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The Hydrogen Burn - Equipment Response Algorithm (HYBER)

Users Guide

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Abstract

The users guide for the Hydrogen Burn Survival algorithm, HYBER, is provided in this report. HYBER (Hydrogen Burn—Equipment Response) is comprised of two self-contained computer programs, DATGEN and SOLVER. These computer codes may be used to estimate the thermal response of safety-related equipment exposed to hydrogen combustion in nuclear reactor containments. The state and composition of the combustion gases are obtained by modeling single or multiple deflagrations in mixtures of hydrogen, steam, carbon monoxide, and air.

This users manual describes the interactive generation of the input data files using DATGEN and discusses the execution of SOLVER. Special usage of the algorithm on IBM Personal Computer (PC) and IBM compatible computer systems is also described. Illustrative examples, including the input data files, are provided to demonstrate some of the capabilities of the algorithm.

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Acknowledgements

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Executive Summary

During a degraded core accident in a nuclear power plant, hydrogen may be released from the reactor system into the containment building. If enough hydrogen accumulates and is ignited, the resulting pressures could be high enough to breach the containment allowing the release of radioactive materials into the environment. Furthermore, the hydrogen burn might produce temperatures inside the building that are high enough to threaten the operation of equipment needed to mitigate the effects of the degraded core accident and return the plant to a safe shutdown condition. To limit the effects of hydrogen burns, many reactor power plants now include deliberate ignition systems to ignite the hydrogen intentionally at low hydrogen concentrations so that the resulting pressures will not pose a threat to the containment. As part of the reactor licensing process, the Nuclear Regulatory Commission requires licensees to provide analyses which show that certain systems and components be able to function during and following hydrogen burning. To support the NRC review of licensee submittals, an equipment survival algorithm named HYBER (Hydrogen Burn—Equipment Response) has been developed as a part of the Hydrogen Burn Survival program at Sandia National Laboratories, Albuquerque, NM.

HYBER is comprised of two self-contained computer programs, DATGEN and SOLVER, developed on the VAX 11/780 and CRAY-1 computers for use on IBM PC and IBM compatible computer systems. These computer codes allow the user to estimate the thermal response of safety-related equipment subject to a combustion and post-combustion gas environment. The environment gas state and composition are obtained by modeling single or multiple hydrogen–carbon monoxide–air combustion processes.

The users guide for the HYBER is provided in this report. The interactive generation of the input data files, using DATGEN, and the execution of SOLVER are discussed. Special usage of the algorithm on IBM PC and IBM compatible systems, using a procedure file named RUN.BAT, is also described. Illustrative examples are provided to demonstrate some of the capabilities of the algorithm. The input files for these examples are included for the users' reference. A companion report, the reference manual to HYBER, describes the theoretical basis for the models used in the HYBER [3].

1 Introduction

One of the potential consequences of a degraded core accident in a nuclear power plant is the generation and release of hydrogen into the reactor containment building. In some accident scenarios, the hydrogen concentration reaches combustible, even detonable, levels. If such a mixture is ignited, the resulting gas pressure could compromise the ability of the reactor building to prevent release of radioactive materials. Furthermore, the high gas temperatures could damage equipment necessary to return the reactor power plant to a safe condition. Evidence indicates that during the March 1978 accident at Three Mile Island Unit II (TMI-2), a hydrogen burn event occurred [1]. The resulting overpressure (28 psig) did not breach the containment, but the containment environment reached temperatures great enough to char and melt some materials [2].

As a result of the increased concern over the possibility of the occurence of hydrogen burns severe enough to threaten containment integrity, deliberate ignition systems have been installed in some reactors . These systems consist of arrays of glow plugs or spark plugs distributed throughout the containment building. In the event of an accident, the system can be activated so that hydrogen which is released will be ignited at low concentrations (less than 10%), resulting in low-energy deflagrations that are less threatening to the containment integrity. This scheme reduces the probability of containment breach but presents the potential of exposing safety-related equipment to repeated hydrogen burns and their attendant thermal environments.

At present, experimental programs and computational studies are being used to predict combustion-induced thermal environments and the effects of such environments on safety-related equipment. The Hydrogen Burn Survival (HBS) Program at Sandia National Laboratories, Albuquerque, NM, (SNLA) was initiated as part of an NRC effort to investigate the survivability of safety-related equipment in either inadvertant or deliberate hydrogen burns. The overall objective of the HBS program is to develop an understanding of (1) the hydrogen burn environment, (2) the applicable heat transfer mechanisms in the burn environment, and (3) the response of equipment exposed to the burn environment. A specific goal is to provide the NRC an independent means to estimate equipment survivability and evaluate analyses submitted by applicants for nuclear power plant licenses. In response to this goal, a set of computer programs, collectively named HYBER, has been developed. HYBER, also referred to herein as

the "algorithm", provides estimates of the thermal environment due to hydrogen deflagrations and the resulting thermal responses of safety-related components. HYBER consists of two programs, DATGEN and SOLVER, which were developed on the VAX 11/780 and CRAY-1 for use on the IBM PC or IBM compatible computer systems employing FORTRAN 77. DATGEN and SOLVER are self-contained, i.e., require no external libraries. DATGEN generates input data files for SOLVER through interactive prompting to the user, and SOLVER performs all calculations to simulate the thermal environment and associated equipment responses. Note that the algorithm can be used for simulating small scale combustion vessel experiments or large scale reactor analyses. However, the users guide is written towards reactor applications.

This report provides documentation for the use of HYBER. A general description of the algorithm and several examples to illustrate the use and capabilities of the codes are included. A procedure file to execute the algorithm on IBM or IBM compatible PC systems is also described. Detailed information for the generation of input files by DATGEN for SOLVER and a source listing of DATGEN and SOLVER (Appendix G) are provided. Details on the models used in SOLVER are given in the algorithm reference manual [3].

To learn how to use HYBER, the user should read in a cursory manner Sections 2 through 6 to get an impression of the features present in the algorithm and carefully study the example problem in Appendix C. The user should then execute HYBER using Appendix C as a guide and duplicating the files in Appendix D when responding to the prompts of DATGEN. Repeating the four cases in Appendix D will demonstrate the capabilities of HYBER. After finishing the four cases, the user may need to re-read Sections 2 through 6 and the reference manual to clarify any remaining questions.

2 General Description of the Algorithm

The algorithm simulates transient heat transfer resulting from single or multiple hydrogen deflagrations in a single-volume combustion vessel. Multiple deflagration scenarios are simulated in HYBER as a series of single deflagrations. HYBER is re-started for each new deflagration using the final gas conditions of the previous deflagration as the initial conditions for the next burn. A deflagration can be simulated as an adiabatic, isochoric, instantaneous energy release or as an energy release to the gas such that the temperature increases at a constant rate. The former simulation allows energy exchange to occur between the combustion products and the vessel and equipment surfaces after the instantaneous energy release, but in the latter simulation, energy exchange is allowed to occur during the combustion period (the length of which is user specified) as well as after combustion. Both models, however, assume that each deflagration is global, i.e., the deflagration occurs uniformly throughout the entire volume of the vessel being considered.

Heat transfer between the hot gas, containment walls, and equipment surface(s) is simulated using models for thermal radiation, convection, steam condensation, and conduction in equipment and containment walls. The radiation model includes surface-to-surface, gas-to-surface, and gas-to-gas radiative energy interchange. The algorithm includes two models to simulate forced convection and two models to simulate condensation on vessel and equipment surfaces. The user selects the models most appropriate for each application. The environment is assumed to be spatially uniform in pressure, temperature, and gas species. In addition, all heat transfer processes are assumed to be independent (non-coupled) and quasi-steady. These assumptions allow a global energy balance to be performed for each time step permitting calculation of the transient values of gas pressure, temperature, and species concentrations.

HYBER also has three engineering models that the user can specify to tailor the algorithm for a specific application. These models include: 1) water-spray cooling, 2) gas flow between upper and lower compartments in ice-condenser pressurized water reactors (PWR), and 3) gas leakage from the containment. A detailed description of these models and all heat and mass transfer models included in the algorithm are presented in the reference manual [3].

The algorithm, in general, operates in two steps. First, appropriate input data files are generated by DATGEN. These files are created through interactive

prompting from DATGEN to the user. Second, SOLVER uses the input files to perform calculations that simulate combustion and post-combustion phenomena. The output files written by SOLVER can be used to continue a simulation such as in a multiple burn sequence. The following section discusses, in detail, step 1 of this procedure. input data file generation.

3 DATGEN

A flow diagram of the data generator is shown in Figure 1. The numbered boxes in this figure will be referred to during the following descriptions of the options of DATGEN available to the user. The flow diagram shows the three basic paths that a user may take when using DATGEN:

1. For the first deflagration of a multiple burn simulation where all data needs to be generated, the path would follow boxes 1-18.

2. For a single burn simulation where all data needs to be generated, the path would follow boxes 1,2,4-18.

3. Often, the user may wish to perform additional simulations using the same containment geometry while changing some options in the heat transfer section (boxes 10-12) or in the combustion section (boxes 14-16). This is referred to as the re-start option and includes both (1) the re-executing of a single burn simulation or the first burn of a multiple burn simulation and (2) the executing of subsequent burns of a continuing multiple burn simulation. Note that re-start for (1) requires only prior containment geometry data while (2) requires prior geometry data as well as heat transfer and engineering systems options.

When the last path is utilized, the re-starts involve interactive prompting from DATGEN to the user. The following features for this option are noteworthy.

- For a single burn re-start, changing an option in the combustion section would require the path to follow boxes 1,2,4,20-22,14-18. The information in boxes 6-13, is read in by DATGEN from the data file for the previous burn simulation. To change options in both the combustion and heat transfer sections, the path would follow boxes 1,2 4,20,21,10-18. The information in boxes 6-9 is written to the new data file for use in SOLVER.

- For a first deflagration of a new multiple burn re-start, the path would follow boxes 1-4,20-22,14-18 to change options only in the combustion section. To change options in both the combustion and heat transfer sections, the path would follow boxes 1-4,20,21,10-18. For the former case, DATGEN read previously generated data for boxes 6-13 and writes this information to the new data file. In the latter case, data for boxes 6-9 are written to the new data file.

- For any re-start after the first deflagration in a multiple burn simulation, the user cannot change the heat transfer options and must follow boxes 1-3,19,23,14-18.

The data generator is organized into several parts. The following sub-sections discuss these different parts as they occur in the code. In the following sections, the user must enter all information in SI units unless otherwise directed by the data generator.

3.1 Preliminary Input

In the Preliminary Input section, the user is prompted for the information shown in boxes 1-5, 19a, and 20a which specify the type of burn simulation. The user is first prompted to enter the time of day and date that the data files are being generated and a title for the simulation (box 1). Second, DATGEN prompts the user to enter the type of burn sequence (single or multiple) to be simulated (box 2). If a single burn is to be considered, the user is offered the option of using geometry and radiative factors from a previous simulation (i.e., re-start for single burn) for the current simulation (box 4). Otherwise, if a multiple burn sequence is to be simulated, DATGEN asks if this is the first deflagration of the sequence (box 3). If this is the first deflagration, then the user is offered the option of using a previously created geometry (box 4). The final prompts for this section are to input the start time and duration of the simulation (box 5, 19a, 20a).

3.2 Containment Geometry Input

After entering the preliminary input, the user must input the dimensions of the containment in which the burn is to be simulated. The user is instructed to enter the containment volume, total surface area, equivalent containment diameter, and number of surfaces comprising the containment walls and components inside the containment (box 6). The number of surfaces is limited to three.

