut-off value, EXACT. Provided that default values of NMAX, NPHI and EXACT are used, the user is recommended to use NIMAX=100 and NITACC=71 when the 2DHT code is run from scratch. In this case, NITACC=71 means that the radiative heat fluxes computed by the radiation model are averaged over the last 30 (i.e., $100-71+1=30$) iterations. The execution of the heat transfer code will be terminated after 100 iterations.

When the user is uncertain about the values he should use for NIMAX and NITACC, in particular when a new run is started from scratch, the following procedures are recommended to follow:

- Run the new boiler set-up with a few iterations but not to activate the Monte-Carlo averaging process. For instance, set NIMAX=10 and NITACC=10. Any input errors detected in this stage should be corrected.

- Run the model with NIMAX approximately equals to 50 but not to activate the averaging process (i.e., NIMAX=50, NITACC=50).
- Check the convergence of the total heat balance as discussed above. If criterion (3) as shown above is not satisfied, carry out continuation runs (without the averaging) until it complies.
- When criterion (3) is fulfilled, carry out a final run with NIMAX approximately equals 40 and NITACC=11.

If the user wants to reduce computational time, the initial model runs may be carried out using a relatively smaller number of beams (e.g., NMAX=1 and NPHI=2). The beam number can be increased starting from the second run and for the final run.

Continuation Runs — A 2DHT continuation run may be required for the following reasons:

- The iteration number (NIMAX) of a preceding run was not sufficient to achieve the convergence of the total heat balance.
- The number of iterations, where the averaging process was performed (i.e., NIMAX-NITACC+1), was not sufficient to obtain the desired smoothing on furnace variables.
- Perturbation of input variables. The user plans a series of model applications and changes model input parameters parametrically .

A continuation run needs a restarting file to provide values of all furnace variables so that the calculations can continue from the end of a preceding run. To create the restarting file, the output control parameter of the preceding run, NWRTE, should be set to 1. In this case, arrays containing values of all furnace variables will be written to an output array (or a restarting) file, normally with a default name OARRcsvs.lll, at the end of the run. In the following it is assumed that the name of the output array file was OARR0101.100.

During model set-up for the continuation run, the input control parameter, NREAD, should be set to 1. The user also has to specify the name of the input array file for the continuation run. The output array file of the previous run is then used as the input array file of the continuation run. For example, the user must copy file OARR0101.100 to file IARR0102.100, to serve as the input array file for the continuation run.

To avoid overwriting output array file OARR0101.100, output array file of the continuation run should have a different name, for example, OARR0102.100. Similar action may be taken to avoid over-writing other output files such as files 2DOT0101.100 and BOILER.DAT. The output array file generated by the continuation run may be used as the input array file of any further continuation runs.

Furnace Operating Parameters — Entering data in this category is quite simple if the user has prepared the furnace operating data a priori.

(a). Fuel type

Fuel type is referred to the burner fuel and is controlled by three input parameters: NGAS, NLIQ, and NSLL in the model. These parameters specify whether the fuel is in gaseous, liquid, or solid form so that 2DINPT can proceed properly in later input sections. Each parameter can be switched on or off by

assigning its value to 1 or 0, respectively. For example, setting NGAS=1, NLIQ=0, and NSLL=0 indicates the furnace being modeled is gas-fired.

When a gaseous or liquid fuel is selected, the model treats the fuel as a solid fuel having very high volatile content. 2DINPT may show that proximate analysis of a gaseous fuel is, for instance, PCFX=0.0001, PVOL=0.9999, PMOI=0.0000 and PASH=0.0001. Setting fixed carbon content to 0.0 (i.e., PCFX=0.0000) could lead to some undefined values during 2DHT execution and should be avoided. When gaseous or liquid fuels are fired, the value of CMCVLS which is used to indicate flame zone soot concentrations should also be set appropriately in later input sections.

The small amount of "fixed" carbon used to simulate the gaseous fuel has no influence on furnace predictions. 2DINPT will set several default parameters to make sure that this carbon is practically all burned while numerical stability is conserved. Some radiation parameters related to the "fixed" carbon will also be set to 0.0 internally to eliminate the "fixed" carbon contribution.

(b). Overall furnace stoichiometry

Overall furnace stoichiometry can be specified by providing values to one of the following three parameters:

- Total wet air flow rate, DMA2W (kg wet/s)
- Overall air number (i.e. air/fuel ratio), AIRNR
- O₂ concentration in flue gas based on complete combustion, FLUO2D (Vol. %, dry).

The other two parameters not chosen for the input should be set to zero.

(c). Temperature of water wall tubes

This input parameter has a name as TOUT, and represents the surface temperature of the furnace walls. TOUT may be estimated from the saturation temperature of a given drum pressure. Normally, a drum saturation temperature plus 30 to 60 K is a good choice. The 30-60 K temperature-addition accounts for heat transfer resistance of the metal, and some finite values of the water-side heat transfer coefficients.

(d). Initial particle size distribution

For coal-fired furnaces, initial particle sizes are described by the use of two parameters: XMN0(L) and CMFR(L). Coal particles are represented by 10 size classes with each class having an average diameter of XMN0(L) and mass fraction CMFR(L), where L is the size index. 2DINPT offers default values for the two inputs. The size distribution can also be derived from data obtained from the mill.

2DINPT requires that the initial particle diameters, XMN0(L), are supplied in order of increasing XMN0(L). 2DINPT will provide a message if this is not the case, and will not proceed until this requirement is satisfied. The code also checks whether mass fractions of the 10 size classes add up to 1.0000. The user is responsible to make sure that each mass fraction corresponds to the intended diameter class.

For oil-fired furnaces, 2DINPT also provides a default size-distribution for the oil droplets. This default is derived from experimental data using a Y-jet, steam atomized nozzle. The user is recommended to use this default. The size distribution of the oil droplets will not influence furnace overall predictions, since the model actually treats the droplets as volatile lumps. The model does not perform ballistic trajectory calculations for the droplets due to its decoupled nature. However, this type of data is necessary for unburned carbon predictions if the fixed carbon content of the oil is high.

Data for initial particle size distribution is not required if the furnaces are gas-fired.

Empirical Model Parameters — In addition to the mean flow field and the heat sink boundary conditions, the user has to provide several empirical model parameters. These parameters are used to describe properties and combustion characteristics of the fuel. 2DINPT offers default values for these empirical parameters.

(a). Inherent sulfur capture

Default value for inherent sulfur capture by ash is 0.0. This parameter only affects the flue gas SO₂ concentration and has little effect on furnace thermal performance predictions. In lignite-fired boilers, inherent capture can be as high as 40 %. In bituminous coal fired boilers the inherent capture is usually much smaller, and an assumption of 0.0 is often justified.

(b). Evaporation of fuel moisture

The percentage of fuel moisture vaporized in mills is important for high moisture coals. When external flue gas recirculation is used for coal drying, 100 % evaporation may be assumed. A more accurate assessment has to be made by the user himself, based on heat and mass balances on the mills. Any assessment of the mill evaporation also has an impact on the temperature of the primary fuel/air mixture, which is also an input.

(c). Constants of char combustion model

Char combustion is described by an Arrhenius' rate equation. The user has to input three reactivity constants, and they are the activation energy, the frequency factor, and the so-called Q-factor. The Q-factor indicates the amount of actual volatile yield with respect to the yield indicated by the proximate analysis. These constants strongly influence predictions of carbon-in-ash percentages, and moderately influence the intensity of heat release near the burner zones.

2DINPT offers sets of default values for three generic coals, namely, a very high volatile western bituminous coal, a high volatile coal, and a medium volatile coal. The default values are often sufficient for heat transfer performance predictions. If the user is interested in more accurate predictions on carbon-in-ash content, it may be necessary to "calibrate" these char parameters based on baseline burnout data. In doing so, it is advisable to keep the activation energy at the default value and to change the frequency factor only, until baseline carbon burnout is matched.

There are limitations on the increase of the frequency factors. Therefore, highly reactive coals also require increases in the Q-factor. Note that some lignites are very reactive, consequently, the Q-factor may have to be increased to 1.8 to match the baseline carbon-in-ash data.

(d). Constant of volatile combustion model

The most important parameter for burner-zone heat-release is the burn-out time of volatiles, TLFMAX. This parameter can be interpreted as an averaged time required for burn-out of a volatile fuel lump down to 0.1 % of its original mass. The constant includes the effect of fuel/air mixing, and effectively determines the locations of visible flames in the furnace. Its value depends on burner design characteristics. The user may need to calibrate this parameter based on baseline data if global flame locations were known.

Past experience has shown that a burn-out time of 0.7 sec (the default value) characterizes fairly well the heat release pattern in medium-sized boiler furnaces. However, a scale effect can be observed. This is shown in Figure 5.3, in which time constants used in previous studies are plotted over full load capacities of the various boilers investigated. Figure 5.3 also shows an empirical relationship for flame extension over capacities based on results from previous modelling studies. The user may use Figure 5.3 in order to determine TLFMAX for a particular application.

Figure 5.3. Volatile burn-out time based on previous modeling studies. Burner capacity based on full-load operation.

Reburn or Co-firing — One major capability of the 2DHT code is that it can model boiler reburning/co-firing applications. To activate the reburning/co-firing application, the user must set the parameter NREB to 1. The current version of the code only allows gaseous fuel as the reburning/co-firing medium, although reservations have been made in the 2DINPT code to allow future inclusion of reburning/co-firing applications involving liquid fuels.

If reburning application is selected, the user needs to input additional parameter values to describe the properties of the reburn fuel. These values include the reburn fuel flow rate, temperature, heat capacity, lower heating value, and moisture content. If part of the boiler flue-gas is recirculated (FGR) and mixed with the reburn jets to enhance jet penetration and mixing, the user also has to specify the FGR flow rates and temperature.

The injection locations of the reburn fuel are described by "the mass injection-profiles" in the J- (or Y-) or I- (or X-) directions, referred to the 2D zone arrangement. Normally for boiler reburning, the reburn fuel is injected into volume-layers in the I-direction (i.e., along the furnace axial direction). As an example, if 60 % of the reburn fuel is injected at zone I=11 and the balance of the reburn fuel injected into zone I=12, the reburn-fuel injection profiles at I=11 is 0.6 and at I=12 is 0.4.

The structure of the 2DHT code allows coal/gas, liquid/gas, and gas/gas co-firing, since reburning actually can be viewed as a process which combines fuel staging and co-firing applications. For fuel co-firing, the user has to treat the "reburn fuel" as the fuel to be co-fired with the fuel through the burners. No additional input is required for the co-firing applications.

Soot Radiation — 2DHT has a simple module to calculate zonal soot concentrations. This module requires specification of a parameter, CMCVLS, to describe the fraction of volatile carbon converted to soot. Default values are 0.1 for high volatile bituminous coals, 0.05 for lignites, and 0.2 for heavy oil flames. Zonal soot concentrations are related to the progress of the volatile burnout through the parameter CMCVLS.

CMCVLS can influence flame emissivities near the burner zones and therefore burner zone heat transfer. A detailed assessment on this parameter is out of the scope. However, the impact of CMCVLS decreases with the increase of boiler size. This is due to the fact that large flames behave like black bodies. Any further increase in soot concentration have less effect on the flame emissivity, except at the tail end of the flame.

Ash Radiation — Ash radiation can be important in furnace sections not occupied by the flame. It's impact on furnace heat transfer depends on ash concentration and optical properties of the ash cloud. The optical properties of the ash cloud are influenced by fuel properties and boiler operating conditions in an extremely complex way. 2DHT has incorporated a gray ash model to account for ash radiation.

The model neglects scattering by ash particles. Gray ash radiation is characterized by a specific ash absorption coefficient, SKASH, in units of $1/((\text{kg}/\text{m}^3) \text{ m})$. The user must specify a value for this parameter. The input program offers a default value of SKASH assessed from the initial coal size distribution. Ash absorption efficiency is assumed to be 0.1 during the default calculation. This efficiency is chosen to be relatively small in order to compensate for the scattering effect, which normally reduces overall radiative heat transfer to boiler heat sinks.

Specification of Radiant Heat Exchangers — 2DINPT allows simulation of radiant heat exchangers in the upper furnace. In this simulation, actual tube banks in a zone layer I is replaced by NSHS(I) number of concentric panels. Each panel has NTUBE(I) number of tubes arranged in shapes of horizontal tori. The panels are spaced equally toward the furnace walls of the 2D model, i.e., the Y-direction.

Actual inputs to simulate the 2D heat exchangers are guided by the 2DINPT code, based on user supplied information describing actual design of the heat exchangers. The user must first decide the locations of the heat exchangers in terms of I-zone layers. A radiant heat exchanger can occupy more than one I-layer. In this case, it becomes necessary to determine the distribution of the heat exchanger surface areas in the various I-layers. Usually, the split ratio should be proportional to the axial zone heights, DX(I).

To simulate the heat exchangers, the user has to choose Option C when 2DINPT displays the text "Heat Extraction by Heat Sinks". No radiant heat exchangers will be simulated if Option A is chosen. Option B allows for consideration of cooling panels arranged on the side walls of small furnaces by refractory lining. Option B has not become available yet and the user should not use this option.

The user then has to specify the lowest I-layer, ISHL, and the highest I-layer, ISHU, of the zone arrangement occupied by the heat exchangers. A cavity-layer can be represented by specifying 0.0 as the heat exchanger surface area. For each occupied layer, the user has to provide the heat exchanger surface area as well as the outer diameter of the heat exchanger tubes. If the tube diameter is not known, any estimation on the order of 0.03 to 0.08 m is sufficient for heat transfer predictions.

2DINPT offers three options for the heat exchanger simulation:

- Option A: in which the user prescribes the number of cylindrical panels, NSHS(I); and the spacing of the panels in the radial direction, DEL(I)
- Option B: in which the user prescribes the number of tubes, TUBE(I), in the X-direction; and the radial panel-spacing DEL(I)
- Option C: in which the user prescribes the longitudinal pitch of the heat exchanger design, ELL(I). ELL(I) is defined as the ratio of tube spacing in the flow direction divided by the tube outer-diameter.

Regardless which option is chosen, 2DINPT will always arrange the panels in a way that they are evenly spaced by DEL(I) in the radial direction, starting from the furnace axis. The spacing between the last panel and the surrounding furnace walls can be larger or smaller than DEL(I). The total surface area is always preserved.

In Options A or B, some arrangements may not be possible for a chosen input parameter. For instance, if the number of panels is too small, the tubes contained in one panel may not fit into the given axial zone height, DX(I). 2DINPT will indicate these situations and allow the user to repeat his inputs with modified specifications.

(a). Heat sink boundary conditions

After the heat exchanger geometrical specifications have been completed, the user moves on to prescribe some physical data concerning characteristics of the heat sink surfaces. These data are:

- Initial gas side surface temperatures, TWSINK(I,J) in K
- Surface emissivities, EWSINK(I,J)
- Ratio of deposit conductivity to thickness, CSSINK(I,J) in kW/m² K
- Temperature of the deposits on the metal side, TOUTSH(I,J).

To input the first three items listed above, the user is suggested to follow the same guidelines as described later for the furnace wall surfaces. The metal side temperature of the deposits can be estimated from the design steam temperature or boiler performance data. In order to take account moderate heat transfer resistances occurred in the metal and the steam side, TOUTSH(I,J) should roughly be the mean steam temperature plus 20 to 50 K.

(b). Convective heat transfer coefficients

Convective heat transfer coefficients, ALSH(I,J) in kW/m², must be prescribed as inputs for every volume zones occupied by the heat sink surfaces. ALSH(I,J) is based on the outer surface of the deposit layer surrounding the tubes.

In most cases, it is sufficient to assume an uniform distribution of ALSH(I,J) over an I-layer. Default value is 0.05 kW/m² K. More accurate values can be obtained by using the input code of the boiler performance model (BPINPT) as a tool. With the parameter ICALUS set to 1, the BPINPT code can calculate convective heat transfer coefficients based on tube geometry, tube arrangement, flow rates, and thermal properties of the flue gas.

Flow Field Prescription — The furnace code 2DHT does not solve momentum equations. Furnace flow distribution has to be prescribed by the user as inputs.

Experience has shown that in many cases details of the flow prescription only have moderate impact on furnace performance predictions, provided that the bulk flow behavior is described properly. This is because the dominate impact of radiation on furnace heat transfer, and the accurate treatment of radiative heat transfer by the 2DHT code.

Guidelines for the flow field set-up will be provided later. These guidelines are based on accumulation of experience gained from numerous isothermal physical modeling, various model applications, and from comparison of predictions with the boiler field data. Users that are new in this area are strongly recommended to acquire some experience in flow field set-up before commencing his formal model applications.

(a). Mass flux definitions

The 2DHT code requires specification of relative mass flux vectors over four boundaries of each of the furnace volume-zones to perform total heat and species mass balances. The term "relative" means that magnitudes of all the vectors are normalized by the total mass flow rate (DMTOT) through the boiler. The relative mass flux vectors used in the 2DHT code, and consequently in the 2DINPT code, are defined in the following way:

- DM1(I,J) is the magnitude of the vector normal to the lower boundary of a volume zone I,J pointing in the positive X-direction.
- DM3(I,J) is the magnitude of the vector normal to the lower boundary of a volume zone I,J pointing in the negative X-direction.
- DM2(I,J) is the magnitude of the vector normal to the inner boundary of a volume zone I,J pointing in the positive Y-direction.

- $DM4(I,J)$ is the magnitude of the vector normal to the inner boundary of volume zone I,J pointing in the negative Y-direction.

These mass fluxes always have positive signs. 2DINPT expects that the user is familiar with the index notation of the various mass flow fluxes.

2DINPT breaks up the input of the relative mass flux distribution into five steps:

- Prescription of the inlet mass flow rates
- Prescription of the outlet mass flow rates
- Prescription of the internal flow distribution
- Superposition of recirculation
- Specification of turbulence.

These five steps are described in the following by order of appearance.

(b). Inlet mass flow rates

The prescription of inlet mass flow rates is only allowed for boundary zones in the $M=1$ and $M=4$ directions. The inlet mass fluxes specified are $DM1(i,j)$ and $DM4(i,j)$. 2DINPT guides the user through all allowable inlet zones, and requests for the inlet mass flow rates.

2DINPT expects that the user can identify inlet zones of burners, overfire air, and any other furnace inlets such as reburning jets. Knowledge on the relative mass fluxes of these inlets is also required. After all inlet mass fluxes have been entered, 2DINPT checks whether their sum adds up to 1.0000. If the sum is smaller than 1.0000, the user will be forced to repeat his inputs.

(c). Outlet mass flow rates

Relative outlet mass fluxes can be prescribed over all volume zone boundaries in directions $M=1$ through $M=4$. However, boiler outlet zones are usually in the $M=3$ direction.

A volume zone can not be prescribed as both an inlet and an outlet zones. If this occurs, the user has to repeat his inputs for the inlet and the outlet mass fluxes.

Three options are available in prescribing the outlet flow distribution over outlet zones at $M=3$:

- Option A: Zone-wise prescription
- Option B: Use profile factors
- Option D: Plug flow distribution.

In Option A, the user prescribes the magnitude of the outlet mass fluxes in the same way as for outlets at $M=1$, $M=2$ or $M=4$.

Options B and D assume that the sum of the total mass fluxes exiting the outlet zones at $M=3$ is 1. Option B uses profile factors to calculate the outlet mass fluxes. Profile factors are normalized velocities of the outlet zones, and have values equal or larger than zero. Based on the factors prescribed and the outlet flow areas, 2DINPT calculates the relative outlet mass fluxes $DM3(i,j)$. The profile factors have to be supplied

in order of increasing J indices and separated by commas or blanks. 2DINPT does not save the values of the outlet profile factors. The user is therefore advised to keep a record of the factors applied. Use of profile factors to describe internal flow distribution will be explained later in this sub-section.

If the user chooses the default Option D, 2DINPT calculates outlet mass fluxes assuming plug flow conditions prevail over the outlet zones at $M=3$. In this case, all profile factors are internally set to 1.0 for the outlet zones at $M=3$. 2DINPT will ask the user to repeat the inputs if it detects that the sums of all inlet and outlet mass fluxes are not equal.

(d). Internal mass flux distribution

Internal mass fluxes are fluxes across individual volume zone boundaries, except those coincide with the 2D boundary zones. Two choices for the input of these internal mass fluxes are available:

- Option A: Direct prescription of $DM1(i,j)$, $DM2(i,j)$, $DM3(i,j)$ and $DM4(i,j)$.
- Option B: Computer aided prescription, where several options are available.

2DINPT checks mass continuity throughout the volume-zone flow-field. Discrepancies will be reported if the option of direct prescription is chosen. The radial mass fluxes will be adjusted if the discrepancies exist and the computer aided option is selected, to satisfy the continuity requirement.

(d-1). Direct prescription

If the user has pre-determined mass fluxes for all the internal zone-boundaries, he may use this option to construct a boiler flow field. Using the 2DINPT to input these mass fluxes is straightforward. The extent of the direct prescription, however, can vary. Some of the possibilities are:

- The user prescribes all mass fluxes of the boiler furnace, except turbulent contributions. The user subsequently uses one of the options offered by the 2DINPT to include the turbulent effect on the mean flow field. This is the most common case.
- The user prescribes all internal mass fluxes, including the turbulent contributions.
- The user prescribes only the forward mass fluxes (potential flow). Later, the user uses the 2DINPT options to superimpose recirculation mass fluxes and turbulent contributions.

Independent of how the direct prescription is performed, mass continuity must be fulfilled for all volume zones. 2DINPT checks for continuity and displays zone indices where continuity is not satisfied. If mass continuity is not preserved, 2DINPT will not proceed until input errors are corrected.

(d-2). Computer-aided prescription

If computer aided prescription is chosen for prescription of the internal mass fluxes, three options are provided for further selection:

- Plug forwarding flow in the positive X-direction (the Default option). The forward flow starts at the first horizontal grid plane downstream of the lowest burner or inlet. All mass fluxes up to the furnace exit are automatically calculated. The user may superimpose recirculation flows on the forwarding plug flow later.

- Option A: The user assigns profile factors of the forward flow. The forward flow starts at the first horizontal grid plane downstream of the lowest burner or inlet. All mass fluxes up to the furnace exit are automatically calculated based on the prescribed profile factors. Later, the user may superimpose recirculations or turbulence on the forward flow.
- Option B: The user prescribes velocity profiles for each horizontal grid plane. The velocities should be normalized by the mean velocity over the largest furnace cross-section. All internal mass fluxes in the furnace are then automatically calculated.
- Default plug flow

Using this option to set-up the forward mass flow field is straightforward and quick. In many cases, a plug flow superimposed with a coarse estimation of the recirculation pattern is sufficient for overall furnace performance predictions. The superposition of the recirculation flow will be discussed later.

- Use of profile factors

Use of the profile factors has been briefly explained before, for the outlet flows at $M=3$. Here, the same technique is used for each horizontal grid plane except at $I=1$ and $I=NX+1$. Figure 5.4 shows an example of the profile factors. Contrary to those of the outlet flows, these factors can have positive and negative values. The user is recommended to use only the positive values, since a negative value would lead to recirculation toward the negative X -direction and is best described in the recirculation section. The absolute magnitude of the factors may differ from plane to plane. Within a particular plan, the forward velocities are determined by the relative magnitude of the profile factors.

Figure 5.4. Specification of forward flow-field using profile factors.

At each I-plane, the factors should be supplied in order of increasing J-indices, separated by commas or blanks. 2DINPT will create a data file with name FORWA.DAT after the input process is completed. This data file will be used for file updating if it exists in the user's working directory. If the user changes profile factors of the forward flow during a file updating session, the contents of file FORWA.DAT will be over-written to reflect the profile modifications.

- Use of normalized velocities

This option allows the user to set up a complete mass flux distribution from scratch. The user must prepare velocity profiles normalized with the mean velocity calculated from the largest horizontal cross-section of the furnace, total mass inputs, and a constant density of 1. Use of negative values for the normalized velocities are acceptable.

When the computer-aided options are exercised to determine internal mass fluxes, 2DINPT displays firstly current values of the normalized velocities in the X-direction. After user inputs are completed, normalized velocities in the Y-direction, as calculated by the 2DINPT, are displayed. Although using the computer-aided options generally ensures mass continuity, a continuity check for every volume zone is still carried out, and the resulting residuals are displayed.

(e). Prescription of Recirculation

2DINPT can superimpose a recirculation flow field on any existing flow distribution regardless the options used for the flow-field creation, or whether recirculation already exists. However, this option is recommended to use for flow fields currently free of recirculation.

2DINPT displays the current strength of recirculation in percent over every horizontal grid planes from $I=2$ to $I=NX$. The recirculation percentage is calculated with respect to the total input mass flow. This percentage may include turbulent flow contributions if the existing flow field had been superimposed with the turbulence. If the existing flow field is initially set up with the computer aided Options D or A, the recirculation strength displayed should be zero (sometimes with small truncation errors).

The user can change the recirculation strength over each specific cross-section. This can be accomplished in two steps:

- Input the percentage of recirculation, or percentage change if recirculation already exists, for a cross-section I.
- Distribute the recirculating mass specified above in terms of profile factors in the positive and negative X-directions.

The differentiation of the recirculating mass flows in positive and negative directions is a fundamental feature of the flow recirculation. Differences between the sums of positive and negative recirculation mass flow rates, over each cross-section I, is always zero. 2DINPT ensures the differences are no more than small round-off errors.

Entering recirculation mass percentage is straightforward, but the following details are worth mentioning. If recirculation already exists at an I-plan and, for example is 15 %, entering a value of 15 % will

increase the total recirculation strength at that plan to 30 %. If a value of -15 % is given and care is taken in prescribing recirculating profile factors, overall recirculation over that section can be eliminated. In general, this practice of using negative recirculation percentages should be avoided, since under certain circumstances it can lead to negative mass flow rates which are not acceptable to the 2DHT code.

The technique of using profile factors is similar to the one described in the determination of the forward flow field. The profile factors in both the positive and the negative X-directions should always be greater or equal to zero. Zero values for either direction indicates the absence of local recirculating zones. At a particular cross-section, at least one profile factor should be larger than zero. A common way to assign the profile factors is to use 0.0 for one direction, and use a value larger than 0.0 for the other direction. This means that the recirculation over one zone boundary is directed either in the positive or the negative directions. 2DINPT, however, allows assignment of positive values to both of the profile factors over a volume zone boundary. In this case, the profile factors simulate a small scale recirculation, which also resemble the simulation of the turbulent exchange as discussed later.

The recirculation flow field is determined by the relative magnitude, rather than by the absolute value of the profile factors. The user is recommended to prepare his data regarding the recirculation strength and the local profiles prior to execution of the 2DINPT. 2DINPT will create a data file with name RECIR.DAT after the input process is completed. This data file will be used for file updating if it exists in the user's working directory. If the user changes profile factors of the recirculating flow during a file updating session, the contents of file RECIR.DAT will be over-written, to reflect the profile modifications.

Some suggestions regarding the recirculation mass percentages and flow patterns are given at the end of this sub-section.

(f). Superposition of Turbulence

The final step in setting up a flow field is superposition of pairs of turbulent mass fluxes on the mean flow at each internal volume-zone boundaries. These turbulent mass fluxes are of equal magnitude but acting in opposite directions, hence continuity is automatically satisfied. Previous modeling experience strongly suggests that this turbulent exchange is important to account for mixing due to large scale fluctuations, which were observed in physical isothermal models or actual boilers.

The turbulent mass fluxes should be normalized with the total mass flow exiting from the boiler, as previously described in setting up the internal mass fluxes. 2DINPT displays the current turbulent fluxes before allowing the user to set up inputs for the turbulent exchange sub-model. The values displayed are the magnitudes of the turbulent mass fluxes in both the X- and the Y-directions.

Even if the user has not prescribed any turbulent fluxes, 2DINPT may show that some volume zone boundaries have turbulent fluxes. These fluxes are caused by the user's input of the recirculation pattern. Note that small scale recirculation over a zone boundary operates just like the turbulent exchange phenomenon. The contribution of the small scale recirculations should not concern the user. He can maintain these fluxes or later erase them with one key stroke.

2DINPT offers several options for superimposing turbulence on the mean mass flux field:

- Option A: The user prefers 2DHT to calculate a default turbulent distribution.
- Option B: The user neglects turbulent exchange .
- Option C: The user prescribes the turbulent fluxes over each internal boundaries.
- Option D: The user keeps the current turbulent field unchanged.

The user is recommended to use option A if he is new in describing the boiler flow field. Option D is also the default, and can be activated by pressing the Return key. The default option will maintain the existing turbulent fluxes unchanged.

In Option A, the user must prescribe two constants for the turbulence sub-model so that 2DHT can calculate and superimpose a turbulent flow field. These two parameters are called CTUR1 and CTUR3. CTUR1 is a proportionality factor to include contributions of the turbulent exchanges calculated from the mean velocities. CTUR3 is another factor for the inclusion of the turbulent effect calculated from the mean velocity over the largest furnace cross-section. Default values for CTUR1 and CTUR3 are 10 % and 5 %, respectively. The user is recommended to use these values. Use of other values requires that the user has gained some experience on how local variable profiles are influenced by the strength of the turbulence effect.

Radiant heat exchangers in the upper furnace can cause damping of large-scale turbulent fluctuations. To account for this damping effect, the user can reduce the values of the turbulent constants by a fractional amount. Default reduction on the values of the turbulent constants is 0.5.

(g). Some recommendations for mass flux prescription

Boiler flow field is very specific to furnace operating conditions and the boiler design. Assessment of actual flow field in an utility boiler is, in most cases, very limited by the availability of the boiler ports. The hostile environment within the boiler also imposes strict limitations on the types of measurement methods that can be applied. Although 3D computational fluid dynamics models are available and useful in many instances, they are still at the state-of-the-art, and are expensive to use in practical boiler designs. As a last resort, many boiler engineers use isothermal physical modeling to fulfill their design requirements.

In a previous modeling study, furnace hopper recirculation was varied from 25 to 100 % with respect to the total furnace flow. The predicted mean furnace exit temperature changes only 25 K for the conditions studied. This is an example to show that the user should not be overly pertained to the absolute accuracy of the flow field.

In many cases, overall thermal performance predictions can be achieved with knowledge of the boiler bulk flow field only. The user may perform, at least in the beginning stage, parametric studies for his particular applications to assess the impact of flow field. He can build up experience gradually, which will be very useful for future flow field specifications. Moreover, if relative boiler performance changes are of the major concern, the user can calibrate his flow field against any available baseline data. He then can use the calibrated flow field to perform model applications, and predict the influence of operational or design changes.

Measurement in physical isothermal models have shown that flow recirculation into the hopper is typically between 40 % to 60 % of the mass fed through the lowest burner level. Horizontal recirculation in corners does not need attention due to the 2D nature of the current model. However, vertical recirculation zones above the upper burner level and also behind the boiler nose plane may be considered. Typical recirculation mass for the former may be 15 % to 30 % of the mass fed to the upper burner level. Recirculation behind the nose plane may be 5 % to 20 % of the total mass flow through the furnace outlet.

With respect to local recirculation profiles, recommendations given below might be useful.

The profiles in tangentially fired boilers depend on the boiler geometry and the firing circle. For small firing circles in relatively narrow and tall boilers, profiles of the forward flow are very likely to show a maximum on the furnace axis at levels above the upper burners. For boilers with large firing circles and wide furnace cross-sections, the minimum in forward flow profiles is likely to extend from the burner level upward, in some cases into the upper furnace. Recirculation into furnace hopper typically starts from outside regions of the hopper, and ends at the circulating vortex in the furnace center.

Hopper recirculation of front- or opposed- fired boilers is most likely to start from the center of the hopper and extends to the edges of the burner inlets at the lower level. For opposed fired boilers, it is also reasonable to assume that the mass flux profiles has a maximum on furnace axis at locations above the upper burner .

Estimation of the forward flow profiles in front fired boilers is difficult, because of the flow asymmetries involved. The best way in this case is to use the plug flow option to describe the forward flow, then superimpose some recirculation on flow field above the upper burners. Hopper recirculation must also be considered.

(h). Modification of existing flow field

2DINPT allows the user to modify an existing flow field. When the user selects flow field modification, all existing mass fluxes will be set to 0.0 except at the inlets and the outlets. New flow field will be recalculated based on information specified in the forward-velocity data-file, FORWA.DAT, and the recirculation data-file, RECIR.DAT. During an interactive session, the user can modify or create these two data files and establish a new flow field. The modified files, FORWA.DAT and RECIR.DAT, will be saved automatically by the code but using the same file names. The user is recommended to save the files FORWA.DAT and RECIR.DAT under different names before commencing any flow field modification.

If the user selects direct flow-field prescription (Option A, see item (d)), during the modification process, he has to enter all mass fluxes one-by-one. This may be time-consuming. It may be easier to use the computer aided option when one needs to modify an existing flow field. If the user changes the inlet mass fluxes or the inlet locations, 2DINPT can detect these changes. In this case, 2DINPT will automatically assume that the user selects flow field modification. The flow field modification procedures are the same as those described above.

Heat Sink Boundary Conditions — 2DINPT differentiates the following types of heat sink surfaces:

- Furnace-wall surface zones, on sections $M=1$ to $M=4$

- Furnace outlet zones, on sections $M=1$ to $M=4$
- Surfaces of heat exchangers embedded in volume zones I, J.

Each of the heat sinks requires the following as inputs:

- Surface emissivities
- Deposit thermal conductivity/thickness ratios on these surfaces, if surface temperatures are calculated by a heat balance equation.

(a). Surface emissivities

Surface emissivity ($EW(*,M)$) depends on material type and surface structure in complex ways. If a surface is covered with ash deposits like in pulverized coal fired boilers, the emissivity of the surface depends strongly on the physical, chemical, and geometric nature of the deposits. Strong dependency of deposit emissivities on deposit temperatures have also been observed. In general, emissivity decreases with the increase of surface temperature. Quantification of the emissivity-temperature relationship is difficult mostly due to the variation of ash compositions associated with the types of coal used, and different furnace operating conditions.

2DINPT requires the user to prescribe surface emissivities for each of the surfaces on sections $M=1$ to $M=4$. An uniform emissivity value is recommended for all surfaces. 2DINPT offers 0.7 as the default value. The 0.7 value has been found to represent emissivities of coal ash deposit quite well. If 2DINPT is used to assign the default value or any other constant emissivity value, the emissivities of the outlet zones are automatically set to 1.0. However, the user may change them.

(b). Temperatures and emissivities of the outlet zones

Heat transfer boundary conditions at the furnace outlet is a complex issue due to the elliptic nature of the problem. Even if convective back-mixing is neglected as does the current code, radiative fluxes can be thrown back into the furnace through the outlets.

2DHT treats the outlet boundary conditions by assigning equivalent radiation surface temperatures, $TW(*,M)$, and equivalent surface emissivities, $EW(*,M)$, to these zones. Since the equivalent temperatures and emissivities depend on individual boiler design (e.g., exit location, screen tubes, backpass geometry, furnace exit temperatures, etc.), only general recommendations are possible and they are listed as below:

- If the spacing of screen tubes is wide or no screen tube is present, the equivalent emissivities may be set to 1.
- For tightly-spaced screen tubes, the equivalent emissivity should be the one used for the furnace wall surface zones (e.g., 0.7).
- The equivalent radiation temperatures $TW(*,M)$ assigned to the outlet zones should not exceed the predicted furnace exit gas temperature. This may require some iterative processes. The user is advised to compare his estimate of the equivalent radiation temperatures with the model predictions. Values of $TW(*,M)$ in the order of $(T_{gas,exit} - 200 \text{ K})$ seem to be reasonable estimations. Also, the temperatures should not be lower than, for example, 50 K plus metal temperatures of the water wall tubes at the furnace exit.

The outlet problem can be circumvented if the heat transfer model is extended beyond the upper furnace exit, and towards the cooler end of the boiler. However, the effort for model set-up and the computation times will increase.

(c). Ash hopper

2DINPT does not consider mass flux of the bottom ash. Ash-hopper outlet is treated in a similar way like the furnace outlet zones, and is typically located at the center of the bottom section where $M=1$. The hopper outlet zone has negligible impact on boiler thermal performance predictions due to its relatively small size. The equivalent emissivity may be set to 1.0 and a temperature less than 400 K may be used for the equivalent radiation temperature.

(d). Ratio of deposit conductivity to thickness

The ratios of deposit conductivity to thickness, $CS(*,M)$, have to be specified for all heat exchanger and wall surfaces on sections $M=1$ to $M=4$. A zone with zero value indicates surface temperature of that zone is an user-specified constant during the furnace heat balance iterations. This ratio is automatically set to 0.0 by the code for outlet zones. Values for wall surfaces on section $M=2$ should always be set to zero. The sequence of specifying $CS(*,M)$ follows the same order as those for surface-zone temperatures and emissivities.

2DINPT offers an uniform distribution of $CS(*,M)$, with values equal to $0.4 \text{ kW/m}^2 \text{ K}$, as default values. The user may change them zone-by-zone. The value of $0.4 \text{ kW/m}^2 \text{ K}$ simulates moderate slagging/fouling conditions of coal-fired boiler furnaces. Larger values of $CS(*,M)$ represent cleaner furnaces. Typical values remain between 0.1 and $0.4 \text{ kW/m}^2 \text{ K}$ for highly slagged boiler sections.