3.3 Thermophysical Properties and Surface Characteristics

Thermophysical properties of the vessel walls and equipment are constant during a simulation. Therefore, the selection of values for these properties must

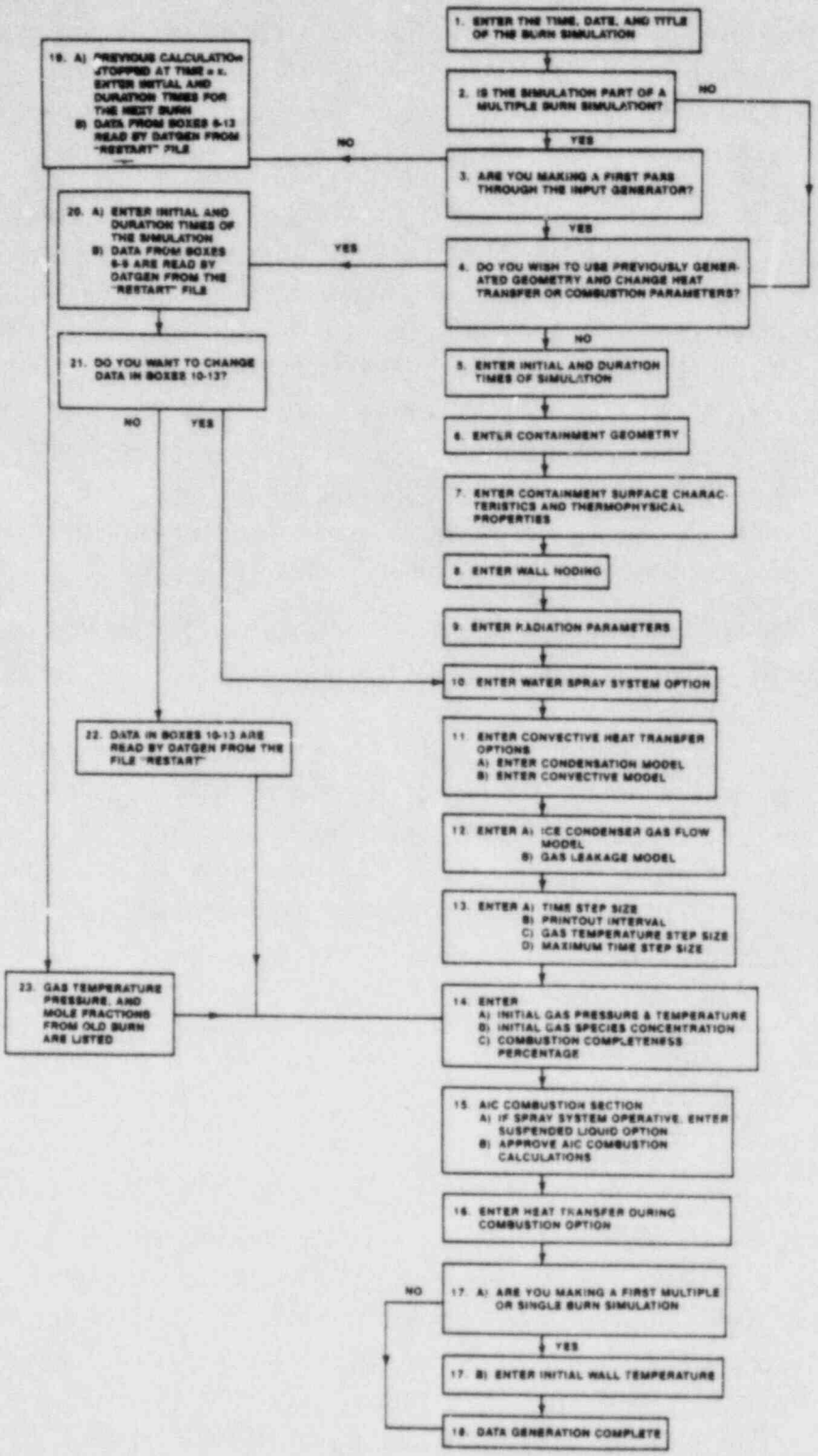

Figure 1. DATGEN flow diagram.

be done with caution and foresight. All properties should be chosen at some average temperature expected for a given simulation. All prompts for the properties listed below will be repeated for each surface if more than one surface has been specified by the user. A table listing sample thermophysical property data is found in Appendix A.

The data generator first prompts the user for the surface area, characteristic length, thermal emissivity of the surface, and the number of materials (3 or less) comprising the wall or equipment. The characteristic length is a physical dimension of the surface that is appropriate for use in convective heat transfer models. The emissivity of each surface must be less than unity since the radiation model will fail if the emissivity is equal to or greater than unity. To simulate heat conduction, each wall or piece of equipment is modeled as a one-dimensional slab (which may have up to 3 layers of different materials) with an insulated back surface. For each material, the user is prompted to enter the material thermal diffusivity, thermal conductivity, and thickness (box 7).

The user next specifies the nodalization for each slab to be used in the conduction model (box 8). When a multi-material (composite) slab is specified, the nodalization for each material must be uniform, i.e., the nodes are equally spaced. The user is prompted for the number of nodes in each material comprising the slab. For a slab comprised of one material, the mesh is divided into two regions; a fine, uniformly-spaced mesh for the front portion of the slab and a coarser, uniformly-spaced mesh for the back portion. The user inputs (1) the fraction of the slab thickness to be represented by a coarse mesh (from the back to the front of the slab), (2) the number of coarse mesh nodes, and, (3) the number of fine mesh nodes. Two options are available in DATGEN for this latter case:

1. Specifying zeros for these three parameters ("0,0,0"), directs the code to internally compute a default slab nodalization based on the slab thickness and thermal diffusivity.

2. If the user specifies the nodalization to be used rather than using default values, thought must be given to the nature of the simulation and the slab material properties. For example, a material with a high thermal diffusivity needs only a coarse mesh to adequately resolve the temperature gradient in the material. However, a material with a low thermal diffusivity may require a relatively fine mesh near the front surface to resolve the temperature changes in the material.

DATGEN writes the nodal arrangement to the screen and asks the user user if the nodalization is satisfactory. If not, the user can start the process over again.

Upon completion of a suitable nodal arrangement in each slab, the user can

specify that the temperatures of various nodal locations are to be written to an output file for the simulation. The user is prompted to specify the number of nodes for which the temperatures (up to 5) are to be saved and the node number(s) representing the spatial location(s).

3.4 Radiative Parameters

In this section, the user is prompted to enter all beam lengths and configuration factors for each surface. The beam lengths must be in units of meters, and the configuration factors are dimensionless (box 9).

The specified beam lengths must obey reciprocity, i.e., the beam length from surface i to surface j must equal the beam length from surface j to surface i. DATGEN checks for reciprocity, indicates if an error exists, and prompts the user to input the correct values. Reciprocity must also hold for the configuration factors, i.e., $A_i F_{i-j} = A_j F_{j-i}$, where A_i, A_j are the surface areas of surface i and surface j and F_{i-j}, F_{j-i} are the configuration factors from surfaces i to j and j to i, respectively. The configuration factors for each surface must also sum to unity, e.g., $F_{1-1} + F_{1-2} + F_{1-3} = 1$. If an error exists in the configuration factor input, the code will prompt the user to enter the correct data.

Methods to compute beam lengths and configuration factors are given in Appendix B; additional descriptions of these concepts are provided in [3].

3.5 Heat Transfer and Engineering System Options

Included in this section are prompts to select heat transfer models and engineering systems to be used in the simulation. Details of the specific prompts are discussed as they occur in DATGEN, shown in boxes 10-12.

3.5.1 Water Spray System

The user is prompted to specify whether or not the water spray system is operative (box 10). If the spray system is operative, the user must enter the distance that the spray droplets fall, that is the distance from the spray nozzle(s) to the base of the vessel, as well as a spatial increment for the fall distance. The spatial increment should be approximately one one-hundredth of the fall distance

and the fall distance must be evenly divisible by the spatial increment. The spray model calculates the amount of heat lost by the gas to the spray droplets by numerically integrating the ordinary differential equation which governs the evaporation rate of the falling droplets [3]. The user is then prompted to enter the flow rate from the spray nozzles (in gallons per minute), the number of drop sizes exiting the nozzles, and the diameter of each drop size in microns. The user can enter up to three drop sizes. Each drop size will comprise a fraction of the total flow rate; this fraction, denoted as "frequency" in DATGEN, must also be entered for each drop size. Reference 4 lists some representative values of the spray parameters discussed above for the Grand Gulf Reactor.

3.5.2 Convective Heat Transfer

If the user wants to include convective heat transfer, a forced convection model and a condensation model must be specified (box 11). Note that condensation occurs only if thermodynamic conditions permit. In the absence of convection and condensation, thermal radiation is the only heat transfer mechanism between the walls and the gas. If no convective heat transfer is desired, convection and condensation heat transfer are neglected.

The user can choose from two condensation models. The first model matches the heat flux incident on the liquid film (convective, condensation and radiative fluxes) with the heat flux across the film. This is accomplished by iteratively varying the film-gas interface temperature. This method may not converge for large mole fractions of steam. In the second model, the interface temperature is assumed to be equal to the wall temperature and the liquid layer conductance is assumed to be infinite. This model requires no iteration and executes faster than the first model. The first model is the more rigorous of the two; however, no significant difference in output has been observed between the two models. The user should use the second model for faster HYBER execution.

After the condensation model has been selected, the user is prompted to choose one of two available forced convection models. The first model is a correlation using the Reynolds numbers for flat plates. This correlation (denoted as RE), is for steady-state laminar or turbulent flow over a flat plate with transition from laminar to turbulent flow occurring at a Reynolds number of 3 (10^5). The input of a free stream gas velocity is required (the input of a characteristic surface length is also required and was entered in Section 3.3). This type of model has previously been used in other reactor containment accident analyses [4,5]. The second model is the Means-Ulrich (MU) correlation which is

for transient forced convection. This correlation does not require the input of a gas velocity and is based on phenomena similar to that which occurs during combustion, i.e., swirling, turbulent, and decaying gas velocities. The data base for the correlation was obtained by venting a high pressure gas reservoir into a closed cylinder and measuring the heat tranfer rate following injection. The correlation requires an equivalent containment diameter (entered in Section 3.2).

The user should execute HYBER several times (using both convective models) to determine the sensitivity of the results to each forced convection model. When using the Reynolds number correlation, the user should also execute HYBER trying different gas velocities to determine the sensitivity of the simulation to this parameter. When the characteristic length of a surface is in doubt, it can also be treated as a parameter in the sensitivity study. For the MU correlation, the equivalent containment diameter can also be varied. Only through varying the input parameters of the forced convection models, can the user gain insight as to the importance of convective phenomena. Section 6 of the reference manual compares experimental results of various scale test facilities with computational results from the two forced convection correlations. The user should refer to this section to gain more understanding of the character of each correlation.

Although a user input is not required, free convective heat transfer is also calculated in SOLVER. The free convection model calculates laminar or turbulent free convection with transition occurring at a Rayleigh number of 10^9 During a burn simulation, SOLVER compares the calculated heat transfer coefficients due to forced and free convection and uses whichever is greater.

3.5.3 Gas Flow in Ice-Condenser Reactors

The ice-condenser reactor gas flow model is designed to simulate gas flow between the lower compartment and the upper compartment in an ice-condenser nuclear power plant only for combustions in the lower compartment (see box 12). The compartments are connected by (1) an ice condenser, which allows flow from the lower compartment to the upper compartment, and (2) fans, which force the gas from the upper compartment to the lower compartment. The lower compartment may have a slightly higher pressure than the upper compartment at some time during the simulation; the fans can be allowed to pump air against this adverse pressure difference (see Figure C-2). Initially both compartments are at the same pressure. When a hydrogen deflagration occurs, the lower compartment pressure becomes higher than the upper compartment pressure, and gas flows only through the ice condenser into the upper compartment. When the pressures

in the compartments become approximately equal, the fans will begin to pump upper compartment gas into the lower compartment, maintaining gas circulation through both compartments. For greater detail, refer to the reference manual [3].

If the user specifies this model to be operative, the volume and gas temperature of the upper compartment, the fan rating in cubic feet per minute, the fan opening area, the ice-condenser inlet area, the temperature of the gas exiting the ice condenser, and the maximum pressure difference against which the fan may operate must be input. Sample input values for this model are given for the Sequoyah reactor in [6].

3.5.4 Gas Leakage from a Combustion Vessel

If the ice-condenser gas flow model is not used, DATGEN prompts the user to specify whether gas leakage (box 12b) is to be modeled. This model simulates inflow or outflow through a small hole in the containment structure [3]. When used, the user must enter the leak area, and the gas pressure and temperature outside of the vessel, i.e., back pressure and temperature for the leak. Note that the ice condenser-fan model and leak models cannot be used simultaneously.

3.6 Time Step and Output Control

All geometry and thermophysical property data and heat transfer options have been entered at this point. The user must now input the initial time step increment to be used in the calculations, the gas-temperature step-size used in time step acceleration, the maximum time step allowed, and print-out intervals (box 13). These parameters are discussed below.

HYBER analyses performed at SNLA have shown that an initial time step of 0.01 to 0.05 second gives reasonable, i.e., numerically stable, results. To minimize execution time, the user should choose 0.05 second as the initial time step but is encouraged to try several values between 0.01 and 0.05 second to compare output results. During each time step, SOLVER performs an energy balance and updates the gas state (gas temperature, pressure, and composition), computes new, net heat fluxes for each surface, and computes the temperature distribution in each wall and piece of equipment. The print interval parameter is used to limit the size of the output files. Specifically, all output is written every n-th time step, where n is the print interval parameter.

If the initial time step size results in excessive execution time, the execution time can be decreased via a time step acceleration option which utilizes the gas-temperature step-size parameter. This option increases the magnitude of the time step whenever the gas temperature decrease per time step during execution is less than the gas-temperature step-size parameter. The time step size is increased by adding the initial time step size to the present time step size. Increasing the step size in such a manner decreases the execution time. A gas-temperature step-size parameter between 0 K and 5 K is recommended. If 0 K is entered for the parameter, the time step will remain constant, i.e., at the initial time step size. The user must also specify the maximum time step to be allowed in the simulation. It is recommended that this value be 5.0 seconds or less. It has been found in analyses using the ice-condenser engineering option, that the time step acceleration can lead to unstable results unless the maximum time step is small (less than 1.0 second). Note that this time step acceleration is allowed to occur only following completion of combustion; the time step remains constant during combustion. In addition, the print interval should be small (less than 5) when using time step acceleration. Otherwise, the output might be too sparse for practical use.

3.7 Combustion Parameters and Options

The user must now enter information pertaining to combustion (box 14). This includes the pre-combustion gas state and composition, combustion completeness, and parameters associated with heat transfer during combustion. An expanded flow diagram of the combustion parameters and options (boxes 14 and 15) is shown in Figure 2. Three combustion processes can be modeled:

- Hydrogen–oxygen combustion
- Carbon monoxide–oxygen combustion
- Hydrogen–carbon monoxide–oxygen combustion

The user is prompted to input the initial gas pressure, temperature, and mole fractions of hydrogen, oxygen, water vapor, nitrogen, carbon dioxide, and carbon monoxide. The initial mole fractions must sum to unity; otherwise, the user is prompted to re-enter the mole fractions. In addition, the initial gas state must be an equilibrium state, i.e., the gas must not be super-saturated. DATGEN compares the steam partial pressure to the saturation value at the initial gas temperature. If the gas is determined to be super-saturated from this comparison, a warning message is provided and the user is prompted to re-enter the initial gas composition.

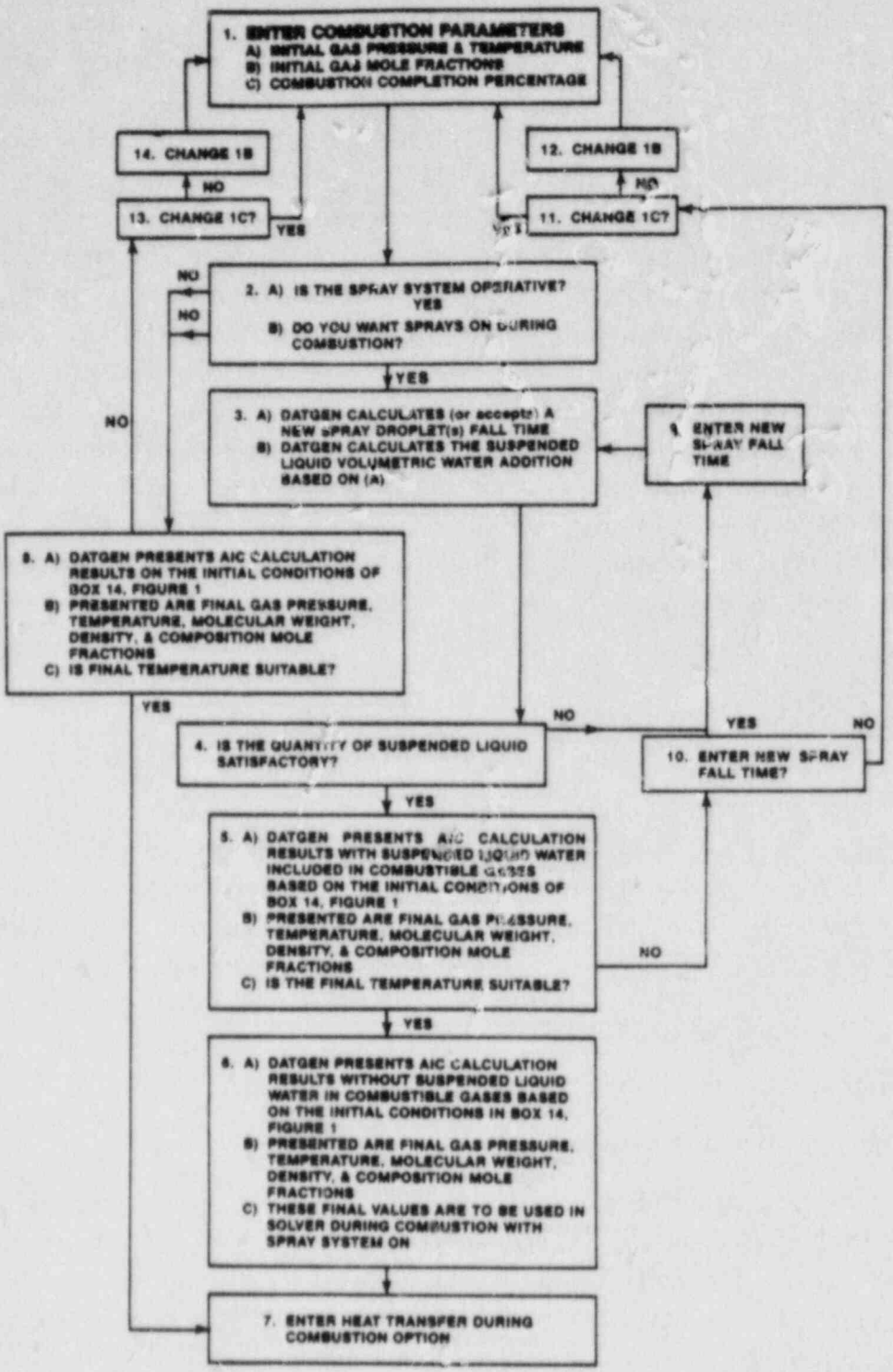

Figure 2. DATGEN combustion diagram

Next, the user is prompted for the combustion completeness. Hydrogen–air combustion is complete if all the hydrogen specified is consumed; otherwise, the combustion is termed incomplete. Completeness is thus defined from 0 to 100 percent. If the combustion is to be incomplete ($< 100\ \%$) , then a completion percentage must be entered. Note that any combustion involving carbon monoxide is always assumed to be complete. Data for combustion completeness versus mole fraction of hydrogen are given in [5,6].

Upon completion of the combustion parameters input (box 14), DATGEN performs adiabatic isochoric combustion (AIC) calculations. The results of the AIC calculation are presented in terms of a peak gas temperature and pressure, species mole fractions, and energy release to the gas and are written to a data file to be used by SOLVER. DATGEN computes one or two AIC calculations depending upon what the user specifies in the combustion options input (boxes 15,16). This feature is explained below.

SOLVER uses the AIC calculation results in one of two ways depending on the user input in the combustion options section (box 16):

1. the user may specify the AIC energy release to the gas to be instantaneous, and SOLVER calculates only post-combustion heat exchange,

2. the user may specify the AIC energy to be released over a user-specified time (the combustion period). SOLVER then releases the AIC energy at a rate which causes the gas temperature to increase at a constant rate during the combustion period. The gas temperature at the end of combustion would agree with the AIC peak gas temperature if the burn were adiabatic. However, since this option also includes heat loss by the gas due to a) radiation, convection, condensation, and b) the engineering systems options, i.e., sprays, if so specified, the peak gas temperature calculated in SOLVER will be less than the AIC gas state.

In DATGEN sprays may be operative in two modes: 1) before, during, and after combustion, or 2) only after combustion. If the sprays are operative (spray option, box 10), the user may specify that sprays are on for mode (1). If so, the effect of the spray droplets entering the combustible gases is included in the combustion calculation (box 15a), i.e., a percentage by volume of the suspended liquid droplets in the gas must be calculated. First, DATGEN calculates the time that an average droplet takes to fall through the fall distance (assuming no initial downward droplet velocity). The fall time is multiplied by the spray volumetric flow rate to obtain the volume of suspended liquid in the gas. From the volume calculated, a percentage (by volume) of the suspended liquid may be calculated. The user may change the percentage (by volume) by entering a new fall distance.

Note that if suspended water is not considered during combustion, then the sprays are assumed to be operative only after completion of the combustion process.

Therefore, the suspended liquid option allows the user to simulate two cases:

1. Sprays on and no suspended liquid simulates an event where the spray system is not operative until after combustion.

2. Sprays on and suspended liquid on simulates an event where the spray system is on prior to and during combustion as well as after combustion.

When sprays are operative during combustion, DATGEN performs two adiabatic isochoric combustion (AIC) calculations (see [3]). The first calculation includes suspended water, providing an estimate of the peak gas temperature, pressure, and species mole fractions. If the user decides that these peak conditions are satisfactory, a second calculation which does not include the suspended water is performed. Comparison of the two AIC calculations shows the user the effect of sprays on the combustion process. The results of the second AIC calculation are written to the input file for SOLVER, and are used in SOLVER with the spray model operative during combustion. For this case, it is required that the combustion occur over a user-specified time period, during which heat loss and condensation can occur. The peak gas state computed in SOLVER will differ somewhat from the first AIC calculation for two reasons:

1. the actual spray model differs from the suspended liquid model in the AIC calculation performed in DATGEN and,

2. the combustion process is non-adiabatic in SOLVER. That is, heat transfer and condensation during the burn will decrease the peak gas state.

If the user does not wish to consider sprays during combustion or if sprays are inoperative (box 10), no questions are asked about suspended liquid, and DATGEN performs a single AIC combustion calculation without suspended liquid.

For sprays operative during combustion, only after combustion, or not operative at all, the user is allowed to modify the pre-combustion conditions (box 14) if the final gas state of the above AIC calculation(s) is not suitable. The following options are available depending upon the combustion scenario being considered.

- The initial gas composition can be modified.

- The hydrogen–air combustion completeness can be modified.

- The spray droplet fall distance and increment can be altered to modify the quantity of suspended water if sprays are operative during combustion.
- Any combination of the above.

By changing any combination of the options listed above, the user may choose the peak gas state from the AIC calculation to match any other simulation or real event. With this capability, HYBER can begin calculations from the same peak gas state of any other event to compare its output against those of another simulation or a real event.

Upon obtaining satisfactory AIC combustion results, DATGEN prompts the user to indicate if heat transfer during combustion (box 16) is to be simulated. If the the answer is no, the AIC combustion energy is released instantaneously to the gas, and SOLVER calculates only a post-combustion heat exchange using the final AIC gas temperature and pressure as the initial gas conditions for the simulation.