(e). Surface zones with constant temperatures

2DINPT treats surface zones where the user specifies surface-temperatures by assigning 0.0 as values of $CS(*,M)$.

Initial Furnace Conditions — The user has to provide initial conditions of the following furnace variables:

- Gas temperatures, $T(I,J)$ in K, for all volume zones
- Surface temperatures, $TW(*,M)$ in K, for all surface zones on wall sections from $M=1$ to $M=4$
- Surface temperatures, $TWSINK(I,J)$ in K, for all heat exchangers surfaces.

These initial conditions are actually used in a 2DHT creation run. For a continuation run (i.e., $NREAD=1$), the initial values are read directly from an "input array file" specified by the user. In this case, initial values of these variables contained in file INPUT.DAT are not used and arbitrary values may be assigned. Initial values of all other furnace variables not listed above are set to $1.0 \text{ e-}5$ in a 2DHT creation run.

2DHT uses a very robust solution algorithm for heat balance calculations. Therefore, a very rough guess on the initial gas and surface temperatures is in most cases sufficient for 2DHT to achieve a convergence solution. However, more realistic initial conditions reduces the number of iterations to achieve convergence solutions.

(a). Gas temperatures

The user can set initial gas temperatures of all volume zones to a default value of 1600 K by pressing D. A similar action allows the user to set the initial volume-zone temperatures to any other constant value. In some lignite-fired boilers where coal has high moisture content, the default value of 1600 K may not be a good guess. A better initial guess should be less than 1600 K. The user can set the initial gas temperatures of each zone although this is not often needed. 2DINPT assigns arbitrary values of 1 K to volume zones which stay outside the boundaries of the chosen 2D zone arrangement.

(b). Wall surface temperatures

The user can set surface temperatures (except the outlet zones) of M=1, M=3, and M=4 walls to the default temperature of 1200 K by pressing D. A similar action allows the user to set initial wall surface temperatures to any other constant value. The use of the default value implies moderate deposits on furnace walls. For boilers with heavy ash deposits, higher initial values should be used.

The user can also specify initial surface temperatures zone-by-zone. An arbitrary value of zero K is assigned to all surface zones on M=2 (i.e., the furnace axis) by default. The user should not change this default setting.

(c). Heat Exchanger surface temperatures

Procedures of setting initial heat exchanger surface temperatures closely resemble those discussed above for setting up the wall surface temperatures.

5.2 Reburning-NO_x-Model Input Code (RBINPT)

RBINPT (Reburning model Input) is an interactive computer code which can be used to prepare an input data file needed to execute the reburning NO_x code RBNOX. The input code operates only in one mode for file updating (or modification), and in its current form does not support file creation. Since the user's manual includes examples of the NO_x model input-files (Volume II), the user can use RBINPT to update any one of the supplied input-files for his reburning NO_x predictions.

This section describes the use of the RBINPT code in detail. The description begins with some background information relating to the code structure. The user is suggested to familiarize himself with the background information provided before concerning too much about the model details. Mode inputs are addressed item by item in later sub-sections.

RBINPT is designed to work on IBM or IBM-compatible personal computers. The code occupies a memory size approximately at 242 kilobytes (KB). The code accepts inputs in upper case only. Consequently, the user is advised to set his keyboard accordingly (i.e., Caps Lock).

During the course of an interactive session, BPINPT communicates with the user through a number of statements in the form of blocks. These blocks usually contain:

- Name, current value(s) and dimension(s) of the input variable(s) associated with the block
- Recommended default value(s)
- Available options and key strokes used to select the options.

Numerical input data can be supplied in any format provided that the number of significant digits is sufficient for the input variable under concern.

File Management

The default input file name is RINPUT.DAT. The default output file name is RBINcsvs.lll, where cs is an user specified case number, vs is an user specified version number, and lll is a character string extracted from a user specified parameter describing the boiler load. For example, if cs is 01, vs is 02, and the specified boiler load is 95.0 % relative to the MCR, the default output file name will be RBIN0102.095. The user can overwrite the default output file name. However, the default input file name is always fixed as RINPUT.DAT. This means that if the user wants to modify an existing file, say RBIN0102.095, he has to copy that file to file RINPUT.DAT first. The objective of this file structure is to prevent accidental overwriting of the input files created earlier.

RBINPT will terminate the user's interactive input session if file RINPUT.DAT does not exist in the same working directory. This is because the code can only be used to update a file as mentioned before.

Upon completion of the heat transfer model runs, some furnace properties predicted by the 2DHT code are transferred to a data file named REBURN.DAT. RBINPT requires the presence of the file REBURN.DAT. If this file does not exist in the same directory, RBINPT will terminate the user's input session. The user is advised to save the file REBURN.DAT under a different name, since it will be overwritten every time 2DHT is executed.

Input Requirement

The amount of inputs requested by the RBINPT code is very limited since most of the inputs are pre-fixed in the code. User supplied inputs can be summarized as follows:

- Input/Output file names, and comments to the cases run
- Flue gas composition, including NO concentration from the burners
- Stoichiometric air ratios of the reburn and over-fire air zones
- Residence times and temperatures of the four reactors used in the RBNOX model.

Input Structure

RBINPT organizes the input requirement into blocks of data and labels them in the form of chapters. The code advances through each of these chapters for the user's inputs. The user may by-pass some of the chapters if no data modification is planned for those chapters.

Typical information displayed for each data input includes: the variable name, current value, a brief explanation of the variable's meaning, any default or recommended values, and a list of options for selection. The user may then select one of these options. The options will generally include: leaving the value(s) unchanged; changing to a value specified by the user; or assigning default values to the variable.

The following paragraphs describe the sequence of these input chapters. The chapter numbers shown may not be consecutive because no user's attention is required on some Chapters.

CHAPTER 1: PARAMETERS OF FILE SPECIFICATION.

The user specifies input/output file names and provide comments to the RBNOX model runs. He can over-write the default output file name provided by the RBINPT code.

Chapters 2 to 5 set the detailed chemical kinetics model for NO_x predictions. The model contains 43 species and 201 reaction mechanisms. Numerical control parameters are also prescribed in these chapters. RBINPT does not allow the user to change parameters listed in these chapters.

CHAPTER 6: PROPERTIES OF FURNACE FLUE GAS.

Here, the user should specify flue gas composition (CO_2 , H_2O , O_2 , N_2 , NO , SO_2) exiting from the furnace burner zone. NO concentration from the burner zone is an user specified input.

CHAPTER 7: PROPERTIES OF REBURN AND OFA JETS.

The user specifies Stoichiometric air Ratios (SR) for the reburn and the Over-Fire Air (OFA) zones. He also provides characteristic mixing times for the reburning and the OFA jets.

CHAPTER 8: REACTOR DEFAULT OPERATING CONDITIONS.

RBINPT has a subroutine to calculate the temperature and residence times of the four PFR reactors (see Section 4.2) used in the Reburning NO_x Model. For each reactor, the default operating conditions are extracted from the user's inputs up to this point, and from the data file REBURN.DAT. RBINPT displays the default information to the user in a tabulated form. No user action is required in this chapter.

CHAPTER 9: SPECIFICATION OF REACTOR RESIDENCE TIMES.

The user can change residence times of the four reactors in this chapter. The default values calculated in Chapter 8 are also shown here for each reactor.

CHAPTER 10: SPECIFICATION OF REACTOR TEMPERATURES.

The user can change the initial and the final temperatures of each reactors in this chapter. For each of the four reactor, RBINPT shows the default values calculated in Chapter 8.

Chapters 9 and 10 appear alternately until the residence time and the temperature specifications are completed for all the four reactors.

Special Key Functions

There are some frequently used keys by the RBINPT code. These keys are: C, D, P, Y, N, and the Return (or Enter). In general, key C designates that the user prefers a "Change" on model inputs. Key D is used for selecting "Default" values. Key P is used to "by-Pass" a chapter or a block of input data. Key Y represents "Yes" and is used only to answer few input prompts. Key N has opposite meaning as compared to key Y discussed here. The Return key is used to advance the interactive input session without changing the value of any existing data- item.

Updating Data Files using RBINPT

To update an input data file, the following steps are suggested to follow:

- Install RBINPT.EXE in the user's working directory.
- Copy the file to be updated to file RINPUT.DAT. The file to be updated may be taken from one of the example files supplied with this user's manual.
- Have file REBURN.DAT available in the same directory. (assuming you have run 2DHT for your boiler)
- Type RBINPT and press "Enter".

The code is now in the proper updating mode. Proceed to data block where changes are to be made by pressing "Return". After reaching the input parameters you want to change, follow procedures as described in the previous sub-section.

The updating mode can also be used to check the input data only. Enter "Return" as many times as required to reach input parameters you want to check. Abnormal termination does not destroy data contained in the input file to be modified, neither in file RINPUT.DAT.

The user has to specify a file name for the updated data-file. RBINPT provides a default name based on the version and case numbers transferred from the 2DHT inputs. The code will also ask the user whether he wants to overwrite an existing file if it has the same name as the default.

Description of Specific Input Items

This section discusses individual input associated the execution of the RBINPT code. With few exceptions, the items discussed will follow the order of appearance as one will experience during execution of the BPINPT code.

Default output file names — There are two of the default output-file-names: one refers to the output file from the input code RBINPT (RBINcvs.111), and the other (RBOTcvs.111) refers to the output file from the reburning NO_x model, RBNOX. For consistency, the file naming notations used here are parallel to those used by the 2DINPT and the 2DHT codes.

Comment block — The comments used by the 2DHT code are transferred to the RBINPT code through the file REBURN.DAT, and offered as default values. The user can change the contents of the comment block here.

Flue gas composition — RBINPT reads flue gas composition from file RINPUT.DAT and displays them as the current values. The user can either select to change, or use the default option to calculate the flue gas composition. If the default option is selected, the user then provides the burner zone stoichiometric air ratio (i.e., SR_1) for RBINPT to calculate the flue composition. Ultimate analysis of the burner fuel and a nominal air composition (21 % O_2 , 79 % N_2 , 50 % relative humidity) are used for the calculation of default flue gas concentrations.

Only selected species are considered in the flue gas stream, and they are CO_2 , H_2O , O_2 , N_2 , NO , and SO_2 . Since the emphasis is on NO predictions, trace species such as CO and unburned hydrocarbons (UHC) from the burner zone are not considered. The user, however, has to prescribe the initial NO concentration from the burners. This initial NO concentration is strongly dependent on the boiler heat release rates and on individual burner designs. In general, the NO data are available from the control room logbook.

RBINPT will warn the user if the initial NO concentration is zero, because in this case NO reduction efficiency has no practical meaning.

Reburn gas composition — Default reburn gas composition is 100 % CH_4 . The user can prescribe the reburn gas composition in terms of volume fractions of twelve species: CO_2 , H_2O , O_2 , N_2 , NO , CH_4 , C_2H_6 , CO , SO_2 , H_2 , C_2H_2 , and C_2H_4 . The inclusion of some trace species here is to insure that if flue gas is recirculated and mixed with the reburn jets, the model can handle the situation. The user may simulate higher order hydrocarbons by representing them with surrogate compounds made of C_2 species (e.g., C_2H_2 , C_2H_4 , C_2H_6), and CO and H_2 . For example, if C_3H_8 is present in the reburn fuel, it may be described as a mixture made from equal moles of CH_4 and C_2H_4 , in prescribing the reburn fuel compositions.

Reburn zone stoichiometric O_2 ratio (SR_2) — This is defined as the amount of available oxygen atoms divided by the required oxygen atoms for complete combustion of C, H, and S. A nominal SR_2 value for many reburning applications is 0.9. RBINPT calculates the reburn fuel flow rate based on the inputs given by the user up to this point.

OFA zone stoichiometric O_2 ratio (SR_3) — SR_3 has a similar meaning as SR_2 is defined but includes the additional effect of the over-fire air jets. A nominal SR_3 value for many reburning applications is 1.2. RBINPT calculates the OFA flow rate based on the user's inputs.

Characteristic mixing times of the reburn and OFA jets — These are the times elapsed starting from the injection of the jets until the jets lost their identities. The mixing time of a jet strongly depends on injector design and on boiler global flow field. It is best be obtained from physical isothermal models. Simple jet entrainment calculations may also help to quantify the jet mixing times. Experience has shown that values between 0.2 to 0.3 sec are good estimates when no data is available.

Reactor default operating conditions — The information displayed includes the SR level, residence time, and the initial and final temperatures of each of the four kinetics reactors. The locations of the reburn and the OFA jets are also shown in terms of 2D zone numbers in the I-direction.

The SR levels shown for reactors 1 and 3 are the inputs given. SR levels at reactors 2 and 4 remain the same as those of reactor 1 and 3, respectively, because no external mass-injection applies to them. The default residence times are calculated from two sources: one from the reburn and OFA characteristic

mixing times, and the other from the mean flue gas residence times calculated by the 2DHT code. The data file REBURN.DAT contains the necessary furnace information for the calculations.

RBINPT uses the furnace mean temperature profile to calculate the default reactor temperatures. Again, file REBURN.DAT contains the furnace temperature information. The initial and final temperatures of the reactors are linearly interpolated from the furnace mean temperatures, based on the residence times established.

Reactor residence times and temperatures — Current reactor residence times and temperatures are displayed, together with the default operating conditions discussed above. The user can select the default operating conditions by pressing D, or change them to any appropriate values if he has additional concerns on these inputs. RBINPT advances through each of the four reactors and prompts for these inputs. When an interactive input-session is completed, RBINPT shows the name of the output file together with other reminders .

5.3 Boiler-Performance-Model Input Code (BPINPT)

BPINPT (Boiler Performance model Input) is an interactive computer code which can be used to prepare an input data file needed to execute the Boiler Performance Model, BPM. The input code can operate in two modes: file creation and file updating (or modification). When the code is in the updating mode, an input data file must exist so that it can be updated.

This section describes the use of the BPINPT code in detail. The description begins with some background information relating to the code structure. The user is suggested to familiarize himself with the background information provided, before moving into too much about the model details. Model inputs are addressed item by item in later sub-sections.

BPINPT is designed to work on IBM or IBM-compatible personal computers. The code occupies a memory size approximately at 285 kilobytes (KB), and accepts inputs in both upper and lower cases.

During the course of an interactive session, BPINPT communicates with the user through a number of statements in the form of blocks. These blocks usually contain:

-Name, current value(s) and dimension(s) of the input variable(s) associated with the block

- Recommended default value(s)
- Brief descriptions of the variable meaning(s)
- User options and key strokes used to select the options.

Numerical input data can be supplied in any format provided that the number of significant digits is sufficient for the input variable under concern.

File Management

The default input file name is BINPUT.DAT. The default output file name is BPINcsvs.lll, where cs is an user specified case number, vs is an user specified version number, and lll is a character string extracted from a user specified parameter describing the boiler load. For example, if cs is 01, vs is 02, and the specified boiler load is 95.0 % relative to the MCR, the default output file name will be

BPIN0102.095. The user can overwrite the default output file name. However, the default input file name is always fixed as BINPUT.DAT. This means that if the user wants to modify an existing file say BPIN0102.095, he has to copy that file to file BINPUT.DAT first. The objective of this file structure is to prevent accidental overwriting of the input files created earlier.

The parameters cs, vs, and lll are those specified during execution of the 2DINPT code. Upon completion of the heat transfer model runs (2DHT), these parameter values are transferred along with other furnace properties predicted by the 2DHT, to a data file named BOILER.DAT. The user is advised to save the file BOILER.DAT under a different name, since it will be over-written every time 2DHT is executed. BPINPT will read the contents of file BOILER.DAT if it exists in the user's working directory. If the file does not exist, the user has to prescribe some furnace variables such as heat absorptions item-by-item, so that the boiler performance model can perform steam side calculations.

Input Requirement

Table 5.3 lists typical inputs of the Boiler Performance Model. These inputs are categorized into three groups in terms of: boiler steam- and air- side operating conditions, inputs passed by the 2D Model, and other wall and heat exchanger parameters. Some comments on the model inputs are also indicated.

Table 5.3. Typical Inputs for the Boiler Performance Model

Operating Parameters

- Steam Inlet Temperatures
Economizer Inlet
Reheater Inlet
- SH and RH Attenuation Temperatures
Spray Water
Control Temperature
- Steam Pressures
Economizer Inlet
Drum Pressure
Primary Superheater Outlet
Secondary Superheater Outlet
Low Temperature Reheater Inlet
High Temperature Reheater Outlet
- Air Heater Parameters
Air Inlet Temperature
Percent of Total Air Flow Through Air Heater
- Reheater Steam Flow
Percent of Superheater Outlet Flow
- Heat Loss (%)
+ Percent of heat transfer from gas to walls and to back pass tube banks which is not received by steam/water. Generally, this parameter is set equal to the design value for radiation heat loss.

Inputs Based Directly On 2D Code Inputs and Results

- Heat Transfer Parameters
Gas temperature at exit of 2D code domain
Heat flux to walls and heat exchangers in 2D code domain
Net furnace heat release
- Flue Gas Parameters
Mass flow rate
Composition
- Fuel Parameters
Mass flow rate
Upper heating value
Lower heating value
Moisture
- Air Parameters
Mass flow rate
Composition

Other Model Input Parameters

- Wall Parameters
Surface area
Total heat transfer coefficient
- Heat Exchanger Parameters
Flow pattern for each tube bank (parallel flow or counterflow)
Heat exchanger surface area
Deposit thickness on heat exchanger tubes
Tube outer diameter
Gas side cross-sectional area
Longitudinal and lateral tube spacing in heat exchangers
Air heater heat transfer coefficient

Input Structure

BPINPT organizes the input data required to execute the boiler performance model (BPM) into a series of input blocks. Typical information displayed with each input data includes: the variable name, it's current value, a brief explanation on the meaning of the variable, any default values, and a list of options for selection. The user may then select one of these options. Available options generally include: leaving the value unchanged, or changing to a user-specified value. For some variables the user has the option of using data in the data file BOILER.DAT.

The following paragraphs describe the sequence of the input blocks and their contents. The description follows in order of variable appearance as one would experience in actual interactive computer session.

(a) Specification of boiler type: tower or two-passes.

Input data for the two types of boilers are similar, but available boiler sections and their order of appearance are different. In particular, the tower boiler may include a "screen" or "triflux" section which

is not available in the two-pass boiler. The two-pass boiler includes a "DRUM/SHW" section which is not available in the tower boiler.

(b) Status of boiler data file.

The user should indicate the status of the input file BINPUT.DAT. The input file can be created from scratch, or updated if an boiler data file already exists.

(c) Specification of boiler sections.

The user selects boiler sections based on the diagrams displayed by the BPINPT. Only sections selected will be included in the boiler model calculations. Using this provision, the boiler performance model (BPM) can be tailored to fit the user's boiler configurations. Any data assigned to a non-existing section will be automatically assigned to the next existing section.

(d) Specification of active attemperators.

The user specifies the model attemperators to simulate actual attemperators in operation. Attemperators affixed to a non-existing boiler section is automatically disconnected. Then, the user has the option to review the specification of the boiler sections and attemperators. He should ensure that the boiler is correctly configured before continuing the session.

(e) Specification of heat exchanger flow patterns.

The user specifies the gas-steam contacting patterns for each boiler section. Two contacting patterns are available: parallel flow and counter flow.

(f) Specification of attemperator control and spray water temperatures.

(g) Specification of inlet and outlet steam pressures.

This is carried out for each heat exchanger section in the boiler. The user must specify the inlet and outlet pressures of the steam path, which include pressures of the superheaters and the reheaters. Steam pressures for other intermediate sections may be assigned by using a program option which interpolates pressures between the boiler sections.

(h) Specification of initial steam/water mass flow rate.

This is carried out for each heat exchanger section in the boiler. The user must specify the economizer inlet mass flow rate, and the fraction of the superheated flow which enters the first reheater. For a tower boiler, the fraction of mass flux from the "S.Heater II" section to the "SH. Sec. Triflx" section is also specified. Mass flows for other intermediate sections may be assigned using the default distribution.

(i) Specification of initial steam inlet and outlet temperatures.

This is carried out for each boiler section. This data block operates in a way similar to the steam pressure block described above.

- (j) Specification of waterwall surface area and heat transfer coefficient for each boiler section.
- (k) Specification of heat exchanger properties.

The user specifies surface area, deposit thickness, deposit thermal conductivity, tube outer diameter, and the gas-side overall heat transfer coefficient for each heat exchanger section. BPINPT offers an option to calculate deposit thermal conductivity as a function of temperature. If this option is selected, the user has no need to specify the deposit conductivity.

The Boiler Performance Model has an option to calculate the overall heat transfer coefficients of the heat exchangers (gas-side). If this option is selected, the user will not be asked for the heat transfer coefficients except for the air heater. Instead, the user has to supply more information such as the gas-side cross sectional area (which should not consider tube blockage), and the longitudinal and lateral pitches of the tube arrangement.

- (l) Specification of air temperature into the air preheater.
- (m) Status of BOILER.DAT file.

The user indicates whether data file BOILER.DAT exists or not. If this file exists, BPINPT will read the contents.

- (n) Coupling of 2D furnace and the boiler sections.

This is a major input block. The user matches the 2D furnace zones with the boiler section numbers as directed by the BPINPT code. He then specifies the beginning section at which the energy balance is to be calculated by the BPM code. The gas-side inlet temperature of that section is also an input. The user then provides an initial temperature for the flue gas entering the air preheater.

Following the above inputs, the user specifies furnace parameters. These parameters include: the heat flux distributions, flue gas composition, fuel flow rate, upper heating value, lower heating value, fuel moisture, net furnace heat release, air flow rate, and air composition. If file BOILER.DAT exists, the values read from the file are shown as default.

- (o) Specification of numerical parameters.

Here, the user defines the convergence criteria of the BPM code. Included are criteria for convergence of boiler heat and mass balances. The maximum number of heat balance iterations is also an input.

Special Key Functions

Frequently used keys in the BPINPT code are similar to those adopted in the 2DINPT and RBINPT codes. Namely, these keys are: C, D, Y, N, and the Return (or Enter). In general, key C designates that the user prefers a "Change" on model inputs, or to "Create" a new input data file. Key D is used for selecting "Default" values. Key Y represents "Yes" and is used to turn on a boiler section. Key N turns a boiler section off. Boiler sections that are turned (or switched) off don't participate in overall boiler steam/gas

energy balance. The Return key is used to advance the interactive input session without changing any existing input values.

File Creation Using BPINPT

The following procedures are necessary for creating a data file to run the Boiler Performance Model:

- Install BPINPT.EXE in the user's working directory
- have file BOILER.DAT ready in the same directory (assuming you have run 2DHT for your boiler).

To start the file creation session, type BPINPT and press Enter. BPINPT will prompt inputs for boiler type, then ask the user whether he wants to create or update a boiler data file. At that stage, the user should press C followed by pressing Return to activate a file creation session.

In the creation session, BPINPT will first create an input data file BINPUT.DAT. All input parameters in this file will be set to zero. Default values will overwrite some of the zeros later. Thus, as the session continues, current input values displayed by the BPINPT will be either zeros or the default values. The user can change these initial settings based on his boiler input data.

Entering wrong data can occur. There are several ways that BPINPT responds to the wrong input:

- The format of the input data is wrong. For example, a character is mistakenly entered and BPINPT expects to read-in a numerical number. Under this circumstance, BPINPT will display the input parameter until an input with correct format is entered.
- BPINPT detects an un-acceptable input-data. In this case BPINPT will not proceed until an acceptable input is given.
- The user enters an input data that he does not intend to do so. In this case, he is recommended to continue the session as if no error had occurred (but takes notes). After the file creation session is completed, he can re-run BPINPT under the update mode (see next section) to correct the errors made. Entering Return frequently in order to proceed to the end of a file creation session is not recommended.

At some stage of the interactive input session, BPINPT will ask whether file BOILER.DAT is available. This file should be created by a 2DHT run, and it contains output data to be coupled with the Boiler Performance Model calculations. If the intended BOILER.DAT file exists, the user should set IFNCE to 1 when BPINPT prompts for the input. If this file is not available, or available but not intended to use, set IFNCE to zero. The user then has to supply the required input data to describe the heat fluxes and operating conditions of the boiler furnace.

Updating Data Files using BPINPT

To update an input data file, the following steps are suggested to follow:

- Install BPINPT.EXE in the user's working directory

- Copy the file to be updated to file BINPUT.DAT
- Have file BOILER.DAT available in the same directory (assuming you have run 2DHT for your boiler)
- Type BPINPT and press "Enter" to start the program
- If possible, do not change the boiler type in an updating session
- Press Return when BPINPT displays the message: "To Update a boiler data file, press: Return"

The code is then in the proper updating mode. Proceed to the data block where changes are to be made by pressing Return. After reaching the input parameters you want to change, follow procedures as described in the earlier sub-section. The updating mode can also be used to check the input data only.

If boiler types are the same, it is possible to use an existing data file as basis to update the file for a new boiler. In this instance, all input parameters should be modified properly. The updating session is concluded in the same way as described for the file creating session. Abnormal termination does not destroy data contained in the old input file (i.e., the input file to be updated), neither in data file BINPUT.DAT.

The user has to specify a file name for the updated data-file. BPINPT provides a default name based on the version and case numbers transferred from the 2DHT inputs. The code will also ask the user whether he wants to overwrite an existing file if it has the same name as the default.

Description of Specific Input Items

This section discusses individual input associated with the execution of the BPINPT code. With few exceptions, the items discussed will follow the order of appearance as one would experience during execution of the BPINPT code.

Boiler Type — The Boiler Performance Code (BPM) can handle two types of boilers:

- Type 1: Tower boiler (boilers with one pass)
- Type 2: Two-passage boiler (boilers with furnace, transition, and convective backpass sections).

Distinction between these two types of boilers was made because different boiler types comprise different contact patterns among steam/water streams and the flue gas flow. Figures 5.5 and 5.6 show the steam/water flow patterns of the Type 1 and Type 2 (IDRUM=0) boilers. The dashed lines represent the water/superheat steam flows, while the dotted lines show the reheat steam flows. Both configurations allow only one reheat stream.

In general, selection of a boiler type to represent the user's particular boiler configuration should be simple. However, the user may have to configure his specific boiler by switching appropriate sections on or off after the boiler type is selected. BPINPT allows the user to switch off the superheater and reheater sections. Experience has shown that by proper maneuvering of these on/off switches, many different designs of boiler steam/water flow patterns can be modeled. For instance, the user can switch off all reheater sections to model boilers without reheat stream. More discussions about the use of these switches will be presented later.

Figure 5.5. Sequence indices of a tower-boiler (ITYPE=1).

Figure 5.6. Sequence indices of a two-pass boiler (ITYPE=1, IDRUM=0).

Default boiler type is Type 2 if the user selects to create a new input-file, but he can change it to Type 1. Although it is possible to change the boiler type during a file updating session, this practice should be avoided. This is because the input-data of the two boiler types are ordered differently, and they must be re-typed anyway.

Drum Section for Type 2 Boilers — Type 2 boiler-configuration has two variations which concern the possibility of having a drum. The drum heat-exchanger section is located in the horizontal transition between the upper furnace and convective back pass. This drum section usually consists of an upper and a lower drums connected by a tube array exposed to the flue gas. The user should set the parameter IDRUM to 1 if this drum section exists.

The message dispatched by the BPINPT code as "The boiler has no drum section" does not mean the boiler has no drum. On the contrary, the current version of the BPINPT code only supports drum boilers (i.e. sub-critical boilers). Since these boiler drums are located outside the enclosure of the water tube walls and do not participate in heat absorption from the flue gas, their graphical display is omitted in Figure 5.6.

The schematic steam/water flow pattern considered by the BPINPT code, if the drum option is selected (IDRUM=1) for a type 2 boiler, is shown in Figure 5.7. Note that the boiler display provided by the BPINPT code does not show any difference as compared to Figure 5.6 where IDRUM was set to 0. However, the change in the sequence numbers of the heat exchangers are worth mentioning.

When BPINPT Code is run in the file-creation mode, IDRUM is set to 0 by default. The user may change this value as necessary. Changing the switch IDRUM during a file updating session is not recommended but feasible. In this case, some input data have to be re-typed due to the change of the heat-exchanger section numbers.

Boiler Heat Exchanger Sections — Both Type 1 and Type 2 boiler-configurations allow a maximum of 12 different heat exchanger sections, including furnace, economizer, and air preheater, to be modeled. These sections are identified by the section index, the section name, and the steam/water (S/W) sequence index.

The section index refers to the order of the heat exchanger sections encountered by the flue gas stream, which exits the furnace and flows to the air preheater. Depending on the boiler type chosen (Type 1 or 2) and whether IDRUM is 0 or 1 (for Type 2 boilers), the same section index can associate itself with different section names. The steam/water sequence index denotes the order of the heat exchanger sections as experienced by the steam/water flows, which start from the economizer, up to the high temperature superheater, or from the low temperature to the high temperature reheaters. The steam/water sequence indices also depend on the boiler type chosen.

Table 5.4 lists the section indices, section names and S/W sequence indices for each of the three boiler variations. This table may best be used with the graphical display as shown in Figures 5.5 to 5.7. Numerical numbers shown in these figures correspond to the steam/water (S/W) sequences. The sequence indices, and the names of the heat exchangers remain unchanged even if some sections are switched off. The S/W sequences displayed by the BPINPT code during an updating run will appear as 0 if a section had been switched off before.

Note that in all three configurations considered, section index 1 is always associated with the furnace, and section indices 11 and 12 are connected with the economizer and air preheater, respectively. Similarly, S/W sequence indices 1 and 2 are always assigned to the economizer and furnace. The last superheater always has the S/W sequence index as 8, the first reheater as index 9, and the last reheater as index 11, regardless they exist or not. The assignment of a S/W sequence index 12 to the air preheater is only nominal and serves no further computational purposes.

Table 5.4. Summary of Boiler Section Indices, Names and Steam/Water Sequence Indices.

Boiler Type: Tower Boiler		
Section Index	Section Name	S/W Sequence Index
1	Furnace	2
2	Screen	3
3	S. Heater III	7
4	S. Heater IV	8
5	R. Heater II	11
6	S. Heater II	5
7	SH. Sec. Triflx	6
8	RH. Sec. Triflx	10
9	S. Heater I	4
10	R. Heater I	9
11	Economizer	1
12	Air Preheater	12
Boiler Type: Two Passes Boiler without Drum Section		
Section Index	Section Name	S/W Sequence Index
1	Furnace	2
2	S. Heater III	6
3	S. Heater IV	7
4	R. Heater III	11
5	S. Heater V	8
6	R. Heater II	10
7	Drum/S. Wall	5
8	S. Heater II	4
9	R. Heater I	9
10	S. Heater I	3
11	Economizer	1
12	Air Preheater	12
Boiler Type: Two Passes Boiler with Drum Section		
Section Index	Section Name	S/W Sequence Index
1	Furnace	2
2	S. Heater III	6
3	S. Heater IV	7
4	R. Heater III	11
5	S. Heater V	8
6	R. Heater II	10
7	Drum/S. Wall	3
8	S. Heater II	5
9	R. Heater I	9
10	S. Heater I	4
11	Economizer	1
12	Air Preheater	12

(a) On-off switches

The existence of a S/W section is controlled by the on/off switch of that section. The user has to answer yes ("Y") or no ("N") to questions asked. When a section is switched on, BPINPT displays the corresponding sequence index as (ON). When a section is switched off, a value of 0 followed by (OFF), will be displayed.

In a file creation run, all S/W switches are set to (ON) by default. In an updating run, previous settings contained in the file BINPUT.DAT prevail. In both cases, the user can switch on or off all boiler heat-exchanger sections but with the following exceptions:

- The furnace section (S/W sequence index 2) must always be "ON".
- At least one superheater should be switched on. All reheaters may be switched off if the boiler is operated without reheat.

If an input data file is updated and new sections are added, appropriate changes should be made to the input data for each section that is switched on.

There is also ad-hoc alternatives to use the on/off switches. For example, boiler sections which do not exist can be treated as sections with very small heat sink surface areas (zero should be avoided), or very small convective heat transfer coefficients. In some cases there may be several switch combinations which can represent a boiler configuration of interest. When these alternatives can be applied to consecutive superheater or reheater sections, the user is recommended to switch-off the section located upstream of an existing attemperator. This approach allows the attemperator to control the temperature of the superheater or reheater outlet steam, if it exists.

If Type 2 boiler without the drum section (IDRUM=0) is chosen, section 7 (S/W Index 5) may be used to simulate a wall section cooled by superheated steam (SHW walls).

(b) Switches for attemperator settings

Up to six attemperators is provided for a Type 1 boiler, and a maximum of four attemperators can be used to model a Type 2 boiler. The locations of these attemperators with respect to the steam/water circuits are shown in Figures 5.5 to 5.7. For both boiler types as discussed, only one attemperator may be assigned to the reheat cycle.

The attemperators are identified by index IA(L), and their on/off status are shown by variable IAC(L). If attemperator L is switched on, the code assigns the value of IA(L) to IAC(L), and displays IAC(L) followed by (ON). If an attemperator is switched off, BPINPT assigns value 0 to IAC(L), and displays IAC(L) followed by (OFF). The graphical display of the steam/water circuits provided by the BPINPT code uses IAC(L) to indicate the attemperator switch-setting (for instance A5 or A0). The heat exchanger section just downstream of the attemperator must be switched on, otherwise the attemperator can not be switched on.

When an input file is being created, the switches of all attemperators are set to "ON" by default. The user can change these switch settings. Setting changes are also possible during a file updating session.

(c) **Attemperation control temperatures**

Attemperation spray flows in the Boiler Performance Model are controlled by differences between control temperatures and the outlet steam temperatures. An attemperator is activated when steam temperature exceeds the control temperature.

For all attemperators in operation, the user has to prescribe the attemperator control temperatures, TMAX(L). No default values are offered. In cases where an attemperator controls the final superheated or reheated steam temperatures, the maximum steam temperatures provided by the boiler manufacture should be used as the control temperature. Besides using switches to select attemperators, the user has the following alternative. All attemperators may be switched on by default. By assigning values of TMAX(L) much higher than the expected steam outlet temperatures, the attemperators effectively are not in operation (i.e., switched off).

(d) **Attemperation spray water temperatures**

The Boiler Performance Model uses TA0 to represent the temperature of the sprayed water in superheat attemperation. Likewise, the sprayed water temperature in reheaters is represented by TA0R. Both are user inputs.

The user should always check the heat balance of the reheat attemperation in the output of the Boiler Performance Model. Boiling of reheat spray at reheater pressure should be avoided. Low values of TA0R may be used to avoid the boiling. If boiling occurs, the calculated results become not reliable.

(e) **Setting of flow indices**

As mentioned in the description of the Boiler Performance Model, heat transferred from the flue gas to the various heat exchanger sections is calculated with the assumption of either parallel or counter flows. Parallel flow is defined as the water or steam temperatures are the lowest at the flue gas inlet. For counter flow, the water or steam temperatures are the highest at the flue gas inlet.

Each heat exchanger, except for the furnace and the air preheater, can be treated as being arranged in parallel or counter flows. The index controlling the selection of flow patterns is IBCP(I), and must be set by the user. Parallel flow is identified by setting IBCP(I)=1, otherwise set IBCP(I)=2 for the counter flow. BPINPT allows these flow indices to be set for existing heat exchanger sections only.

During a file creation session, BPINPT assigns 0 to flow indices by default. The user has to specify flow indices for his particular boiler arrangements. Typically, heat exchangers in hotter boiler sections are designed for the parallel flow, and those in colder sections are for the counter flow. If the user has doubts about the contacting patterns of a particular section, he may apply the above rule. The impact of an incorrectly assigned flow index on overall steam predictions is usually very small.

Steam/water Pressure Distributions in Boiler — The steam/water pressure distributions in the boiler are not calculated but inputs. Setting up the inlet and outlet pressures of each heat exchanger section can be easily accomplished by the BPINPT code.

In general, the inlet pressures of the feedwater and cold reheat, and the outlet pressures of the superheated and reheated steam are known. These pressures, in unit of MPa, are inputs. The code will interpolate intermediate pressures for all other sections. Alternatively, the user can prescribe all intermediate pressures section-by-section. Only sub-critical pressures can be used. If the feedwater inlet pressure is larger than the critical value of 22.089 MPa, BPINPT will display a warning message until a sub-critical pressure is used.

BPINPT assumes that the inlet pressure of a section is equal to the outlet pressure of a previous section. This assumption implies that pressure drops between two tube banks are neglected. Typical sequences in specifying the pressure distributions are described below.

In step 1, the user supplies the feedwater inlet, the final superheater outlet, the cold reheat inlet, and the final reheat outlet pressures regardless these sections exist or not. When a boiler is operated without reheat, a default reheat pressure of 3.5 MPa is assigned to all reheat sections although it is not used.

In step 2, BPINPT displays the outlet pressures before interpolation, which may be ignored by pressing "Return" to proceed. The interpolated outlet pressure distributions will then be displayed. Note that sections which were switched off impose no pressure drops.