When heat transfer during combustion is specified, the user is prompted to enter a flame speed and burn length, which define the combustion time period. (Flame speed data as a function of hydrogen concentration are given in [6,7].) The AIC energy is released in a manner to cause a constant rate of increase to the gas temperature. The resulting temperature rate of increase is not constant, however, due to heat loss and condensation during the combustion process. The maximum gas temperature calculated in SOLVER will always be less than the AIC gas temperature. The initial gas state and composition for the simulation are those entered for the pre-combustion conditions used in the AIC calculation in DATGEN. Note that if the ice-condenser gas flow model is operative or if sprays are operative during combustion, DATGEN automatically specifies that heat transfer during combustion is occurring, and the user must enter flame speed and burn length.

3.8 Final Input

For single deflagration simulations and the initial deflagrations of multiple burn simulations, the user must input the initial wall temperature (box 17). The initial wall temperature must be greater than 283 K . Initial wall temperatures must always be entered for any single burn simulation, but need not be entered after the first deflagration of a multiple burn simulation. In the latter case, the final wall temperatures of the previous deflagration are automatically stored as the initial wall temperatures for the next deflagration.

At this point, all data generation is complete. DATGEN has created two input files for SOLVER. The two files are named "NRCDAT" and "NRCDAT.NOD" NRCDAT contains the time, date, and title of the simulation and all of the data that has been entered above by the user. NRCDAT.NOD contains geometrical and thermophysical information required by the conduction model in SOLVER.

4 SOLVER

The data files generated in DATGEN are used in SOLVER, which performs the numerical simulation of the specified combustion scenario. Figure 3 shows the computational framework in SOLVER. Specific details of the computational models and organization of SOLVER are given in the reference manual [3]. Since the user cannot influence the operation of SOLVER except through the inputs generated in DATGEN, only the output generated by SOLVER is discussed in this manual.

4.1 SOLVER Execution

The first operation performed in SOLVER is the data initialization. In this part of the code, the data generated in DATGEN is read and echo-printed to the screen of the terminal. This is provided so that the user is aware of which simulation is to be performed. Since SOLVER is not an interactive code, the input cannot be modified after execution has commenced. A check is included in the data initialization section to insure that the data are in the correct format. This is provided since a format error (i.e., omission of variables or inclusion of extraneous variables) could be introduced if the user edited the "NRCDAT" file. Editing NRCDAT is a quick and convenient method to change parameters of a simulation without executing DATGEN.

After the data initialization is complete, the numerical simulation begins. During the execution, informative messages are written to the screen to indicate execution progress, e.g., completion of combustion and completion of simulation messages. When the simulation is completed, a set of messages indicating the types of output files generated from this simulation is written to the screen. These output files are described below.

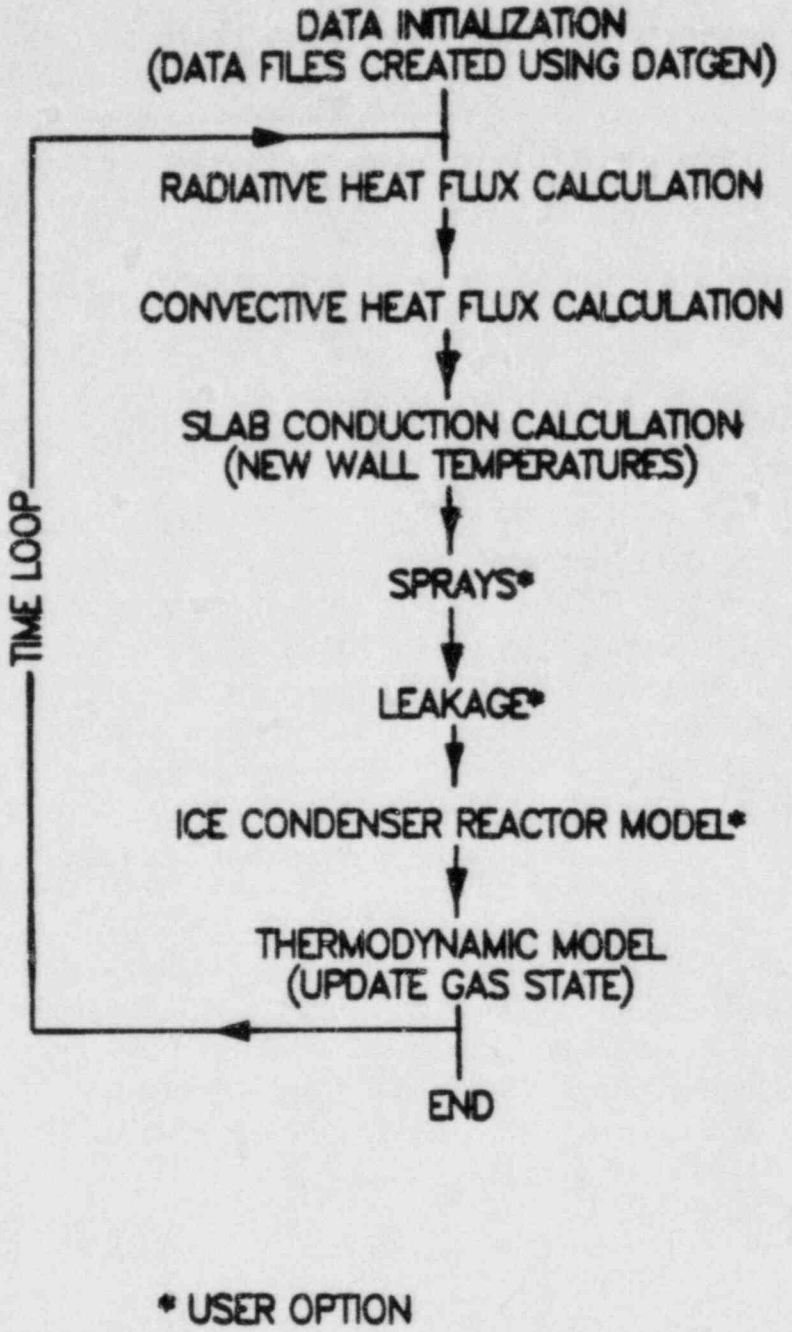

Figure 3. SOLVER execution procedure.

4.2 Output

When the execution of SOLVER is complete, several files are created by SOLVER:

1. OUTPUT
2. FLUX
3. ENERGY
4. TEMPS1 - optional (see box 8 description in Section 3.3)
5. TEMPS2 - optional (see box 8 description in Section 3.3)
6. TEMPS3 - optional (see box 8 description in Section 3.3)
7. OLDWALL - optional (written if part of a multiple burn simulation)
8. OLDDAT - optional (written if part of a multiple burn simulation)
9. FLOWS - optional (written if ice-condenser or leak option specified)

The output files TEMPS1, TEMPS2, and TEMPS3 contain temperatures of slabs 1, 2, and 3, respectively, at the nodes designated by the user. Since the user has the option to save nodal temperatures of any or all slabs, these three files may or may not be created by DATGEN. OUTPUT, FLUX, and ENERGY are always created. The files OLDWALL and OLDDAT are generated if the user specifies that the simulation is part of a multiple burn sequence. These files are used in re-start procedures. The file FLOWS is generated only if the leak or ice-condenser engineering models are included in the analysis. Below are summary descriptions of these files and of the output data provided.

4.2.1 OUTPUT

The file OUTPUT provides gas state and composition, surface temperatures, and indications of whether condensation was occurring and whether forced or free convection was occurring. The header to OUTPUT contains:

1) ST	- the simulation title
2) P1	- initial gas pressure
3) T1	- initial gas temperature
4) H21	- initial gas hydrogen mole fraction
5) H2O1	- initial gas water vapor mole fraction
6) CO21	- initial gas carbon dioxide mole fraction
7) CO1	- initial gas carbon monoxide mole fraction
8) COMPL1	- completion percentage of the burn
9) VPH2OL	- suspended liquid water percentage

The following items are written to OUTPUT at the user-specified print interval.

10) TIME - time during simulation
11) PGAS - gas pressure during simulation
12) TGAS - gas temperature during simulation
13) FRACT - fraction of spray that has evaporated
14) TS1 - surface temperature of surface 1 during simulation
15) TS2 - surface temperature of surface 2 during simulation
16) TS3 - surface temperature of surface 3 during simulation
17) MFS - mole fraction of steam in gas
18) CONDF - condensation flag (true or false) to indicate if condensation is occurring on a surface during simulation
19) CONVF - convection flag (Forced, Natural or Blank) to indicate the type of convection or if convection is occurring during simulation

Note that items 15 and 16 are given only when two or three surfaces are used.

4.2.2 FLUX

The output file FLUX contains net radiative and convective heat fluxes in W/m^2 for each surface during the entire simulation. The header for this file is the same as that described in 4.2.1. The file FLUX contains:

1) ST, P1, T1, H21, H2O1, CO21, CO1, COMPL1, VPH2OL, TIME
2) HFRC1, HFRC2, HFRC3 - convective and condensation heat flux to surfaces 1,2,3
3) HFR1, HFR2, HFR3 - radiative heat flux to surfaces 1,2,3

Customary sign conventions are used for the fluxes. That is, a negative sign on a radiative flux indicates a net flux into the surface, and a positive sign on a convective flux indicates a net flux into the surface.

4.2.3 ENERGY

The output file ENERGY provides integrated net radiative and convective heat fluxes for the post-combustion time period. The header for this file is the same as that described in 4.2.1. The file ENERGY contains:

1) ST, P1, T1, H21, H2O1, CO21, CO1, COMPL1, VPH2OL, TIME

2) HFRC1, HFRC2, HFRC3 - convective and condensation energy depositions for surfaces 1,2,3
3) HFR1, HFR2, HFR3 - net radiative energy depositions for surfaces 1,2,3

4.2.4 TEMPS1,TEMPS2,TEMPS3

The files TEMPS1, TEMPS2, and TEMPS3 contain temperatures of nodes specified in box 8 for each surface. The header consists only of the simulation title. The files contain:

1) ST,TIME
2) NODE n - nodal location where n is the node number
3) TW - wall temperature at node n during simulation

4.2.5 FLOWS

If the simulation includes either the ice-condenser or leak engineering model, then the file FLOWS is created to indicate the gas state for the compartment and for either the environment or upper compartment depending upon the model specified. In addition, the flow rates between compartments (or between the compartment and environment for the leak model) are also given. The header for this file is the same as that described in 4.2.1. The file FLOWS contains:

1) ST, P1, T1, H21, H2O1, CO21, CO1, COMPL1, VPH2OL, TIME
2) TIME
3) PGAS(L.C.),PGAS(U.C.),TGAS(L.C.),TGAS(U.C.),
   MASFL(L.C.),MASFL(U.C.)
   (for ice-condenser engineering option)
   or
3) PGAS(COMP),PGAS(ENV.),TGAS(COMP),TGAS(ENV.),
   MASFL(OUT),MASFL(INTO)
   (for leak option)

where PGAS - gas pressure
TGAS - gas temperature
MASFL - mass flow rate
L.C. - lower compartment
U.C. - upper compartment
COMP - compartment identifier
ENV. - environment

4.2.6 OLDWALL

If the simulation is part of a multiple burn scenario, the file OLDWALL is created for use in re-start simulations. It has the simulation title as a header. The final temperature distributions for each slab are given, but not labeled. This file is read in by SOLVER in re-start analyses and is not intended for inspection by the user.

4.2.7 OLDDAT

If the simulation is part of a multiple burn scenario, the file OLDDAT is created for use in re-start simulations. It has the simulation title as a header. The initial and final gas conditions are given, but not labeled. This file is used only in re-start analyses in DATGEN and is not intended for inspection by the user.

5 Re-start Options

HYBER has three types of re-start capabilities. The first allows the user to read-in previously generated combustion vessel geometry and to change heat transfer, engineering systems, and/or combustion specifications. Using this option, the user does not have to re-input geometry and radiative parameter data. This option may be used for new single burn simulations or for the first burn of a multiple burn scenario. The second re-start option allows the user to simulate any burn after the first of a continuing multiple burn scenario. Results from each burn are used in the succeeding burn. In the second re-start option, geometry and radiative parameters and heat transfer and engineering system options cannot be changed during the course of the multiple burn simulation. For the two re-start options above, DATGEN interacts with the user, i.e., DATGEN prompts the user for information concerning the simulation. Note that when the re-start option is exercised, the data generation file NRCDAT (created in a previous burn simulation) is renamed RESTART. The third re-start option may be used in place of the two options above. The third option allows the user to edit the data file NRCDAT previously generated by DATGEN. The advantage of this option is that the user need not go through the prompting process required by DATGEN. Instead the edited data file is read directly by SOLVER. Further details of the options are discussed below.

5.1 Re-start for a New Single Burn or for the First Burn of a Multiple Burn Scenario

When beginning a new multiple or single burn simulation, the user may wish to use old geometry and heat transfer and engineering options. Upon executing DATGEN for a new single burn re-start, the user should enter: (1) the time, date, and burn simulation title, (2) that the simulation is a single burn, and (3) that previous geometry data will be used (boxes 1,2,4). For a new multiple burn scenario, the user should enter: (1) the time, date, and burn simulation title, (2) that the simulation is a multiple burn, (3) that a new multiple burn is being run (first pass), and (4) that old geometry and heat transfer and engineering systems options will be used (boxes 1-4). In both cases, the user must say "yes" to box 4 to begin the re-start option, and the user must enter the initial and duration times of the simulation (box 20). DATGEN then reads the RESTART file data to obtain the old geometry data (boxes 6-9). The user is then prompted about whether the heat transfer and engineering systems options and/or the time step and output control parameters (box 21) are to be modified. If the

answer is "yes", then the user must enter (1) the heat transfer and engineering system options, (2) time step and output control parameters, (3) combustion options and parameters, (4) the heat transfer during combustion option, and (5) the initial wall temperatures (boxes 10-17). If the answer is "no", DATGEN reads the RESTART file data to obtain the old heat transfer and engineering system options and time step and output control parameters (boxes 10-13). The user must then enter the combustion options and parameters, the heat transfer during combustion option, and the initial wall temperatures (boxes 14-17).

5.2 Re-start for any Burn after the First of a Continuing Multiple Burn

The following procedure is used in DATGEN in order to generate the input files for any deflagration after the first deflagration of a continuing multiple burn analysis. The user should enter (1) the time, date, and burn simulation title, (2) that the simulation is a multiple burn scenario, and (3)that the burn being simulated is not the first of the multiple burn scenario being run, i.e., not the first pass through the input generator DATGEN (boxes 1-3). For this re-start option, the time at which the previous burn ended (obtained from the file OLDDAT) is written to the screen, and the user enters the initial and duration times of the current burn (box 19). DATGEN then automatically reads the RESTART file data to obtain the old geometry, heat transfer and engineering system options, and time step and output control parameters (boxes 6-13). For this re-start option, the heat transfer and engineering system options selected for the first burn of the continuing multiple burn are always the same in succeeding burns. The final gas state and composition from the previous burn are read from the file OLDDAT (box 23) and are written to the screen for use in selecting the initial conditions for the current combustion process. The user determines the new gas state by specifying the gas state and composition. Note that the new gas state should not differ significantly from the final gas state of the previous simulation; the only justifiable differences would be due to steam injection and hydrogen release, each of which are treated as step inputs in these analyses. The remainder of the data generation follows the description presented in Section 3.

5.3 Re-start by Editing Existing Data Files

Upon completion of DATGEN two data files (NRCDAT and NRCDAT.NOD) are created for use by SOLVER. Both of these data files may be edited for use by SOLVER in lieu of using DATGEN to create the identical file(s). Examples of NRCDAT and NRCDAT.NOD are in sections D.1.a-c . Editing the existing data files requires caution on the part of the user and should only be attempted by a user experienced in using HYBER. Any edit which accidently alters the format

of the data file will cause a fatal error generation in SOLVER and cause HYBER to terminate execution.

While every option described in section 3 may be edited, some options should not be changed by editing but by using DATGEN to interactively change the options (see 5.a and 5.b). The user should not change the following options by editing the data files: 1) containment geometries, 2) surface (or slab) nodding for the slab temperature distributions, 3) configuration factors and beam lengths, and 4) surface thermophysical properties. Options 1 and 3 should not be edited because the user may not maintain reciprocity for the beam lengths and configuration factors which will cause erroneous HYBER output. Options 2 and 4 should not be edited because NRCDAT.NOD (which contains geometrical and thermophysical data required by the conduction model in SOLVER) can only be created by a subroutine contained in DATGEN.

This editing option is intended to allow the user to change: 1) the burn type (single or multiple), 2)the simulation initial and duration times, 3) surface length scales and emissivities, 4) heat transfer and engineering system options, 5) time step and output control, 6) combustion options and parameters, and 7) initial wall temperatures. A typical example NRCDAT data file for a multiple burn simulation (base case, first burn), is provided in section D.1.1 . As an example of the edit option, one could change the time step size from .05 to .01 second, by changing the line marked with '**********' from 5.0000001E-02 to .01.

Note that the edited version of NRCDAT must always be on disk 1 with DATGEN when using this option on the IBM personal computer (see next section).

6 Algorithm Usage on the IBM Personal Computer

HYBER may be used with the IBM PC or any IBM compatible operating with a Microsoft Fortran-77 software package. The PC must be equipped with two disk drives (denoted A and B) in order to operate the algorithm, given the sizes of the two computer codes, DATGEN and SOLVER. Further, to execute the algorithm, the user needs to have at least three disks, two of which hold the compiled computer codes and one which can be used to store algorithm-generated results. The PC must also be booted up with the Disk Operating System (DOS) disk. Additional details on the IBM PC system are given in [8].

Disk number one, labeled DATGEN, contains the compiled computer code DATGEN and is operated from drive A. The purpose of DATGEN is to generate data files which contain information pertinent to the simulation. The data files are generated by DATGEN as described above. Containment geometry, heat transfer correlation data, and combustion data are stored in data file NRCDAT, and thermal conduction nodalization information are stored in data file NRCDAT-.NOD.

Disk number two, labeled SOLVER, contains the compiled version of SOLVER, and is placed in drive B. SOLVER reads the data files created by DATGEN and performs the combustion and post-combustion heat transfer calculations. After completing the heat transfer calculations, SOLVER writes the output files described in Section 4.

A procedure file named "RUN.BAT" is provided to coordinate operations associated with executing the algorithm. A listing of this file is given in Appendix F. The file RUN.BAT is located on disk number one with DATGEN and performs the following functions:

1. RUN.BAT transfers files created by DATGEN or edited by the user on disk 1 to SOLVER on disk 2.

2. RUN.BAT transfers files from disk 2 to disk 1 to allow a re-start option for single or multiple burns.

3. RUN.LAT tells the user how to store the SOLVER output files on disk 3. During a multiple burn, the old output files from a previous simulation are erased on disk 2 as new output files are created during subsequent simulations; therefore, the old output files must be stored on a new disk.

4. RUN.BAT tells the user how to start another execution of DATGEN and SOLVER for subsequent burn simulations.

6.1 Algorithm Execution Using RUN.BAT

To begin algorithm execution on the IBM PC, the user must enter "RUN PROGNAM SOLVER FILNAM", where "PROGNAM" is a user-specified name which indicates whether 1) DATGEN will be used interactively for a first-time execution of HYBER or for a re-start from section 5.1 or 5.2, or 2) a re-start by editing is to be used from section 5.3 . For option (1), "PROGNAM" is replaced by DATGEN, and for (2), "PROGNAM" is replaced by DATFIL. "FILNAM" is a user-specified name describing the deflagration to be simulated. For example, REACB1 is the name assigned to the first deflagration of the multiple burn example problem shown in Appendix C (section 3.2). After entering the RUN statement above, the interactive prompting described in section 3 will commence. If DATGEN is used interactively, upon completion of DATGEN execution, RUN.BAT transfers the files NRCDAT and NRCDAT.NOD to disk 2 and renames these data files "DATA" and "NODES", respectively. If the re-start by file editing is being used, then the edited version of NRCDAT and a previous version of NRCDAT.NOD are transferred by RUN.BAT to disk 2 and are renamed "DATA" and "NODES", respectively. The PC is then instructed by RUN.BAT to begin executing SOLVER.

When SOLVER completes execution, the output files OUTPUT, FLUX, ENERGY, TEMPS1, TEMPS2, TEMPS3, and FLOWS will be renamed by RUN.BAT as they are transferred to disk 3. Each file will receive FILNAM as its new name with a three letter suffix to identify each file. For the base case, OUTPUT, FLUX, ENERGY, TEMPS1, TEMPS2, TEMPS3, and FLOWS are renamed REACB1.OUT, REACB1.FLX, REACB1.NRG, REACB1.TS1, REACB1.TS2, REACB1.TS3, and REACB1.FLO, respectively. Note that the suffix designation will be the same regardless of the name selected. The suffix designations were selected to resemble the output file names given in section 4.2 as shown below:

1. .OUT - OUTPUT
2. .FLX - FLUX
3. .NRG - ENERGY
4. .TS1 - TEMPS1
5. .TS2 - TEMPS2
6. .TS3 - TEMPS3
7. .FLO - FLOWS

6.2 RUN.BAT Post-Processing

When SOLVER execution is completed, RUN.BAT begins file manipulations. For single burn simulations, the file DATA is transferred to disk 1 and is renamed RESTART. With RESTART, the user may begin interactive re-starts described in section 5.1 . For multiple burn simulations, after finishing the first deflagration of a multiple burn scenario, the file DATA is transferred to disk 1 and named "RESTART". The geometry, thermophysical and radiative parameters, and heat transfer and engineering systems options in RESTART are re-input during an interactive re-start with DATGEN described in section 5.2. To allow for a continuing multiple burn re-start, OLDDAT is transferred to disk 1 to use the final values of the previous burn for the next burn to be simulated. Also, OLDWALL is copied into a file named "OLDWALT" on disk 2, so that the final slab temperature distributions can be used as initial values in the next deflagration analysis.

Although file(s) are always created after SOLVER finishes execution to allow interactive re-starts, the user may ignore these files and perform a re-start by editing NRCDAT.

Following the completion of SOLVER execution, RUN.BAT copies the output files onto disk 1. The user is then instructed to place a new formatted disk into drive B, and the output files are copied from disk 1 in drive A to disk 3 in drive B using the output name FILNAM (with the three letter suffixes described above) in the execution statement: RUN PROGNAM SOLVER FILNAM. After the output files are saved, RUN.BAT tells the user how to start another simulation.

7 Algorithm Usage on the VAX 11/780 Computer

HYBER was developed primarily on the VAX 11/780 and CRAY-1 computer systems, but the only difference between the VAX/CRAY and IBM versions of the algorithm is the logical units which specify the interactive input/output files. To convert the algorithm to a different system, the user needs only to modify one line in DATGEN and one line in SOLVER. These changes are described in the introduction in the source listing of each code. (See Appendix G for the listing of DATGEN and SOLVER.)

To facilitate use of the algorithm on the VAX system, an interactive procedure file has been developed. A listing of this file, "RUNALG.COM", is given in Appendix F. RUNALG.COM performs operations similar to those performed by the IBM procedure file. Since RUNALG.COM is interactive, its operation is self-explanatory and is not described herein.

8 Example Programs

All of the options of DATGEN and SOLVER have been presented. A detailed example problem is provided in Appendix C to demonstrate the actual prompts and sample user responses for a fictitious reactor containment. (This example is known as the "base case"). Note that Appendix C is intended to be used as a tutorial and the user is urged to execute HYBER using the data files in Appendix D after reading through Appendix C. The computer prompts are shown in type-set capital letters, and the user inputs are shown in lower-case characters surrounded by the symbols, < >, e.g. <user input>. The symbol, < >, also indicates that the return key must be pressed to input the data. Note that this example is presented for execution on an IBM PC and includes statements from RUN.BAT, the previously described procedural file for the IBM operating system.