In step 3, the user can change outlet pressures of each operating sections provided he has the detailed information. The changes can be made in order of increasing S/W sequence index. The user may overwrite values of the superheat and reheat outlet pressures if he wishes. Care should be given to the outlet pressure of the furnace (S/W Sequence Index 2), because it also is the boiler drum pressure.

In step 4, BPINPT displays the inlet pressures for all sections based on either the interpolated or the calculated outlet pressures. At this stage it is still possible to modify the outlet pressures. However, the feedwater and reheat inlet pressures can not be modified. The user has to terminate his interactive session appropriately, then execute BPINPT under the updating mode to achieve the objective.

Initial Conditions — The Boiler Performance Model solves heat and mass balances iteratively. Therefore, initial conditions of the iterated variables must be provided. The iterated variables include:

- Steam/water mass flux distributions
- Steam/water temperature distributions
- Flue gas temperature distributions.

BPINPT assists the user in estimating initial conditions of these variables.

(a) Steam/water mass flux distribution

This includes two major items: the feedwater flow rate into the economizer, and a ratio obtained by dividing the cold-reheat mass-flow to the superheat steam flow. Both quantities are usually known, and their values depend on boiler load, boiler design, and plant operation.

BPINPT uses the feedwater flow rate and the reheat ratio to suggest a default distribution for initial water or steam mass-flow rates, regardless the settings of the switches. It also assumes that all attemperator

spray flows are zero initially. The user has the freedom to change the default distribution. However, it is strongly recommended that the default distribution is used.

If the boiler is operated without reheat, the prescription of the reheat ratio is replaced by another parameter named as FMSA0(3). This parameter is defined as the inlet mass-flow-rate of the medium-pressure-turbine divided by the superheated steam flow. Since this version of the Boiler Performance Code does not consider cycle analysis, an arbitrary value for FMSA0(3) may be provided.

Special user action is required for Type 1 boiler operated under the triflux mode (ITRIX=1). In this case the user has to prescribe a ratio, FRE6, defined as the steam mass-flow entering the superheater triflux section (S/W sequence index 6) divided by the steam mass-flow leaving the superheater II section (S/W sequence index 5). In practice, this ratio simulates a valve which controls metal temperatures in the triflux section. Values on the order of 0.075 might be used if the ratio is not known.

(b) Initial steam/water temperatures

BPINPT estimates initial water or steam temperature distribution based on user's inputs on feedwater, cold reheat, and final superheat and reheat temperatures. Based on the temperature values mentioned above, BPINPT interpolates outlet temperatures for each heat exchanger that is switched on. Non-operating heat exchanger has the same outlet temperature as that of a preceding one, if it is activated. Inlet temperature is assigned by the code assuming that it equals to the outlet temperature of a previous section. Hence, the code does not consider heat losses between the various sections. The user can change the default values of the initial outlet temperatures section-wise, although it is not recommended. In case the boiler is operated without reheat, an arbitrary reheat temperature of 600 K is assigned to all reheat sections, although these sections don't exist.

For Type 1 boiler operated with the triflux mode (ITRIX=1), BPINPT prescribes the outlet temperature of the Superheater II section (S/W sequence index 5) as the inlet temperature of the SH/Triflux section (S/W sequence index 6). Initial guess on outlet steam temperature of the SH/Triflux section should be 50 K higher than the inlet temperature.

(c) Initial flue gas temperatures

This item is discussed briefly here because BPINPT requests inputs on initial flue gas temperatures later. Default initial values are interpolated from two inputs: furnace exit temperature, and the flue gas inlet temperature of the air preheater.

Specification of Heat Sink Boundary Conditions — BPINPT requires three types of input data in this category from the user as follows:

- Geometric data of the heat sinks
- Heat transfer coefficients
- Fouling specifications.

Here, the heat sinks include the internal tube banks, and the wall tubes surrounding the tube banks. Unless otherwise stated, the heat sink data have to be provided only for the existing sections downstream of the

user defined inlet plane at which the BPM code starts to solve the flue gas heat balance. This inlet plane is usually the upper furnace exit.

(a) Projected wall surface area

Projected wall surface area is the sum of all wall tube surfaces surrounding a particular heat exchanger section projected on a plane in unit of m^2 . These surfaces are usually water cooled. If Type 2 boiler is chosen and operated without a drum section ($\text{IDRUM}=0$), but with section 7 switched on, the surrounding surfaces are considered to be steam-cooled. BPINPT does not require projected surface area of the air preheater (Section 12).

BPINPT does not require this type of data for boiler sections which are located upstream of the user-defined inlet plane, where flue gas heat balances are not solved by the Boiler Performance Model. Note also that the code does not require any heat sink specifications for the furnace walls.

The effect of wall surfaces, which are located downstream of the upper furnace exit, is usually small on total heat absorbed. Therefore, these surfaces sometimes may be neglected in steam calculations. In this instance, the projected surface area surrounding the various sections can be set to zero. For Type 1 boiler operated under the Triflux mode ($\text{ITRIX}=1$), the projected wall area of the superheater triflux section (S/W sequence index 6) must be set to zero. BPINPT does not allow a non-zero input for the triflux section.

(b) Projected wall heat transfer coefficients

Wall heat transfer coefficients for various heat exchanger sections are user input. These coefficients, in unit of $\text{kW/m}^2 \text{K}$, should combine components of the convective and the radiative transfers. BPINPT offers a default value of $0.0350 \text{ kW/m}^2 \text{K}$ for any existing sections. Default values displayed for sections where flue gas heat balance is not solved can be ignored (similar to the projected wall surface area — see above). The user can change the default values, or prescribe individual coefficients for each existing sections.

(c) Fouling of projected wall surfaces

Fouling of the wall surfaces surrounding the heat exchanger sections are not explicitly considered by the BPINPT code. However, a fouling effect may be lumped into the heat transfer coefficients prescribed for these surfaces.

(d) Wall heat losses

Wall heat losses are handled in an engineering manner. The total wall-heat-loss is prescribed as a fraction of the heat transferred to all water walls, which include the furnace and the back pass walls, by an input parameter XLOSS0 . It is assumed that fractional losses are the same for each boiler sections. The total wall-heat-loss corresponds to the sum of radiation and unaccounted heat losses. Typical values of XLOSS0 range between 0.015 and 0.02.

(e) Heat exchanger surface areas

This is the actual surface area (m^2) of the heat exchanger tubes. These data can be found from boiler blue prints, and must be provided for all existing tube banks including the air preheater.

(f) Fouling of heat exchanger surfaces

The following inputs are necessary to incorporate the influence of ash fouling:

- Equivalent deposit thickness (m) on tubes
- Conductivity of deposits (kW/m K)
- Outer diameter (m) of the clean tubes.

This type of data have to be provided for sections which are switched on, and located downstream of the user-defined inlet plane.

(f-1) Deposit thickness

Deposit thickness must be interpreted as an average, as if the tube banks were covered completely and evenly by the ash deposits. Choosing an appropriate deposit thickness should also consider another parameter: deposit thermal conductivity, which will be described next. The user should keep in mind that the most important parameter in the heat transfer calculation is the ratio of deposit conductivity to thickness, commonly called as $k/\Delta s$ ratio here. The $k/\Delta s$ ratio represents the thermal conductance of the deposit-layers.

Default deposit thicknesses is 0.0005 m. If the default deposit-conductivity (0.0008 kW/m K) is used, thermal conductance of the deposit is 1.6 $\text{kW/m}^2 \text{ K}$. Experience suggests that the 1.6 conductance value represents rather clean tubes, and smaller values should be applied if the tubes are dirty. Heat sink surfaces in boilers are seldom completely clean. Therefore, BPINPT does not allow zero as deposit thickness.

(f-2) Thermal Conductivity

BPINPT offers two options to specify the thermal conductivities of the deposits on the heat exchanger tube banks:

- Prescription of the conductivities section-by-section ($\text{ITC}=0$)
- Use default calculation based on deposit temperatures ($\text{ITC}=1$).

In a file creation run, ITC is set to zero by default. If the user selects $\text{ITC}=0$, BPINPT suggests a default value of 0.0008 kW/mK for all sections that were switched-on. The code does not allow zero as the input. If the user selects $\text{ITC}=1$, BPINPT proceeds to the next input data block. It should be mentioned that the temperature-dependent distribution ($\text{ITC}=1$) is only typical of partially sintered deposits. Depending on physical states and many other factors, different deposit behaviors are quite possible. In these cases it may be better to use the option $\text{ITC}=0$, and prescribe the conductivity values section-by-section.

(f-3) Tube outer diameters

This input serves for two purposes. Firstly, it provides necessary data for detailed calculation of heat conduction through the deposit layers. Secondly, it allows the code to provide default values of convective heat transfer coefficients.

In many cases, information about tube diameters is not available. For such cases, BPINPT offers a default value of 0.0550 m as typical tube diameters. This default value is normally sufficient for engineering calculations. However, caution is advised if the option of automatic calculation of heat transfer coefficients is exercised. This is because the default coefficients calculated strongly depend on the specified tube diameters. BPINPT does not accept zero as tube diameters.

Contrary to entering values of deposit thickness and conductivities, the tube diameters and convective heat transfer coefficients (discussed next) have to be furnished in order of the Section Index, instead of the S/W Sequence Index.

(g) Convective Heat Transfer Coefficients

Convective heat transfer coefficients ($\text{kW/m}^2 \text{K}$) are important model parameters for steam calculations. BPINPT offers two options to determine these coefficients:

- Prescription of these coefficients section-by-section (ICALUS=0)
- Automatic calculation based on geometric and thermal properties of each section (ICALUS=1).

In a file creation run, ICALUS is set to zero by default but may be modified later. Independent of which option is chosen, the heat transfer coefficient of the air preheater is an input.

When a user selects options, he should keep the following in mind. The option of automatic calculation (ICALUS=1) is recommended only when the tube diameters and the geometry of the tube arrangements are known for each sections. Furthermore, current version of the BPINPT takes no radiation effects into account. The calculated heat transfer coefficients are purely due to convection. This can lead to under-estimation of actual heat transferred to boiler sections, if the flue gas temperatures are still high (for instance, above 800 K) at the boiler back pass.

The second option (ICALUS=0) has the advantage that radiation effects can be lumped into the coefficients so that more realistic overall heat-transfer coefficients are represented. Generally, estimation of these overall coefficients is difficult. However, in many cases, these coefficients can be deduced from baseline boiler operating conditions. For other performance evaluations, the user can use values concluded from the baseline operating conditions but corrected for Reynolds number dependencies.

(g-1) Option ICALUS=0

No default values will be offered by the BPINPT if this option is selected, since the heat transfer coefficients depends on a particular boiler design and operation. However, typical values are within the range of $0.04 \text{ kW/m}^2 \text{K}$ to $0.08 \text{ kW/m}^2 \text{K}$.

The heat transfer coefficient for the economizer may depend on the surface area defined for that section (e.g., whether the fin surface is included or not). This coefficient should be defined for surface area which

is actually considered. Similar argument holds for the air preheater. In determining the coefficient of the air preheater, the user is advised not to be over-scrupulous. This coefficient does not influence boiler efficiency calculations, since the efficiency is based on the steam/water heat absorptions and the assumed wall losses.

BPINPT does not allow zero as the heat transfer coefficients of existing sections. Therefore, the user also has to supply arbitrary values for sections upstream of the user-defined inlet plan.

(g-2) Option ICALUS=1

Under this option, the user only has to provide heat transfer coefficient of the air preheater. Coefficients for other sections are calculated automatically. However, the following information is required :

- Cross-sectional areas (m^2) perpendicular to the flow direction at mean heat exchanger elevations or locations.
- Longitudinal pitches, ELL(I), of the tube banks
- Lateral pitches, EBB(I), of the tube banks.

No default values are offered since the above quantities are boiler specific. Zero is not permitted as inputs for the existing sections. Arbitrary values have to be provided for sections upstream of the user-defined inlet plane.

The cross-sectional areas should exclude tube blockage. If this area varies in the flue gas flow direction, an average value may be used. The longitudinal pitch is the ratio of the tube outer diameter divided by tube spacing in the flow direction. The lateral pitch is the ratio of tube outer diameter divided by tube spacing in directions perpendicular to the gas flow. BPM considers in-line tube-banks only. Therefore, staggered tube-banks should be treated as if the tubes were arranged in-line.

Coupling with the 2D Furnace Heat Transfer Code — This coupling is provided by the data file BOIEFF.DAT generated from 2DHT runs. The file has information needed for a subsequent run of the Boiler Performance Model.

If BOIEFF.DAT exists, the following input data will automatically be transferred to BPINPT:

- Inlet flue gas temperature (K) at which BPM commences iterative solution of the flue gas heat balance
- Heat fluxes (kW) to all boiler sections upstream of the inlet plan where BPM begins flue gas heat balance calculations
- Total flue gas mass flow rate (kg/s)
- Flue gas composition (Vol. Frac., wet), including CO_2 , H_2O , N_2 and O_2
- Total fuel flow rate, FMFUEL (kg wet/s)
- Upper heating value, HUSW (kJ/kg wet)
- Lower heating value, HLOW (kJ/kg dry)
- Fuel moisture, PMOI (kg/kg wet)
- Net furnace heat release, FHR (kW)
- Air flow rate, FMAPH (kg wet/s)
- Air composition (Vol. Frac., wet), including CO_2 , H_2O , N_2 and O_2 .

The data file BOILER.DAT does not include the air inlet temperature, TAPHI(K), of the air preheater. This particular variable has to be supplied by the user.

The user can over-write all input data listed above. Also, entering these data manually is required if the file BOILER.DAT does not exist. This means that BPINPT may be applied under the condition that a preceding run of 2DHT is not executed. The availability of the BOILER.DAT file is indicated by a parameter defined as IFNCE. Setting IFNCE to 0 means the manual input; otherwise the code assumes the data file BOILER.DAT exists. IFNCE is set to 0 by default in a file creation run.

(a) Section index to begin gas side heat balance

BPINPT requires the user to specify a section index (not the S/W Sequence Index), JGSHB, to indicate the first active heat exchanger. This section index JGSHB defines the reference section at which the BPM code commences iterative solutions for the flue gas heat balance.

Since the domain of the 2DHT calculations usually stops at the upper furnace exit, JGSHB should be the section index of the first active heat exchanger following the upper furnace exit, provided the option IFNCE=1 was selected. If IFNCE=0 was selected, the user may assign any section index to JGSHB, except Index 2 of the furnace. In this case, BPINPT expects the user to supply the input data normally provided by the BOILER.DAT file.

(b). Option IFNCE=1

To ensure correct data transfer from file BOIEFF.DAT to BPINPT, the user has to map I-Indices of the heat exchangers used in the 2DHT with the section indices of those used in the BPINPT. This mapping is required for all heat exchangers with section indices smaller than the JGSHB. Normally, all superheater and reheater sections downstream of the upper furnace exit plan have to be mapped.

As the first step of the mapping procedure, the user has to provide the I-index, IEX, of the 2DHT zone layer, which locates in front of the heat exchanger with the section index JGSHB. IEX usually equals NX, which is the last zone number of the 2D zone arrangement. Overlapping of the 2D zone arrangement with the heat exchanger sections used in the BPINPT code is acceptable. However, a gap between the last I-layer used in the 2DHT and the section with index JGSHB is not allowed.

In the second step, the user has to prescribe the lower and upper I-indices of the 2DHT zone arrangement for all heat exchanger sections with section indices smaller than the JGSHB (except the furnace). The Boiler Performance Model will not calculate flue gas heat balances for these sections, but reads heat fluxes from the data file BOILER.DAT. For heat exchanger sections, considered by the BPINPT, the lower and upper indices can both be set to zero. Zero also constitutes default settings during file creation. If the last I-layer of the 2D zone arrangement (layer NX) is located just in front of the first existing heat exchanger section, the user has no need to carry out the mapping as described.

(c) Option IFNCE=0

If file BOIEFF.DAT does not exist, the user has to provide the furnace data as already discussed.

BPINPT offers no default values and all of the furnace inputs are set to zero in a file creation run.

(d) Initial gas temperatures

Independent of whether option IFNCE=1 or IFNCE=0 is used, an initial value of flue gas inlet temperature is required for each existing section. BPINPT offers these initial values to the user.

BPINPT approximates the initial temperatures based on the inlet gas temperature of the section with the index JGSHB, and on the air preheater inlet temperature as provided by the user. BPINPT interpolates and extrapolates inlet temperatures for all sections except the furnace. The furnace inlet temperature is not needed, but is set to 400 K only for cosmetic reasons. Inlet temperature of an inactive section is set to the value of the next existing downstream section, in the direction of the flue gas flow. The user can change the default distributions. However, this is only recommended when a better distribution is known, for instance, output from a preceding run is available.

(e) Flue gas mass flux distribution

Flue gas mass flux is displayed for each section as a constant. Changing the flue gas mass flux to account for leakage effects is not acceptable to the code.

Numerical and Output Control Parameters — These parameters control numerical accuracy of the user's runs, and the extent of output information he prefers.

(a) Convergence criteria

Two parameters have to be provided by the user to control the execution of the Boiler Performance Model. The execution of the BPM will be terminated when those criteria are met. These two parameters are:

- Maximum difference in temperatures (K) of the flue gas exiting the economizer, between two successive sub-iterations.
- Maximum difference in superheated steam mass flows (kg/s) between two successive sub-iterations .

Typical values for the temperature difference is 0.01 K, and 0.01 kg/sec is suggested for the mass flow difference.

(b) Maximum number of iterations

The objective of this input is to prevent endless code execution when convergence solution can not be found. The iterative processes carried out in the BPM will be terminated when an user-prescribed maximum iteration number is reached, even if the convergence criteria have not been met. Typically, a number between 5 and 10 is sufficient for boiler steam/gas energy iterations.

(c) Output control parameters

These parameters control the amount of information that will be stored in the output file generated by the BPM code. Selection of output level 2 will give more steam/gas information than the one generated by level 1.

Chapter 6

6.0 DESCRIPTION OF OUTPUTS

This chapter describes the format and the physical meanings of various output files generated by the three main codes (2DHT, RBNOX, and BPM). The objective of this chapter is to assist the user to interpret the results of the model predictions. The three main codes generate outputs in the following two forms:

- Screen displays — These displays are outputs directed to the user's computer terminal screen, to inform the user about the progress of the codes execution. All three main codes generate screen displays if the user exercise them.
- Disk files — These files contain model predictions, and are written to the computer's hard disk with names specified by the user. In general, the user may print these files and extract the kind of engineering information he wants.

The description of the outputs are presented in Sections 6.1, 6.2 and 6.3, respectively, for the 2DHT, RBNOX, and the BPM codes.

6.1 Outputs from the 2DHT Code

Outputs from the 2DHT code include screen display and files such as 2DOTcsvs.lll, OARRcsvs.lll, BOILER.DAT, and REBURN.DAT. These outputs are discussed item-by-item in the following sub-sections. Note again that "cs" is the user-specified case number and "vs" is the version number provided, lll indicates boiler load relative to the boiler's maximum continuous rating.

Screen Display

The screen display shows the progress of the code convergence by displaying error percentages of furnace energy balance. The iteration number and the furnace heat balance information immediately after the code completed an iterative calculation will be shown on the screen. In this way, the user can track the status of the code execution and if necessary, estimate the time required to complete the run. The screen display can be captured in the form of disk files and later be printed. Volume II includes the captured 2DHT screen displays for five example cases. The messages displayed on the screen are actually abbreviated from an output disk-file (2DOTcsvs.lll), which is discussed in the next sub-section thoroughly. The user should refer to the next sub-section to gain knowledge of interpreting the 2DHT screen display.

File 2DOTcsvs.lll

This is the file which contains the 2DHT furnace performance predictions, and is most likely to be dealt with by the user. Listing 6.1 is an example indicating the contents of this file. The size of this file is determined by the user's choice in setting the value of the parameter LOUTPUT (see Section 5.1). The output shown in Listing 6.1 was generated by the default option, for a reburning case. The size of this file will increase considerably if the user selects higher output levels (e.g., LOUTPUT=4), to obtain comprehensive output information at each iterative cycle. In this case, it is important to ensure that enough disk space is available to avoid abnormal termination. Setting output level to 1 generates the most concise 2DOTcsvs.lll output file.

File 2DOTcsvs.lll normally is saved in computer hard disks. However, the user can direct this file to his terminal screen by setting the input parameter FHDOPT to "CON" during the 2DINPT interactive session. In this instance, the output file 2DOTcsvs.lll will not be saved in disks but displayed on the computer screen only. If the user is also interested in obtaining a copy of the output file while viewing the file on the screen, he can perform on-line printing by pressing the "ctrl" and the "print scrn" keys *simultaneously then release them before* he executes the 2DHT code. The user may find that the outputs displayed on the screen are difficult to read, due to the wrapping of the output lines to fit the 80 display-column found in most of the computer screens.

Table 6.1 was prepared to describe the 2DOTcsvs.lll output file such as the one shown in Listing 6.1. The outputs shown in the Listing were grouped into "blocks" of information and each block was labeled by a numeral. To interpret a block of the output information, the user may refer to Table 6.1 and locate the description of that block by matching the "Index of Output Block" in the table with the numeral shown in Listing 6.1. Table 6.1 then shows the user the variable names, units, and the physical meanings of the variables for that block. A block of information may not appear in the output file if the output level (LOUTPUT) is set low. Table 6.1 reminds the user about this by showing the output levels required in a separate column. If the required output level is 4 and the user sets the level to 1, then that block of output information will not be included in the output file 2DOTcsvs.lll.

File OARRcsvs.lll

The 2DHT code can also generate an "output array file" with a default name as OARRcsvs.lll in the disk, depending on the user's choice (NWRTE=1, see Section 4.1). This file has a size of about 164 KB, and contains all variable values concluded upon the completion of a 2DHT run. If used, the output array file will set the initial furnace-temperature and heat-flux profiles to the values saved, so that a new run can start its iterative calculation from there. This file may be used to continue the execution of a run that has not converged, or to provide better initial conditions for a new run. The file will not be discussed and shown here since it consists of numerical numbers only, and the user need not to know the details.

File REBURN.DAT

2DHT generates this additional file only when the reburning option is activated (NREB=1). This file contains necessary furnace time-temperature and fuels information needed by the reburning NO_x model, RBNOX. File REBURN.DAT must be present during the RBINPT interactive input sessions. The format of this file is shown in Volume II for Case 2 example, but will not be discussed here since it consists of numerical numbers only and the user need not to know the details.

File BOILER.DAT

This output file is generated by the 2DHT code every time the code is executed, even though the user may not plan to use the file for subsequent boiler performance modeling. BOILER.DAT contains furnace operation and performance data, including lower and upper heating values, furnace gas temperatures, net heat fluxes to furnace walls and radiant heat exchangers, and total furnace heat release. This file may be used during the interactive BPINPT input sessions. The format of file is shown in Volume II for the five example cases, but will not be discussed here since it consists of numerical numbers only and the user need not to know the details.

Listing 6.1. Output generated by the 2DHT code.

* GENERAL INFORMATION *

BOILER NAME: BOILER 1
CASE NUMBER: 02
VERSION NUMBER: 01
THERMAL LOAD: .30.0 % OF FULL LOAD

* INPUT/OUTPUT *

NREAD: 0
NWRITE: 1

NAME OF INPUT DATA FILE: 2DIN0201.100 (copied to 2DINPT.DAT)
NAME OF INPUT ARRAY FILE: IARR0201.100
NAME OF OUTPUT ARRAY FILE: OARR0201.100
NAME OF GRAPHICS OUTPUT FILE: GRAF
NAME OF OUTPUT DATA FILE: 2DOT0201.100
OUTPUT LEVEL: DEFAULT

* USER'S COMMENTS *

c UPDATE INPUT DATA FILE 2DIN0101.100 FOR OIL FIRING AT 75% LOAD WITH
c GAS REBURNING
c
c
c
c
c
c
c

HIGV
HUGVW
SFLOW

NET CAL. VALUE OF REBURN FUEL
GROSS CAL. VALUE OF REBURN FUEL
ATOMIZING STEAM IN BURNER FUEL

31785.6992
39382.1992
0.0000

KJ/M3N GAS DRY
KJ/M3N GAS WET
KG-STEAM/SEC

MASS CONCENTRATION OF GASEOUS SPECIES IN KG/KG WET

CO2	H2O	N2	O2	VOL	SO2	ASH	CHAR	SOOT
0.1878	0.0846	0.7130	0.0136	0.0000	0.0010	0.0000	0.0000	0.0000

CONCENTRATION OF GASEOUS SPECIES IN VOL. FRACTION WET

CO2	H2O	N2	O2	VOL	SO2
0.1224	0.1347	0.7302	0.0122	0.0000	0.0005

CONCENTRATION OF GASEOUS SPECIES IN VOL. FRACTION DRY

CO2	H2O	N2	O2	VOL	SO2
0.1415	0.0000	0.8439	0.0141	0.0000	0.0005

SO2 CONCENTRATION IN PPM MASS 1027.

SO2 CONCENTRATION IN PPM VOL WET 460.

SO2 CONCENTRATION IN PPM VOL DRY 531.

HEAT CAPACITY OF COMBUSTION SPECIES (KJ/KG-K)

	CO2	H2O	N2	O2	VOL	SO2	ASH	CHAR	SOOT
AT 493.15K	0.9319689	1.9024371	1.0447987	0.9416904	2.5248535	0.6756042	0.8373599	1.0724180	0.9727679
AT 376.15K	0.8821020	1.8765520	1.0403634	0.9260021	2.3311000	0.6448221	0.8373600	0.9819483	0.8222868
AT 298.25K	0.8434441	1.8582036	1.0395815	0.9173627	2.2140925	0.6205368	0.8373599	0.9184768	0.7111416
AT 1800.00K	1.2005430	2.3140147	1.1634477	1.0747626	4.3484931	0.8270922	0.8373600	1.6863927	1.5045161
AT 900.00K	1.0583812	2.0220246	1.0806181	0.9992388	3.2324150	0.7527937	0.8373600	1.3415941	1.3412676
AT 573.15K	0.9621025	1.9230694	1.0497636	0.9533783	2.6651895	0.6944230	0.8373600	1.1309191	1.0638425

MEAN HEAT CAPACITIES OF SOME INPUT/OUTPUT STREAMS

INPUT STREAM	TEMPERATURE (K)	MEAN Cp (KJ/KG-K)
AIR	376.15	1.0222045
AIR	493.15	1.0294459
FLUE GAS	573.15	1.1055170
FLUE GAS	900.00	1.1546530
FLUE GAS	1800.00	1.2662147

MASS BALANCE FOR VOLUME ZONES

NR	I	J	MCONIN KG/S	MCONNT KG/S	MDIFIN KG/S	MDIFNT KG/S	MTOTIN KG/S	MTOTEX KG/S	MTOTNT KG/S
1	1		14.266	0.000	14.803	0.000	29.068	29.068	0.000
1	2		14.266	0.000	17.624	0.000	31.889	31.889	0.000
2	1		14.266	0.000	16.213	0.000	30.478	30.478	0.000
2	2		26.946	0.000	39.128	0.000	66.074	66.074	0.000
2	3		19.021	0.000	28.859	0.000	47.880	47.880	0.000
3	1		6.340	0.000	11.321	0.000	17.661	17.661	0.000
3	2		14.266	0.000	31.110	0.000	45.376	45.376	0.000
3	3		19.021	0.000	50.854	0.000	69.875	69.875	0.000
3	4		6.149	0.000	22.110	0.000	28.259	28.259	0.000
4	1		4.755	0.000	11.613	0.000	16.368	16.368	0.000
4	2		12.056	0.000	33.513	0.000	45.569	45.569	0.000
4	3		19.316	-0.006	49.537	0.000	68.853	68.847	-0.006
4	4		17.974	0.006	28.687	0.000	46.661	46.667	0.006
5	1		2.210	0.000	12.337	0.000	14.547	14.547	0.000
5	2		5.762	0.006	35.104	0.000	40.866	40.872	0.006
5	3		24.418	0.000	44.517	0.000	68.935	68.935	0.000
5	4		24.511	-0.006	25.930	0.000	50.440	50.435	-0.006
6	1		3.292	0.000	21.490	0.000	24.782	24.782	0.000
6	2		6.126	0.000	65.451	0.000	71.578	71.578	0.000
6	3		33.367	0.000	75.389	0.000	108.757	108.757	0.000
6	4		28.525	0.000	41.445	0.000	69.971	69.971	0.000
7	1		3.581	0.000	20.492	0.000	24.072	24.072	0.000
7	2		7.185	0.000	59.340	0.000	66.525	66.525	0.000
7	3		39.378	-0.006	56.414	0.000	95.792	95.786	-0.006
7	4		22.278	0.006	30.985	0.000	53.263	53.269	0.006
8	1		2.164	0.000	16.485	0.000	18.648	18.648	0.000
8	2		8.359	0.000	50.576	0.000	58.935	58.935	0.000
8	3		34.698	0.006	53.610	0.000	88.308	88.313	0.006
8	4		16.273	-0.006	28.080	0.000	44.353	44.347	-0.006
9	1		6.080	0.000	13.335	0.000	19.415	19.415	0.000
9	2		22.150	0.000	42.362	0.000	64.512	64.512	0.000
9	3		49.200	0.000	64.797	0.000	113.998	113.998	0.000
9	4		21.983	0.000	26.615	0.000	48.598	48.598	0.000
10	1		6.080	0.000	9.556	0.000	15.636	15.636	0.000
10	2		18.234	0.000	28.664	0.000	46.898	46.898	0.000
10	3		33.535	0.000	41.858	0.000	75.393	75.393	0.000
11	1		6.080	0.000	6.469	0.000	12.549	12.549	0.000
11	2		18.234	0.000	19.403	0.000	37.637	37.637	0.000
11	3		33.535	0.000	35.684	0.000	69.219	69.219	0.000
12	1		6.080	0.000	6.469	0.000	12.549	12.549	0.000
12	2		18.234	0.000	19.403	0.000	37.637	37.637	0.000
12	3		33.535	0.000	35.684	0.000	69.219	69.219	0.000
13	1		6.080	0.000	9.795	0.000	15.875	15.875	0.000
13	2		18.234	0.000	22.730	0.000	40.964	40.964	0.000
13	3		33.535	0.000	35.684	0.000	69.219	69.219	0.000
14	1		14.462	0.000	14.825	0.000	29.287	29.287	0.000
14	2		51.769	0.000	32.790	0.000	84.559	84.559	0.000
14	3		33.535	0.000	17.842	0.000	51.377	51.377	0.000
15	1		26.032	0.000	14.969	0.000	41.001	41.001	0.000
15	2		43.387	0.000	49.536	0.000	92.922	92.922	0.000
16	1		26.032	0.000	14.969	0.000	41.001	41.001	0.000
16	2		43.387	0.000	49.536	0.000	92.922	92.922	0.000
17	1		14.462	0.000	11.498	0.000	25.961	25.961	0.000
17	2		43.387	0.000	34.495	0.000	77.882	77.882	0.000
18	1		14.462	0.000	11.498	0.000	25.961	25.961	0.000
18	2		43.387	0.000	34.495	0.000	77.882	77.882	0.000
19	1		14.462	0.000	5.749	0.000	20.211	20.211	0.000
19	2		43.387	0.000	17.247	0.000	60.634	60.634	0.000