The example of Appendix C should be repeated by the first-time user of the algorithm so that the options presented in this manual can be reviewed. Additional sample input data files and summary results are provided in Appendix D. These examples include:

- Example #1: Multiple burn simulation – base case
- Example #2: Multiple burn simulation with spray systems operative
- Example #3: Multiple burn simulation which includes the ice-condenser engineering model
- Example #4: Multiple burn simulation with gas leakage from the containment

The user is advised to repeat the examples in Appendix C and D on the PC to gain familiarity with the algorithm.

9 Error Messages

9.1 Error Messages in DATGEN

Some of the thermophysical property data used in the algorithm are tabulated, e.g., saturation temperature versus pressure are given for some number of pressure values. Linear interpolation is performed to find the desired property value. Occasionally, the dependent variable is outside the range of the tabulated data. If so, a diagnostic message indicating that the user is operating outside of the data range is provided and the program execution is terminated.

9.2 Error Messages in SOLVER

1. The iterative condensation model is allowed 50 iterations to equalize the heat fluxes. If more than 50 iterations are required, SOLVER tells the user that the model does not converge and the program is terminated.

2. The same error listed for DATGEN above can also occur in SOLVER, i.e., some gas and liquid thermophysical property data are obtained via linear interpolation, and as such, are subject to limits of the data base.

10 Reference Manual

This report is not intended to describe the theoretical basis and engineering assumptions incorporated in the development of the algorithm models. A companion report to this users' guide, the algorithm reference manual [3], provides this information and comparisons between experimental results and algorithm predictions. The user should carefully read through the users' guide and consult the reference manual if questions about DATGEN or SOLVER are not resolved in this manual.

References

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   Reference Manual for HYBER, the Hydrogen Burn—Equipment Response Algorithm, Sandia National Laboratories, SAND83-2579, February, 1984
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8. **IBM Disk Operating System by Micro-Soft, Inc., 1st Ed.**
   January, 1983 Version 2.00

Appendix A: Thermophysical and Radiative Property Data

Table 1. Thermophysical Property Data

Material	Composition	Thermophysical Properties*			
	(%)	Density (kg/m^3)	Specific Heat (J/kg-K)	Thermal Conductivity (W/m-K)	Thermal Diffusivity (m^2/s)
Aluminum Duraluminum	94-96 Al 3-5 Cu Trace Mg	2787	833	164	6.676
Copper Aluminum	95Cu, 5Al	8666	410	83	2.330
Steel					
Carbon	1.5 C	7753	486	36	0.970
Chrome	5 Cr	7833	460	40	1.110
Tungsten	1 W	7913	448	66	1.858
Tungsten	5 W	807	435	54	1.525
Concrete,dry		2000	837	0.128	0.049

* Values shown are for 293 K

Table 2. Normal Emissivity Data

Substance	State of Surface	Temperature (K)	Normal Emissivity
Aluminum	Polished plate	296	0.040
		498	0.039
	Rolled,polished	443	0.039
	Rough plate	298	0.070
Brass	Oxidized	611	0.22
	Polished	292	0.05
		573	0.032
	Tarnished	329	0.202
Chromium	Polished	423	0.058
Copper	Black oxidized	293	0.780
	Lightly tarnished	293	0.037
	Polished	293	0.030
Steel	Polished	313	0.94
	Ground sheet	1213	0.520
Enamel			
White	Rough	293	0.9
Black	Bright	298	0.876
Oil Paint		273-473	0.885

The user is encouraged to consult the following references if different materials are required, if a different average temperature is applicable, or if different surface treatments are specified:

References

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Handbook of Thermodynamic Tables and Charts, McGraw-Hill Book Co., New York, 1976
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Appendix B. Beam Lengths and Configuration Factors

B.1 Mean Beam Lengths

The mean beam length is a measure of the thickness of the gas between two surfaces. Geometrically, the beam length is the average distance between two surfaces. Several mean beam length relations for simple geometries are provided in the reference by Siegel and Howell [1] given below, and this reference should be consulted for details on the mean beam length concept. Closed form solutions do not exist for most geometries.

An often used approximation for the mean beam length from an optically thin gas volume to its entire boundary is:

$$L_{e,o} = 4V/A, \tag{b.1}$$

where V is the gas volume, A is the bounding surface area, and $L_{e,o}$ is the mean beam length. For an optically thick gas,

$$L_e = 0.9L_{e,o}. \tag{b.2}$$

The optical thickness is a measure of the ability of a given path length of gas to attenuate radiation traveling through the path length. Note that this approximation is useful only for a single surface combustion vessel.

If more than one surface is to be modeled in a vessel, the following method is suggested to calculate the mean beam length from surface i to surface j (see Eq.(b.3) below). This method consists of calculating the distance from every point of surface i to every point on surface j. Each "point" can be approximated by a small surface area element. First, calculate the length (ray) from each surface element of surface i to each surface element of surface j. Second, sum the product of the area of the surface element k (of surface i) and the sum of all the ray lengths that eminate from surface element k, over the number of surface elements

comprising surface i. Third, sum the product of the number of rays eminating from a surface element and the surface element area, over the number of surface elements in surface i. Finally, the mean beam length is computed by dividing the summation from step two by the summation from step three. Note that beam length accuracy will increase as the number of surface elements are increased. In some instances, however, the results computed in SOLVER are rather insensitive to beam lengths. For these cases, any increase in beam length accuracy obtained by increasing the number of surface area elements is unwarranted.

$$BL_{i-j} = \frac{\sum_{k=1}^{K}(A_k \sum_{l=1}^{L} L_{k-l})}{\sum_{k=1}^{K} A_k k} \qquad (b.3)$$

Note that reciprocity must exist for beam lengths, i.e., the beam length from surface i to surface j must equal the beam length from surface j to i. Flat and convex surfaces do not "see" themselves; therefore, beam lengths for such surfaces to themselves are zero.

The above explanation for beam length calculations may be clarified through an example. The fictitious nuclear reactor containment structure used in Appendices C and D is provided in Figure 4. Surfaces 1 and 2 of Figure 4 are each divided into four elements: a,b,c,d for surface 1 and e,f,g,h for surface 2. The mean beam length from surface 1 to 2 would be calculated as follows. First, calculate the lengths from a to h,g,f,e; b to h,g,f,e; c to h,g,f,e; and d to h,g,f,e. Second, calculate the product of each element area of surface 1 and the sum of all of the lengths from that element to all elements on surface 2. Then sum this product for each element of surface 1. Third, calculate the product of the number of lengths from each element of surface 1 with the surface area of that element. Then sum the products for each element of surface 1. The mean beam length is computed by dividing the summation from step two by the summation from step three.

In summary,

1) Calculate $L_{a,b,c,d-e}, L_{a,b,c,d-f}, L_{a,b,c,d-g}, L_{a,b,c,d-h}$

2) Calculate $A_i(L_{i-e} + L_{i-f} + L_{i-g} + L_{i-h})$ $(i = a - d)$

3) Calculate $\sum_{i=a}^{d} A_i(L_{i-e} + L_{i-f} + L_{i-g} + L_{i-h})$

4) Calculate $n_a A_a$, $n_b A_b$, $n_c A_c$, and $n_d A_d$.

5) Calculate $\sum_{i=a}^{d} n_i A_i$

6) Divide result of step 3 by result of step 5

where

L_{i-j}	is the length from element i of surface 1 to element j of surface 2,
A_i	is the surface area of element i in surface 1
n_i	is the number of lengths originating from element i of surface 1 to all elements of surface 2.

A user may be able to estimate beam lengths for the containment simulation by visual inspection and omit the extensive beam length calculations. This method is the least desirable but, in some instances, the user may have no alternative.

No matter which method is used, the user is encouraged to execute HYBER and vary the beam lengths for the same simulation to determine the sensitivity of HYBER to beam length input.

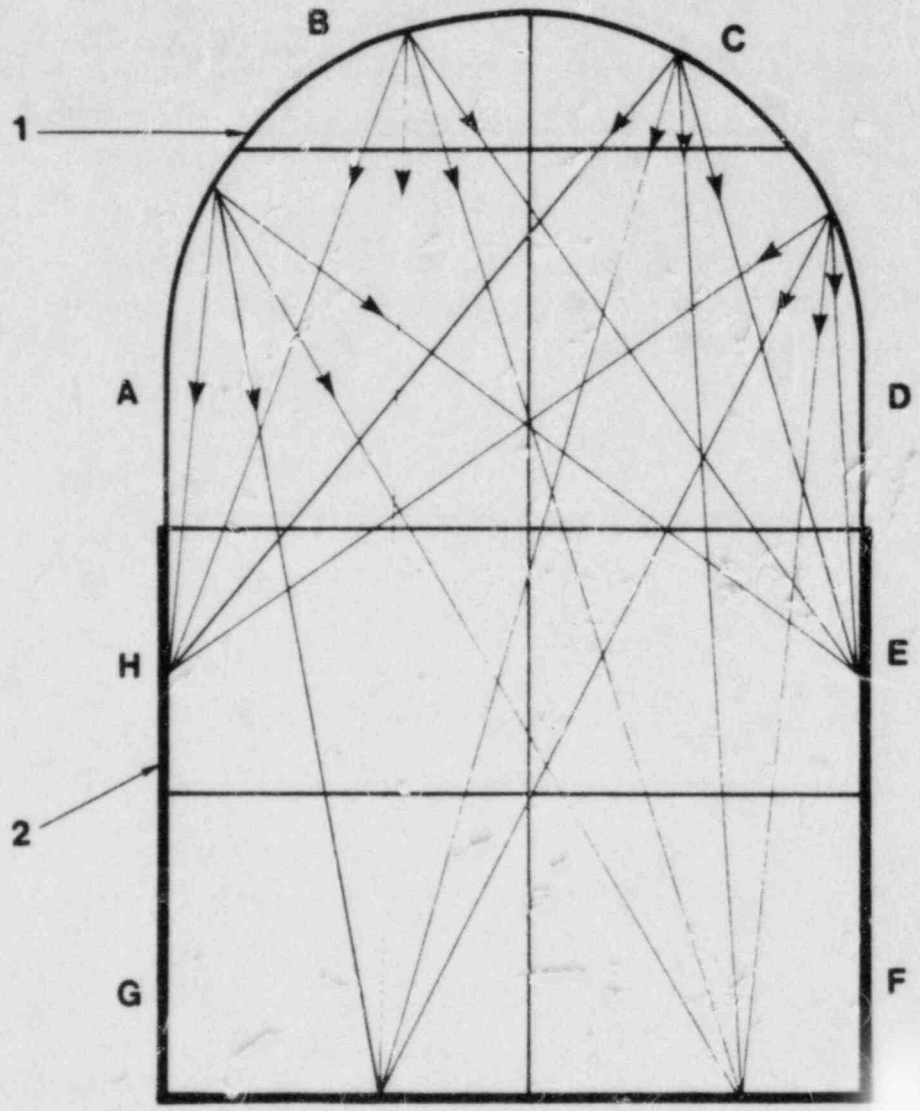

Figure 4. Mean beam length grid for a fictitious containment building.

B.2 Configuration Factors

Techniques to compute configuration fa :ors are found in References [1] and [2]. The purpose of this section is to demonstrate how to use configuration factor reciprocity and algebra to compute all required configuration factors from "n" known configuration factors, where n is 3 for 3 surfaces and 1 for 2 surfaces. For a single surface, the configuration factor must be unity.