TOTAL MASS BALANCE FOR THE FURNACE VOLUME

INCLUDING SYMMETRICAL FLUXES IF EXISTING: 1193.72 0.00 1720.98 0.00

2914.702914.70 0.00

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iter. no. = 1, act.err. = 705.7140 %, avg.err. = 705.7140 %, 20 it.err. = 705.7140 %, hb.err. = -75.4073 %
iter. no. = 2, act.err. = -70.0213 %, avg.err. = 317.8463 %, 20 it.err. = 317.8463 %, hb.err. = 15.7280 %
iter. no. = 3, act.err. = -39.4965 %, avg.err. = 198.7321 %, 20 it.err. = 198.7321 %, hb.err. = 11.6893 %
iter. no. = 4, act.err. = -29.3348 %, avg.err. = 141.7153 %, 20 it.err. = 141.7153 %, hb.err. = 8.6393 %
iter. no. = 5, act.err. = -23.1255 %, avg.err. = 108.7472 %, 20 it.err. = 108.7472 %, hb.err. = 5.8732 %
iter. no. = 6, act.err. = -18.6358 %, avg.err. = 87.5167 %, 20 it.err. = 87.5167 %, hb.err. = 4.2228 %
iter. no. = 7, act.err. = -13.8597 %, avg.err. = 73.0343 %, 20 it.err. = 73.0343 %, hb.err. = 2.8306 %
iter. no. = 8, act.err. = -13.0660 %, avg.err. = 62.2718 %, 20 it.err. = 62.2718 %, hb.err. = 3.2780 %
iter. no. = 9, act.err. = -9.3933 %, avg.err. = 54.3090 %, 20 it.err. = 54.3090 %, hb.err. = 1.8173 %
iter. no. = 10, act.err. = -6.7552 %, avg.err. = 48.2026 %, 20 it.err. = 48.2026 %, hb.err. = 1.0997 %
iter. no. = 11, act.err. = -5.4984 %, avg.err. = 43.3207 %, 20 it.err. = 43.3207 %, hb.err. = 1.2046 %
iter. no. = 12, act.err. = -3.4600 %, avg.err. = 39.4223 %, 20 it.err. = 39.4223 %, hb.err. = 0.7902 %
iter. no. = 13, act.err. = -3.8765 %, avg.err. = 36.0916 %, 20 it.err. = 36.0916 %, hb.err. = 1.4963 %
iter. no. = 14, act.err. = -3.8696 %, avg.err. = 33.2373 %, 20 it.err. = 33.2373 %, hb.err. = 0.8328 %
iter. no. = 15, act.err. = -2.1690 %, avg.err. = 30.8768 %, 20 it.err. = 30.8768 %, hb.err. = 0.6775 %
iter. no. = 16, act.err. = -1.8329 %, avg.err. = 28.8325 %, 20 it.err. = 28.8325 %, hb.err. = 0.3978 %
iter. no. = 17, act.err. = -0.9136 %, avg.err. = 27.0827 %, 20 it.err. = 27.0827 %, hb.err. = -0.1321 %
iter. no. = 18, act.err. = -0.6881 %, avg.err. = 25.5399 %, 20 it.err. = 25.5399 %, hb.err. = 0.4587 %
iter. no. = 19, act.err. = -0.9538 %, avg.err. = 24.1455 %, 20 it.err. = 24.1455 %, hb.err. = 0.9868 %
iter. no. = 20, act.err. = -1.3709 %, avg.err. = 22.8697 %, 20 it.err. = 22.8697 %, hb.err. = 0.8215 %
iter. no. = 21, act.err. = -0.1442 %, avg.err. = 21.7738 %, 20 it.err. = -12.4233 %, hb.err. = 0.0308 %
iter. no. = 22, act.err. = -0.2166 %, avg.err. = 20.7742 %, 20 it.err. = -8.9330 %, hb.err. = 0.8322 %
iter. no. = 23, act.err. = -0.8257 %, avg.err. = 19.8351 %, 20 it.err. = -6.9995 %, hb.err. = 0.1173 %
iter. no. = 24, act.err. = -1.5573 %, avg.err. = 18.9437 %, 20 it.err. = -5.6106 %, hb.err. = 0.4712 %
iter. no. = 25, act.err. = -1.4825 %, avg.err. = 18.1267 %, 20 it.err. = -4.5285 %, hb.err. = 0.8269 %
iter. no. = 26, act.err. = -2.6069 %, avg.err. = 17.3292 %, 20 it.err. = -3.7270 %, hb.err. = 0.6853 %
iter. no. = 27, act.err. = -0.6906 %, avg.err. = 16.6618 %, 20 it.err. = -3.0686 %, hb.err. = 0.3819 %
iter. no. = 28, act.err. = -2.0593 %, avg.err. = 15.9932 %, 20 it.err. = -2.5182 %, hb.err. = 0.9449 %
iter. no. = 29, act.err. = -0.6019 %, avg.err. = 15.4210 %, 20 it.err. = -2.0787 %, hb.err. = 0.5361 %
iter. no. = 30, act.err. = 0.3434 %, avg.err. = 14.9184 %, 20 it.err. = -1.7237 %, hb.err. = -0.2475 %
iter. no. = 31, act.err. = -0.3739 %, avg.err. = 14.4251 %, 20 it.err. = -1.4675 %, hb.err. = 0.7398 %
iter. no. = 32, act.err. = -1.3256 %, avg.err. = 13.9329 %, 20 it.err. = -1.3608 %, hb.err. = 0.5460 %
iter. no. = 33, act.err. = -0.3667 %, avg.err. = 13.4995 %, 20 it.err. = -1.1853 %, hb.err. = -0.1499 %
iter. no. = 34, act.err. = -0.9636 %, avg.err. = 13.0742 %, 20 it.err. = -1.0400 %, hb.err. = 0.3763 %
iter. no. = 35, act.err. = -0.6010 %, avg.err. = 12.6834 %, 20 it.err. = -0.9616 %, hb.err. = 0.5455 %
iter. no. = 36, act.err. = -1.2601 %, avg.err. = 12.2961 %, 20 it.err. = -0.9330 %, hb.err. = 0.3606 %
iter. no. = 37, act.err. = -0.2126 %, avg.err. = 11.9581 %, 20 it.err. = -0.8979 %, hb.err. = 0.8199 %
iter. no. = 38, act.err. = -1.1227 %, avg.err. = 11.6138 %, 20 it.err. = -0.9196 %, hb.err. = 0.1300 %
iter. no. = 39, act.err. = 0.4322 %, avg.err. = 11.3271 %, 20 it.err. = -0.8503 %, hb.err. = 0.1555 %
iter. no. = 40, act.err. = 0.7414 %, avg.err. = 11.0625 %, 20 it.err. = -0.7447 %, hb.err. = -0.2481 %
iter. no. = 41, act.err. = -1.5781 %, avg.err. = 10.7542 %, 20 it.err. = -0.8164 %, hb.err. = 1.0582 %
iter. no. = 42, act.err. = -0.4698 %, avg.err. = 10.4869 %, 20 it.err. = -0.8291 %, hb.err. = 0.0187 %
iter. no. = 43, act.err. = -2.1871 %, avg.err. = 10.1922 %, 20 it.err. = -0.8971 %, hb.err. = 0.6512 %
iter. no. = 44, act.err. = -0.5961 %, avg.err. = 9.9470 %, 20 it.err. = -0.8491 %, hb.err. = 0.2580 %
iter. no. = 45, act.err. = 0.7398 %, avg.err. = 9.7424 %, 20 it.err. = -0.7380 %, hb.err. = -0.0610 %
iter. no. = 46, act.err. = -1.7188 %, avg.err. = 9.4932 %, 20 it.err. = -0.6936 %, hb.err. = 0.7809 %
iter. no. = 47, act.err. = -1.3488 %, avg.err. = 9.2626 %, 20 it.err. = -0.7265 %, hb.err. = 0.1436 %
iter. no. = 48, act.err. = -1.6842 %, avg.err. = 9.0345 %, 20 it.err. = -0.7077 %, hb.err. = 0.9826 %
iter. no. = 49, act.err. = 0.2956 %, avg.err. = 8.8561 %, 20 it.err. = -0.6628 %, hb.err. = -0.5288 %
iter. no. = 50, act.err. = 1.7096 %, avg.err. = 8.7132 %, 20 it.err. = -0.5945 %, hb.err. = -0.4847 %
iter. no. = 51, act.err. = -1.4575 %, avg.err. = 8.5138 %, 20 it.err. = -0.6487 %, hb.err. = 0.1577 %
iter. no. = 52, act.err. = 1.8115 %, avg.err. = 8.3849 %, 20 it.err. = -0.4918 %, hb.err. = -0.4767 %
iter. no. = 53, act.err. = 2.9490 %, avg.err. = 8.2823 %, 20 it.err. = -0.3261 %, hb.err. = -0.2175 %
iter. no. = 54, act.err. = -2.6470 %, avg.err. = 8.0799 %, 20 it.err. = -0.4102 %, hb.err. = 1.1017 %
iter. no. = 55, act.err. = -1.9531 %, avg.err. = 7.8975 %, 20 it.err. = -0.4778 %, hb.err. = 0.7294 %
iter. no. = 56, act.err. = -0.8579 %, avg.err. = 7.7412 %, 20 it.err. = -0.4577 %, hb.err. = -0.2129 %
iter. no. = 57, act.err. = 0.5276 %, avg.err. = 7.6146 %, 20 it.err. = -0.4207 %, hb.err. = 0.0268 %
iter. no. = 58, act.err. = 0.4505 %, avg.err. = 7.4911 %, 20 it.err. = -0.3421 %, hb.err. = -0.0250 %
iter. no. = 59, act.err. = -0.9526 %, avg.err. = 7.3480 %, 20 it.err. = -0.4113 %, hb.err. = 0.5432 %
iter. no. = 60, act.err. = -1.2558 %, avg.err. = 7.2046 %, 20 it.err. = -0.5112 %, hb.err. = 0.2582 %
iter. no. = 61, act.err. = 2.3973 %, avg.err. = 7.1258 %, 20 it.err. = -0.3124 %, hb.err. = -0.8371 %
iter. no. = 62, act.err. = -1.4258 %, avg.err. = 6.9879 %, 20 it.err. = -0.3602 %, hb.err. = 0.8995 %
iter. no. = 63, act.err. = -1.9249 %, avg.err. = 6.8464 %, 20 it.err. = -0.3471 %, hb.err. = 0.0788 %
iter. no. = 64, act.err. = -0.4467 %, avg.err. = 6.7324 %, 20 it.err. = -0.3396 %, hb.err. = 0.2565 %
iter. no. = 65, act.err. = 1.3057 %, avg.err. = 6.6489 %, 20 it.err. = -0.3113 %, hb.err. = -0.6331 %
iter. no. = 66, act.err. = 0.6445 %, avg.err. = 6.5580 %, 20 it.err. = -0.1932 %, hb.err. = -0.0227 %
iter. no. = 67, act.err. = 0.0906 %, avg.err. = 6.4614 %, 20 it.err. = -0.1212 %, hb.err. = 0.2569 %
iter. no. = 68, act.err. = -0.1653 %, avg.err. = 6.3640 %, 20 it.err. = -0.0452 %, hb.err. = 0.0896 %
iter. no. = 69, act.err. = -0.6212 %, avg.err. = 6.2627 %, 20 it.err. = -0.0911 %, hb.err. = -0.3088 %
iter. no. = 70, act.err. = 0.2669 %, avg.err. = 6.1771 %, 20 it.err. = -0.1632 %, hb.err. = -0.2699 %
iter. no. = 71, act.err. = 1.4276 %, avg.err. = 6.1102 %, 20 it.err. = -0.0190 %, hb.err. = -0.9385 %
iter. no. = 72, act.err. = 1.4092 %, avg.err. = 6.0449 %, 20 it.err. = -0.0391 %, hb.err. = 0.8430 %
iter. no. = 73, act.err. = -0.8604 %, avg.err. = 5.9503 %, 20 it.err. = -0.2295 %, hb.err. = -0.1694 %
iter. no. = 74, act.err. = -0.4473 %, avg.err. = 5.8639 %, 20 it.err. = -0.1196 %, hb.err. = 0.0858 %
iter. no. = 75, act.err. = -0.0909 %, avg.err. = 5.7845 %, 20 it.err. = -0.0265 %, hb.err. = -0.0885 %
iter. no. = 76, act.err. = 0.1777 %, avg.err. = 5.7107 %, 20 it.err. = 0.0253 %, hb.err. = 0.4451 %
iter. no. = 77, act.err. = -0.9739 %, avg.err. = 5.6239 %, 20 it.err. = -0.0497 %, hb.err. = -0.2381 %
iter. no. = 78, act.err. = -0.3900 %, avg.err. = 5.5468 %, 20 it.err. = -0.0918 %, hb.err. = 0.2054 %
iter. no. = 79, act.err. = -0.8747 %, avg.err. = 5.4655 %, 20 it.err. = -0.0879 %, hb.err. = -0.2362 %
iter. no. = 80, act.err. = 0.0416 %, avg.err. = 5.3977 %, 20 it.err. = -0.0230 %, hb.err. = 0.3899 %
iter. no. = 81, act.err. = -0.9760 %, avg.err. = 5.3190 %, 20 it.err. = -0.1917 %, hb.err. = -0.0722 %
iter. no. = 82, act.err. = -0.3480 %, avg.err. = 5.2499 %, 20 it.err. = -0.1378 %, hb.err. = 0.2355 %
iter. no. = 83, act.err. = -1.1740 %, avg.err. = 5.1725 %, 20 it.err. = -0.1002 %, hb.err. = -0.2261 %
iter. no. = 84, act.err. = -0.5736 %, avg.err. = 5.1041 %, 20 it.err. = -0.1066 %, hb.err. = -0.0400 %
iter. no. = 85, act.err. = -0.1191 %, avg.err. = 5.0426 %, 20 it.err. = -0.1778 %, hb.err. = 0.1628 %
iter. no. = 86, act.err. = -0.5528 %, avg.err. = 4.9776 %, 20 it.err. = -0.2377 %, hb.err. = -0.1162 %
iter. no. = 87, act.err. = -0.7549 %, avg.err. = 4.9117 %, 20 it.err. = -0.2800 %, hb.err. = -0.3187 %
iter. no. = 88, act.err. = 0.0448 %, avg.err. = 4.8564 %, 20 it.err. = -0.2695 %, hb.err. = 0.0756 %
iter. no. = 89, act.err. = 0.5367 %, avg.err. = 4.8078 %, 20 it.err. = -0.2116 %, hb.err. = 0.3532 %
iter. no. = 90, act.err. = -0.9923 %, avg.err. = 4.7434 %, 20 it.err. = -0.2745 %, hb.err. = -0.6999 %
iter. no. = 91, act.err. = 1.1851 %, avg.err. = 4.7043 %, 20 it.err. = -0.2866 %, hb.err. = 0.7609 %
iter. no. = 92, act.err. = -0.9255 %, avg.err. = 4.6431 %, 20 it.err. = -0.4034 %, hb.err. = -0.6967 %
iter. no. = 93, act.err. = 1.8286 %, avg.err. = 4.6128 %, 20 it.err. = -0.2689 %, hb.err. = 1.2086 %
iter. no. = 94, act.err. = -2.4073 %, avg.err. = 4.5382 %, 20 it.err. = -0.3669 %, hb.err. = -1.5557 %
iter. no. = 95, act.err. = 1.7928 %, avg.err. = 4.5093 %, 20 it.err. = -0.2727 %, hb.err. = 1.1996 %
iter. no. = 96, act.err. = -0.9999 %, avg.err. = 4.4519 %, 20 it.err. = -0.3316 %, hb.err. = -0.7204 %
iter. no. = 97, act.err. = 0.5497 %, avg.err. = 4.4116 %, 20 it.err. = -0.2554 %, hb.err. = 0.3490 %
iter. no. = 98, act.err. = 0.0232 %, avg.err. = 4.3669 %, 20 it.err. = -0.2348 %, hb.err. = -0.0593 %
iter. no. = 99, act.err. = 0.0462 %, avg.err. = 4.3232 %, 20 it.err. = -0.1887 %, hb.err. = -0.0512 %

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THE DISTRIBUTION OF SPSU in m**2/kg AFTER 100 ITERATIONS

18

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J= 4 0.000E-01 0.000E-01 2.284E+02 2.205E+02 2.165E+02 2.199E+02 2.289E+02 2.355E+02 2.571E+02 0.000E-01
J= 3 0.000E-01 2.314E+02 2.301E+02 2.263E+02 2.246E+02 2.271E+02 2.299E+02 2.347E+02 2.461E+02 2.475E+02

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J= 2	2.322E+02	2.316E+02	2.307E+02	2.294E+02	2.297E+02	2.315E+02	2.335E+02	2.369E+02	2.432E+02	2.449E+02
J= 1	2.321E+02	2.319E+02	2.318E+02	2.316E+02	2.326E+02	2.340E+02	2.353E+02	2.380E+02	2.418E+02	2.431E+02
	I= 1	I= 2	I= 3	I= 4	I= 5	I= 6	I= 7	I= 8	I= 9	I=10
J= 4	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 3	2.484E+02	2.488E+02	2.490E+02	2.491E+02	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 2	2.457E+02	2.462E+02	2.468E+02	2.480E+02	2.480E+02	2.480E+02	2.480E+02	2.480E+02	2.480E+02	2.480E+02
J= 1	2.437E+02	2.443E+02	2.455E+02	2.472E+02	2.475E+02	2.476E+02	2.476E+02	2.476E+02	2.476E+02	2.476E+02
	I=11	I=12	I=13	I=14	I=15	I=16	I=17	I=18	I=19	

THE DISTRIBUTION OF UBRT in Fraction of Input fixed-C AFTER 100 ITERATIONS

19

J= 4	0.000E-01	0.000E-01	8.167E-01	9.340E-01	1.001E+00	9.460E-01	8.275E-01	7.499E-01	5.675E-01	0.000E-01
J= 3	0.000E-01	7.749E-01	7.927E-01	8.461E-01	8.698E-01	8.366E-01	8.035E-01	7.513E-01	6.428E-01	6.271E-01
J= 2	7.654E-01	7.722E-01	7.847E-01	8.025E-01	7.997E-01	7.791E-01	7.587E-01	7.235E-01	6.632E-01	6.458E-01
J= 1	7.661E-01	7.688E-01	7.708E-01	7.732E-01	7.634E-01	7.495E-01	7.363E-01	7.095E-01	6.727E-01	6.595E-01
	I= 1	I= 2	I= 3	I= 4	I= 5	I= 6	I= 7	I= 8	I= 9	I=10
J= 4	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 3	6.179E-01	6.135E-01	6.112E-01	6.101E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 2	6.370E-01	6.315E-01	6.269E-01	6.176E-01	6.174E-01	6.177E-01	6.176E-01	6.175E-01	6.175E-01	6.175E-01
J= 1	6.536E-01	6.475E-01	6.370E-01	6.239E-01	6.211E-01	6.210E-01	6.208E-01	6.208E-01	6.207E-01	6.207E-01
	I=11	I=12	I=13	I=14	I=15	I=16	I=17	I=18	I=19	

THE DISTRIBUTION OF PO2 in Vol. Fraction, Wet AFTER 100 ITERATIONS

20

J= 4	0.000E-01	0.000E-01	1.094E-02	3.188E-02	5.381E-02	3.751E-02	1.106E-02	6.993E-03	3.959E-02	0.000E-01
J= 3	0.000E-01	9.517E-03	1.012E-02	1.091E-02	1.350E-02	8.541E-03	3.928E-03	3.450E-03	1.653E-02	1.423E-02
J= 2	9.227E-03	9.349E-03	9.429E-03	9.416E-03	7.599E-03	4.729E-03	2.845E-03	3.490E-03	9.572E-03	1.003E-02
J= 1	9.172E-03	9.166E-03	8.755E-03	7.988E-03	6.011E-03	4.073E-03	3.469E-03	3.924E-03	6.894E-03	7.535E-03
	I= 1	I= 2	I= 3	I= 4	I= 5	I= 6	I= 7	I= 8	I= 9	I=10
J= 4	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 3	1.388E-02	1.382E-02	1.381E-02	1.381E-02	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 2	9.965E-03	1.011E-02	1.055E-02	1.222E-02	1.219E-02	1.210E-02	1.211E-02	1.212E-02	1.212E-02	1.212E-02
J= 1	7.721E-03	8.145E-03	9.272E-03	1.118E-02	1.157E-02	1.158E-02	1.158E-02	1.159E-02	1.159E-02	1.159E-02
	I=11	I=12	I=13	I=14	I=15	I=16	I=17	I=18	I=19	

THE DISTRIBUTION OF FULO in kg/(kg,mixture) AFTER 100 ITERATIONS

21

J= 4	0.000E-01	0.000E-01	5.899E-02	5.965E-02	5.982E-02	5.873E-02	5.453E-02	5.214E-02	4.197E-02	0.000E-01
J= 3	0.000E-01	5.868E-02	5.882E-02	5.917E-02	5.908E-02	5.803E-02	5.643E-02	5.410E-02	4.863E-02	4.885E-02
J= 2	5.856E-02	5.862E-02	5.868E-02	5.866E-02	5.807E-02	5.694E-02	5.570E-02	5.394E-02	5.101E-02	5.072E-02
J= 1	5.854E-02	5.854E-02	5.842E-02	5.814E-02	5.733E-02	5.630E-02	5.542E-02	5.412E-02	5.231E-02	5.190E-02
	I= 1	I= 2	I= 3	I= 4	I= 5	I= 6	I= 7	I= 8	I= 9	I=10
J= 4	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 3	4.885E-02	4.885E-02	4.885E-02	4.885E-02	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 2	5.070E-02	5.063E-02	5.042E-02	4.962E-02	4.965E-02	4.970E-02	4.969E-02	4.969E-02	4.969E-02	4.969E-02
J= 1	5.183E-02	5.164E-02	5.108E-02	5.015E-02	4.997E-02	4.997E-02	4.997E-02	4.997E-02	4.997E-02	4.997E-02
	I=11	I=12	I=13	I=14	I=15	I=16	I=17	I=18	I=19	

THE DISTRIBUTION OF VOLO in Number of Vol. Lumps Released AFTER 100 ITERATIONS

22

J= 4	0.000E-01	0.000E-01	2.000E+00	2.095E+03	3.129E+03	3.137E+03	1.400E+01	0.000E-01	0.000E-01	0.000E-01
J= 3	0.000E-01	0.000E-01	0.000E-01	8.000E+00	1.900E+01	1.600E+01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 2	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 1	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
	I= 1	I= 2	I= 3	I= 4	I= 5	I= 6	I= 7	I= 8	I= 9	I=10
J= 4	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 3	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 2	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 1	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
	I=11	I=12	I=13	I=14	I=15	I=16	I=17	I=18	I=19	

THE DISTRIBUTION OF SO2 in Vol. Fraction, Wet AFTER 100 ITERATIONS

23

J= 4	0.000E-01	0.000E-01	5.343E-04	4.822E-04	4.156E-04	4.461E-04	4.798E-04	4.703E-04	3.792E-04	0.000E-01
J= 3	0.000E-01	5.317E-04	5.331E-04	5.382E-04	5.289E-04	5.246E-04	5.094E-04	4.887E-04	4.396E-04	4.416E-04
J= 2	5.301E-04	5.310E-04	5.324E-04	5.324E-04	5.264E-04	5.154E-04	5.039E-04	4.878E-04	4.611E-04	4.583E-04
J= 1	5.299E-04	5.300E-04	5.296E-04	5.277E-04	5.195E-04	5.097E-04	5.014E-04	4.893E-04	4.727E-04	4.689E-04
	I= 1	I= 2	I= 3	I= 4	I= 5	I= 6	I= 7	I= 8	I= 9	I=10
J= 4	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 3	4.415E-04	4.414E-04	4.413E-04	4.413E-04	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 2	4.581E-04	4.574E-04	4.555E-04	4.481E-04	4.483E-04	4.487E-04	4.486E-04	4.486E-04	4.486E-04	4.486E-04
J= 1	4.683E-04	4.665E-04	4.614E-04	4.528E-04	4.511E-04	4.511E-04	4.510E-04	4.510E-04	4.510E-04	4.510E-04
	I=11	I=12	I=13	I=14	I=15	I=16	I=17	I=18	I=19	

UNBURN FIXED CARBON AT FURNACE EXIT = 61.81% AFTER 100 ITERATIONS

24
25

ATOM OUTFLOW IN KG/S :

C= 2.964584 H= 0.547796 N= 41.244461 O= 13.062082
S= 0.029583 A= 0.000297
SUM= 57.848804

ATOM INFLOW IN KG/S :

C= 2.965163 H= 0.547721 N= 41.244305 O= 13.061593
S= 0.029724 A= 0.000297
SUM= 57.848804

ATOM BALANCE -> (OUT-IN)/IN IN % :

C= -0.019515 H= 0.013625 N= 0.000379 O= 0.003746
S= -0.475400 A= -0.055321
SUM= 0.000000

26
27

ENERGY BALANCE FOR VOLUME ZONES AND TOTAL FURNACE EFFICIENCY AFTER 100 ITERATIONS

28, 28a

I	J	TPSAD	TEX	RHO	OLD	CP	EX	QCONIN	QCONNT	QDIFIN	QDIFNT	QCHEIN	QCHENT	QGRADIN	QGRADNT	QTOTIN	QTOTEX	QTOTNT	TNEW	
		K	K		KG/M3	KJ/KGK	KW	KW	KW	KW	KW	KW	KW	KW	KW	KW	KW	KW	K	
1	1	1391.6	1380.1	0.	0.25469	1.21673	38719.	-454.	0.	0.	0.	0.	0.	12484.	454.	51203.	51203.	0.	1380.	
2	1	1416.6	1413.7	0.	0.24863	1.22078	41626.	-119.	0.	0.	0.	0.	0.	13445.	119.	55071.	55071.	0.	1414.	
3	1	1496.8	1492.5	0.	0.23547	1.23027	26056.	-105.	0.	0.	0.	0.	0.	14482.	105.	40538.	40538.	0.	1493.	
4	1	1569.9	1566.8	0.	0.22423	1.23930	25917.	-183.	0.	0.	0.	0.	0.	14703.	183.	40621.	40621.	0.	1567.	
5	1	1631.2	1625.8	0.	0.21591	1.24773	24180.	-82.	0.	0.	0.	0.	-29.	10055.	111.	34236.	34265.	0.	1626.	
6	1	1661.0	1654.7	0.	0.21192	1.25306	42114.	12.	0.	0.	0.	0.	-93.	16414.	80.	58528.	58620.	0.	1655.	
7	1	1665.4	1653.8	0.	0.21188	1.25425	41049.	-119.	0.	0.	0.	0.	-93.	12521.	211.	53570.	53662.	0.	1654.	
8	1	1645.1	1636.9	0.	0.21391	1.25269	31368.	-93.	0.	0.	0.	0.	-124.	12318.	217.	43685.	43809.	0.	1637.	
9	1	1605.2	1594.7	0.	0.21942	1.24717	31611.	-215.	0.	0.	0.	0.	-62.	13364.	277.	44974.	45036.	0.	1595.	
10	1	1557.2	1513.8	0.	0.23111	1.23793	24434.	-904.	0.	157.	0.	0.	0.	9190.	778.	33624.	33655.	0.	1514.	
11	1	1483.1	1444.1	0.	0.24228	1.22981	18355.	-671.	0.	266.	0.	0.	0.	9469.	405.	27824.	27824.	0.	1444.	
12	1	1425.5	1394.1	0.	0.25094	1.22372	17367.	-537.	0.	247.	0.	0.	0.	8928.	290.	26295.	26295.	0.	1394.	
13	1	1374.1	1372.3	0.	0.25489	1.22068	20854.	-39.	0.	0.	0.	0.	0.	8850.	39.	29704.	29704.	0.	1372.	
14	1	1315.1	1310.2	0.	0.26689	1.21232	36132.	-198.	0.	0.	0.	0.	0.	7806.	198.	43938.	43938.	0.	1310.	
15	1	1269.1	1250.1	0.	0.27969	1.20450	48053.	-1038.	0.	520.	0.	0.	0.	8182.	518.	56235.	56235.	0.	1250.	
16	1	1233.3	1214.5	0.	0.28789	1.19983	46100.	-1020.	0.	482.	0.	0.	0.	7601.	538.	53701.	53701.	0.	1215.	
17	1	1181.8	1129.3	0.	0.30961	1.18828	27424.	-1783.	0.	1350.	0.	0.	0.	6770.	433.	34194.	34194.	0.	1129.	
18	1	1110.2	1065.3	0.	0.32822	1.17928	24995.	-1509.	0.	1118.	0.	0.	0.	5806.	391.	30801.	30801.	0.	1065.	
19	1	1065.3	1042.6	0.	0.33538	1.17601	18285.	-591.	0.	343.	0.	0.	0.	7531.	248.	25815.	25815.	0.	1043.	
1	2	1380.5	1343.1	0.	0.26171	1.21216	41995.	-1602.	0.	391.	0.	0.	0.	35501.	1211.	77495.	77495.	0.	1343.	
2	2	1387.7	1381.6	0.	0.25443	1.21672	87648.	-546.	0.	0.	0.	0.	0.	38305.	546.	125952.	125952.	0.	1382.	
3	2	1469.8	1458.3	0.	0.24106	1.22569	65237.	-713.	0.	0.	0.	0.	0.	41112.	713.	106350.	106350.	0.	1458.	
4	2	1570.0	1566.5	0.	0.22441	1.23798	71929.	-380.	0.	0.	0.	0.	-71.	43868.	451.	115797.	115868.	0.	1566.	
5	2	1651.6	1644.9	0.	0.21354	1.24834	68494.	212.	0.	0.	0.	0.	-593.	30422.	380.	98916.	99509.	0.	1645.	
6	2	1681.9	1676.2	0.	0.20930	1.25499	123676.	108.	0.	0.	0.	0.	0.	49457.	783.	173133.	174025.	-1.	1676.	
7	2	1683.2	1679.0	0.	0.20868	1.25809	115139.	428.	0.	0.	0.	0.	0.	38554.	559.	153692.	154679.	-1.	1679.	
8	2	1667.8	1662.2	0.	0.21059	1.25658	100563.	452.	0.	0.	0.	0.	0.	38009.	506.	138572.	139530.	-1.	1662.	
9	2	1614.3	1607.0	0.	0.21764	1.24780	105431.	-69.	0.	0.	0.	0.	0.	40274.	687.	145705.	146322.	-1.	1607.	
10	2	1567.5	1554.1	0.	0.22503	1.24172	73994.	-853.	0.	0.	0.	0.	0.	30029.	884.	104024.	104054.	0.	1554.	
11	2	1520.6	1485.0	0.	0.23551	1.23388	56926.	-1809.	0.	574.	0.	0.	0.	29611.	1266.	86537.	86568.	0.	1485.	
12	2	1457.9	1420.9	0.	0.24612	1.22633	53722.	-1900.	0.	530.	0.	0.	0.	27090.	1370.	80812.	80812.	0.	1421.	
13	2	1389.4	1379.6	0.	0.25348	1.22118	54644.	-545.	0.	0.	0.	0.	0.	26266.	545.	80910.	80910.	0.	1380.	
14	2	1307.2	1303.9	0.	0.26812	1.21116	103387.	-379.	0.	0.	0.	0.	0.	23273.	378.	126660.	126660.	0.	1304.	
15	2	1265.1	1240.6	0.	0.28182	1.20304	108384.	-3030.	0.	1100.	0.	0.	0.	23643.	1930.	132027.	132027.	0.	1241.	
16	2	1215.6	1191.6	0.	0.29340	1.19659	102289.	-2942.	0.	998.	0.	0.	0.	21335.	1944.	123624.	123624.	0.	1192.	
17	2	1164.9	1122.8	0.	0.31137	1.18721	80529.	-4276.	0.	2820.	0.	0.	0.	19789.	1457.	100318.	100318.	0.	1123.	
18	2	1106.1	1069.9	0.	0.32679	1.17976	74558.	-3651.	0.	2409.	0.	0.	0.	17513.	1242.	92071.	92071.	0.	1070.	
19	2	1069.9	1046.8	0.	0.33398	1.17646	55204.	-1796.	0.	911.	0.	0.	0.	22651.	885.	77854.	77854.	0.	1047.	
2	3	1387.8	1345.7	0.	0.26123	1.21220	63515.	-2714.	0.	615.	0.	0.	0.	65564.	2099.	129080.	129080.	0.	1346.	
3	3	1407.7	1403.9	0.	0.25045	1.21885	94494.	-320.	0.	0.	0.	0.	-42.	71050.	361.	165544.	165586.	0.	1404.	
4	3	1583.5	1565.5	0.	0.22466	1.23642	102028.	5865.	0.	0.	0.	0.	-7940.	78775.	2074.	180802.	188742.	0.	1566.	
5	3	1699.1	1661.1	0.	0.21158	1.24821	108464.	8809.	0.	0.	0.	0.	-12420.	54757.	3611.	163221.	175641.	0.	1661.	
6	3	1727.4	1703.0	0.	0.20612	1.25707	182518.	9544.	0.	0.	0.	0.	-12742.	90095.	3197.	272613.	285354.	-1.	1703.	
7	3	1731.5	1693.9	0.	0.20671	1.26427	166829.	2200.	0.	0.	0.	0.	-4753.	69583.	2553.	236412.	241165.	-1.	1694.	
8	3	1692.2	1674.9	0.	0.20883	1.26162	151873.	1509.	0.	0.	0.	0.	-3691.	69246.	2181.	221119.	224809.	-1.	1675.	
9	3	1598.6	1586.3	0.	0.22033	1.24351	181369.	1230.	0.	0.	0.	0.	-3320.	69359.	2089.	250728.	254048.	-1.	1586.	
10	3	1564.5	1542.5	0.	0.22660	1.23880	117448.	-1229.	0.	332.	0.	0.	-1082.	53080.	1978.	170528.	171609.	0.	1542.	
11	3	1505.2	1461.6	0.	0.23915	1.22961	102956.	-3934.	0.	1148.	0.	0.	-201.	51182.	2987.	154138.	154338.	0.	1462.	
12	3	1427.5	1388.7	0.	0.25170	1.22100	95781.	-3613.	0.	1063.	0.	0.	-31.	46595.	2582.	142376.	142407.	0.	1389.	
13	3	1360.9	1327.3	0.	0.26333	1.21349	89571.	-3122.	0.	978.	0.	0.	0.	42693.	2143.	132264.	132264.	0.	1327.	
14	3	1327.3	1280.3	0.	0.27301	1.20755	64166.	-3234.	0.	1097.	0.	0.	0.	39330.	2137.	103496.	103496.	0.	1280.	
3	4	1453.2	1395.6	0.	0.25199	1.21735	38664.	-909.	0.	592.	0.	0.	-1397.	33872.	1714.	72536.	73933.	0.	1396.	
4	4	1607.7	1474.3	0.	0.23746	1.23086	53490.	14062.	0.	455.	0.	0.	-36.	-20281.	39222.	5765.	92676.	112993.	0.	1474.
5	4	1586.7	1471.2	0.	0.23662	1.23738	54982.	18235.	0.	274.	0.	0.	-54.	-22134.	30815.	3625.	85743.	107931.	0.	1471.
6	4	1642.8	1553.4	0.	0.22441	1.24982	89268.	20508.	0.	473.	0.	0.	-54.	-29524.	46709.	8543.	135923.	165501.	0.	1553.
7	4	1648.2	1607.3	0.	0.21606	1.28311	83985.	5487.	0.	410.	0.	0.	0.	-8852.	31084.	2955.	115069.	123920.	0.	1607.
8	4	1691.3	1636.2	0.	0.21292	1.26976	73247.	2110.	0.	438.	0.	0.	0.	-4352.	32011.	1804.	105258.	109610.	0.	1636.
9	4	1501.0	1479.4	0.	0.23593	1.22280	68440.	1756.	0.	539.	0.	0.	0.	-3336.	27334.	1041.	95774.	99110.	0.	1479.

HEAT BALANCE FOR VOLUME ZONES: 4.11E+06 3.93E+04 0. 2.3E+04-1.4E+02-1.4E+05 1.8E+06 7.9E+04 6.0E+06 6.1E+06-9.1E+00

-28b

ABSOLUTE AND RELATIVE RESIDUALS AFTER 100 ITERATIONS

I	J	DTMAX	I	J	RDIMAX	I	J	DQMAX	I	J	RDQMAX	DQTOTAL	RDQTOTAL
K	K	K	K	K	K	K	K	KW	K	K	K	KW	K
7	1	0.00	7	1	0.000	8	3	-0.7	8	1	0.000	-9.1	0.000

29

HEAT FLUX TO ADDITIONAL HEAT SINKS IN KW

CONVECTIVE FLUX RADIATIVE FLUX TOTAL FLUX
15842.3271 21289.3789 37131.7070

30

SURFACE TEMPERATURES OF ADDITIONAL HEAT SINKS IN K --- represented by TWSINK(I,J)

TWSINK(10,) = 911.89 0.00
TWSINK(11,) = 843.14 835.60 831.04
TWSINK(12,) = 834.44 821.48 810.45
TWSINK(13,) = 0.00 0.00 797.67
TWSINK(14,) = 0.00 0.00 788.54
TWSINK(15,) = 838.99 847.88
TWSINK(16,) = 833.35 837.07
TWSINK(17,) = 804.51 805.64
TWSINK(18,) = 796.30 799.82
TWSINK(19,) = 798.42 792.34

31

MEAN FURNACE EXIT TEMPERATURE = 1045.78K AFTER 100 ITERATIONS ← 32
TOTAL FURNACE EFFICIENCY = 66.5870 % WITH 140710. KW HEAT RELEASE AND 11572. KW SENSIBLE INPUT

CHEM. HEAT OUTFLOW IN KW : ← 33a
FUEL= 6.2 SULF.= 0.0 SUM = 6.2

SENS. HEAT OUTFLOW IN KW : ← 33b
EXT.= 50876.0 REC. = 0.0 SUM = 50876.0

OUTFLUX TO HEAT SINKS IN KW : ← 33c
RAD.= 78771.0 CONV.= 22629.3 SUM = 101400.3

TOTAL HEAT OUTFLOW : ← 33d
152282.5 KW ← 34a

CHEM. HEAT INFLOW IN KW : ← 34b
FUEL= 140873.8 EVAP.= -143.5 CALC.= 0.0 SUM = 140730.3

SENS. HEAT AIR INFLOW IN KW : ← 34c
SEC.= 10553.1 PRIM.= 0.0 TRANS.= 0.0 SUM = 10553.1

SENS. HEAT FUEL INFLOW IN KW : ← 34d
DRY = 466.9 H2OG = 8.6 SUM = 475.5

SENS. HEAT SORBENT INFLOW IN KW : ← 34e
CAO = 0.0 H2OG = 0.0 CO2G = 0.0 SUM = 0.0

SENS. HEAT BURNER-STEAM INFLOW IN KW: 0.0 ← 34f

SENS. HEAT FLUE GAS INFLOW IN KW: 543.6 ← 34g
TOTAL HEAT INFLOW : 152302.5 KW ← 35

GAS ZONE HEAT BALANCE : ←
HEAT BALANCE -> OUT - IN : -20.0 KW
HEAT BALANCE -> (OUT-IN)/IN : -0.013101 %

ENERGY BALANCE FOR SURFACE ZONES AFTER 100 ITERATIONS ← 36, 36a, 36b

I	J	M	TOLDW K	QCONIN KW	QCONNT KW	QDIFIN KW	QDIFNT KW	QRADIN KW	QRADNT KW	QTOTIN KW	QTOTEX KW	QTOTN KW	TNEWW K
1	2	1	701.1	0.	903.	118.	-118.	905.	-785.	1023.	1023.	0.	701.1
2	3	1	733.3	0.	2254.	208.	-208.	2311.	-2047.	2519.	2519.	0.	733.3
3	4	1	720.9	0.	1024.	116.	-116.	1033.	-908.	1149.	1149.	0.	720.9

SURFACE ZONE HEAT BALANCE : 0.0E-01 4.2E+03 4.4E+02-4.4E+02 4.2E+03-3.7E+03 4.7E+03 4.7E+03-9.7E-05

ABSOLUTE AND RELATIVE RESIDUALS AFTER 100 ITERATIONS ← 37

I	J	M	DTMAX K	I	J	M	RDTHAX %	I	J	M	DQMAX KW	I	J	M	RDQMAX %	DQTOTAL KW	RDQTOTAL %
3	4	1	0.00	3	4	1	0.000	1	2	1	0.0	1	2	1	0.000	0.0	0.000

ENERGY BALANCE FOR SURFACE ZONES AFTER 100 ITERATIONS ← 38, 38a, 38b

I	J	M	TOLDW K	QCONIN KW	QCONNT KW	QDIFIN KW	QDIFNT KW	QRADIN KW	QRADNT KW	QTOTIN KW	QTOTEX KW	QTOTN KW	TNEWW K
14	3	3	732.8	0.	1123.	186.	-186.	1201.	-937.	1387.	1387.	0.	732.8
9	4	3	843.6	0.	1084.	109.	-109.	1209.	-975.	1318.	1318.	0.	843.6

SURFACE ZONE HEAT BALANCE : 0.0E-01 2.2E+03 2.9E+02-2.9E+02 2.4E+03-1.9E+03 2.7E+03 2.7E+03-1.1E-04

ABSOLUTE AND RELATIVE RESIDUALS AFTER 100 ITERATIONS ← 39

I	J	M	DTMAX K	I	J	M	RDTHAX %	I	J	M	DQMAX KW	I	J	M	RDQMAX %	DQTOTAL KW	RDQTOTAL %
9	4	3	0.00	9	4	3	0.000	9	4	3	0.0	9	4	3	0.000	0.0	0.000

ENERGY BALANCE FOR SURFACE ZONES AFTER 100 ITERATIONS ← 40, 40a, 40b

I	J	M	TOLDW K	QCONIN KW	QCONNT KW	QDIFIN KW	QDIFNT KW	QRADIN KW	QRADNT KW	QTOTIN KW	QTOTEX KW	QTOTN KW	TNEWW K
1	2	4	694.6	0.	1914.	273.	-273.	1905.	-1641.	2178.	2178.	0.	694.6
2	3	4	718.0	0.	3777.	408.	-408.	3835.	-3369.	4243.	4243.	0.	718.0
3	4	4	731.4	0.	4698.	477.	-477.	4776.	-4222.	5253.	5253.	0.	731.4
4	4	4	797.4	0.	6821.	455.	-455.	7100.	-6365.	7555.	7555.	0.	797.4
5	4	4	833.0	0.	5190.	274.	-274.	5475.	-4916.	5749.	5749.	0.	833.0
6	4	4	850.8	0.	8777.	473.	-473.	9256.	-8304.	9728.	9728.	0.	850.8
7	4	4	817.2	0.	5806.	409.	-409.	6021.	-5397.	6430.	6430.	0.	817.2
8	4	4	790.0	0.	5040.	438.	-438.	5146.	-4602.	5584.	5584.	0.	790.0
9	4	4	753.6	0.	4593.	430.	-430.	4679.	-4163.	5109.	5109.	0.	753.6
10	3	4	741.2	0.	2938.	332.	-332.	2944.	-2606.	3276.	3276.	0.	741.2
11	3	4	765.0	0.	1872.	311.	-311.	1974.	-1560.	2285.	2285.	0.	765.0
12	3	4	726.0	0.	1398.	296.	-296.	1437.	-1101.	1733.	1733.	0.	726.0
13	3	4	710.9	0.	1213.	276.	-276.	1246.	-938.	1522.	1522.	0.	710.9
14	3	4	701.4	0.	1099.	259.	-259.	1132.	-840.	1391.	1391.	0.	701.4
15	2	4	652.6	0.	396.	206.	-206.	361.	-190.	567.	567.	0.	652.6
16	2	4	646.3	0.	335.	191.	-191.	309.	-144.	500.	500.	0.	646.3
17	2	4	628.7	0.	266.	183.	-183.	239.	-83.	422.	422.	0.	628.7
18	2	4	625.2	0.	213.	164.	-164.	201.	-49.	366.	366.	0.	625.2
19	2	4	647.2	0.	724.	197.	-197.	761.	-528.	957.	957.	0.	647.2