For illustrative purposes, the containment geometry in Appendix C is considered and the piece of equipment (surface 3) is located within the containment. Surface 1 is the concrete and surface 2 is the steel liner. The user has computed the configuration factors for surface 3 to surface 1 from methods described in [1,2]. Surface 3 is known to be a flat plate so that F_{3-3} is zero. The following are known.

$$F_{3-1} = 0.4$$

$$F_{3-3} = 0.0$$

$$A_1 = 600.m^2$$

$$A_2 = 400.m^2$$

$$A_3 = 0.25m^2$$

F_{m-n} is the configuration factor from surface m to surface n and A_k is the surface area for surface k. Note that starting the calculations with the smallest surface is the easiest procedure to use.

Since the sum of the configuration factors from a surface to all others must sum to unity, the configuration factor from 3 to 2 is

$$F_{3-2} = 1. - F_{3-3} - F_{3-1} = 0.6$$

From reciprocity ($A_i F_{i-j} = A_j F_{j-i}$),

$$F_{1-3} = A_3/A_1 F_{3-1} = 1.667E-4$$

$$F_{2-3} = A_3/A_2F_{2-3} = 3.74E-4$$

One other configuration factor needs to be calculated to complete the containment configuration factors. Assume that $F_{2-1} = 0.6$ is known. Therefore, because configuration factors for a surface must sum to unity:

$$F_{2-2} = 1 - F_{2-1} - F_{2-3} = 0.399625$$

Then:

$$F_{1-2} = A_2/A_1F_{2-1} = 0.4$$

and

$$F_{1-1} = 1 - F_{1-2} - F_{1-3} = 0.599833$$

Thus, the configuration factors for this problem have been completely determined.

References

1. **Siegel, R., and J. R. Howell,**
Thermal Radiation Heat Transfer, 2nd Edition, McGraw-Hill Book Co., New York, 1981.
2. **Hottel, H. C., and A. F. Sarofim,**
Radiative Transfer, McGraw-Hill Book Co., New York, 1967.

Appendix C. Detailed Example Problem

C.1 Description of Reactor Geometry

In the example problem to be discussed in this appendix and in the examples of Appendix D, a small, fictitious containment building, shown in Figure 5, is considered. This containment has a volume of 5000 m^3, a surface area of 1000 m^2, and an equivalent diameter of 17 m. The inner-wall containment consists of two materials, concrete and steel, which are assumed to have surface areas of 600 m^2 and 400 m^2, respectively. Note that this containment volume may be either an upper or lower compartment of an ice-condenser reactor containment. If this region is assumed to be the lower compartment of an ice-condenser reactor, then the upper compartment is assumed to have an open volume of 10000 m^3, and the ice-condenser open area connecting the two regions is assumed to be 2.0 m^2. (A schematic of this configuration is provided in Figure 6.) Note that both geometries are assumed to have a water spray system which may or may not be operative.

A piece of safety-related equipment is assumed to be located in the containment building. This equipment has an exposed front surface area of 0.25 m^2, and is modeled as a composite slab of two materials separated by an air gap with the back surface insulated. Representations for the equipment and the steel and concrete slabs comprising the reactor containment are given in Figure 7. All other geometry, thermophysical property specifications for the materials, and all radiative parameters are given in the example to follow. These data are also summarized in the data file for this example given in section D.1. The particular example problem to be developed in the following sections is example 1 of Appendix D (refer to the appendix for a description of this problem). When alternative options are described in the following sections, the data presented will be taken from the other three examples included in Appendix D. Included in this example is the interactive output from HYBER when used on an IBM PC.

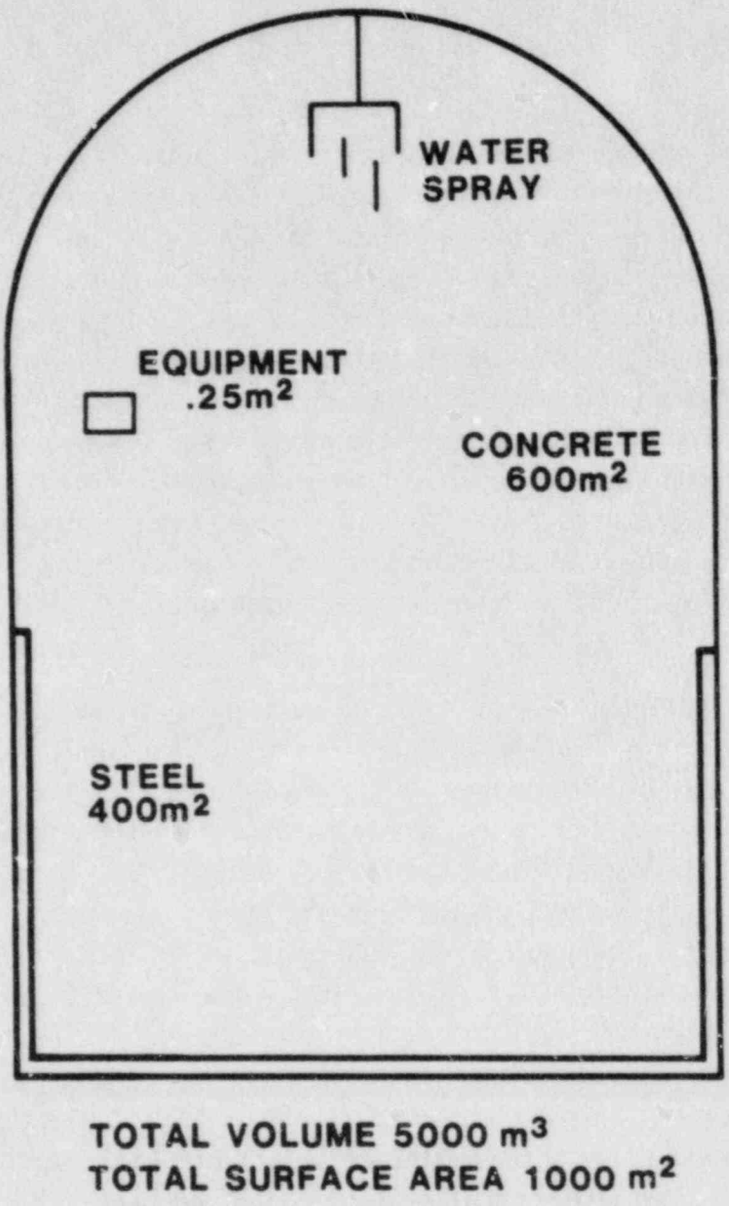

Figure 5. Schematic of fictitious containment geometry used in 'base case'.

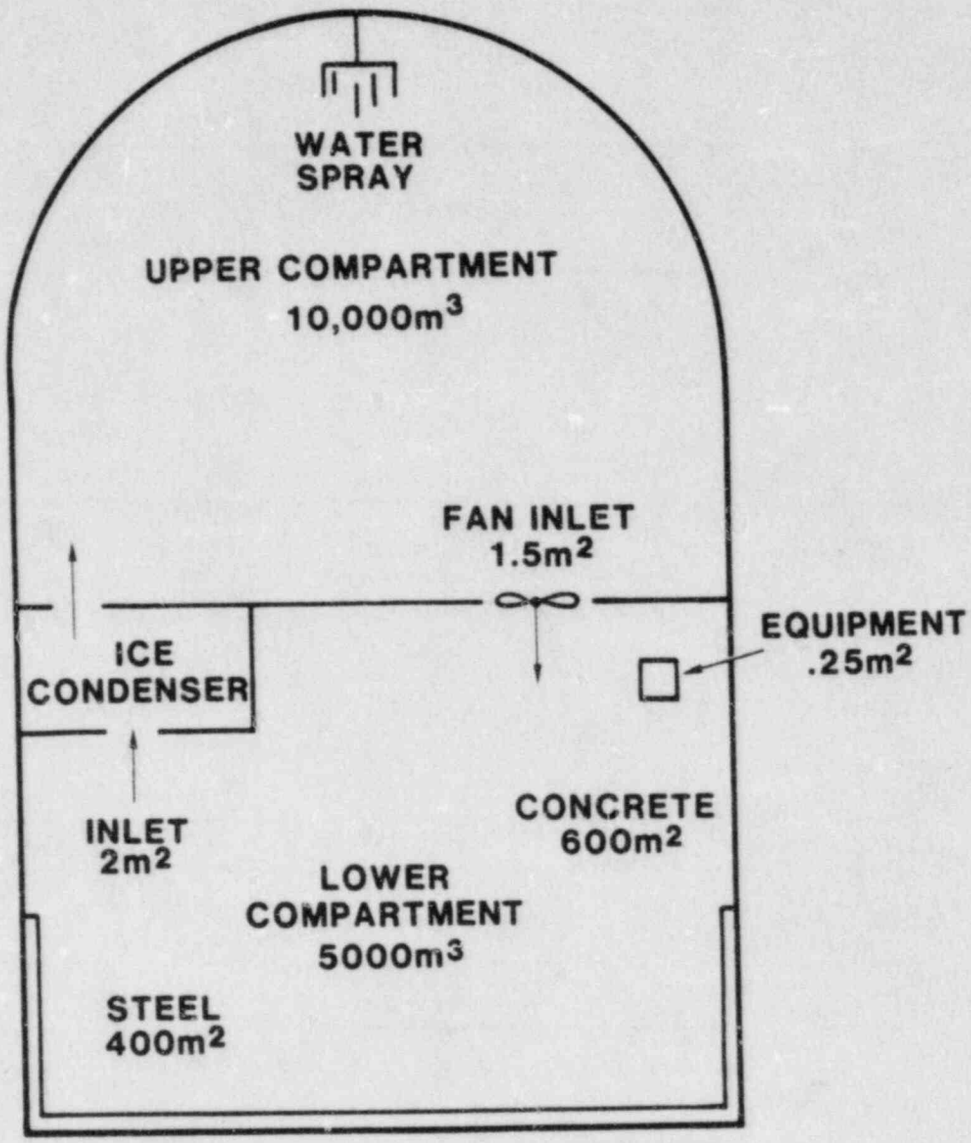

Figure 6. Schematic of fictitious ice-condenser reactor containment.

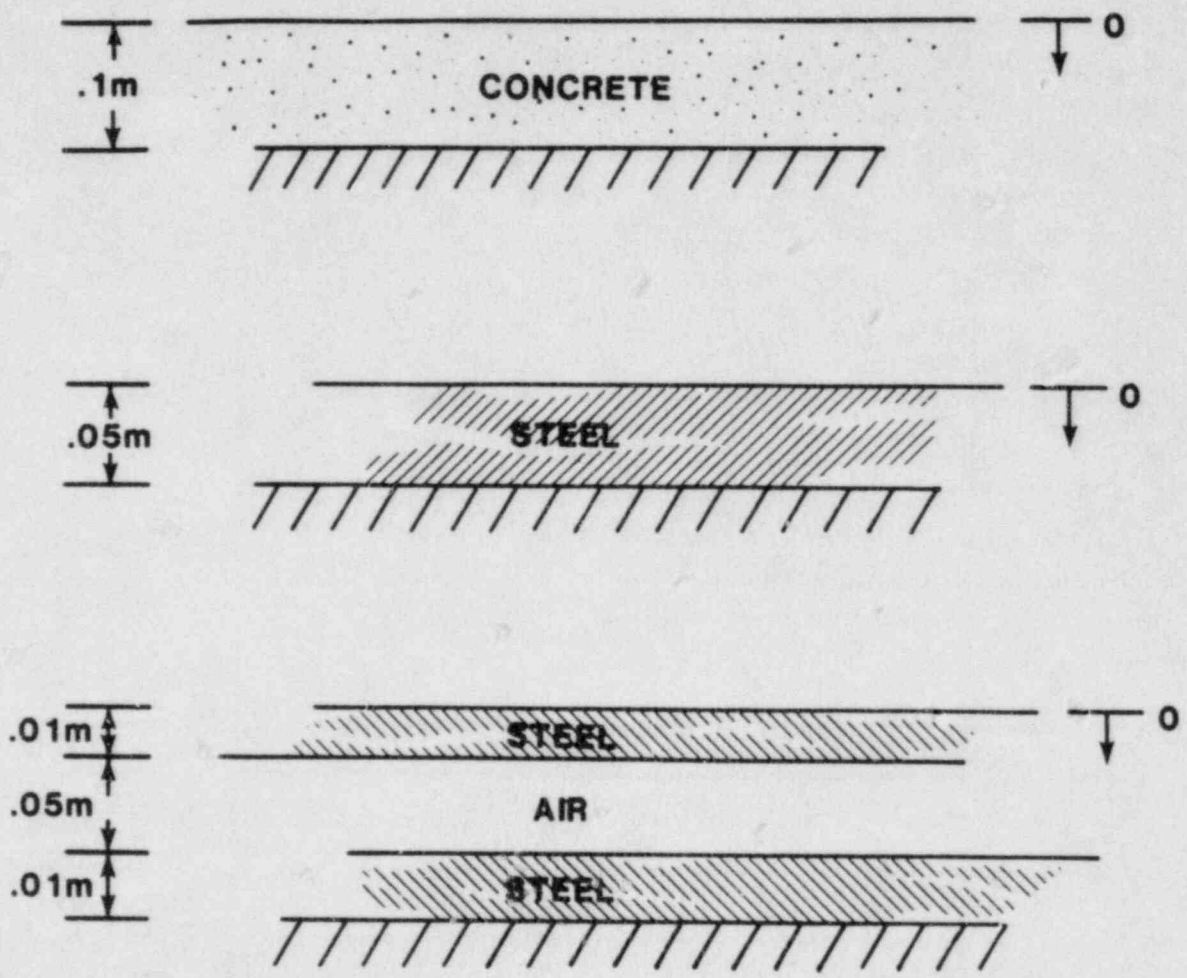

Figure 7. Cross-sections of slabs modeled in example problems.