SURFACE ZONE HEAT BALANCE : 0.0E-01 5.7E+04 6.1E+03-6.1E+03 5.9E+04-5.1E+04 6.5E+04 6.5E+04-1.2E-03

ABSOLUTE AND RELATIVE RESIDUALS AFTER 100 ITERATIONS ← 41

I	J	M	DTMAX K	I	J	M	RDTHAX %	I	J	M	DQMAX KW	I	J	M	RDQMAX %	DQTOTAL KW	RDQTOTAL %
19	2	4	0.00	19	2	4	0.000	2	3	4	0.0	18	2	4	0.000	0.0	0.000

THE DISTRIBUTION OF T in K AFTER 100 ITERATIONS ← 42

J=	4	3	2	1	I=	1	2	3	4	5	6	7	8	9	I=10
J= 4	0.000E-01	0.000E-01	1.396E+03	1.474E+03	1.471E+03	1.553E+03	1.607E+03	1.636E+03	1.479E+03	0.000E-01					
J= 3	0.000E-01	1.346E+03	1.404E+03	1.566E+03	1.661E+03	1.703E+03	1.694E+03	1.675E+03	1.586E+03	1.542E+03					
J= 2	1.343E+03	1.382E+03	1.458E+03	1.566E+03	1.645E+03	1.676E+03	1.679E+03	1.662E+03	1.607E+03	1.554E+03					
J= 1	1.380E+03	1.414E+03	1.493E+03	1.567E+03	1.626E+03	1.655E+03	1.654E+03	1.637E+03	1.595E+03	1.514E+03					

4344

I= 1	I= 2	I= 3	I= 4	I= 5	I= 6	I= 7	I= 8	I= 9	I=10
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I=11	I=12	I=13	I=14	I=15	I=16	I=17	I=18	I=19
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I= 1 I= 2 I= 3 I= 4 I= 5 I= 6 I= 7 I= 8 I= 9 I=10

I=11	I=12	I=13	I=14	I=15	I=16	I=17	I=18	I=19
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46

J= 4	0.000E-01	0.000E-01	1.397E+03	2.032E+04	2.202E+04	2.805E+04	8.852E+03	1.231E+03	1.383E+01	0.000E-01
J= 3	0.000E-01	0.000E-01	4.149E+01	7.800E+03	1.242E+04	1.271E+04	9.681E+02	1.383E+01	1.383E+01	0.000E-01
J= 2	0.000E-01	0.000E-01	0.000E-01	5.532E+01	3.458E+02	1.660E+02	1.383E+01	0.000E-01	0.000E-01	0.000E-01
J= 1	0.000E-01	0.000E-01	0.000E-01	0.000E-01	1.383E+01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
	I= 1	I= 2	I= 3	I= 4	I= 5	I= 6	I= 7	I= 8	I= 9	I=10

J= 4	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 3	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 2	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 1	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
	I=11	I=12	I=13	I=14	I=15	I=16	I=17	I=18	I=19	

THE DISTRIBUTION OF VOL in kg/(kg,mixture) AFTER 100 ITERATIONS

47

J= 4	0.000E-01	0.000E-01	1.210E-05	6.494E-03	1.364E-02	9.210E-03	1.111E-03	7.713E-06	0.000E-01	0.000E-01
J= 3	0.000E-01	0.000E-01	0.000E-01	5.962E-05	7.790E-04	1.887E-04	2.142E-05	3.873E-06	0.000E-01	0.000E-01
J= 2	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.511E-05	9.557E-06	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 1	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
	I= 1	I= 2	I= 3	I= 4	I= 5	I= 6	I= 7	I= 8	I= 9	I=10

J= 4	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 3	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 2	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
J= 1	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
	I=11	I=12	I=13	I=14	I=15	I=16	I=17	I=18	I=19	

THE DISTRIBUTION OF TW in K AFTER 100 ITERATIONS

48

J= 4	7.209E+02
J= 3	7.333E+02
J= 2	7.011E+02
J= 1	3.500E+02

M1= 1

THE DISTRIBUTION OF QIN in kW/m**2 AFTER 100 ITERATIONS

49

J= 4	1.266E+02
J= 3	1.432E+02
J= 2	1.031E+02
J= 1	1.385E+02

M1= 1

THE DISTRIBUTION OF QW in kW/m**2 AFTER 100 ITERATIONS

50

J= 4	-8.782E+01
J= 3	-9.776E+01
J= 2	-7.201E+01
J= 1	-1.376E+02

M1= 1

THE DISTRIBUTION OF TW in K AFTER 100 ITERATIONS

51

J= 4	8.436E+02
J= 3	7.328E+02
J= 2	8.000E+02
J= 1	8.000E+02

M3= 1

THE DISTRIBUTION OF QIN in kW/m**2 AFTER 100 ITERATIONS

52

J= 4	1.482E+02
J= 3	7.442E+01
J= 2	3.216E+01
J= 1	3.662E+01

M3= 1

THE DISTRIBUTION OF QW in kW/m**2 AFTER 100 ITERATIONS

53

J= 4	-9.301E+01
J= 3	-4.870E+01
J= 2	-8.939E+00
J= 1	-1.340E+01

M3= 1

THE DISTRIBUTION OF TW in K AFTER 100 ITERATIONS

54

M4= 1	6.946E+02	7.180E+02	7.314E+02	7.974E+02	8.330E+02	8.508E+02	8.172E+02	7.900E+02	7.536E+02	7.412E+02
	I= 1	I= 2	I= 3	I= 4	I= 5	I= 6	I= 7	I= 8	I= 9	I=10
M4= 1	7.650E+02	7.260E+02	7.109E+02	7.014E+02	6.526E+02	6.463E+02	6.287E+02	6.252E+02	6.472E+02	

	I=11	I=12	I=13	I=14	I=15	I=16	I=17	I=18	I=19	
THE DISTRIBUTION OF QIN in kW/m**2 AFTER 100 ITERATIONS										55
M4= 1	9.504E+01	1.240E+02	1.398E+02	2.216E+02	2.675E+02	2.890E+02	2.443E+02	2.088E+02	1.659E+02	1.490E+02
	I= 1	I= 2	I= 3	I= 4	I= 5	I= 6	I= 7	I= 8	I= 9	I=10
M4= 1	9.272E+01	6.750E+01	5.854E+01	5.320E+01	2.168E+01	1.854E+01	1.357E+01	1.143E+01	3.249E+01	
	I=11	I=12	I=13	I=14	I=15	I=16	I=17	I=18	I=19	
THE DISTRIBUTION OF QW in kW/m**2 AFTER 100 ITERATIONS										56
M4= 1	-6.682E+01	-8.550E+01	-9.625E+01	-1.491E+02	-1.775E+02	-1.918E+02	-1.649E+02	-1.431E+02	-1.140E+02	-1.041E+02
	I= 1	I= 2	I= 3	I= 4	I= 5	I= 6	I= 7	I= 8	I= 9	I=10
M4= 1	-6.155E+01	-4.597E+01	-3.990E+01	-3.614E+01	-1.662E+01	-1.407E+01	-1.056E+01	-8.474E+00	-2.166E+01	
	I=11	I=12	I=13	I=14	I=15	I=16	I=17	I=18	I=19	
iter. no.=100, act.err.= 0.0672 %, avg.err.= 4.2807 %, 20 it.err.= -0.1875 %, hb.err.= -0.0131 %										57
BALANCE OF TOTAL RADIATIVE EXCHANGE										58
NUMBER OF BEAMS = 354960										
SUM OF EMITTED RADIATION (KW) :										
VOLUME ZONES	1.918E+06									
WALL SECTIONS	2.439E+04									
			M=1	M=2	M=3	M=4		TOTAL		
			5.146E+02	7.609E+03	8.707E+02	1.540E+04		1.942E+06		
SUM OF ABSORBED RADIATION (KW) :										
VOLUME ZONES	1.875E+06									
WALL SECTIONS	6.659E+04									
			M=1	M=2	M=3	M=4		TOTAL		
			4.828E+03	0.000E-01	2.967E+03	5.880E+04		1.942E+06		
SUM OF NET EMITTED RADIATION (KW) :										
VOLUME ZONES	4.218E+04									
WALL SECTIONS	-4.220E+04									
			M=1	M=2	M=3	M=4		TOTAL		
			-4.313E+03	7.609E+03	-2.096E+03	-4.340E+04		-1.496E+01		
ERROR OF RADIATIVE ENERGY BALANCE -7.704E-04 %										59
TOTAL HEAT BALANCE :										60
HEAT TO FURNACE WALLS IN KW :										
RAD.=	56670.1	CONV.=	6787.2	SUM =	63457.3					
HEAT TO FURNACE EXIT IN KW :										
RAD.=	168.1	CONV.=	0.0	SUM =	168.1					
HEAT TO FURNACE HOPPER IN KW :										
RAD.=	575.2	CONV.=	0.0	SUM =	575.2					
HEAT FLUXES TO ZONAL HEAT EXCHANGERS IN KW :										61
ZONE I	BY RADI.	BY CONV.	SUM							
10	1839.1	156.5	1995.6							
11	4402.4	1676.1	6078.5							
12	3661.4	1544.4	5205.7							
13	1357.8	702.6	2060.4							
14	1165.9	652.3	1818.2							
15	2716.3	1414.1	4130.4							
16	2206.1	1289.4	3495.5							
17	1953.6	3986.9	5940.4							
18	1588.4	3362.8	4951.2							
19	398.5	1057.3	1455.8							
CLOSURE OF TOTAL HEAT BALANCE :										62
HEAT FLUX FROM FLUE GAS : 101400.3 KW										
HEAT FLUX TO HEAT SINKS : 101332.2 KW										
DIFFERENCE : -68.1 KW										
ACT. PERCENTAGE ERROR : 0.067176 %										
AVG. PERCENTAGE ERROR : 4.280663 %										
AVG. ERROR OF LAST 20 IT. : -0.187462 %										
I INDEX	X-CO-ORDINATE	NET NORM. MASS FLUX	MEAN TEMP.	MEAN RES. TIME	SUM OF RES. TIME					63
-	M	-	K	Sec	Sec					
1	0.988	0.2466	1343.11	0.6020	1.6432					
2	2.964	0.5754	1374.98	0.6086	1.0379					
3	4.912	0.5754	1440.12	0.7336	0.3668					
4	6.772	0.5489	1546.61	0.6634	0.3317					
5	8.247	0.6221	1600.37	0.3587	0.8427					
6	9.722	0.9348	1647.36	0.3622	1.2032					
7	11.314	0.9619	1664.76	0.2685	1.5185					
8	12.700	0.8578	1660.81	0.3023	1.8040					
9	14.185	1.0000	1593.71	0.3145	2.1124					
10	15.608	1.0000	1543.17	0.1966	2.3679					
11	16.919	1.0000	1467.13	0.2229	2.5777					
12	18.279	1.0000	1399.44	0.2337	2.8059					
13	19.640	1.0000	1348.62	0.2425	3.0440					
14	21.000	1.0000	1305.51	0.2533	3.2919					
15	22.501	1.0000	1244.88	0.1336	3.4853					
16	24.144	1.0000	1197.37	0.1387	3.6214					
17	25.834	1.0000	1124.47	0.1560	3.7688					
18	27.570	1.0000	1068.72	0.1641	3.9288					
19	29.592	1.0000	1045.78	0.2230	4.1224					
MEAN GAS SPECIES CONCENTRATION ALONG FURNACE :										64

I	X-CO-ORD.	CO2	H2O	N2	O2	VOL	SO2
-	M	VOL% WET	VOL% WET	VOL% WET	VOL% WET	VOL% WET	VOL% WET
1	0.988	12.8839	12.8788	73.2591	0.9253	0.0000	0.0529
2	2.964	12.8802	12.8614	73.2667	0.9388	0.0000	0.0529
3	4.912	12.8721	12.8269	73.2717	0.9758	0.0003	0.0531
4	6.772	12.5438	12.4881	73.2604	1.4449	0.2107	0.0521
5	8.247	11.8646	11.8970	73.0581	2.4288	0.7023	0.0492
6	9.722	12.1350	12.3066	72.8505	1.9146	0.7437	0.0497
7	11.314	12.8089	13.2329	72.2874	0.6285	0.9914	0.0510
8	12.700	12.7745	13.6077	72.5812	0.4826	0.5047	0.0493
9	14.185	12.1794	13.3583	73.0001	1.3531	0.0633	0.0458
10	15.608	12.2275	13.4526	73.0199	1.2420	0.0122	0.0458
11	16.919	12.2353	13.4709	73.0244	1.2220	0.0016	0.0458
12	18.279	12.2299	13.4701	73.0268	1.2274	0.0000	0.0457
13	19.640	12.2103	13.4593	73.0324	1.2524	0.0000	0.0456
14	21.000	12.2385	13.4752	73.0227	1.2179	0.0000	0.0458
15	22.501	12.2443	13.4783	73.0183	1.2132	0.0000	0.0458
16	24.144	12.2400	13.4761	73.0189	1.2192	0.0000	0.0458
17	25.834	12.2400	13.4762	73.0181	1.2200	0.0000	0.0458
18	27.570	12.2399	13.4762	73.0175	1.2206	0.0000	0.0458
19	29.592	12.2399	13.4762	73.0175	1.2206	0.0000	0.0458

OTHER MEAN QUANTITIES ALONG FURNACE :

I	X-CO-ORD.	CARBON	TOT. FUEL	VOLATILE	SO2	CAO
-	M	IN ASH	HEAT REL.	HEAT REL.	REDUCTION	UTIL.
1	0.988	39.6596	0.0000	0.0000	0.0000	0.0000
2	2.964	39.8560	0.0001	0.0000	0.0000	0.0000
3	4.912	40.3654	1.0212	1.2352	0.0000	0.0000
4	6.772	41.8043	21.1298	25.4276	0.0000	0.0000
5	8.247	43.2646	46.1386	55.3088	0.0000	0.0000
6	9.722	42.9461	76.8787	90.4513	0.0000	0.0000
7	11.314	41.4741	87.3030	98.8955	0.0000	0.0000
8	12.700	40.6436	93.7800	99.9644	0.0000	0.0000
9	14.185	39.2276	98.9875	99.9881	0.0000	0.0000
10	15.608	38.6403	99.7992	99.9881	0.0000	0.0000
11	16.919	38.3220	99.9638	99.9881	0.0000	0.0000
12	18.279	38.1543	99.9858	99.9881	0.0000	0.0000
13	19.640	38.0610	99.9858	99.9881	0.0000	0.0000
14	21.000	37.9958	99.9858	99.9881	0.0000	0.0000
15	22.501	37.9755	99.9858	99.9881	0.0000	0.0000
16	24.144	37.9671	99.9858	99.9881	0.0000	0.0000
17	25.834	37.9622	99.9858	99.9881	0.0000	0.0000
18	27.570	37.9592	99.9858	99.9881	0.0000	0.0000
19	29.592	37.9584	99.9858	99.9881	0.0000	0.0000

Table 6.1. Description of output generated by the 2DHT code.

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
1	1,2,3,4, Default	GENERAL INFORMATION		
			%	Boiler name Case number Version number Thermal load as % of boiler full load
2	1,2,3,4, Default	INPUT/OUTPUT		Input/output control parameters
		NREAD NWRITE		Switch (0 or 1) to read initial values of iterated variables from an input array file for continuation runs Switch (0 or 1) to write an output array file for continuation runs Name of input data file Note: Input data file for 2DHT has to be named as 2DINPT.DAT. Name of input array file Name of output array file "Name of Graphics Output File" is not used by the code. Name of output data file generated by 2DHT Output level selected by the user
3	1,2,3,4, Default	USER'S COMMENTS		User's comments on the case. Note: User can specify up to ten lines of comments with a maximum of 78 characters per line.

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
4	1,2,3,4, Default	SUMMARY OF INPUT PARAMETERS		
		FUEL TYPE		Gas, liquid or solid
		TOTAL FUEL FLOW	kg wet/s	Total wet fuel flow rate including reburn fuel
		TOTAL AIR FLOW	kg wet/s	Total wet air flow rate
		EXCESS AIR	%	Total excess air in percentage
		O2-CONTENT OF FLUE GAS	Vol. % dry	Oxygen concentration in flue gas assuming complete fuel burnout
		SEC. AIR TEMPERATURE	K	Temperature of secondary air or over-fired air
		PRIM. MIXTURE TEMPERATURE	K	Temperature of burner fuel and primary air mixture
		AMOUNT OF PRIM. AIR	%	Amount of primary air in percentage of burner fuel stoichiometric air
		ATOMIZING STEAM FLOW	$\frac{\text{kg steam}}{\text{kg dry fuel}}$	Mass flow rate of atomizing steam divided by burner fuel dry flow rate
5	1,2,3,4, Default	FUEL PROPERTY		Fuel analysis and heating values based on mixture of burner and reburn fuels
5a	1,2,3,4, Default	CFIX VOL MOI ASH	kg/kg wet kg/kg wet kg/kg wet kg/kg wet	Proximate analysis (corrected for Q-factor and inherent sulfur capture) Fixed carbon mass fraction on wet basis Volatile mass fraction on wet basis Moisture mass fraction on wet basis Ash mass fraction on wet basis
		C H N O S ASH	kg/kg dry kg/kg dry kg/kg dry kg/kg dry kg/kg dry kg/kg dry	Ultimate analysis (corrected for inherent sulfur capture) Mass fraction of carbon element on dry basis Mass fraction of hydrogen element on dry basis Mass fraction of nitrogen element on dry basis Mass fraction of oxygen element on dry basis Mass fraction of sulfur element on dry basis Ash mass fraction on dry basis
5b	1,2,3,4, Default			Heating values based on mixture of burner and reburn fuels
			kJ/kg dry	Lower (net) heating value

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
5c	1,2,3,4, Default			Heating values of burner fuel
			kJ/kg wet Kj/kg dry	Upper (gross) heating value Lower (net) heating value
6	1,2,3,4, Default	REBURNING		Reburn information Note: This block is displayed only when the reburning option is selected.
		REBURN OR COFIRING		Reburning switch, on (YES) or off (NO)
		FUEL TYPE		Reburning fuel type (gas only)
		FUEL FLOW	kg dry/s	Reburn fuel flow rate on dry basis
		FGR FLOW	kg/s	Recirculated flue gas flow rate
		FUEL TEMPERATURE	K	Reburn fuel temperature
		FGR TEMPERATURE	K	Temperature of recirculated flue gas
7	1,2,3,4, Default	ASH RADIATION		Parameters of ash radiative properties used in the radiation model
		CLOUD SPECIFIC ABSORPTION COEFFICIENT	$\frac{1}{(\text{kg/m}^3) \text{ m}}$	Ash specific absorption coefficient
		CLOUD SPECIFIC SURFACE AREA	m ² /kg	Specific surface area of ash cloud
		SCATTERING		Scattering switch, always off (NO)
		ABSORPTION EFFICIENCY	fraction	Absorption efficiency of ash cloud
		SCATTERING EFFICIENCY	fraction	This option is not used by the 2DHT code.

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
8	1,2,3,4, Default	NUMERICAL PARAMETERS		Parameters related to numerical accuracy of the model
		NMAX		Number of cells in dividing the largest linear dimension of a volume zone
		NPHI		Number of sub-divisions on polar angle between 0 and π
		EXACT		Fraction of beam energy fluxes with respect to a reference flux, below which beam tracking is terminated
		NO. OF ITERATIONS		Maximum number of iterations on total heat balance
		NO. OF AVERAGED ITERATIONS		Number of averaged iterations on total heat balance
		WEIGHTING FACTOR FOR HEAT FLUXES OF A PREVIOUS RUN		This option is not used by the code.
9	4,Default	STOICHIO-METRIC CALCULATION AT COMPLETE COMBUSTION		Overall stoichiometric calculation for complete combustion
9a	4,Default	O2MINT	kg/kg dry	Ratio of stoichiometric O2 mass flow to total fuel mass flow of burner and reburn fuels
		AIRMNT	kg/kg dry	Ratio of stoichiometric air mass flow to total fuel mass flows of burner and reburn fuels
		AIRNR		Air number (actual air to fuel ratio)
		H2OFUT	kg/kg dry	Fuel moisture per unit of dry fuel
		H2OA2	kg/kg dry	Air moisture per unit of dry air
		FUTOT	kg dry/s	Total dry fuel mass flow rate including burner and reburn fuels
		DMA	kg dry/s	Total dry air mass flow rate
		DMH2O	kg/s	Total input mass flow rate of water
		DMTOT	kg/s	Total input mass flow rate including recirculated flue gas
		HL	kJ/kg dry	Lower (net) heating value of fuel mixture

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
9b	4, Default	O2MINV	kg/kg dry	Stoichiometric O2 requirements of "volatile" fuels
		AIRMINV	kg/kg dry	Stoichiometric air requirements of "volatile" fuels
		FUS	kg dry/s	Total mass flow rate of burner fuel on dry basis
		FUSW	kg wet/s	Total mass flow rate of burner fuel on wet basis
		FUG	kg dry/s	Total mass flow rate of reburn fuel on dry basis
		FUGW	kg wet/s	Total mass flow rate of reburn fuel on wet basis
		FUGV	Nm ³ /s	Total volumetric flow rate of reburn fuel on dry basis
		FUGVW	Nm ³ /s	Total volumetric flow rate of reburn fuel on wet basis
		DMA2	kg dry/s	Total mass flow rate of dry air
		DMA2W	kg wet/s	Total mass flow rate of wet air
		DMA2V	Nm ³ /s	Total volumetric flow rate of dry air
		DMAVW	Nm ³ /s	Total volumetric flow rate of wet air
		DMCG	Nm ³ /s	Total volumetric flow rate of dry flue (combustion) gas
		DMCGW	Nm ³ /s	Total volumetric flow rate of wet flue (combustion) gas
		HLS	kJ/kg dry	Lower (net) heating value of burner fuel on dry basis
		HUSW	kJ/kg wet	Upper (gross) heating value of burner fuel on wet basis
		HLG	kJ/kg dry	Lower (net) heating value of reburn fuel on dry basis
		HUGW	kJ/kg wet	Upper (gross) heating value of reburn fuel on wet basis
		HLGV	kJ/Nm ³ s	Lower (net) heating value of reburn fuel on dry volumetric basis
		HUGVW	kJ/Nm ³ s	Upper (gross) heating value of reburn fuel on wet volumetric basis
		SFLOWF	kg/s	Atomizing steam flow rate accompanied with burner fuel

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
10	3,4, Default			Mass concentration of flue gas species, based on complete combustion and wet basis
		CO2	kg/kg wet	CO2 mass concentration
		H2O	kg/kg wet	H2O mass concentration
		N2	kg/kg wet	N2 mass concentration
		O2	kg/kg wet	O2 mass concentration
		VOL	kg/kg wet	Volatile mass concentration (It is always zero due to the assumption of complete combustion. Actual values are later calculated by combustion model.)
		SO2	kg/kg wet	SO2 mass concentration
		ASH	kg/kg wet	Ash concentration (Sulfur inherently captured by ash is considered part of the ash.)
		CHAR	kg/kg wet	Char concentration (It is always zero due to the assumption of complete combustion. Actual values are later calculated by combustion model.)
		SOOT	kg/kg wet	Soot concentration (It is always zero due to the assumption of complete combustion. Actual values are later calculated by combustion model.)

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
11	3,4, Default			Volumetric concentrations of flue gas species based on complete combustion and wet basis
		CO2	Vol. Frac. Wet	CO2 concentration
		H2O	"	H2O concentration
		N2	"	N2 concentration
		O2	"	O2 concentration
		VOL	"	Volatile concentration (It is always zero due to the assumption of complete combustion. Actual values are later calculated by combustion model.)
		SO2	"	SO2 concentration (Sulfur inherently captured by ash is not released to the gas stream.)
12	1,2,3,4, Default			Volumetric concentration of flue gas species based on complete combustion and dry basis
		CO2	Vol. Frac. Dry	CO2 concentration
		N2	"	N2 concentration
		O2	"	O2 concentration
		VOL	"	Volatile concentration (It is always zero due to the assumption of complete combustion. Actual values are later calculated by combustion model.)
		SO2	"	SO2 concentration (Sulfur inherently captured by ash is not released to the gas stream.)
13	1,2,3,4, Default			Flue gas SO2 concentration in ppm, based on complete combustion Note: Sulfur inherently captured by ash is not released to the gas stream.
		SO2 IN PPM MASS	ppm	SO2 mass concentration
		SO2 IN PPM VOL WET	ppm	SO2 volumetric concentration on wet basis
		SO2 IN PPM VOL DRY	ppm	SO2 volumetric concentration on dry basis

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
14	4,Default			Mean specific heat capacities of combustion species at various temperatures Note: The mean specific heat capacity is referenced to 298.15 K.
		CO2	kJ/kg K	Mean specific heat capacity of CO2
		H2O	kJ/kg K	Mean specific heat capacity of H2O
		N2	kJ/kg K	Mean specific heat capacity of N2
		O2	kJ/kg K	Mean specific heat capacity of O2
		VOL	kJ/kg K	Mean specific heat capacity of volatiles (CH4)
		SO2	kJ/kg K	Mean specific heat capacity of SO2
		ASH	kJ/kg K	Mean specific heat capacity of ash
		CHAR	kJ/kg K	Mean specific heat capacity of char
		SOOT	kJ/kg K	Mean specific heat capacity of soot
15	1,2,3,4, Default			Mean heat capacities of some input/output steams at various temperatures
		INPUT STREAM		Air or flue gas
		TEMPERATURE	K	Temperatures of primary mixture, secondary air and FGR specified for the current run, and temperatures at 900 and 1800 K which are assigned by the code
		MEAN CP	kJ/kg K	Mean specific heats of air or flue gas

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
16	4,Default	MASS BALANCE FOR VOLUME ZONES		Examination of mass continuity at each volume zone (I,J)
		I J		Volume zone (I,J)
		MCONIN	kg/s	Mean convective mass flow rate entering volume zone (I,J)
		MCONNT	kg/s	Difference between mean convective mass flow rates leaving and entering volume zone (I,J) Note: Values other than zero indicate violations of continuity, but small errors due to machine round-off can be tolerated.
		MDIFIN	kg/s	Mass flow rate entering volume zone (I,J) due to turbulent exchange or small scale recirculation
		MDFNT	kg/s	Difference between mass fluxes leaving and entering volume zone (I,J) due to turbulent exchange or small scale recirculation Note: Values other than zero indicate violations of continuity, but small errors due to machine round-off can be tolerated.
		MTOTIN	kg/s	Total convective and turbulent mass flow rate entering volume zone (I,J)
		MTOTEX	kg/s	Total convective and turbulent mass flow rate leaving volume zone (I,J)
		MTOTNT	kg/s	Difference between total (convective and turbulent) mass flow rates entering and leaving volume zone (I,J) Note: Values other than zero indicate local mass continuity is violated, but small errors due to machine round-off can be tolerated.

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
17	4,Default	(MCONIN)	kg/s	Sum of mean convective mass flow rate entering each volume zone
		(MCONNT)	kg/s	Sum of differences of mean convective mass flow rates leaving and entering each volume zone Note: Values other zero indicate violations of continuity, but small errors due to machine round-off can be tolerated.
		(MDIFIN)	kg/s	Sum of mass flow rates entering each volume zone due to turbulent transport Note: Overall strength of turbulent exchange is shown by comparing with MCONIN defined above.
		(MDFNT)	kg/s	Sum of differences between turbulent mass flow rates leaving and entering each volume zone Note: Values other than zero indicate violations of continuity, but small errors due to machine round-off can be tolerated.
		(MTOTIN)	kg/s	Sum of total convective and turbulent flow rates entering each volume zone
		(MTOTEX)	kg/s	Sum of total convective and turbulent flow rates leaving each volume zone
		(MTOTNT)	kg/s	Sum of differences between total convective and turbulent mass flow rates leaving and entering each volume zone Note: Values other than zero indicate local continuity is violated, but small errors due to machine round-off can be tolerated.
				Zonal distributions of combustion model variables
18	3,4, Default	SPSU	m ² /kg	Zonal distribution of specific surface area of char particle cloud after the last iteration of overall heat balance
19	2,3,4, Default	UBRT	fraction	Zonal distribution of unburned fixed carbon as a fraction of total fixed carbon input after the last iteration of overall heat balance
20	2,3,4, Default	PO2	Vol. Fraction Wet	Zonal distribution of O2 concentration on volumetric wet basis after the last iteration of overall heat balance
21	3,4, Default	FULO	kg/kg mixture	Zonal concentration of un-reacted or reacted fuel mass after the last iteration of overall heat balance
22	3,4, Default	VOL0	Number of lumps	Number of volatile fuel lumps released into volume zone (I,J) during the last iteration of overall heat balance Note: Summation of the lumps over all volume zones equals total number of lumps prescribed by the user.

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
23	2,3,4, Default	SO2	Vol. Fraction Wet	Zonal distribution of SO2 concentration on a volumetric wet basis after the last iteration of overall heat balance Note: Sulfur captured by ash is not released to the gas stream.
24	see below			Progress of fixed carbon burnout
	4 1,2,3, Default	UNBURNED FIXED CARBON AT FURNACE EXIT	%	Mean unburned fixed carbon at 2D model furnace exit as a percentage of total fixed carbon input For output level 4, unburned fixed carbon is printed during every sub-iteration of combustion model and every iteration of overall heat balance. For output levels of 1, 2, 3, and default, unburned fixed carbon is printed for the final sub-iteration of combustion model and the final iteration of overall heat balance.
				Check of atom mass balances
25	4,Default	ATOM OUTFLUX		Total atom mass fluxes leaving furnace after the last iteration
		C H N O S A SUM	kg/s kg/s kg/s kg/s kg/s kg/s kg/s	Carbon element Hydrogen element Nitrogen element Oxygen element Sulfur element Ash Sum of the above atom out-fluxes
26	4,Default	ATOM INFLUX		Total atom mass fluxes entering the furnace after the last iteration of overall energy balance
		C H N O S A SUM	kg/s kg/s kg/s kg/s kg/s kg/s kg/s	Carbon element Hydrogen element Nitrogen element Oxygen element Sulfur element Ash Sum of the above atom in-fluxes

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
27	1,2,3,4, Default	ATOM BALANCE		Relative percentage difference in atom mass balances after the last iteration of overall energy balance
		C	%	Carbon element
		H	%	Hydrogen element
		N	%	Nitrogen element
		O	%	Oxygen element
		S	%	Sulfur element
		A	%	Ash
		SUM	%	Overall atom mass fluxes balance Note: Values other than zero indicate violations of species and/or overall mass balances. Small errors due to machine round-off can be tolerated. Large values indicate errors of some model input parameters.
28	4,Default			Overall energy balance for volume zones Note: This block is printed only when NGPRI is set to one.

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
28a	4,Default	ENERGY BALANCE		Detailed output of variables involved in volume zone energy balances after the last iteration of overall energy balance
		TPSAD	K	Adiabatic zonal temperature
		TEX	K	Zonal gas temperature of the previous iteration
		RHOG OLD	kg/m ³	Flue gas density at temperature TEX
		CP EX	kJ/kg K	Mean specific heat of mixture in volume zone (I,J) at temperature TEX, referenced to 298.15 K
		QCONIN	kW	Sensible heat transported into volume zone (I,J)
		QCONNT	kW	Difference between sensible heat transported out of and into volume zone (I,J)
		QDIFIN	kW	Convective heat flux entering volume zone (I,J) from adjacent surfaces or boundary areas, including radiant heat exchanger surfaces
		QDIFNT	kW	Difference between convective heat fluxes leaving and entering volume zone (I,J) including the effect of radiant heat exchangers
		QCHEIN	kW	Heat sink term in volume zone (I,J) due to vaporization of fuel moisture
		QCHENT	kW	Difference between chemical-heat source and sink terms in volume zone (I,J) Note: Chemical heat source term includes heat gained by char and volatile combustion.
		QRADIN	kW	Radiative heat absorbed by volume zone (I,J)
		QRADNT	kW	Difference between radiative fluxes emitted and absorbed by volume zone (I,J)
		QTOTIN	kW	Total energy gain by volume zone (I,J) from in-fluxes and heat sources
		QTOTEX	kW	Total energy losses by volume zone (I,J) due to out-fluxes and heat sinks
		QTOTNT	kW	Difference between total energy gains and losses in volume zone (I,J) Note: Values other than zero indicate violations of local volume zone energy balance. If differences persist after a large number of iterations, setup of some model parameters may be incorrect.
		TNEW	K	New gas temperature of volume zone (I,J) obtained from solution of energy balance equation

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
28b	4,Default	SUM OF ENERGY BALANCE	.	Overall heat balance for all volume zones after the last iteration
		(QCONIN)	kW	Sum of sensible heat transported into each volume zone
		(QCONNT)	kW	Sum of differences between sensible heat transported out of and into each volume zone
		(QDIFIN)	kW	Sum of convective heat fluxes entering each volume zone from adjacent surfaces or boundary areas, including radiant heat exchanger surfaces
		(QDIFNT)	kW	Sum of differences between convective heat fluxes leaving and entering each volume zone including the effect of radiant heat exchangers
		(QCHEIN)	kW	Sum of heat sink terms in each volume zone due to vaporization of fuel moisture
		(QCHENT)	kW	Sum of differences between source and sink terms of chemical heat in each volume zone Note: Chemical heat source term includes heat gained by char and volatile combustion.
		(QRADIN)	kW	Sum of radiative heat absorbed by each volume zone
		(QRADNT)	kW	Sum of differences between radiative fluxes emitted and absorbed by each volume zone
		(QTOTIN)	kW	Sum of total energy gained by each volume zone through in-fluxes and heat sources
		(QTOTEX)	kW	Sum of total energy losses by each volume zone due to out-fluxes and heat sinks
		(QTOTNT)	kW	Sum of differences between total energy gains and losses in each volume zone Note: Values other than zero indicate local violations of volume zone energy balance. If differences persist after large number of iterations, setup of some model parameters may be incorrect.

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
29	4,Default	ABSOLUTE AND RELATIVE RESIDUALS		Maximum variations of energy balance solutions between the last two consecutive iterations Note: This block is printed only when NGPRI is set to one.
		I J		Volume zone (I,J) where the maximum occurs
		DTMAX	K	Maximum zonal temperature variation at volume zone (I,J) between the last two consecutive iterations
		RDTMAX	%	Maximum zonal temperature variation relative to the current temperature of volume zone (I,J) between the last two consecutive iterations
		DQMAX	kW	Maximum difference on heat gains and losses at volume zone (I,J) between the last two consecutive iterations
		RDQMAX	%	Maximum percentage difference on heat gains and losses relative to the heat gained by volume zone (I,J) between the last two consecutive iteration
		DQTOTAL	kW	Sum of differences on heat losses and gains of all volume zones
		RDOTOTAL	%	Percentage difference on total heat losses and gains relative to the sum of energy gained by all volume zones
30	3,4, Default	HEAT FLUXES TO ADDITIONAL HEAT SINKS		Heat fluxes to radiant heat exchangers
		Convective Flux	kW	Sum of convective heat fluxes to all radiant heat exchangers
		Radiative Flux	kW	Sum of net radiative heat fluxes to all radiant heat exchangers
		Total Flux	kW	Sum of convective and net radiative fluxes to all radiant heat exchangers
31	3,4, Default	SURFACE TEMPERATURES OF ADDITIONAL HEAT SINKS		Surface temperatures of radiant heat exchangers embedded in volume zone (I,J) after the last iteration Note: Volume zones without the presence of radiant heat exchangers are assigned with zero temperatures.
		TWSINK(IJ)	K	Heat exchanger surface temperatures at volume zone (I,J)

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
32	1,2,3,4, Default			Furnace thermal performance predictions
		Mean Furnace Exit Temp.	K	Mean furnace exit gas temperature after each iteration of total energy balance
		Total Furnace Efficiency	%	Furnace efficiency based on net fuel heat release rate and sensible heat input
		Heat Release	kW	Net fuel heat release in furnace (i.e., heat release due to combustion minus latent heat required for evaporation)
		Sensible Input	kW	Total sensible heat entering furnace Note: For output levels 3 and 4, this block is printed for every iteration. For output levels 1 and 2, this block is printed only for the last iteration.
				Discrimination of overall furnace heat balance into in and out heat fluxes based on chemical heat, sensible heat and heat sinks
33a	3,4, Default	CHEM. HEAT OUTFLUX		Out-fluxes of chemically bonded heat
		FUEL	kW	Heat in unburned char Note: In this output block, 2DHT assumes that volatiles are burned completely.
		SULF.	kW	This option is not used by the code.
		SUM	kW	Sum of out-fluxes via chemically bonded heat
33b	3,4, Default	SENS. HEAT OUTFLUX		Out-fluxes of sensible heat
		EXT.	kW	Sensible heat carried by flue gas at 2D model furnace exit
		REC.	kW	This option is not used by the code.
		SUM	kW	Sum of sensible heats defined by the above two items
33c	3,4, Default	OUTFLUX TO HEAT SINKS		Out-fluxes to heat sinks
		RAD.	kW	Total net radiative fluxes to wall surfaces, boundary areas, and radiant heat exchanger surfaces
		CONV.	kW	Total net convective fluxes to wall surfaces, boundary areas, and radiant heat exchanger surfaces
		SUM	kW	Sum of the above two items
33d	3,4, Default	TOTAL HEAT OUTFLUX	kW	Sum of total heat out-fluxes based on chemical heat, sensible heat, and heat sinks

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
34a	3,4, Default	CHEM. HEAT INFLUX		In-fluxes of chemically bonded heat
		FUEL	kW	Heat input calculated based on lower (net) heating value
		EVAP.	kW	Heat needed for evaporation of fuel moisture within the furnace (negative sign)
		CALC.	kW	This option is not used by the code.
		SULF	kW	This option is not used by the code.
		SUM	kW	Sum of chemically bonded heat in-fluxes
34b	3,4, Default	SENS. HEAT AIR INFLUX		In-fluxes of air sensible heat
		SEC.	kW	Sensible heat carried by secondary air into the furnace
		PRIM.	kW	Sensible heat carried by primary air into the furnace
		TRANS.	kW	This option is not used by the code.
		REC.	kW	Sensible heat carried by flue gas recirculated into the furnace
		SUM	kW	Sum of all sensible heat in-fluxes from air, including externally recirculated flue gas
34c	3,4, Default	SENS. HEAT FUEL INFLUX		In-fluxes of fuel sensible heat
		DRY	kW	Sensible heat of dry burner fuel
		H2OG	kW	Sensible heat of fuel moisture
		SUM	kW	Sum of the above two items
34d	3,4, Default	SENS. HEAT SORBENT INFLUX	kW	This option is not used by the code.
34e	3,4, Default	SENS. HEAT BURNER-STEAM INFLUX	kW	Sensible heat carried into the furnace by atomizing steam of the burner fuel
34f	3,4, Default	SENS. HEAT FLUE GAS INFLUX	kW	Sensible heat carried into the furnace by recirculated flue gas
34g	3,4, Default	TOTAL HEAT INFLUX	kW	Sum of heat in-fluxes based on chemical heat, and sensible heats of air, fuel, atomizing steam and recirculated flue gas

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
35	see below	GAS ZONE HEAT BALANCE		Heat balance for furnace volume zones
	1,2 3,4, Default	OUT-IN (OUT-IN)/IN	kW %	<p>Difference between all heat out-fluxes and in-fluxes</p> <p>Percentage difference of heat out-fluxes and in-fluxes relative to total heat in-fluxes</p> <p>Note: For output levels 1 and 2, this output block is printed only at the last iteration of the heat balance.</p> <p>For output levels 3 and 4, this output block is printed for every iteration.</p>
36	4,Default			Overall energy balance for surface zone on M=1, where surface temperatures are calculated by the code

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
36a	4,Default	SURFACE ZONE HEAT BALANCE OF M=1		Detailed output of variables involved in surface zone energy balance on wall section M=1 after the last iteration of overall heat balance Note: This block is printed only when NWPRI is set to one.
		I J M		Surface zone (I,J) on wall section M=1
		TOLDW	K	Surface zone temperature obtained from previous sub-iteration of surface zone heat balance
		QCONIN	kW	Heat flux transported from water side of surface layer towards the gas stream in furnace (usually zero)
		QCONNT	kW	Difference between heat fluxes transported from furnace gas stream into surface layer and from surface layer towards furnace gas stream. Note: This value is identical with net heat flux conducted through deposit layer.
		QDIFIN	kW	Heat flux transported to surface layer by convection from adjacent volume zone
		QDIFNT	kW	Difference between convective heat fluxes transported from surface into adjacent volume zone and from adjacent volume zone to surface
		QRADIN	kW	Radiative heat flux absorbed by surface zone
		QRADNT	kW	Difference between radiative heat fluxes emitted and absorbed by surface zone
		QTOTIN	kW	Total heat fluxes entering surface zone
		QTOTEX	kW	Total heat fluxes leaving surface zone
		QTOTN	kW	Difference between heat fluxes entering and leaving a surface zone Note: Values other than zero indicate violations of local surface zone heat balance. If differences persist after a large number of iterations, setup of some model parameters may be incorrect.
		TNEWW	K	New surface temperatures obtained from solution of surface energy

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
36b	4,Default	SUM OF SURFACE ENERGY BALANCE OF M=1		Sum of surface zone energy balance on wall section M=1
		(QCONIN)	kW	Sum of heat fluxes transported from water side of surface layer towards the furnace gas stream for surface zones of M=1
		(QCONNT)	kW	Sum of differences between heat fluxes transported from furnace gas stream into surface layer and from surface layer towards furnace gas stream for surface zones of M=1
		(QDIFIN)	kW	Sum of heat flux transported to surface layer by convection from adjacent volume zone for surface zones of M=1
		(QDIFNT)	kW	Sum of differences between convective heat fluxes transported from surface into adjacent volume zone and from adjacent volume zone to surface zones on M=1
		(QRADIN)	kW	Sum of radiative heat fluxes absorbed by surfaces zone on M=1
		(QRADNT)	kW	Sum of differences between radiative heat fluxes emitted and absorbed by surface zones on M=1
		(QTOTIN)	kW	Sum of absorbed and convective heat fluxes towards surface zones on M=1
		(QTOTEX)	kW	Sum of total heat fluxes from surface zones on M=1
		(QTOTN)	kW	Sum of differences between heat fluxes leaving and entering surface zones on M=1 Note: Values other than zero indicate violations of local surface zone heat balance. If differences persist after a large number of iterations, setup of some model parameters may be incorrect.
37	4,Default	ABSOLUTE AND RELATIVE RESIDUALS		Maximum variation of energy balance solutions found at surface zone (I,J) on wall section M=1 between the last two consecutive iterations Note: This block is printed only when NWPRI is set to one. Output descriptions are similar to those discussed in Output Block 29.

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
38	4,Default			Overall energy balance for surface zones on M=3, where surface temperatures are calculated by the code
38a, 38b	4,Default	SURFACE ZONE HEAT BALANCE OF M=3		Detailed output of variables involved in surface zone energy balance on wall section M=3 after the last iteration of overall heat balance Note: This block is printed only when NWPRI is set to one. Output descriptions of this block are similar to those entailed in Output Blocks 36a and 36b.
39	4,Default	ABSOLUTE AND RELATIVE RESIDUALS		Maximum variation of energy balance solutions found at surface zone (I,J) on wall section M=3 between the last two consecutive iterations Note: This block is printed only when NWPRI is set to one. Output descriptions of this block are similar to those entailed in Output Block 29.
40	4,Default			Overall energy balance for surface zones on M=4, where surface temperatures are calculated by the code
40a, 40b	4,Default	SURFACE ZONE HEAT BALANCE OF M=4		Detailed output of variables involved in surface zone energy balance on wall section M=4 after the last iteration of overall heat balance Note: This block is printed only when NWPRI is set to one. Output descriptions of this block are similar to those discussed in Output Blocks 36a and 36b.
41	4,Default	ABSOLUTE AND RELATIVE RESIDUALS		Maximum variation of energy balance solutions found at surface zone (I,J) on wall section M=4 between the last two consecutive iterations Note: This block is printed only when NWPRI is set to one. Output descriptions of this block are similar to those discussed in Output Block 29.
42	2,3,4, Default	T	K	Gas temperatures of each volume zone (I,J) after the last iteration of overall heat balance Note: Volume zones outside the furnace boundaries are assigned with zero gas temperatures.
43	3,4, Default			Zonal mass concentrations of all combustion species after the last iteration of overall heat balance
		CO2 H2O N2 O2 VOL SO2 ASH CHAR SOOT	kg/kg kg/kg kg/kg kg/kg kg/kg kg/kg kg/kg kg/kg kg/kg	Mass concentration of CO2 Mass concentration of H2O Mass concentration of N2 Mass concentration of O2 Mass concentration of VOL Mass concentration of SO2 Mass concentration of ash Mass concentration of char particles Mass concentration of soot particles Note: The sum of all mass concentrations in each volume zone (I,J) is always one since nitrogen was calculated by the difference.

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
				Zonal distributions of other variables in overall furnace heat balance after the last iterations
44	3,4, Default	QG	kW/m ³	Distribution of volumetric net heat fluxes by radiation Note: Values with positive sign indicate that more radiation is emitted by volume zone (I,J) than received. Values with negative sign indicate that more radiation is absorbed by volume zone (I,J) than emitted.
45	3,4, Default	TRES	second	Calculated zonal residence times based on mass fluxes leaving zone (I,J)
46	3,4, Default	VOHR	kW	Distribution of zonal heat release rate resulted from combustion of volatiles Note: The volatile heat distributions can be used as an indication of actual flame extension.
47	3,4, Default	VOL	kg/kg	Distribution of zonal mass concentrations of unburned volatile matters Note: Small difference between values in this block and values in Output Block 43 is due to the fact that the soot concentration is included here.
				Variables of boundary surfaces on wall sections M=1, 3, and 4 after the last iteration
48	3,4, Default	TW for M=1	K	Temperatures of deposit surfaces or boundary areas at section M=1
49	3,4, Default	QIN for M=1	kW/m ²	Density of incident radiative heat fluxes on surfaces of section M=1
50	3,4, Default	QW for M=1	kW/m ²	Density of net total radiative and convective heat fluxes on surfaces of section M=1
51	3,4, Default	TW for M=3	K	Temperatures of deposit surfaces or boundary areas on section M=3
52	3,4, Default	QIN for M=3	kW/m ²	Density of incident radiative heat fluxes on surfaces of section M=3
53	3,4, Default	QW for M=3	kW/m ²	Density of net total radiative and convective heat fluxes on boundary surfaces of section M=3
54	3,4, Default	TW for M=4	K	Temperatures of deposit surfaces or boundary areas at section M=4
55	3,4, Default	QIN for M=4	kW/m ²	Density of incident radiative heat fluxes on surfaces of section M=4
56	3,4, Default	QW for M=4	kW/m ²	Density of net total radiative and convective heat fluxes on surfaces of section M=4

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
57	see below			Progress of code convergence shown in terms of overall heat balances at each iteration
	1,2,3,4, Default and on Terminal Screen	act.err.	%	The error percentage is defined as: $\frac{(\text{Heat fluxes from flue gas}) - (\text{Heat fluxes to heat sinks})}{\text{Heat fluxes from flue gas}}$
		avg.err	%	Actual percentage error averaged over the first to the current iterations Note: Values at the end of a run do not necessarily reflect the convergence of the run, since it may inherit large energy balance errors from the beginning of a run.
		20 it.err	%	Actual percentage error averaged over the last 20 iterations, starting from the current iteration Note: If iteration number is less 20, this error message is the same as the actual percentage error averaged over the first to the current iterations. If this value is within $\pm 1\%$, quasi-convergence is achieved and the averaging process can be started.
		hb.err	%	Heat balance error of gas zones (same meaning as shown in Output Block 35)
58	4,Default	BALANCE OF TOTAL RADIATIVE EXCHANGE		Detailed balance of radiative heat exchange for furnace volumes, surfaces, and boundary areas
		NUMBER OF BEAMS		Number of beams actually tracked during the last non-averaged iteration or during all averaged iterations
		SUM OF EMITTED RADIATION		Sum of radiation emitted during the last non-averaged iteration or during all averaged iterations
		VOLUME ZONES	kW	Radiative heat fluxes emitted by all volume zones
		WALL SECTIONS	kW	Radiative heat fluxes emitted by all surfaces including radiant heat exchangers
		M=1,M=2,M=3, M=4	kW	Radiative heat fluxes emitted by wall sections on M=1,2,3, and 4 Note: Values for M=2 and 4 include the fluxes emitted by radiant heat exchangers.
		TOTAL	kW	Total radiation emitted by volume zones and wall surfaces

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
		SUM OF ABSORBED RADIATION		Sum of radiation absorbed during the last non-averaged iteration or during all averaged iterations
		VOLUME ZONES	kW	Radiative heat fluxes absorbed by all volume zones and radiant heat exchangers
		WALL SECTIONS	kW	Radiative heat fluxes absorbed by all wall sections
		M=1, M=2, M=3, M=4	kW	Radiative heat fluxes absorbed by wall sections of M=1, 2, 3, and 4
		TOTAL	kW	Total radiation absorbed by volume zones and wall sections
		SUM OF NET EMITTED RADIATION		Difference between radiation emitted and absorbed during the last non-averaged iteration or during all averaged iterations
		VOLUME ZONES	kW	Net heat fluxes emitted by volume zones
		WALL SECTIONS	kW	Net heat fluxes emitted by wall sections
		M=1, M=2, M=3, M=4	kW	Net heat fluxes emitted by wall sections of M=1, 2, 3, and 4
		TOTAL	kW	Total net radiative heat flux emitted by the furnace Note: Values other than zero indicate violations of overall radiative energy balance. Small errors due to machine round-off can be tolerated.
59	1,2,3,4, Default	ERROR OF RADIATIVE ENERGY BALANCE	%	Percentage difference of net radiative heat fluxes emitted by the system relative to total emitted radiation of the last non-averaged iteration or of all averaged iterations. Note: Values other than zero indicate violation of radiative heat balance. Errors within $\pm 0.1\%$ can be tolerated because they are likely due to round-off errors. Large errors indicate that the geometric set-up is incorrect.

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
60	3,4, Default	TOTAL HEAT BALANCE		Detailed overall furnace heat balance
		HEAT TO FURNACE WALLS		Heat fluxes to furnace wall surfaces
		RAD.	kW	Net radiative heat fluxes
		CONV.	kW	Net convective heat fluxes
		SUM	kW	Sum of net radiative and convective heat fluxes to furnace wall surfaces
		HEAT TO FURNACE EXIT		Heat fluxes to boundary surfaces at the exit
		RAD.	kW	Net radiative heat fluxes
		CONV.	kW	Net convective heat fluxes
		SUM	kW	Sum of net radiative and convective heat fluxes to furnace exit
		HEAT TO FURNACE HOPPER		Heat fluxes to furnace boundary surfaces of the hopper
		RAD.	kW	Net radiative heat fluxes
		CONV.	kW	Net convective heat fluxes
		SUM	kW	Sum of net radiative and convective heat fluxes to furnace boundary surfaces
61	3,4, Default	HEAT FLUXES TO ZONAL HEAT EXCHANGERS		Heat fluxes to radiant heat exchangers allocated in the volume zone layers
		Zone I		Index of volume zone layer in axial direction
		BY RADL.	kW	Net radiative heat fluxes absorbed by heat exchangers in zone layer I
		BY CONV.	kW	Convective heat fluxes absorbed by heat exchangers in zone layer I
		SUM	kW	Total net radiative and convective heat fluxes absorbed by heat exchangers in zone layer I

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
62	1,2,3,4, Default	CLOSURE OF TOTAL HEAT BALANCE		Furnace heat balance at the last iteration
		HEAT FLUX FROM FLUE GAS	kW	Total heat fluxes extracted from flue gas
		HEAT FLUX TO HEAT SINKS	kW	Total heat fluxes received by heat sinks
		DIFFERENCE	kW	Difference between total heat fluxes received by heat sinks and total heat fluxes extracted from flue gas
		ACT. PERCENTAGE ERROR	%	Actual percentage error of overall furnace heat balance at the last iteration Note: For definition, see Output Block 57.
		AVG. PERCENTAGE ERROR	%	Actual percentage error of overall furnace heat balance averaged over the first till the last iterations Note: For definition, see Output Block 57.
		AVG. ERROR OF LAST 20 IT.	%	Actual percentage error of overall furnace heat balance averaged over the last 20 iterations Note: For definition, see Output Block 57. Note: A 2DHT run is considered converged when both the actual percentage error and the percentage error averaged over the last 20 iterations are within $\pm 1\%$.
63	1,2,3,4, Default			Mean time-temperature profile in volume zone layers along furnace axial direction
		I INDEX		Index of volume zone layer in axial direction
		X-CO-ORDINATE	m	Axial distance to the center of volume zone layer I
		MEAN NORM MASS FLUX		Mean normalized mass flux leaving volume zone layer I
		MEAN TEMP.	K	Mass-weighted mean temperature of volume zone layer I
		MEAN RES. TIME	second	Mean residence time of the furnace gas in volume zone layer I

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
64	1,2,3,4, Default	MEAN GAS SPECIES CONCENTRATION		Mean volumetric concentration of gaseous species in volume zone layers along furnace axial direction
		I X-CO-ORD. CO2 H2O N2 O2 VOL SO2	 m Vol.% wet Vol.% wet Vol.% wet Vol.% wet Vol.% wet Vol.% wet	Index of volume zone layer in axial direction Axial distance to the center of volume zone layer I CO2 volumetric concentration H2O volumetric concentration N2 volumetric concentration O2 volumetric concentration Volatile volumetric concentration SO2 volumetric concentration Note: Sulfur inherently captured by ash is not released to the gas stream.
65	1,2,3,4, Default	OTHER MEAN QUANTITIES ALONG FURNACE		Mean data predicted by combustion model in volume zone layers along furnace axial direction
		I X-CO-ORD. CARBON IN ASH TOT. FUEL HEAT REL. VOLATILE HEAT REL. SO2 REDUCTION CAO UTIL.	 m % % % % %	Index of volume zone layer in axial direction Axial distance to the center of volume zone layer I Mean unburned fixed carbon in ash in layer I Fuel heat release in layer I as percentage of total fuel heat input Volatile heat release in layer I as percentage of total volatile heat input This option is not used by the code. This option is not used by the code.

6.2 Outputs from the RBNOX Code

The RBNOX code generates two kinds of outputs as discussed below.

Screen Display

The screen display generated by the RBNOX code shows the progress of the kinetics calculations for the four plug flow reactors (PFR) used. At the beginning of any reactor calculation, a message is displayed to inform the user which reactor is currently being handled by the RBNOX code. For example, the message " — RXR NO 1. : REBURNING REACTOR — " indicates the code is handling the first reactor where the reburning gas is being injected. The other three reactors are called as "RICH ZONE REACTOR", "OVER-FIRED-AIR REACTOR", and "QUENCHING REACTOR", respectively, for reactors numbered from 2 to 4 (see Figure 4.11). The screen display also indicates the current integration location (x) and the step size (dx), if a previous step size is doubled or halved. Again, this screen message is abbreviated from an output file RBOTcsvs.111, which will be discussed in detail in the next sub-section. The user may find that if the step size is reduced (or halved) very often, the computational time will increase. This normally occurs at very high reactor temperatures (say greater than 2000 K), and is outside the temperature windows of general boiler reburning applications.

File RBOTcsvs.111

This is the file which contains the reburning NOX predictions, and is most likely to be dealt with by the user. Listing 6.2 is an example indicating the contents of this output file. The description of this output file follows the same format as shown for the 2DHT code outputs. The outputs shown in the Listing are grouped into "blocks" of information and each block is labeled by a numeral. Table 6.2 is a corresponding table to interpret the contents of the Listing. To interpret a block of the output information, the user may refer to Table 6.2 and locate the description for that block by matching the "Index of Output Block" with the numeral shown in Listing 6.2. Table 6.2 then shows the user the variable names, units, and the physical meanings of the variables for that block. If the outputs contain the same information that was repeated for every iteration cycle, the labeling shown in Listing 6.2 uses the output blocks of the last iteration.

Listing 6.2. Output generated by the RBNOX code.

BOILER REBURNING NOX MODEL (RBNOX) OUTPUTS
OUTPUT FILE NAME: RBOT0201.075

1

1a

*
* USER'S COMMENTS *
*

1b

C.OIL FIRING WITH GAS REBURN AT 75% LOAD
C.SR1=1.1 SR2=0.9 SR3=1.06
C.0.24 SECONDS MIXING TIME FOR OFA AND RBN FUEL
C.
C.
C.
C.
C.
C.
C.

645

----- RXR NO. 1 : REBURNING REACTOR -----

page 1

2

2a

irxr= 1
iprt= 0
x= 0.000000E+00 cm
dx= 0.300000E-07 cm
p= 0.100000E+01 atm
dpdx= 0.000000E+00 atm/cm
tausr= 0.000000E+00 sec

TEMPERATURE(K) = 1656.06 ENTHALPY(CAL/G)=-2.444E+02 VELOCITY(CM/SEC)= 1.000E+00 CP(CAL/G-K) = 3.291E-01
DENSITY(G/CC) = 2.131E-04 MOLE/GM-TOTAL = 3.454E-02 AREA(CM2) = 1.000E+00 H.T.(CAL/CC-S) = 0.000E-01

2b

MASS INFLUX(XMDOTE,GM/SEC)= 1.000E-01 ENERGY INFLU X(QDOTE,CAL/SEC)= 0.000E-01 TE(K)= 3.000E+02 RHOE(G/CC)= 0.000E-01
OFRE= 1.000E-16 FEXTNAL= 2.131E-04

2c

I	SPECIES	MASS FRXN		MOLE FRXN		NET RATE	DADT(I)	ALPHA E(I)	ALPHA A(I)	ALPHA F(I)	#N
		(OVERALL)	(GAS/SOLID)	(OVERALL)	(GAS/SOLID)	(MOLE/CC-S)	(FRXN/S)				
1	H2	6.9628E-18	6.9628E-18	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
2	O2	1.9356E-02	1.9356E-02	1.7513E-02	1.7513E-02	0.0000E-01	0.0000E-01	0.0000E-01	7.2784E-03	6.0486E-04	0
3	HO	5.8742E-17	5.8742E-17	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
4	O	5.5261E-17	5.5261E-17	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
5	H	3.4814E-18	3.4814E-18	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
6	H2O	7.3200E-02	7.3200E-02	1.1764E-01	1.1764E-01	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	4.0630E-03	0
7	CO2	1.9227E-01	1.9227E-01	1.2649E-01	1.2649E-01	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	4.3688E-03	0
8	HO2	1.1400E-16	1.1400E-16	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
9	H2O2	1.1748E-16	1.1748E-16	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
10	CO	9.6744E-17	9.6744E-17	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
11	CH4	5.5409E-17	5.5409E-17	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
12	CH3	5.1928E-17	5.1928E-17	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0

3

13	CH2	4.8446E-17	4.8446E-17	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
14	CH	4.4965E-17	4.4965E-17	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
15	C2H4	9.6893E-17	9.6893E-17	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
16	C2H6	1.0386E-16	1.0386E-16	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
17	C2H5	1.0037E-16	1.0037E-16	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
18	C2H3	9.3411E-17	9.3411E-17	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
19	C	4.1484E-17	4.1484E-17	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
20	C2H2	8.9930E-17	8.9930E-17	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
21	C2H	8.6448E-17	8.6448E-17	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
22	CH2O	1.0371E-16	1.0371E-16	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
23	CH3O	1.0719E-16	1.0719E-16	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
24	CHO	1.0023E-16	1.0023E-16	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
25	N	4.8381E-17	4.8381E-17	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	1
26	NO	6.2185E-04	6.2185E-04	6.0000E-04	6.0000E-04	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	2.0723E-05	1
27	N2	7.1333E-01	7.1333E-01	7.3720E-01	7.3720E-01	0.0000E-01	0.0000E-01	0.0000E-01	2.7381E-02	2.5462E-02	0
28	NO2	1.5890E-16	1.5890E-16	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	1
29	N2O	1.5202E-16	1.5202E-16	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	2
30	NH3	5.8825E-17	5.8825E-17	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	1
31	NH2	5.5344E-17	5.5344E-17	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	1
32	NH	5.1862E-17	5.1862E-17	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	1
33	HN2	1.0024E-16	1.0024E-16	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	2
34	N2H2	1.0372E-16	1.0372E-16	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	2
35	HNO	1.0712E-16	1.0712E-16	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	1
36	CN	8.9864E-17	8.9864E-17	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	1
37	NCO	1.4512E-16	1.4512E-16	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	1
38	CHN	9.3346E-17	9.3346E-17	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	1
39	HNCO	1.4861E-16	1.4861E-16	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	1
40	HOCN	1.4861E-16	1.4861E-16	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	1
41	SO2	1.2187E-03	1.2187E-03	5.5080E-04	5.5080E-04	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	1.9023E-05	0
42	SO3	2.7652E-16	2.7652E-16	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0
43	HSO3	2.7999E-16	2.7999E-16	1.0000E-16	1.0000E-16	0.0000E-01	0.0000E-01	0.0000E-01	3.4659E-18	3.4538E-18	0

MOLE FRACTION OF FIXED NITROGEN IN GAS PHASE = 6.000E-04

3a

4

Step size increased at: x= 0.300E-07 dx= 0.600E-07
Step size increased at: x= 0.900E-07 dx= 0.120E-06
Step size increased at: x= 0.210E-06 dx= 0.240E-06
Step size increased at: x= 0.450E-06 dx= 0.480E-06
Step size increased at: x= 0.930E-06 dx= 0.960E-06
Step size increased at: x= 0.189E-05 dx= 0.192E-05
Step size increased at: x= 0.381E-05 dx= 0.384E-05
Step size increased at: x= 0.765E-05 dx= 0.768E-05
Step size increased at: x= 0.153E-04 dx= 0.154E-04
Step size increased at: x= 0.307E-04 dx= 0.307E-04

4a

Step size reduced at: x= 0.921E-04 dx= 0.307E-04 ideqn= 3 delmax= 0.119E+00 qm= 0.251E-07 savea= 0.158E-07
restart at: x= 6.141E-05 dx= 1.536E-05
Step size reduced at: x= 0.768E-04 dx= 0.154E-04 ideqn= 3 delmax= 0.584E-01 qm= 0.204E-07 savea= 0.158E-07
restart at: x= 6.141E-05 dx= 7.680E-06
Step size increased at: x= 0.998E-04 dx= 0.154E-04
Step size increased at: x= 0.192E-03 dx= 0.307E-04
Step size reduced at: x= 0.124E-02 dx= 0.307E-04 ideqn= 5 delmax= 0.520E-01 qm= 0.252E-07 savea= 0.200E-07
restart at: x= 1.206E-03 dx= 1.536E-05
Step size increased at: x= 0.176E-02 dx= 0.307E-04
Step size increased at: x= 0.191E-02 dx= 0.614E-04
Step size increased at: x= 0.216E-02 dx= 0.123E-03
Step size increased at: x= 0.253E-02 dx= 0.246E-03

4b

Step size increased at: x= 0.302E-02 dx= 0.492E-03
Step size increased at: x= 0.400E-02 dx= 0.800E-03

REACH MAX. at X= 2.400E-01

4c

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page 2

----- RXR NO. 1 : REBURNING REACTOR -----

irxr= 1
iprt= 402
x= 0.240001E+00 cm
dx= 0.800000E-03 cm
p= 0.100000E+01 atm
dpdx= 0.000000E+00 atm/cm
tausr= 0.000000E+00 sec

TEMPERATURE(K) = 1662.07 ENTHALPY(CAL/G)=-2.741E+02 VELOCITY(CM/SEC)= 1.000E+00 CP(CAL/G-K) = 3.385E-01
DENSITY(G/CC) = 2.070E-04 MOLE/GM-TOTAL = 3.542E-02 AREA(CM2) = 1.042E+00 H.T.(CAL/CC-S) = 0.000E-01

MASS INFLUX(XMDOTE,GM/SEC)= 1.051E-05 ENERGY INFLU X(QDOTE,CAL/SEC)= 0.000E-01 TE(K)= 5.450E+02 RHOE(G/CC)= 3.775E-04
OFRE= 1.000E-16 FEXTNAL= 2.131E-04

I	SPECIES	MASS FRXN (OVERALL)	MASS FRXN (GAS/SOLID)	MOLE FRXN (OVERALL)	MOLE FRXN (GAS/SOLID)	NET RATE (MOLE/CC-S)	DADT(I) (FRXN/S)	ALPHA E(I)	ALPHA A(I)	ALPHA F(I)	#N
1	H2	7.6342E-04	7.6342E-04	1.0690E-02	1.0690E-02	5.6107E-07	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
2	O2	2.9771E-07	2.9771E-07	2.6264E-07	2.6264E-07	-1.1748E-10	0.0000E-01	5.9232E-18	7.2784E-03	6.0486E-04	0
3	HO	3.1794E-06	3.1794E-06	5.2771E-06	5.2771E-06	1.8387E-09	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
4	O	1.8674E-09	1.8674E-09	3.2947E-09	3.2947E-09	-5.3595E-13	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
5	H	3.2747E-07	3.2747E-07	9.1712E-06	9.1712E-06	-1.0104E-09	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
6	H2O	8.7154E-02	8.7154E-02	1.3656E-01	1.3656E-01	3.8361E-07	0.0000E-01	5.9232E-18	3.4659E-18	4.0630E-03	0
7	CO2	1.8152E-01	1.8152E-01	1.1643E-01	1.1643E-01	-7.4206E-07	0.0000E-01	2.9616E-04	3.4659E-18	4.3688E-03	0
8	HO2	1.0314E-11	1.0314E-11	8.8211E-12	8.8211E-12	-5.4569E-15	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
9	H2O2	1.0180E-11	1.0180E-11	8.4486E-12	8.4486E-12	-4.2941E-15	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
10	CO	2.1595E-02	2.1595E-02	2.1764E-02	2.1764E-02	1.1047E-06	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
11	CH4	1.0701E-03	1.0701E-03	1.8830E-03	1.8830E-03	-4.9026E-07	0.0000E-01	5.5678E-02	3.4659E-18	3.4538E-18	0
12	CH3	2.0640E-05	2.0640E-05	3.8754E-05	3.8754E-05	4.8869E-10	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
13	CH2	1.5048E-08	1.5048E-08	3.0284E-08	3.0284E-08	3.8147E-13	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
14	CH	5.2964E-12	5.2964E-12	1.1485E-11	1.1485E-11	-3.5590E-15	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
15	C2H4	1.6476E-05	1.6476E-05	1.6579E-05	1.6579E-05	-5.5269E-09	0.0000E-01	5.9232E-04	3.4659E-18	3.4538E-18	0
16	C2H6	1.5740E-06	1.5740E-06	1.4777E-06	1.4777E-06	-1.1992E-08	0.0000E-01	1.1846E-03	3.4659E-18	3.4538E-18	0
17	C2H5	1.1879E-09	1.1879E-09	1.1539E-09	1.1539E-09	-3.7519E-12	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
18	C2H3	6.1427E-09	6.1427E-09	6.4115E-09	6.4115E-09	-1.2793E-11	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
19	C	7.4581E-14	7.4581E-14	1.7529E-13	1.7529E-13	1.4337E-17	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
20	C2H2	6.3635E-04	6.3635E-04	6.8991E-04	6.8991E-04	7.9144E-08	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
21	C2H	3.0270E-09	3.0270E-09	3.4139E-09	3.4139E-09	2.3509E-11	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
22	CH2O	3.4766E-05	3.4766E-05	3.2685E-05	3.2685E-05	-4.3430E-11	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
23	CH3O	1.3320E-07	1.3320E-07	1.2116E-07	1.2116E-07	-7.4185E-11	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
24	CHO	4.2009E-09	4.2009E-09	4.0866E-09	4.0866E-09	-1.4795E-11	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
25	N	1.2172E-10	1.2172E-10	2.4531E-10	2.4531E-10	3.7263E-14	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
26	NO	4.2407E-04	4.2407E-04	3.9894E-04	3.9894E-04	-5.6465E-09	0.0000E-01	5.9232E-18	3.4659E-18	2.0723E-05	1
27	N2	7.0547E-01	7.0547E-01	7.1086E-01	7.1086E-01	5.6438E-10	0.0000E-01	1.4808E-03	2.7381E-02	2.5462E-02	0
28	NO2	7.7869E-10	7.7869E-10	4.7779E-10	4.7779E-10	-2.4480E-14	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
29	N2O	1.2534E-07	1.2534E-07	8.0385E-08	8.0385E-08	2.5593E-12	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	2
30	NH3	4.5792E-06	4.5792E-06	7.5899E-06	7.5899E-06	5.0106E-10	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
31	NH2	9.2441E-09	9.2441E-09	1.6285E-08	1.6285E-08	1.2009E-12	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
32	NH	3.3119E-10	3.3119E-10	6.2263E-10	6.2263E-10	3.9587E-14	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
33	HN2	1.3592E-10	1.3592E-10	1.3220E-10	1.3220E-10	-3.8296E-14	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	2
34	N2H2	4.3182E-14	4.3182E-14	4.0591E-14	4.0591E-14	-3.6807E-18	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	2

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35	HNO	1.4941E-08	1.4941E-08	1.3598E-08	1.3598E-08	-3.8878E-12	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
36	CN	7.9850E-10	7.9850E-10	8.6635E-10	8.6635E-10	7.0705E-13	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
37	NCO	6.6287E-11	6.6287E-11	4.4534E-11	4.4534E-11	-4.3715E-16	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
38	CHN	7.2920E-05	7.2920E-05	7.6166E-05	7.6166E-05	4.0066E-09	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
39	HNCO	4.9508E-07	4.9508E-07	3.2482E-07	3.2482E-07	6.3504E-12	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
40	HOCN	1.8616E-07	1.8616E-07	1.2214E-07	1.2214E-07	6.4632E-13	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
41	SO2	1.2044E-03	1.2044E-03	5.3071E-04	5.3071E-04	2.7845E-13	0.0000E-01	5.9232E-18	3.4659E-18	1.9023E-05	0
42	SO3	3.8638E-09	3.8638E-09	1.3623E-09	1.3623E-09	-6.4001E-14	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
43	HSO3	7.1295E-12	7.1295E-12	2.4827E-12	2.4827E-12	-2.1445E-13	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0

MOLE FRACTION OF FIXED NITROGEN IN GAS PHASE = 4.833E-04

PLUG FLOW REACTOR (CONTINUED WITH SAME CHEMISTRY) ←

6

Step size increased at: x= 0.300E-07 dx= 0.600E-07
 Step size increased at: x= 0.900E-07 dx= 0.120E-06
 Step size increased at: x= 0.210E-06 dx= 0.240E-06
 Step size increased at: x= 0.450E-06 dx= 0.480E-06
 Step size increased at: x= 0.930E-06 dx= 0.960E-06
 Step size increased at: x= 0.189E-05 dx= 0.192E-05
 Step size increased at: x= 0.381E-05 dx= 0.384E-05
 Step size increased at: x= 0.765E-05 dx= 0.768E-05
 Step size increased at: x= 0.153E-04 dx= 0.154E-04
 Step size increased at: x= 0.307E-04 dx= 0.307E-04
 Step size increased at: x= 0.614E-04 dx= 0.614E-04
 Step size increased at: x= 0.123E-03 dx= 0.123E-03
 Step size increased at: x= 0.246E-03 dx= 0.246E-03
 Step size increased at: x= 0.491E-03 dx= 0.492E-03
 Step size increased at: x= 0.983E-03 dx= 0.983E-03
 Step size increased at: x= 0.197E-02 dx= 0.110E-02

REACH MAX. at X= 3.318E-01

----- RXR NO. 2 : RICH ZONE REACTOR -----

page 3

irxr= 2
 iprt= 315
 x= 0.331764E+00 cm
 dx= 0.110300E-02 cm
 p= 0.100000E+01 atm
 dpdx= 0.000000E+00 atm/cm
 tausr= 0.000000E+00 sec

TEMPERATURE(K) = 1627.26 ENTHALPY(CAL/G)=-2.812E+02 VELOCITY(CM/SEC)= 1.000E+00 CP(CAL/G-K) = 3.371E-01
 DENSITY(G/CC) = 2.106E-04 MOLE/GM-TOTAL = 3.556E-02 AREA(CM2) = 1.024E+00 H.T.(CAL/CC-S) = 0.000E-01

MASS INFLUX(XMDOTE,GM/SEC)= 0.000E-01 ENERGY INFLU X(QDOTE,CAL/SEC)= 0.000E-01 TE(K)= 5.450E+02 RHOE(G/CC)= 3.775E-04
 OFRE= 1.000E-16 FEXTNAL= 2.131E-04

I	SPECIES	MASS FRXN		MOLE FRXN		NET RATE	DADT(I)	ALPHA E(I)	ALPHA A(I)	ALPHA F(I)	#N
		(OVERALL)	(GAS/SOLID)	(OVERALL)	(GAS/SOLID)						
1	H2	8.1878E-04	8.1878E-04	1.1422E-02	1.1422E-02	8.9132E-09	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
2	O2	1.3138E-08	1.3138E-08	1.1547E-08	1.1547E-08	-1.7615E-13	0.0000E-01	5.9232E-18	7.2784E-03	6.0486E-04	0
3	HO	2.4462E-06	2.4462E-06	4.0450E-06	4.0450E-06	-7.8174E-10	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
4	O	1.2309E-09	1.2309E-09	2.1637E-09	2.1637E-09	3.4686E-13	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0

5	H	2.8957E-07	2.8957E-07	8.0794E-06	8.0794E-06	7.1564E-10	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
6	H2O	8.9099E-02	8.9099E-02	1.3909E-01	1.3909E-01	-6.9356E-09	0.0000E-01	5.9232E-18	3.4659E-18	4.0630E-03	0
7	CO2	1.7402E-01	1.7402E-01	1.1120E-01	1.1120E-01	5.2596E-09	0.0000E-01	2.9616E-04	3.4659E-18	4.3688E-03	0
8	H02	1.2989E-12	1.2989E-12	1.1067E-12	1.1067E-12	7.4088E-17	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
9	H2O2	8.2790E-12	8.2790E-12	6.8451E-12	6.8451E-12	1.7390E-15	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
10	CO	2.8257E-02	2.8257E-02	2.8371E-02	2.8371E-02	-1.4785E-09	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
11	CH4	4.4183E-06	4.4183E-06	7.7456E-06	7.7456E-06	-5.0353E-11	0.0000E-01	5.5678E-02	3.4659E-18	3.4538E-18	0
12	CH3	7.2404E-08	7.2404E-08	1.3544E-07	1.3544E-07	-4.3665E-13	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
13	CH2	4.4364E-10	4.4364E-10	8.8951E-10	8.8951E-10	2.2898E-16	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
14	CH	1.8367E-13	1.8367E-13	3.9677E-13	3.9677E-13	1.0359E-16	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
15	C2H4	1.1387E-07	1.1387E-07	1.1416E-07	1.1416E-07	2.3565E-13	0.0000E-01	5.9232E-04	3.4659E-18	3.4538E-18	0
16	C2H6	2.7235E-11	2.7235E-11	2.5473E-11	2.5473E-11	-8.1884E-17	0.0000E-01	1.1846E-03	3.4659E-18	3.4538E-18	0
17	C2H5	8.8055E-14	8.8055E-14	8.5214E-14	8.5214E-14	2.0181E-16	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
18	C2H3	8.8181E-10	8.8181E-10	9.1696E-10	9.1696E-10	1.4398E-12	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
19	C	3.2192E-15	3.2192E-15	7.5378E-15	7.5378E-15	-1.3191E-19	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
20	C2H2	6.7482E-04	6.7482E-04	7.2889E-04	7.2889E-04	-1.7024E-09	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
21	C2H	2.2954E-09	2.2954E-09	2.5791E-09	2.5791E-09	-1.8382E-11	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
22	CH2O	1.7660E-07	1.7660E-07	1.6541E-07	1.6541E-07	-1.7018E-12	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
23	CH3O	4.1467E-10	4.1467E-10	3.7578E-10	3.7578E-10	6.0569E-14	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
24	CHO	3.7013E-10	3.7013E-10	3.5872E-10	3.5872E-10	3.5608E-12	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
25	N	1.2724E-10	1.2724E-10	2.5546E-10	2.5546E-10	-1.9237E-14	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
26	NO	3.1890E-04	3.1890E-04	2.9888E-04	2.9888E-04	-1.3233E-09	0.0000E-01	5.9232E-18	3.4659E-18	2.0723E-05	1
27	N2	7.0552E-01	7.0552E-01	7.0824E-01	7.0824E-01	8.0486E-10	0.0000E-01	1.4808E-03	2.7381E-02	2.5462E-02	0
28	NO2	4.1376E-10	4.1376E-10	2.5293E-10	2.5293E-10	-5.2499E-15	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
29	N2O	2.2083E-07	2.2083E-07	1.4110E-07	1.4110E-07	-7.5483E-13	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	2
30	NH3	1.0597E-05	1.0597E-05	1.7498E-05	1.7498E-05	8.1976E-12	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
31	NH2	1.7130E-08	1.7130E-08	3.0066E-08	3.0066E-08	-9.0289E-13	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
32	NH	5.7293E-10	5.7293E-10	1.0731E-09	1.0731E-09	-6.7167E-15	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
33	HN2	2.2347E-10	2.2347E-10	2.1654E-10	2.1654E-10	2.0723E-14	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	2
34	N2H2	1.8161E-13	1.8161E-13	1.7007E-13	1.7007E-13	1.1739E-17	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	2
35	HNO	1.3829E-08	1.3829E-08	1.2540E-08	1.2540E-08	1.8633E-12	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
36	CN	5.8744E-10	5.8744E-10	6.3498E-10	6.3498E-10	-3.6227E-13	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
37	NCO	5.8887E-11	5.8887E-11	3.9414E-11	3.9414E-11	1.6740E-16	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
38	CHN	7.2557E-05	7.2557E-05	7.5503E-05	7.5503E-05	-2.9057E-10	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
39	HNCO	6.1498E-07	6.1498E-07	4.0198E-07	4.0198E-07	-2.2861E-12	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
40	HOCN	1.4924E-07	1.4924E-07	9.7547E-08	9.7547E-08	-8.9193E-13	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	1
41	SO2	1.2044E-03	1.2044E-03	5.2873E-04	5.2873E-04	-1.0982E-13	0.0000E-01	5.9232E-18	3.4659E-18	1.9023E-05	0
42	SO3	3.4057E-09	3.4057E-09	1.1963E-09	1.1963E-09	-4.7699E-15	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0
43	HSO3	6.8400E-12	6.8400E-12	2.3730E-12	2.3730E-12	1.1459E-13	0.0000E-01	5.9232E-18	3.4659E-18	3.4538E-18	0

MOLE FRACTION OF FIXED NITROGEN IN GAS PHASE = 3.927E-04

PLUG FLOW REACTOR (CONTINUED WITH SAME CHEMISTRY)

Step size increased at: x= 0.300E-07 dx= 0.600E-07
Step size increased at: x= 0.900E-07 dx= 0.120E-06
Step size increased at: x= 0.210E-06 dx= 0.240E-06
Step size increased at: x= 0.450E-06 dx= 0.480E-06
Step size increased at: x= 0.930E-06 dx= 0.960E-06
Step size increased at: x= 0.189E-05 dx= 0.192E-05
Step size reduced at: x= 0.381E-05 dx= 0.192E-05 ideqn= 2 delmax= 0.197E+00 qm= 0.208E-07 savea= 0.105E-07
restart at: x= 1.890E-06 dx= 9.600E-07
Step size reduced at: x= 0.285E-05 dx= 0.960E-06 ideqn= 2 delmax= 0.984E-01 qm= 0.156E-07 savea= 0.105E-07
restart at: x= 1.890E-06 dx= 4.800E-07
Step size increased at: x= 0.525E-05 dx= 0.960E-06
Step size increased at: x= 0.110E-04 dx= 0.192E-05

Step size increased at: x= 0.225E-04 dx= 0.384E-05
 Step size increased at: x= 0.456E-04 dx= 0.768E-05
 Step size increased at: x= 0.916E-04 dx= 0.154E-04
 Step size increased at: x= 0.168E-03 dx= 0.307E-04
 Step size increased at: x= 0.353E-03 dx= 0.614E-04
 Step size increased at: x= 0.721E-03 dx= 0.123E-03
 Step size reduced at: x= 0.170E-02 dx= 0.123E-03 ideqn= 12 delmax= 0.534E-01 qm= 0.292E-07 savea= 0.231E-07
 restart at: x= 1.582E-03 dx= 6.144E-05
 Step size increased at: x= 0.281E-02 dx= 0.123E-03
 Step size increased at: x= 0.392E-02 dx= 0.246E-03
 Step size increased at: x= 0.465E-02 dx= 0.492E-03
 Step size reduced at: x= 0.106E-01 dx= 0.492E-03 ideqn= 11 delmax= 0.506E-01 qm= 0.545E-07 savea= 0.729E-07
 restart at: x= 1.006E-02 dx= 2.458E-04
 Step size increased at: x= 0.174E-01 dx= 0.492E-03
 Step size increased at: x= 0.179E-01 dx= 0.800E-03

REACH MAX. at X= 2.403E-01

----- RXR NO. 3 : OVER-FIRED-AIR REACTOR -----

page 4

irxr= 3
 iprt= 413
 x= 0.240324E+00 cm
 dx= 0.800000E-03 cm
 p= 0.100000E+01 atm
 dpdx= 0.000000E+00 atm/cm
 tausr= 0.000000E+00 sec

TEMPERATURE(K) = 1582.37 ENTHALPY(CAL/G)=-2.847E+02 VELOCITY(CM/SEC)= 1.000E+00 CP(CAL/G-K) = 3.300E-01
 DENSITY(G/CC) = 2.212E-04 MOLE/GM-TOTAL = 3.481E-02 AREA(CM2) = 1.147E+00 H.T.(CAL/CC-S) = 0.000E-01

MASS INFLUX(XMDOTE,GM/SEC)= 0.000E-01 ENERGY INFLU X(QDOTE,CAL/SEC)= 0.000E-01 TE(K)= 3.000E+02 RHOE(G/CC)= 1.172E-03
 OFRE= 1.000E-16 FEXTNAL= 2.131E-04

I	SPECIES	MASS FRXN		MOLE FRXN		NET RATE	DADT(I)	ALPHA E(I)	ALPHA A(I)	ALPHA F(I)	#N
		(OVERALL)	(GAS/SOLID)	(OVERALL)	(GAS/SOLID)	(MOLE/CC-S)	(FRXN/S)				
1	H2	7.6378E-07	7.6378E-07	1.0883E-05	1.0883E-05	-2.2157E-09	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
2	O2	1.3980E-02	1.3980E-02	1.2550E-02	1.2550E-02	-2.7364E-09	0.0000E-01	7.2784E-03	7.2784E-03	6.0486E-04	0
3	HO	6.4511E-05	6.4511E-05	1.0896E-04	1.0896E-04	-9.9232E-09	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
4	O	1.2000E-06	1.2000E-06	2.1545E-06	2.1545E-06	1.7798E-09	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
5	H	8.7575E-09	8.7575E-09	2.4958E-07	2.4958E-07	1.7846E-10	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
6	H2O	8.2308E-02	8.2308E-02	1.3124E-01	1.3124E-01	7.0724E-09	0.0000E-01	3.4659E-18	3.4659E-18	4.0630E-03	0
7	CO2	1.8754E-01	1.8754E-01	1.2241E-01	1.2241E-01	6.6143E-09	0.0000E-01	3.4659E-18	3.4659E-18	4.3688E-03	0
8	HO2	4.5511E-08	4.5511E-08	3.9608E-08	3.9608E-08	4.1318E-12	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
9	H2O2	9.1762E-09	9.1762E-09	7.7494E-09	7.7494E-09	6.7735E-12	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
10	CO	3.1868E-05	3.1868E-05	3.2682E-05	3.2682E-05	-6.6143E-09	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
11	CH4	1.6043E-19	1.6043E-19	2.8727E-19	2.8727E-19	2.1815E-20	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
12	CH3	1.5035E-19	1.5035E-19	2.8727E-19	2.8727E-19	8.2708E-20	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
13	CH2	1.4027E-19	1.4027E-19	2.8727E-19	2.8727E-19	-1.8102E-18	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
14	CH	1.3019E-19	1.3019E-19	2.8727E-19	2.8727E-19	-1.0935E-17	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
15	C2H4	2.8054E-19	2.8054E-19	2.8727E-19	2.8727E-19	6.4037E-18	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
16	C2H6	3.0070E-19	3.0070E-19	2.8727E-19	2.8727E-19	-2.5264E-20	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
17	C2H5	2.9062E-19	2.9062E-19	2.8727E-19	2.8727E-19	-6.3746E-18	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
18	C2H3	2.7046E-19	2.7046E-19	2.8727E-19	2.8727E-19	-2.9618E-18	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
19	C	1.2011E-19	1.2011E-19	2.8727E-19	2.8727E-19	-2.8365E-19	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
20	C2H2	2.8737E-18	2.8737E-18	3.1705E-18	3.1705E-18	1.6262E-17	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
21	C2H	2.5030E-19	2.5030E-19	2.8727E-19	2.8727E-19	-1.3839E-17	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0

22	CH2O	1.5364E-16	1.5364E-16	1.4698E-16	1.4698E-16	7.6209E-19	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
23	CH3O	3.1035E-19	3.1035E-19	2.8727E-19	2.8727E-19	-5.4237E-19	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
24	CHO	1.3526E-14	1.3526E-14	1.3390E-14	1.3390E-14	1.1153E-15	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
25	N	2.2277E-13	2.2277E-13	4.5685E-13	4.5685E-13	-9.0862E-16	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
26	NO	1.7696E-04	1.7696E-04	1.6940E-04	1.6940E-04	-5.2994E-12	0.0000E-01	3.4659E-18	3.4659E-18	2.0723E-05	1
27	N2	7.1487E-01	7.1487E-01	7.3301E-01	7.3301E-01	4.0738E-12	0.0000E-01	2.7381E-02	2.7381E-02	2.5462E-02	0
28	NO2	2.7026E-07	2.7026E-07	1.6875E-07	1.6875E-07	6.2526E-12	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
29	N2O	6.8198E-08	6.8198E-08	4.4509E-08	4.4509E-08	-4.5728E-12	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	2
30	NH3	9.0927E-13	9.0927E-13	1.5336E-12	1.5336E-12	-3.5628E-16	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
31	NH2	4.5557E-14	4.5557E-14	8.1673E-14	8.1673E-14	-1.9933E-17	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
32	NH	9.2304E-14	9.2304E-14	1.7659E-13	1.7659E-13	-7.2510E-17	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
33	HN2	3.8499E-13	3.8499E-13	3.8105E-13	3.8105E-13	-2.0152E-16	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	2
34	N2H2	5.3791E-19	5.3791E-19	5.1454E-19	5.1454E-19	-4.1355E-22	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	2
35	HNO	2.9807E-10	2.9807E-10	2.7607E-10	2.7607E-10	4.6532E-14	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
36	CN	2.6019E-19	2.6019E-19	2.8727E-19	2.8727E-19	-4.5742E-18	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
37	NCO	1.8647E-16	1.8647E-16	1.2748E-16	1.2748E-16	1.2105E-18	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
38	CHN	6.2668E-17	6.2668E-17	6.6609E-17	6.6609E-17	4.0656E-18	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
39	HNCO	7.5775E-14	7.5775E-14	5.0591E-14	5.0591E-14	-1.1158E-17	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
40	HOCN	3.4898E-16	3.4898E-16	2.3299E-16	2.3299E-16	-2.8738E-20	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
41	SO2	1.0185E-03	1.0185E-03	4.5672E-04	4.5672E-04	9.4936E-11	0.0000E-01	3.4659E-18	3.4659E-18	1.9023E-05	0
42	SO3	5.7366E-06	5.7366E-06	2.0583E-06	2.0583E-06	-1.0861E-10	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
43	HSO3	2.1154E-10	2.1154E-10	7.4962E-11	7.4962E-11	1.3678E-11	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0

MOLE FRACTION OF FIXED NITROGEN IN GAS PHASE = 1.697E-04

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PLUG FLOW REACTOR (CONTINUED WITH SAME CHEMISTRY)

Step size increased at: x= 0.300E-07 dx= 0.600E-07
 Step size increased at: x= 0.900E-07 dx= 0.120E-06
 Step size increased at: x= 0.210E-06 dx= 0.240E-06
 Step size increased at: x= 0.450E-06 dx= 0.480E-06
 Step size increased at: x= 0.930E-06 dx= 0.960E-06
 Step size increased at: x= 0.189E-05 dx= 0.192E-05
 Step size increased at: x= 0.381E-05 dx= 0.384E-05
 Step size increased at: x= 0.765E-05 dx= 0.768E-05
 Step size increased at: x= 0.153E-04 dx= 0.154E-04
 Step size increased at: x= 0.307E-04 dx= 0.307E-04
 Step size increased at: x= 0.614E-04 dx= 0.614E-04
 Step size increased at: x= 0.123E-03 dx= 0.123E-03
 Step size increased at: x= 0.246E-03 dx= 0.246E-03
 Step size increased at: x= 0.491E-03 dx= 0.492E-03
 Step size increased at: x= 0.983E-03 dx= 0.983E-03
 Step size increased at: x= 0.197E-02 dx= 0.197E-02
 Step size increased at: x= 0.393E-02 dx= 0.393E-02
 Step size increased at: x= 0.786E-02 dx= 0.680E-02

REACH MAX. at X= 2.040E+00

10

irxr= 4
 iprt= 317
 x= 0.203987E+01 cm
 dx= 0.679600E-02 cm
 p= 0.100000E+01 atm

----- RXR NO. 4 : QUENCHING REACTOR -----

11
 page 5

dpdx= 0.000000E+00 atm/cm
tausr= 0.000000E+00 sec

TEMPERATURE(K) = 1045.78 ENTHALPY(CAL/G)=-4.562E+02 VELOCITY(CM/SEC)= 1.000E+00 CP(CAL/G-K) = 3.067E-01
DENSITY(G/CC) = 3.348E-04 MOLE/GM-TOTAL = 3.481E-02 AREA(CM2) = 7.581E-01 H.T.(CAL/CC-S) = 0.000E-01

MASS INFLUX(XMDOTE,GM/SEC)= 0.000E-01 ENERGY INFLU X(QDOTE,CAL/SEC)= 0.000E-01 TE(K)= 3.000E+02 RHOE(G/CC)= 1.172E-03
OFRE= 1.000E-16 FEXTNAL= 2.131E-04

I	SPECIES	MASS FRXN		MOLE FRXN		NET RATE	DADT(I)	ALPHA E(I)	ALPHA A(I)	ALPHA F(I)	#N
		(OVERALL)	(GAS/SOLID)	(OVERALL)	(GAS/SOLID)	(MOLE/CC-S)	(FRXN/S)				
1	H2	2.8199E-10	2.8199E-10	4.0185E-09	4.0185E-09	-1.2934E-13	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
2	O2	1.3983E-02	1.3983E-02	1.2553E-02	1.2553E-02	-1.9403E-11	0.0000E-01	7.2784E-03	7.2784E-03	6.0486E-04	0
3	HO	2.1818E-07	2.1818E-07	3.6853E-07	3.6853E-07	-3.5867E-11	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
4	O	2.1867E-10	2.1867E-10	3.9264E-10	3.9264E-10	1.0976E-12	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
5	H	8.7632E-14	8.7632E-14	2.4976E-12	2.4976E-12	8.2298E-17	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
6	H2O	8.2349E-02	8.2349E-02	1.3131E-01	1.3131E-01	8.1066E-12	0.0000E-01	3.4659E-18	3.4659E-18	4.0630E-03	0
7	CO2	1.8759E-01	1.8759E-01	1.2245E-01	1.2245E-01	3.0888E-13	0.0000E-01	3.4659E-18	3.4659E-18	4.3688E-03	0
8	HO2	4.7575E-10	4.7575E-10	4.1407E-10	4.1407E-10	-1.6343E-13	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
9	H2O2	3.7570E-10	3.7570E-10	3.1730E-10	3.1730E-10	2.6569E-14	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
10	CO	3.4278E-08	3.4278E-08	3.5156E-08	3.5156E-08	-3.0885E-13	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
11	CH4	2.7081E-18	2.7081E-18	4.8495E-18	4.8495E-18	1.4338E-21	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
12	CH3	1.5035E-19	1.5035E-19	2.8729E-19	2.8729E-19	3.0708E-20	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
13	CH2	1.4027E-19	1.4027E-19	2.8729E-19	2.8729E-19	-3.6165E-18	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
14	CH	1.3019E-19	1.3019E-19	2.8729E-19	2.8729E-19	-2.2136E-17	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
15	C2H4	2.2021E-18	2.2021E-18	2.2551E-18	2.2551E-18	4.9830E-19	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
16	C2H6	3.0070E-19	3.0070E-19	2.8729E-19	2.8729E-19	2.5900E-23	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
17	C2H5	2.9062E-19	2.9062E-19	2.8729E-19	2.8729E-19	-4.9527E-19	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
18	C2H3	2.7046E-19	2.7046E-19	2.8729E-19	2.8729E-19	-6.8713E-20	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
19	C	1.2011E-19	1.2011E-19	2.8729E-19	2.8729E-19	-4.3297E-19	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
20	C2H2	4.2154E-17	4.2154E-17	4.6510E-17	4.6510E-17	3.4629E-17	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
21	C2H	2.5030E-19	2.5030E-19	2.8729E-19	2.8729E-19	-3.5736E-17	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
22	CH2O	1.1276E-18	1.1276E-18	1.0789E-18	1.0789E-18	3.5572E-19	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
23	CH3O	3.1035E-19	3.1035E-19	2.8729E-19	2.8729E-19	-3.1585E-20	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
24	CHO	2.9019E-19	2.9019E-19	2.8729E-19	2.8729E-19	-3.0718E-18	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
25	N	8.1342E-19	8.1342E-19	1.6682E-18	1.6682E-18	7.3533E-20	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
26	NO	1.7588E-04	1.7588E-04	1.6838E-04	1.6838E-04	-1.9739E-11	0.0000E-01	3.4659E-18	3.4659E-18	2.0723E-05	1
27	N2	7.1487E-01	7.1487E-01	7.3305E-01	7.3305E-01	1.2383E-15	0.0000E-01	2.7381E-02	2.7381E-02	2.5462E-02	0
28	NO2	1.9422E-06	1.9422E-06	1.2127E-06	1.2127E-06	1.9739E-11	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
29	N2O	1.3481E-08	1.3481E-08	8.7987E-09	8.7987E-09	-1.2370E-15	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	2
30	NH3	2.6356E-17	2.6356E-17	4.4456E-17	4.4456E-17	1.2002E-20	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
31	NH2	1.6024E-19	1.6024E-19	2.8729E-19	2.8729E-19	-2.7057E-20	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
32	NH	1.5016E-19	1.5016E-19	2.8729E-19	2.8729E-19	-1.1808E-19	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
33	HN2	1.0742E-18	1.0742E-18	1.0632E-18	1.0632E-18	4.5271E-21	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	2
34	N2H2	3.0032E-19	3.0032E-19	2.8729E-19	2.8729E-19	-6.8170E-23	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	2
35	HNO	3.7031E-12	3.7031E-12	3.4300E-12	3.4300E-12	-2.4477E-17	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
36	CN	2.6019E-19	2.6019E-19	2.8729E-19	2.8729E-19	-4.6461E-18	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
37	NCO	4.2019E-19	4.2019E-19	2.8729E-19	2.8729E-19	2.5388E-18	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
38	CHN	3.7718E-17	3.7718E-17	4.0093E-17	4.0093E-17	3.1145E-18	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
39	HNCO	1.1774E-16	1.1774E-16	7.8616E-17	7.8616E-17	1.1796E-19	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
40	HOCN	4.6043E-17	4.6043E-17	3.0743E-17	3.0743E-17	6.6709E-24	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	1
41	SO2	1.0018E-03	1.0018E-03	4.4923E-04	4.4923E-04	-4.5696E-11	0.0000E-01	3.4659E-18	3.4659E-18	1.9023E-05	0
42	SO3	2.6675E-05	2.6675E-05	9.5715E-06	9.5715E-06	2.5674E-11	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0
43	HSO3	2.2646E-10	2.2646E-10	8.0253E-11	8.0253E-11	2.0022E-11	0.0000E-01	3.4659E-18	3.4659E-18	3.4538E-18	0

MOLE FRACTION OF FIXED NITROGEN IN GAS PHASE = 1.696E-04

Table 6.2. Description of output generated by the RBNOX code.

Index of Output Block	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
1			Case information
1a	OUTPUT FILE NAME		Name of output file specified by the user
1b	USER'S COMMENTS		User's comments on the case Note: A maximum of 10 lines and 78 characters per line can be used.
2			Initial conditions of Reactor #1
2a	irxr iprt x dx p dpdx tausr	 cm cm atm atm/cm sec	Reactor number Print station Current stream tube location where integration is being performed Note: Since the stream tube velocity is set to 1 cm/sec by the code, this variable becomes the reactor residence time (i.e., 1 cm = 1 sec). Step size Reactor pressure Reactor pressure gradient This option is not used by the code.
2b	TEMPERATURE ENTHALPY VELOCITY CP DENSITY MOLE/GM-TOTAL AREA H.T.	K cal/g cm/sec cal/g K g/cc mole/gm-total cm ² cal/cc sec	Temperature of reacting gases Enthalpy of reacting gases Velocity of the stream tube Heat capacity of reacting gases Density of reacting gases Mole number per gram of reacting gases Cross-sectional area of the stream tube This option is not used by the code.

Index of Output Block	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
2c	MASS INFLUX	xmdote,gm/sec	Mass influx introduced by the external stream
	ENERGY INFLUX	qdote,cal/sec	Energy influx introduced by the external stream
	TE	K	Temperature of the external stream Note: Actual value is shown later.
	RHOE	g/cc	Density of the external stream Note: Actual value is shown later.
	OFRE FEXTNAL		This option is not used by the code. Injection intensity of the external stream Note: This variable is used only for debugging purposes.
3			Species concentrations in Reactor #1
	I		Species index
	SPECIES		Species name
	MASS FRXN	fraction	Species mass fractions - Overall : overall species mass fractions, including any solid species Gas/solid: species mass fractions reported seperately for gaseous and solid phases Note: Since no solid-phase species are present, the mass fractions of "Overall" and "Gas/solid" remain the same.
	MOLE FRXN	fraction	Species mole fractions - The meaning is similar to "Species mass fractions" discussed above, except that the unit is in mole for this variable.
	NET RATE		Species formation rates
	DADT	fraction/sec	This option is not used by the code.
	ALPHA E	mole/g	Compositions of reburn fuel or over fire air (OFA) Note: A small number in the order of 10^{-18} is assigned to all species which are not included in the reburn or OFA jets.
	ALPHA A ALPHA F #N	mole/g mole/g moles	Compositions of air Compositions of flue gas leaving burner zones Mole number of nitrogen atom in species I
3a	MOLE FRACTION OF FIXED NITROGEN	fraction	Molar concentration of the total fixed nitrogen (TFN) species (including all species that the value of variable "#N" in Output Block 3 is not zero)
4			Numerical information

Index of Output Block	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
4a			Step size was doubled from 0.240e-06 to 0.48e-06 at $x = 0.450 \text{ e-06}$.
4b			Step size was reduced by half from 0.307e-04 to 1.536e-05 at $x = 0.921\text{e-04}$. Variable of "idenqn" is the species index that caused the reduction of the step size by half. In the current case, species #3 is "HO". Note: Variables of "delmax", "qm", and "savea" are printed out only for debugging purposes. User can ignore them.
4c	REACH MAX. at X= 2.405e-01		The integration reaches the reactor residence time specified by the user. Note: The value of X shown is equivalent to time in second.
5			Thermodynamics and species concentrations at the exit of Reactor #1 Note: Meanings of all variables shown below are similar to those defined in Output Blocks 2 and 3.
6	PLUG FLOW REACTOR		Starts kinetics calculations in Reactor #2 Note: All reaction mechanisms are the same as listed in the input file. The user is not allowed to change the chemical kinetics mechanisms. Initial conditions of Reactor #2 are actually the exit conditions of Reactor #1.
7			Thermodynamics and species concentrations at the exit of Reactor #2 Note: Meanings of all variables shown below are similar to those defined in Output Blocks 2 and 3.
8	PLUG FLOW REACTOR		Starts kinetics calculations in Reactor #3 Note: All reaction mechanisms are the same as listed in the input file. The user is not allowed to change the chemical kinetics mechanisms. Initial conditions of Reactor #3 are actually the exit conditions of Reactor #2.
9			Thermodynamics and species concentrations at the exit of Reactor #3 Note: Meanings of all variables shown below are similar to those defined in Output Blocks 2 and 3.
10	PLUG FLOW REACTOR		Starts kinetics calculations in Reactor #4 Note: All reaction mechanisms are the same as listed in the input file. The user is not allowed to change the chemical kinetics mechanisms. Initial conditions of Reactor #4 are actually the exit conditions of Reactor #3.
11			Thermodynamics and species concentrations at the exit of Reactor #4 Note: Meanings of all variables shown below are similar to those defined in Output Blocks 2 and 3.
12	MOLE FRACTION OF FIXED NITROGEN IN GAS PHASE		Final TFN concentration in unit of mole fraction Note: This value times 10^6 is the TFN concentration in unit of ppm.

6.3 Outputs from the BPM Code

The BPM code generates screen display and a file called BPOTcsvs.lll as outputs. The following two sub-sections discuss these outputs.

Screen Display

The screen display generated by the execution of the BPM code is an exact copy of the output file BPOTcsvs.lll, which is written as a computer disk file. The user is suggested to refer to the next sub-section to interpret the screen messages shown. Since the execution time of the BPM code normally only lasts several minutes and the screen display is quite informative, the user may realize that it is difficult to comprehend the information displayed. This screen display may be good only to indicate the status of the BPM code execution.

File BPOTcsvs.lll

This is the file which contains the boiler steam- and gas-side performance predictions, and is most likely to be dealt with by the user. Listing 6.3 is an example indicating the contents of this output file. The description of this output file follows the same format as shown for the 2DHT code outputs. The outputs shown in the Listing are grouped into "blocks" of information and each block is labeled by a numeral. Table 6.3 is a corresponding table to interpret the contents of the Listing. To interpret a block of the output information, the user may refer to Table 6.3 and locate the description for that block by matching the "Index of Output Block" with the numeral shown in Listing 6.3. Table 6.3 then shows the user the variable names, units, and the physical meanings of the variables for that block. If the outputs contain the same information that was repeated for every reactor, the labeling shown in Listing 6.3 uses the output blocks of the first reactor.

Listing 6.3. Output generated by the BPM code.

OUTPUTS FROM BOILER PERFORMANCE MODEL (BPM)

Output File Name: BPOT0201.075

1

2

UNITS:

Temperature (T): K Heat Flux (Q): KJ/S Deposit thickness : M
Mass Flow : KG/S Work/power : KW Thermal conductivity: KW/M/K
Heat capacity : KJ/KG/K Enthalpy(H) : KJ/KG H.T. coefficient : KW/M2/K

STEAM/GAS PROPERTIES:

Sec.	Tg,in	Tg,out	Ts,in	Hs,in	Ts,out	Hs,out	Qsteam	Qw.wall	Qgas	Steam Fl.	Qg.loss	Qsteam,t
2	480.73	1490.17	522.60	1080.58	604.84	2659.50	63139.98	63139.98	63457.26	47.00	317.25	50.23
6	1490.17	1197.37	664.05	3008.59	813.15	3449.10	21954.66	0.00	22788.68	49.84	0.00	17.47
11	1197.37	951.00	613.15	3122.71	776.78	3478.27	15315.01	2987.77	18394.74	43.07	91.97	12.18
4	951.00	679.97	604.84	2659.50	672.14	3040.01	17884.22	1160.85	19140.75	47.00	95.70	14.23
1	679.97	567.14	489.15	922.91	522.60	1080.58	7410.50	129.18	7577.57	47.00	37.89	5.90
SUM							125704.37	67417.77	131359.00		542.85	100.00

ENERGY BALANCE:

Section	Qg,in	Qg,out	Qs,in	Qs,out	Qw.wall	Qloss	Qsum
6	85097.56	62308.89	149947.14	171901.81	0.00	0.00	834.00
11	62308.89	43914.15	134504.11	149819.12	2987.77	91.97	-0.02
4	43914.15	24773.40	124996.33	142880.55	1160.85	95.70	-0.02
1	24773.40	17195.83	43376.93	50787.44	129.18	37.89	0.00

AIR PREHEATER:

Section	Tg,in	Tg,out	Ta,in	Ta,out	Qg,in	Qg,out	Qa,in	Qa,out	Qsum
12	567.14	549.82	338.00	359.25	17195.83	16053.28	2138.11	3280.66	0.00

ATTEMPERATION:

SECTION	A.	M. FL.	Max. Temp	Ta,in	Ta,out	Qa,in	Qa,out	Ta,w	Qa,w	Qsum
6		2.840	813.150	674.131	664.051	143230.266	155643.531	489.150	2620.765	-9792.5010

MASS FLOW RATES:

Flue Gas Mass Flow (KG/S): 57.849
Air Flow into Air Preheater (KG/S): 52.570

FOULING AND SLAGGING:

Section	Dep. Thickness	Dep. Conductivity	Tot. H.T. Coefficient	Dep. Temp.
11	0.0029	0.0004	0.0334	786.498
4	0.0048	0.0004	0.0351	733.255
1	0.0035	0.0003	0.0369	564.733

BOILER HEAT BALANCE:

Flux to lower furn. walls	63457. kW	Flux absorb. by SH cycle	114667. kW
Flux to conv. sections	67902. kW	Flux absorb. by RH cycle	15315. kW
Wall heat losses	-543. kW		
Flux transferred to W/S	130816. kW	Flux received by W/S	129982. kW

Cross Check on W/S Heat Balance	
Flux out of SH	171902. kW
Flux out of RH	149819. kW
Flux into ECO	-43377. kW
Flux into RH	-134504. kW
Flux into attemperators	-2621. kW
Flux received by W/S	141219. kW
ERROR OF W/S HEAT BALANCE	-11237. kW
REL. ERR. OF W/S BALANCE	-8.6450 %

ITERB= 1 Error of boil. heat balance: -10403. kW
 Rel. error of heat balance: -7.9524 %
 Net Boiler Efficiency: 92.2645 %
 Gross Boiler Efficiency: 86.0518 %

UNITS:

Temperature (T): K	Heat Flux (Q): KJ/S	Deposit thickness: M
Mass Flow: KG/S	Work/power: KW	Thermal conductivity: KW/M/K
Heat capacity: KJ/KG/K	Enthalpy(H): KJ/KG	H.T. coefficient: KW/M2/K

STEAM/GAS PROPERTIES:

Sec.	Tg,in	Tg,out	Ts,in	Hs,in	Ts,out	Hs,out	Qsteam	Qw.wall	Qgas	Steam Fl.	Qg.loss	Qsteam, %
2	480.73	1490.17	525.76	1096.15	604.84	2659.50	63139.98	63139.98	63457.26	43.09	317.29	49.92
6	1490.17	1197.37	653.34	2948.61	813.15	3449.10	22840.79	0.00	22788.68	45.64	0.00	18.06
11	1197.37	953.20	609.94	3115.72	793.15	3514.09	15154.40	2985.03	18234.33	38.04	91.17	11.98
4	953.20	682.35	604.84	2659.50	681.60	3074.42	17878.88	1164.18	19138.79	43.09	95.69	14.14
1	682.35	568.75	489.15	922.91	525.76	1096.15	7464.85	130.10	7633.13	43.09	38.17	5.90
SUM							126478.90	67419.29	131252.19		542.32	100.00

ENERGY BALANCE:

Section	Qg,in	Qg,out	Qs,in	Qs,out	Qw.wall	Qloss	Qsum
6	85097.56	62308.89	134567.83	157408.62	0.00	0.00	-52.12
11	62308.89	44074.56	118526.69	133681.09	2985.03	91.17	3.72
4	44074.56	24935.77	114596.03	132474.92	1164.18	95.69	0.02
1	24935.77	17302.63	39767.77	47232.62	130.10	38.17	0.01

AIR PREHEATER:

Section	Tg,in	Tg,out	Ta,in	Ta,out	Qg,in	Qg,out	Qa,in	Qa,out	Qsum
12	568.75	551.32	338.00	359.40	17302.63	16152.01	2138.11	3288.73	0.00

ATTEMPERATION:

SECTION	A. M. FL.	Max. Temp	Ta,in	Ta,out	Qa,in	Qa,out	Ta,w	Qa,w	Qsum
6	2.548	813.150	681.450	653.337	132452.875	134261.000	489.150	2351.830	543.7053
11	0.130	793.150	613.150	609.941	118385.742	118555.977	489.150	120.198	-50.0368

MASS FLOW RATES:

Flue Gas Mass Flow (KG/S):	57.349
Air Flow into Air Preheater (KG/S):	52.570

FOULING AND SLAGGING:

Section	Dep. Thickness	Dep. Conductivity	Tot. H.T. Coefficient	Dep. Temp.
11	0.0029	0.0004	0.0335	790.849
4	0.0048	0.0004	0.0352	735.622
1	0.0035	0.0003	0.0369	566.266

BOILER HEAT BALANCE:

Flux to lower furn. walls	63457. kW	Flux absorb. by SH cycle	115604. kW
Flux to conv. sections	67795. kW	Flux absorb. by RH cycle	15154. kW
Wall heat losses	-542. kW		
Flux transferred to W/S	130710. kW	Flux received by W/S	130758. kW

Cross Check on W/S Heat Balance	
Flux out of SH	157409. kW
Flux out of RH	133681. kW
Flux into ECO	-39768. kW
Flux into RH	-118406. kW
Flux into attemperators	-2472. kW
Flux received by W/S	130443. kW
ERROR OF W/S HEAT BALANCE	315. kW
REL. ERR. OF W/S BALANCE	0.2407 %

ITERB= 2 Error of boil. heat balance: 266. kW
 Rel. error of heat balance: 0.2038 %
 Net Boiler Efficiency: 92.8154 %
 Gross Boiler Efficiency: 86.5656 %

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UNITS:

Temperature (T): K Heat Flux (Q): KJ/S Deposit thickness : M
 Mass Flow : KG/S Work/power : KW Thermal conductivity: KW/M/K
 Heat capacity : KJ/KG/K Enthalpy(H) : KJ/KG H.T. coefficient : KW/M2/K

STEAM/GAS PROPERTIES:

Sec.	Tg,in	Tg,out	Ts,in	Hs,in	Ts,out	Hs,out	Qsteam	Qw.wall	Qgas	Steam Fl.	Qg.loss	Qsteam, %
2	480.73	1490.17	525.73	1096.02	604.84	2659.50	63139.98	63139.98	63457.26	43.12	317.29	49.94
6	1490.17	1197.37	653.73	2950.86	813.15	3449.10	22790.05	0.00	22788.68	45.74	0.00	18.03
11	1197.37	953.25	610.62	3117.19	793.15	3514.09	15153.65	2985.19	18231.07	38.18	91.16	11.99
4	953.25	682.33	604.84	2659.50	681.54	3074.21	17883.29	1164.27	19143.26	43.12	95.72	14.14
1	682.33	568.74	489.15	922.91	525.73	1096.02	7464.57	130.08	7632.80	43.12	38.16	5.90
SUM							126431.54	67419.51	131253.08		542.32	100.00

ENERGY BALANCE:

Section	Qg,in	Qg,out	Qs,in	Qs,out	Qw.wall	Qloss	Qsum
6	85097.56	62308.89	134976.23	157766.28	0.00	0.00	-1.37
11	62308.89	44077.81	119015.63	134169.28	2985.19	91.16	1.08
4	44077.81	24934.56	114681.60	132564.89	1164.27	95.72	-0.02
1	24934.56	17301.76	39797.46	47262.03	130.08	38.16	-0.01

AIR PREHEATER:

Section	Tg,in	Tg,out	Ta,in	Ta,out	Qg,in	Qg,out	Qa,in	Qa,out	Qsum
12	568.74	551.31	338.00	359.39	17301.76	16151.20	2138.11	3288.66	0.00

ATTEMPERATION:

SECTION	A. M. FL.	Max. Temp	Ta,in	Ta,out	Qa,in	Qa,out	Ta,w	Qa,w	Qsum
6	2.620	813.150	681.534	653.732	132564.578	134968.203	489.150	2417.838	14.2134
11	0.098	793.150	613.150	610.616	118918.836	119024.023	489.150	90.859	-14.3288

MASS FLOW RATES:

Flue Gas Mass Flow (KG/S): 57.849
 Air Flow into Air Preheater (KG/S): 52.570

FOULING AND SLAGGING:

Section	Dep. Thickness	Dep. Conductivity	Tot. H.T. Coefficient	Dep. Temp.
11	0.0029	0.0004	0.0335	791.020
4	0.0048	0.0004	0.0352	735.620
1	0.0035	0.0003	0.0369	566.252

BOILER HEAT BALANCE:

Flux to lower furn. walls	63457. kW	Flux absorb. by SH cycle	115557. kW
Flux to conv. sections	67796. kW	Flux absorb. by RH cycle	15154. kW
Wall heat losses	-542. kW		
Flux transferred to W/S	130711. kW	Flux received by W/S	130711. kW

Cross Check on W/S Heat Balance
 Flux out of SH 157766. kW
 Flux out of RH 134169. kW
 Flux into ECO -39797. kW
 Flux into RH -118925. kW
 Flux into attemperators -2509. kW
 Flux received by W/S 130705. kW
 ERROR OF W/S HEAT BALANCE 6. kW
 REL. ERR. OF W/S BALANCE 0.0049 %

ITERB= 3 Error of boil. heat balance: 6. kW
 Rel. error of heat balance : 0.0047 %
 Net Boiler Efficiency : 92.7819 %
 Gross Boiler Efficiency : 86.5343 %

=====

UNITS:

Temperature (T): K Heat Flux (Q): KJ/S Deposit thickness : M
 Mass Flow : KG/S Work/power : KW Thermal conductivity: KW/M/K
 Heat capacity : KJ/KG/K Enthalpy(H) : KJ/KG H.T. coefficient : KW/M2/K

STEAM/GAS PROPERTIES:

Sec.	Tg,in	Tg,out	Ts,in	Hs,in	Ts,out	Hs,out	Qsteam	Qw.wall	Qgas	Steam Fl.	Qg.loss	Qsteam, %
2	480.73	1490.17	525.73	1096.02	604.84	2659.50	63139.98	63139.98	63457.26	43.12	317.29	49.94
6	1490.17	1197.37	653.74	2950.91	813.15	3449.10	22788.75	0.00	22788.68	45.74	0.00	18.02
11	1197.37	953.24	610.61	3117.18	793.15	3514.09	15154.72	2985.19	18231.14	38.18	91.16	11.99
4	953.24	682.33	604.84	2659.50	681.54	3074.21	17883.25	1164.27	19143.20	43.12	95.72	14.14
1	682.33	568.74	489.15	922.91	525.73	1096.02	7464.56	130.08	7632.79	43.12	38.16	5.90
SUM							126431.27	67419.51	131253.08		542.32	100.00

ENERGY BALANCE:

Section	Qg,in	Qg,out	Qs,in	Qs,out	Qw.wall	Qloss	Qsum
6	85097.56	62308.89	134984.23	157772.98	0.00	0.00	-0.07
11	62308.89	44077.75	119019.73	134174.45	2985.19	91.16	0.07
4	44077.75	24934.55	114681.50	132564.75	1164.27	95.72	-0.03
1	24934.55	17301.76	39797.43	47261.98	130.08	38.16	-0.01

AIR PREHEATER:

Section	Tg,in	Tg,out	Ta,in	Ta,out	Qg,in	Qg,out	Qa,in	Qa,out	Qsum
12	568.74	551.31	338.00	359.39	17301.76	16151.20	2138.11	3288.66	0.00

ATTEMPERATION:

SECTION	A.	M. FL.	Max. Temp	Ta,in	Ta,out	Qa,in	Qa,out	Ta,w	Qa,w	Qsum
6		2.622	813.150	681.536	653.740	132564.750	134983.984	489.150	2419.667	0.4321
11		0.096	793.150	613.150	610.610	118930.742	119020.133	489.150	88.700	-0.6908

MASS FLOW RATES:

Flue Gas Mass Flow (KG/S):	57.849
Air Flow into Air Preheater (KG/S):	52.570

FOULING AND SLAGGING:

Section	Dep. Thickness	Dep. Conductivity	Tot. H.T. Coefficient	Dep. Temp.
11	0.0029	0.0004	0.0335	791.018
4	0.0048	0.0004	0.0352	735.620
1	0.0035	0.0003	0.0369	566.252

BOILER HEAT BALANCE:

Flux to lower furn. walls	63457. kW	Flux absorb. by SH cycle	115556. kW
Flux to conv. sections	67796. kW	Flux absorb. by RH cycle	15155. kW
Wall heat losses	-542. kW		
Flux transferred to W/S	130711. kW	Flux received W/S	130711. kW

Cross Check on W/S Heat Balance	
Flux out of SH	157773. kW
Flux out of RH	134174. kW
Flux into ECO	-39797. kW
Flux into RH	-118931. kW
Flux into attemperators	-2508. kW
Flux received by W/S	130711. kW
ERROR OF W/S HEAT BALANCE	0. kW
REL. ERR. OF W/S BALANCE	0.0001 %

ITERB= 4	Error of boil. heat balance:	0. kW
	Rel. error of heat balance :	0.0001 %
	Net Boiler Efficiency :	92.7817 %
	Gross Boiler Efficiency :	86.5342 %

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UNITS:

Temperature (T): K	Heat Flux (Q): KJ/S	Deposit thickness : M
Mass Flow : KG/S	Work/power : KW	Thermal conductivity: KW/M/K
Heat capacity : KJ/KG/K	Enthalpy(H) : KJ/KG	H.T. coefficient : KW/M2/K

STEAM/GAS PROPERTIES:

Sec.	Tg,in	Tg,out	Ts,in	Hs,in	Ts,out	Hs,out	Qsteam	Qw.wall	Qgas	Steam Fl.	Qg.loss	Qsteam, %
2	480.73	1490.17	525.73	1096.02	604.84	2659.50	63139.98	63139.98	63457.26	43.12	317.29	49.94
6	1490.17	1197.37	653.74	2950.91	813.15	3449.10	22788.71	0.00	22788.68	45.74	0.00	18.02
11	1197.37	953.24	610.61	3117.18	793.15	3514.09	15154.79	2985.19	18231.15	38.18	91.16	11.99
4	953.24	682.33	604.84	2659.50	681.54	3074.21	17883.23	1164.27	19143.19	43.12	95.72	14.14
1	682.33	568.74	489.15	922.91	525.73	1096.02	7464.56	130.08	7632.79	43.12	38.16	5.90
SUM							126431.27	67419.51	131253.08		542.32	100.00

ENERGY BALANCE:

Section	Qg,in	Qg,out	Qs,in	Qs,out	Qw.wall	Qloss	Qsum
6	85097.56	62308.89	134984.42	157773.14	0.00	0.00	-0.04
11	62308.89	44077.73	119019.67	134174.47	2985.19	91.16	0.01
4	44077.73	24934.55	114681.48	132564.72	1164.27	95.72	-0.03
1	24934.55	17301.75	39797.42	47261.98	130.08	38.16	-0.01

AIR PREHEATER:

Section	Tg,in	Tg,out	Ta,in	Ta,out	Qg,in	Qg,out	Qa,in	Qa,out	Qsum
12	568.74	551.31	338.00	359.39	17301.75	16151.20	2138.11	3288.66	0.00

ATTEMPERATION:

SECTION	A.	M. FL.	Max. Temp	Ta,in	Ta,out	Qa,in	Qa,out	Ta,w	Qa,w	Qsum
6		2.622	813.150	681.536	653.741	132564.719	134984.422	489.150	2419.711	0.0081
11		0.096	793.150	613.150	610.609	118931.062	119019.687	489.150	88.609	-0.0164

MASS FLOW RATES:

Flue Gas Mass Flow (KG/S):	57.849
Air Flow into Air Preheater (KG/S):	52.570

FOULING AND SLAGGING:

Section	Dep. Thickness	Dep. Conductivity	Tot. H.T. Coefficient	Dep. Temp.
11	0.0029	0.0004	0.0335	791.018

4	0.0048	0.0004	0.0352	735.620
1	0.0035	0.0003	0.0369	566.252

BOILER HEAT BALANCE:

Flux to lower furn. walls	63457. kW	Flux absorb. by SH cycle	115556. kW
Flux to conv. sections	67796. kW	Flux absorb. by RH cycle	15155. kW
Wall heat losses	-542. kW		
Flux transferred to W/S	130711. kW	Flux received by W/S	130711. kW

Cross Check on W/S Heat Balance

Flux out of SH	157773. kW
Flux out of RH	134174. kW
Flux into ECO	-39797. kW
Flux into RH	-118931. kW
Flux into attemperators	-2508. kW
Flux received by W/S	130711. kW
ERROR OF W/S HEAT BALANCE	0. kW
REL. ERR. OF W/S BALANCE	0.0000 %

ITERB= 5 Error of boil. heat balance: 0. kW
Rel. error of heat balance : 0.0000 %
Net Boiler Efficiency : 92.7817 %
Gross Boiler Efficiency : 86.5342 %

THIS IS TYPE 2 BOILER CONFIGURATION

Table 6.3. Description of output generated by the BPM code.

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
1	1,2	Boiler Output File Name:		User-specified output file name
2	1,2			Generic boiler schematics Left: Type 1 boiler (one pass) Right: Type 2 boiler (two passes)
3	1	UNITS		Units for physical properties used in the code
4	1	STEAM/GAS PROPERTIES		Properties of boiler heat transfer sections Note: Air preheater section is discussed in Block 6.
		Sec.		Sequence index according to steam/water flow path Note: Only existing sections are assigned with indices.
		Tg,in	K	Temperature of flue gas entering the section
		Tg,out	K	Temperature of flue gas leaving the section Note: For Type 1 boiler, the gas inlet and outlet temperatures of two triflux sections (S/W indices 6 and 10) remain the same.
		Ts,in	K	Temperature of steam/water entering the section
		Hs,in	kJ/kg	Enthalpy of steam/water entering the section
		Ts,out	K	Temperature of steam/water leaving the section
		Hs,out	kJ/kg	Enthalpy of steam/water leaving the section
		Qsteam	kW	Heat absorbed by steam/water in the section
		Qw,wall	kW	Heat absorbed by water walls surrounding the section
		Qgas	kW	Heat transferred from flue gas to water walls, steam/water heat exchangers in the gas path, and losses to the atmosphere
		Steam Fl.	kg/s	Steam/water flow rates through the section
		Qg,loss	kW	Heat lost through walls surrounding the section
		Qsteam,%	%	Heat absorption relative to total heat absorbed by both furnace water walls and heat exchangers in the gas path

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
		(Qsteam)	kW	Sum of Qsteam in each section Note: Heat absorbed by water walls surrounding the heat exchanger sections is not included.
		(Qw,wall)	kW	Sum of heat absorbed by furnace water walls, and by water walls surrounding the heat exchanger sections
		(Qgas)	kW	Sum of heat fluxes transferred from flue gas to water walls, steam/water heat exchangers in the gas path, and losses to the atmosphere
		(Qg,loss)	kW	Sum of heat lost through furnace water walls and water walls surrounding the heat exchanger sections
		(Qsteam,%)	%	Sum of relative heat absorptions by various sections Note: Total must be 100 %.
5	1	ENERGY BALANCE		Detailed check of steam and gas side energy balances Note: Furnace and air preheater sections are not included.
		Section		Sequence index according to steam/water flow path Note: Only existing sections are assigned with indices.
		Qg,in	kW	Sensible heat of flue gas entering the section
		Qg,out	kW	Sensible heat of flue gas leaving the section
		Qs,in	kW	Heat carried by steam/water entering the section
		Qs,out	kW	Heat carried by steam/water leaving the section
		Qw,wall	kW	Heat absorbed by water walls surrounding the section
		Qloss	kW	Heat lost to the atmosphere through water walls surrounding the section
		Qsum	kW	Difference between heat released from flue gas, and sum of heat absorbed by steam/water and heat lost to the atmosphere Note: Values other than zero indicate violations of the sectional heat balance. Round-off errors within ± 1 kW can be tolerated. Large errors indicate unrealistic set-up of some model parameters.

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
6	1	AIR PREHEATER		Gas and air side heat balances of air preheater
		Section	-	Sequence index according to steam/water flow path Note: Only existing sections are assigned with indices.
		Tg,in	K	Temperature of flue gas entering air preheater
		Tg,out	K	Temperature of flue gas leaving air preheater
		Ta,in	K	Temperature of air entering air preheater
		Ta,out	K	Temperature of air leaving air preheater
		Qg,in	kW	Sensible heat of flue gas entering air preheater
		Qg,out	kW	Sensible heat of flue gas leaving air preheater
		Qa,in	kW	Sensible heat of air entering air preheater
		Qa,out	kW	Sensible heat of air leaving air preheater
		Qsum	kW	Differences between heat released from flue gas and heat absorbed by air Note: Air leakage is not considered in the BPM code.

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
7	1	ATTEMPER- ATION		Detailed check of attemperator heat balance
		Section	-	Attemperator sequence index Note: Output is made only when attemperation flows are greater than zero.
		A. M. FL.	kg/s	Attemperation (Spray) mass flow rate
		Max. Temp	K	Maximum steam outlet temperature allowed for the heat exchanger section following the attemperator (i.e., User-specified attemperator control temperature)
		Ta,in	K	Steam temperature before addition of spray water
		Ta,out	K	Steam temperature after addition of spray water
		Qa,in	kW	Steam heat flux before entering attemperator
		Qa,out	kW	Steam heat flux leaving attemperator (i.e., after addition of spray water)
		Ta,w	K	Attemperator spray-water temperature
		Qa,w	kW	Heat gained by attemperation spray-water from superheated steam
		Qsum	kW	Difference between heat gained by attemperator and heat lost from superheated steam Note: Values larger than zero indicate violation of attemperator heat balance. This is normally due to incomplete convergence. If values greater than 1 kW persist, some model parameters may be unrealistic.
8	1	MASS FLOW RATES		
		Flue Gas Mass Flow	kg/s	Mass flow rate of flue gas through the boiler
		Air Flow into Air Preheater	kg/s	Mass flow rate of total air into air preheater

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
9	1	FOULING AND SLAGGING		Properties related to slagging and fouling of heat exchanger sections
		Section		Sequence index according to steam/water flow path Note: Air preheater and boiler sections where heat fluxes are calculated by the 2DHT code are not included in the display.
		Dep. Thickness	m	User-specified deposit thickness of the section
		Dep. Conductivity	kW/m/K	Thermal conductivity of deposit layers (either calculated by the BPM code or specified by the user)
		Tot. H.T. Coefficient	kW/M ² /K	Overall heat transfer coefficient from gas to steam/water
		Dep. Temp.	K	Gas side deposit surface temperatures
10	1	BOILER HEAT BALANCE		
		Flux to lower furn. walls	kW	Heat flux to furnace water walls (usually obtained from a 2DHT run)
		Flux to conv. sections	kW	Heat flux to convective sections including water walls surrounding heat exchanger sections
		Wall heat losses	kW	Heat lost through furnace walls and other water wall sections (negative sign)
		Flux transferred to W/S	kW	Net total heat excluding the wall heat losses transferred from flue gas to steam/water
		Flux absorb. by SH cycle	kW	Sum of heat fluxes received by SH cycle
		Flux absorb by RH cycle	kW	Sum of heat fluxes received by RH cycle
		Flux received by W/S	kW	Total heat fluxes received by steam/water cycle

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
11	1	Cross Check on W/S Heat Balance		
		Flux out of SH	kW	Heat flux carried by steam leaving last superheater section
		Flux out of RH	kW	Heat flux carried by steam leaving last reheater section
		Flux into ECO	kW	Heat flux of feedwater entering economizer (negative sign)
		Flux into RH	kW	Heat flux of cold reheat water entering first reheater section (negative sign)
		Flux into attemperators	kW	Heat flux of spray water entering attemperator (negative sign)
		Flux received by W/S	kW	Total heat fluxes received by steam/water (i.e., summation of the above positive and negative fluxes in the current block)
		Error of W/S HEAT BALANCE	kW	Difference of heat absorptions between values of "Flux received by W/S" reported in Blocks 10 and 11.
		REL. ERR. OF W/S BALANCE	%	Heat balance error relative to value of "Flux received by W/S" reported in Block 10
12	1			Errors of boiler heat balance
		ITERB		Iteration number of boiler heat balances
		Error of boil. heat balance	kW	Difference between values of "Flux transferred to W/S" reported in Block 10 and "Flux received by W/S" reported in Block 11
		Rel. error of heat balance	%	Error of boiler heat balance relative to the value of "Flux transferred to W/S" reported in Block 10 Note: Errors of the boiler heat balance are due to incomplete convergence and round-off errors. If errors larger than several kW's persist, set-up of model parameters may be incorrect.
13	1			Boiler efficiencies
		Net Boiler Efficiency	%	Net boiler efficiency defined as percentage ratio of steam/water heat absorptions to fuel heat input based on the lower heating value
		Gross Boiler Efficiency	%	Gross boiler efficiency defined as percentage ratio of steam/water heat absorptions to fuel heat input based on the upper heating value

Index of Output Block	Output Levels	Name of Output Variable or Block	Physical Dimension	Description of Output Block or Output Variable
14	1,2			Major performance predictions displayed in a configured boiler diagram
				Boiler type Heat exchanger section names S/W sequence indices for existing sections Indices for attemperators in service Feedwater inlet mass flow rate Final superheat mass flow rate Cold-reheat inlet mass flow rate Final reheat mass flow rate Lower furnace gas exit temperatures Economizer gas exit temperature Air preheater gas exit temperature

Chapter 7

7.0 REFERENCES

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**PREDICTIVE MODELLING
OF BOILER FOULING**

**SPONSORED BY:
U.S. DEPARTMENT OF ENERGY
PITTSBURGH ENERGY TECHNOLOGY CENTER**

ECONOMIC IMPACT OF FOULING ON POWER GENERATION

IMPROVED FOULING CONTROL

- **WILL REDUCE THE ESTIMATED HUNDREDS OF MILLIONS OF DOLLARS TO OPERATING COSTS**
- **WILL ALLOW UTILITIES MUCH MORE FLEXIBILITY IN THEIR SELECTION OF COALS**
- **WILL REDUCE THE EMISSION OF ACID RAIN PRECURSORS, NO_x, SO_x, AS WELL AS CO₂.**
- **1% DECREASE IN HEAT RATE = \$1 MILLION PER YEAR - SAVINGS \$3 MILLION PER YEAR**

NATIONAL CONTEXT ~\$400 MILLION PER YEAR

**FOULING: A COMPLEX INTERACTION OF GAS FLOW,
MINERAL TRANSPORT AND ADHESION
MECHANISMS**

**CENTRAL MODEL STRUCTURE - AN ADEQUATE
DESCRIPTION OF GAS FLOW FIELD IN THE VICINITY OF THE
HEAT EXCHANGER STRUCTURE INCLUDING MINERAL
TRANSPORT BEHAVIOR, NUCLEATION, CONDENSATION AND
AGGLOMERATION**

**PRIMARY OBJECTIVE OF THIS EFFORT IS THE
DEVELOPMENT OF A COMPREHENSIVE NUMERICAL MODEL
DESCRIBING THE TIME EVOLUTION OF FOULING UNDER
REALISTIC HEAT EXCHANGER CONDITIONS**

L5558

Figure 1 Representative Qualitative Flow Field Vectors and Isotherms with Fouled Tubes

- **SPATIAL EVOLUTION OF GAS STOICHIOMETRY AND GAS AND MINERAL TEMPERATURE NON-UNIFORM ON ENTRY INTO THE HEAT EXCHANGER TUBE BUNDLES**

- **MECHANISMS OF MINERAL SPECIES EVOLUTION FROM COAL**

- **MECHANISMS OF PARTICLE TRANSPORT TO DEPOSIT SURFACES**

- **MECHANISMS OF ADHERENCE AND REMOVAL OF PARTICLES TRANSPORTED TO DEPOSIT SURFACES**

- **MECHANISMS OF GROSS DETACHMENT (SPALLING) OF PREVIOUSLY BUILT UP DEPOSITS**

- **PARTICLE TRANSPORT MECHANISMS (SIZE)**

INERTIAL IMPACTION ($>10\mu$)

TURBULENT EDDY DIFFUSION ($0.1\mu - 5\mu$)

BROWNIAN DIFFUSION ($0.1\mu - 0.05\mu$)

THERMOPHORESIS ($\sim 0.5\mu$)

- **SMOOTH VS ROUGH TUBE SURFACES**

CHAOTIC DEPOSIT DEVELOPMENT

- **BALANCE OF ADHERENCE VS REMOVAL
FORCES - LOWER MELTING INORGANIC COMPOUNDS
(NA) CONTENT AND FORMATION OF GLUE-ASSISTED
PARTICLE CAPTURE MECHANISMS**

- **DIFFUSIVE BONDING OR SINTERING OF DEPOSITED
PARTICLES**

DESCRIPTION OF THE FLOW AND TURBULENCE FIELD IN A DEEP TUBE BANK

- **QUALITATIVE AT BEST PRESENTLY VIA k - ϵ TYPE MODELS**
- **COHERENT STRUCTURES - ENERGY SPECTRUM**
- **RANGE OF SCALES IN A TURBULENT FLOW SCALE WITH $Re^{3/4}$ (1-D)**
- **LARGE EDDY SIMULATION (LES) VS DES**
 - a) **LARGE EDDIES INTERACT STRONGLY WITH MEAN FLOW**
 - b) **TRANSPORT PROCESSES ARE DUE TO LARGE EDDIES**
 - c) **LARGE EDDY STRUCTURE STRONGLY INFLUENCED BY THE GEOMETRY AND NATURE OF FLOW**
 - d) **LARGE EDDY APPROXIMATE CONVECTIVE TIME SCALE**

- **COMPUTATIONAL REQUIREMENTS OF DES**

$$N \approx (6RE_M)^{9/4} \text{ E.G. } N \approx 5 \times 10^{10} \text{ AND}$$

$$K\Delta T = 2 \times 10^3 \text{ FOR } RE = 10^4$$

- **LES REQUIRES EXISTENCE OF INERTIAL SUBRANGE**

- **SIMULATION OF WALL BOUNDED FLOWS**

$$N \simeq 0.06 \text{ } RE_M^2$$

- **SPECTRAL/ITERATIVE METHODS FOR LES TRANSFORM ALGORITHMS**

- **PRACTICAL IMPLEMENTATION OF SPECTRAL TECHNIQUES IN COMPLICATED GEOMETRIES - COST AND FLEXIBILITY**

DEVELOPMENT OF GLOBAL SPECTRAL ELEMENTS

FILTERED FORM OF THE TRANSPORT EQUATIONS

NATURE AND STRUCTURE OF SUB-GRID MODELS

INHOMOGENEOUS FLOWS AND SAMPLE VOLUME

DESCRIPTION OF PHYSICOCHEMICAL PROCESSES IN DEEP TUBE BANKS

- **SULFATE SALT DEPOSITION VIA CLASSICAL VAPOUR
DIFFUSION - DESCRIPTION OF NUCLEATION/
AGGLOMERATION**
- **PARTICLE TRANSPORT MECHANISMS INCLUDING
INERTIAL IMPACTION, EDDY DIFFUSION, THERMO/
ELECTRO PHORETIC DIFFUSION, BROWNIAN
DIFFUSION, ETC.**
- **TYPICAL SIZE RANGE IN A BOILER
0.1 μ - 40 μ**
- **ALGORITHMIC CONSIDERATIONS REGARDING THE
STRUCTURE OF COMPREHENSIVE FOULING MODEL**

**MATHEMATICAL TRACTABILITY VS PHYSICAL
REALISM**

**DEVELOPMENT OF A GENERAL MULTI-PHASE
MULTI-SPECIES TRANSPORT ALGORITHM
FOR FOULING**

CURRENT EFFORT: MULTI-YEAR, LOGICALLY STRUCTURED EVOLUTION

- **LES OF SINGLE PHASE, NON-ISOTHERMAL FLOW
CHARACTERISTICS IN A TUBE BUNDLE**
- **MULTI-SPECIES, MULTI-PHASE TRANSPORT IN A
PASSIVE GAS AEROTHERMAL FIELD**
- **DEPOSITION (ADHERENCE VS REMOVAL) SUB-MODULE
DEVELOPMENT**
- **COUPLING OF MS, MP TRANSPORT AND DEPOSITION
MODELS WITH LES OF FLOW AND HEAT TRANSFER IN A
TUBE BUNDLE**
- **DEVELOPMENT OF REALISTIC ENGINEERING
CORRELATIONS**

Task 2 - Parameter Variation Studies and Development of Engineering Correlations

b) Description of realistic approach conditions (including temporal variation) into the tube bank.

c) Derivation of realistic engineering correlations regarding fouling from above refined predictions.

Task 3 - Management and Reporting

d) Program management and reporting

Figure 2.3 displays the relevant schedule.

1.5 STATEMENT OF WORK

ARL will perform the following tasks in order to accomplish the objectives and goals of the project.

PHASE I

Task 1

Perform semi-quantitative evaluations of solution and algorithmic details of HLS techniques applicable to flow in and around a tube bundle.

Task 2

Assess (quantitatively) HLS predictions for flow and turbulence characteristics of related, simpler problems.

Task 3

Reformulate the algorithm to predict flow details around a cylinder in an isothermal, but otherwise representative environment.

Task 4

Predict heat transfer characteristics for the problem in Task 3.

Task 5

Generalize the algorithm to predict flow, turbulence and heat transfer details for multi-tube configurations including in-line and staggered arrangements.

Task 6

Provide project management and financial control with the required technical and financial reports and documentation.

PHASE II

Task 1

Develop an appropriate multi-phase, multi-specie transport algorithm for a "frozen" gas aerothermal field.

Task 2

Develop sub-modules for surface related processes including adherence and removal.

Task 3

Provide project management and financial control with the required technical and financial reports and documentation.

PHASE III

Task 1

Extend the algorithm to couple multi-species, multi-phase transport and deposition models with a comprehensive HLS of flow and heat transfer in a tube bundle for a representative case.

Task 2

Perform pertinent parameter variation studies and develop improved engineering correlations to model fouling in practical boiler configurations and operating environments.

Task 3

Provide project management and financial control with the required technical and financial reports and documentation.

- iib) Deposition (adherence vs removal) sub-module development.
- iiia) Coupling of multi-species, multi-phase transport and deposition models with a comprehensive higher level simulation of flow and heat transfer in a tube bundle for an idealized case.
- iiib) Description of realistic engineering correlations regarding fouling from above refined predictions.

The multi-year nature of the effort is clearly evident in the above breakdown. It is readily seen that the first year's activity is designed to provide comprehensive description of the flow details (including heat transfer) in a tube bundle in the absence of complicating issues like particle and multi-species transport to the surface. Work planned in later years systematically introduces computational modules for the various physicochemical processes involved, to finally arrive at a comprehensive model that can yield engineering predictions for the fouling process. A detailed description comprising the various sub/tasks involved in accomplishing this Phase I objective is now provided.

1.4.1 Task Description of Phase I and Schedule

Phase I - Higher Level Simulation of Single Phase, Non-Isothermal Flow Characteristics in a Tube Bundle

Tasks

1. Semi-quantitative evaluation of various solution and algorithm details of HLS techniques applicable to flow in a tube bundle.
2. Detailed quantitative assessment of HLS predictions concerning flow and turbulence characteristics of related, simpler problems.
3. Algorithm reformulation to predict flow details around a single cylinder in an isothermal, but otherwise representative environment.

4. Prediction of heat transfer characteristics for the problem outlined in 3.
5. Generalization of the algorithm to predict flow, turbulence and heat transfer details for multi-tube configurations including in-line and staggered arrangements.
6. Program management, reporting and documentation.

A brief, qualitative description is now provided to delineate the nature and extent of the activities involved in this phase. Figure 2.1 displays the schedule for executing the tasks discussed below.

Task 1 - Semi-Quantitative Evaluation of Various Solution and
Algorithmic Details of HLS Techniques Applicable to Flow in a Tube Bundle

As HLS applications in the past have concentrated on resolving the turbulence details of semi-idealized, geometrically simple flow problems including flat plate, channel flow, flow between Taylor cylinders, applications involving configurational and physical complexity comparable to those in typical tube banks are rare. Hence, this task is designed to critically evaluate the computational and algorithm requirements of HLS such that adequate resolution of the flow and turbulence characteristics can be obtained for use in the description of the various physicochemical processes involved. As such this task delineates the critical accuracy bounds for the fluid mechanics description, as well as establishing comparable criteria for the remaining module development effort. It also provides for a greater insight into the physical and mathematical nature of the dominant transport mechanisms.

PHASE 1
HIGHER LEVEL SIMULATION OF SINGLE PHASE, NON-ISOTHERMAL
FLOW CHARACTERISTICS IN A TUBE BUNDLE

P1840

△ DENOTES MILESTONE

Figure 2.1 Proposed Work Schedule for Phase I

PHASE 2
DEVELOPMENT AND INTEGRATION OF MODULES FOR FLOW
AND VARIOUS COMPONENT PHYSICOCHEMICAL PROCESS DETAILS
INCLUDING DEPOSITION FOR A MULTI-TUBE CONFIGURATION

P1168

△ DENOTES MILESTONE

Figure 2.2 Proposed Work Schedule for Phase II

PHASE 3
COMPREHENSIVE PREDICTIONS OF PRACTICAL BOILER FOULING

P1169

△ DENOTES MILESTONE

Figure 2.3 Proposed Work Schedule for Phase III

PROGRESS TO DATE

- **DETAILED PROJECT WORK PLAN HAS BEEN PREPARED AND SUBMITTED FOR PETC'S APPROVAL**
- **SEMI-QUANTITATIVE EVALUATIONS OF APPLICABLE SOLUTION METHODOLOGIES (LES) HAS BEEN COMPLETED**
- **QUANTITATIVE ASSESSMENT OF LES OF RELATED, SIMPLER PROBLEMS HAS BEEN COMPLETED**
- **ALGORITHM REFORMUALTION AND APPLICATION TO PREDICT FLOW, TURBULENCE AND HEAT TRANSFER DETAILS AROUND SINGLE AND MULTI CYLINDER TUBE BANKS CURRENTLY IN PROGRESS**
- **VISITS TO YALE, STANFORD AND PRINCETON**
- **NEKTON SPECTRAL ELEMENT CODE**
- **RNG TECHNIQUES TO MODEL SUB GRID SCALE EFFECTS**

SPECTRAL ELEMENT METHOD

- **NEKTON - SOLVER FOR UNSTEADY NAVIER STOKES AND ENERGY EQUATIONS VIA THE SPECTRAL ELEMENT METHOD**
- **SPECTRAL ELEMENT - A HIGH ORDER FINITE ELEMENT METHOD (LOCAL ISOPARAMETRIC MAPPINGS, VARIATIONAL FORMULATION) EMPLOYING HIGH-ORDER POLYNOMIAL EXPANSIONS USING TENSOR-PRODUCT LAGRANGIAN INTERPOLANTS THROUGH LEGENDRE COLLOCATION POINTS**
- **HIGH ACCURACY WITH RELATIVELY FEW GRID POINTS DUE TO HIGH ORDER INTERPOLATION, AUTOMATIC CLUSTERING, MINIMAL NUMERICAL DIFFUSION AND DISPERSION**
- **GENERAL, ARBITRARY GEOMETRY TREATMENT VIA MACRO-ELEMENT DOMAIN DECOMPOSITION**
- **EFFICIENT, ADVANCED PRE-CONDITIONED ITERATIVE INVERSION PROCEDURES REQUIRING MINIMAL STORAGE**
- **GENERAL FRAMEWORK TO INCORPORATE A WIDE RANGE OF COMPLEX PHYSICAL PHENOMENA, E.G. TURBULENCE VIA RNG PROCEDURES**

A comparison of the Nusselt number (heat transfer rate) predicted by NEKTON (solid symbols) with experimental results (open symbols). Here Nu is the Nusselt number, Re is the Reynolds number, and Pr is the Prandtl number.

Instantaneous Streamlines for Flow Past a Cylinder

BPM 3.0

BOILER PERFORMANCE MODELING SOFTWARE

developed for the

PITTSBURGH ENERGY TECHNOLOGY CENTER

by

**Burns and Roe Company
Energy Systems Technology Division**

HISTORY OF BPM

- Initially developed by Burns and Roe in 1983 to support boiler specialist.
- First uses considered conversion of oil-design units to coal firing.
- DOE funded additional development to add flexibility needed to analyze performance of alternate fuels.
- DOE provided further funding to facilitate use by non-experts for screening purposes. (Includes 4 typical sample models.)
- Used in numerous PETC studies regarding alternate coal-derived fuels and acid rain control.
- Release 2.0 now available through NESC at Oak Ridge.
- Release 3.0 being presented here and submitted to NESC.

USES OF BPM

- Predict performance of an existing boiler with different fuel.
- Predict performance after boiler modification.
- Design modifications for fuel conversion (e.g., switch to low sulfur fuel).
- Review of manufacturer's design for new boilers.
- Efficiency calculation and optimization.

CAPABILITIES OF BPM 3.0

- FUELS -

- Oil.
- Natural Gas.
- Coal (including coal derived fuels such as CWS).

CAPABILITIES OF BPM 3.0 - BOILER CONFIGURATIONS -

- Wall-fired.
- Tilting tangential burners.
- Division walls.
- Radiant steam-cooled surfaces.
- Subcritical or supercritical pressure.
- Drum or once-through.
- Separate module for analyzing PSU industrial-type boiler.

CAPABILITIES OF BPM 3.0

- CONVECTIVE PASS CONFIGURATIONS -

- Single reheat, double reheat or no reheat.
- Attemperator, gas recirculation, split back-pass or burner tilt steam temperature control.
- Radiant/convective upper furnace heat transfer surfaces.

BPM PERFORMANCE PREDICTIONS

- Boiler efficiency.
- Fuel burn rate.
- Fuel slagging characteristics.
- Furnace exit gas temperature.
- Steam temperature profile.
- Gas temperature profile.
- Gas flow rate.
- Gas velocity profile.
- Air preheating requirements.
- Includes intelligent Results Analyzer.

OUTLINE OF CALCULATION SEQUENCE

- Heat-to-steam.
- Combustion/Boiler Efficiency calculation.
- Furnace performance.
- Convective pass performance (includes upper furnace).
- Air heater performance.

Heat to Steam Calculation

Combustion/Boiler Efficiency Calculation

Lower Furnace Calculation

Convective Pass Calculation

Air Heater Calculation