C.2 Input Data File Generation Using DATGEN

A detailed example of the first deflagration of a multiple burn simulation is presented for example problem 1 of Appendix D (designated as the "base case"). User-input is bracketed by the symbols < > which signify that the return key must be depressed after typing in the response. Computer output is shown in capital letters.

To begin execution of the algorithm codes, the user must begin with line 1 below:

```
<RUN DATGEN SOLVER REACB1>                                    (1)
A>REM DATGEN IS IN DRIVE A, SOLVER SHOULD BE IN DRIVE B       (2)
A>PAUSE STRIKE A KEY WHEN READY                               (3)
<carriage return>                                             (4)
A>IF DATGEN == DATFIL GOTO JKL                                (5)
A>A:DATGEN.EXE                                                (6)
DATA INPUT GENERATOR FOR NRC ALGORITHM CODE                   (7)
WHAT IS THE TIME (INPUT CHARACTER STRING)                     (8)
<12:00 PM >                                                   (9)
WHAT IS THE DATE (INPUT CHARACTER STRING < 10)                (10)
<14 MAR 84>                                                   (11)
INPUT ONE LINE DESCRIPTOR FOR DATA SET - 80 COL MAX           (12)
<EXAMPLE #1 - MULTIPLE BURN SIMULATION - BASE CASE-1st BURN>  (13)
```

Lines 1-11 are part of the preliminary data input and are self-explanatory. Line 5 checks to see if DATGEN is being used interactively. JKL is an internal code label located after line 6. Since line 5 is false, program control is transferred to line 6, and DATGEN will execute interactively with the user. Lines 7-12 correspond to box 1 of the flow chart. Note that the simulation name, "FILNAM2," for this analysis is REACB1 and that all output files will be named "REACB1.***", where "***" are given in Section 4.1.

```
IS THIS PART OF A MULTIPLE BURN SIMULATION?                   (1)
1=YES 0=NO                                                    (2)
<1>                                                           (3)
IS THIS THE FIRST PASS THROUGH THE INPUT GENERATOR            (4)
FOR MULTIPLE BURN ANALYSES (0=NO, 1=YES)                      (5)
```

```
<1>                                                              (6)
DO YOU WANT TO USE PREVIOUSLY GENERATED GEOMETRY                 (7)
DECKS AND CHANGE THE HEAT TRANSFER                               (8)
OR COMBUSTION CALCULATION. (0=N,1=Y)                             (9)
<0>                                                             (10)
```

A multiple burn simulation is chosen (lines 1-3). Lines 4-6 (box 3 of the flow chart) show that a first deflagration is to performed, and that the geometry and heat transfer options must be specified (lines 6-10) since a previously generated data file does not exist. Note that if this were to be a single burn simulation without re-start, a negative response to prompts 1-2 would be required. The prompt of lines 4-5 would then be omitted and the data generation would proceed from line 7.

```
ENTER INITIAL TIME FOR THIS BURN,(S)                             (1)
< 0 >                                                            (2)
ENTER DURATION OF SIMULATION (S)                                 (3)
< 100 >                                                          (4)
UNLESS OTHERWISE SPECIFIED, DATA MUST BE INPUT IN SI UNITS       (5)
ENTER VOLUME (M3) AND AREA (M2)                                  (6)
ENTER DIAMETER (M) OF CONTAINMENT                                (7)
< 5000,1000,17 >                                                 (8)
ENTER NUMBER OF SURFACES                                         (9)
MAXIMUM NUMBER OF SURFACES LIMITED TO THREE                     (10)
< 3 >                                                           (11)
```

Lines 1-4 correspond to box 5 and lines 5-11 to box 6 of the flow chart.

```
**** MATERIAL PROPERTY DATA INPUT SECTION *****                  (1)

THERMAL DIFFUSIVITY UNITS OF M2/S                                (2)
THERMAL CONDUCTIVITY UNITS OF W/M-K                              (3)
ALL LENGTHS, THICKNESSES, AND AREAS GIVEN IN M, M2               (4)
SURFACE EMISSIVITY VALUES < 1.0                                  (5)
NOTE THAT PROPERTY VALUES SHOULD BE EVALUATED                    (6)
AT SOME MEAN TEMPERATURE EXPECTED FROM ANALYSIS                  (7)

MATERIAL AND GEOMETRY INPUTS FOR SURFACE  =  1                   (8)
```

```
INPUT SURFACE AREA, CHARACTERISTIC LENGTH, AND THERMAL          (9)
EMISSIVITY                                                      (10)
<600,10,.8>                                                     (11)
ENTER NUMBER OF MATERIALS (3 OR LESS) COMPRISING SLAB           (12)
<1>                                                             (13)
*** NOTE -- INPUT MATERIAL DATA IN ORDER FURTHEST FROM          (14)
FRONT SURFACE                                                   (15)
ENTER THERMAL DIFFUSIVITY, THERMAL CONDUCTIVITY,                (16)
AND THICKNESS FOR COMPOSITE MATERIAL I=1                        (17)
<5E-7, 1,.1>                                                    (18)
```

Lines 1-18 comprise box 7 of the flow chart, and lines 13-18 will change if a composite slab is specified, as shown below for the piece of equipment:

```
ENTER NUMBER OF MATERIALS (3 OR LESS) COMPRISING SLAB           (12)
<3>                                                             (a)
**** NOTE -- INPUT MATERIAL DATA IN ORDER FURTHEST FROM         (b)
FRONT SURFACE                                                   (c)
ENTER THERMAL DIFFUSIVITY, THERMAL CONDUCTIVITY, AND            (d)
THICKNESS FOR COMPOSITE MATERIAL I=1                            (e)
<1E-5, 55, 1E-2 >                                               (f)
ENTER THERMAL DIFFUSIVITY, THERMAL CONDUCTIVITY, AND            (g)
THICKNESS FOR COMPOSITE MATERIAL I=2                            (h)
< 5E-6, 10, .05 >                                               (i)
ENTER THERMAL DIFFUSIVITY, THERMAL CONDUCTIVITY, AND            (j)
THICKNESS FOR COMPOSITE MATERIAL I=3                            (k)
< 2E-5, 65, 1E-2 >                                              (l)
```

Note that when specifying a slab with more than one material, lines b-c instruct the user to input material data in the order from the back surface of the slab to the front surface. Therefore, lines j-l are for the layer facing the gas (material 3), and lines d-f are for the rear, insulated layer (material 1).

The next section deals with assigning nodal coordinates for the slab. The options for assigning nodes will be shown below and are discussed in Section 3.3 of the user's guide. For a single-material slab (the concrete containment in this example), the output is shown below:

```
<5E-7, 1., .1>                                                    (18)
FOR SINGLE MATERIAL SLABS, THE MESHING MAY BE VARIABLE
OR UNIFORM                                                        (19)
ENTER FRACTION OF WALL THICKNESS TO BE COVERED                    (20)
BY A COARSE MESH, NO. OF COARSE NODES AND NO. OF FINE             (21)
NODES FOR SURFACE 1          DEFAULT INPUT- 0.,0,0                (22)
< .75, 6, 10 >                                                    (23)


NODE NO. = 1  MATERIAL TYPE = 1 POSITION = .1000  BACK SURF       (24)
NODE NO. = 2  MATERIAL TYPE = 1 POSITION = .0875                  (25)
NODE NO. = 3  MATERIAL TYPE = 1 POSITION = .0750                  (26)
NODE NO. = 4  MATERIAL TYPE = 1 POSITION = .0625                  (27)
NODE NO. = 5  MATERIAL TYPE = 1 POSITION = .05                    (28)
NODE NO. = 6  MATERIAL TYPE = 1 POSITION = .0375                  (29)
NODE NO. = 7  MATERIAL TYPE = 1 POSITION = .0250 NODE CHANGE      (30)
NODE NO. = 8  MATERIAL TYPE = 1 POSITION = .0225                  (31)
NODE NO. = 9  MATERIAL TYPE = 1 POSITION = .0200                  (32)
NODE NO. = 10 MATERIAL TYPE = 1 POSITION = .0175                  (33)
NODE NO. = 11 MATERIAL TYPE = 1 POSITION = .0150                  (34)
NODE NO. = 12 MATERIAL TYPE = 1 POSITION = .0125                  (35)
NODE NO. = 13 MATERIAL TYPE = 1 POSITION = .0100                  (36)
NODE NO. = 14 MATERIAL TYPE = 1 POSITION = .0075                  (37)
NODE NO. = 15 MATERIAL TYPE = 1 POSITION = .0050                  (38)
NODE NO. = 16 MATERIAL TYPE = 1 POSITION = .0025                  (39)
NODE NO. = 17 MATERIAL TYPE = 1 POSITION = .0     FRONT SURF      (40)

IS THE NODING SUITABLE (0=N 1=Y)                                  (41)
< 1 >                                                             (42)
INPUT HOW MANY NODAL TEMPS (<6) WILL BE SAVED                     (43)
< 0 >                                                             (44)
```

If 0 were entered in line 42, the code would begin again at line 19, and the user would have to re-input line 23. The nodal spacing in lines 24-40 is variable (changing between nodes 6 and 7). A uniform nodalization may be specified by entering <0,0,n> at line 23, where n is the number of uniform nodes desired. The print-out would be similar to lines 24-40 but the number of nodes and spacing would be different, depending on the value of n. If the default value <0,0,0> were entered at line 23, DATGEN would select a nodal arrangement for the user which would also be similar to lines 24-40 but with a different number of

nodes and nodal spacing. Lines 43-47 allow the user to store temperature values at any 5 (or less) locations in the material as shown below.

```
INPUT HOW MANY NODAL TEMPS (<6) WILL BE SAVED                    (43)
< 5 >                                                            (44)
INPUT NODAL NUMBERS FOR SPATIAL LOCATIONS WHERE THE              (45)
TEMPERATURE VS TIME DATA IS TO BE SAVED                          (46)
< 17,12,7,5,1 >                                                  (47)
```

The nodalization prompts and output for a composite slab used to configure the piece of equipment are shown below:

```
<?E-5, 65, 1E-2>                                                 (l)
THE NODING FOR EACH MATERIAL IN THE COMPOSITE SLAB IS TO
BE UNIFORM.                                                      (m)
HOW MANY NODES IN COMPOSITE MATERIAL I=1                         (n)
< 6 >                                                            (o)
HOW MANY NODES IN COMPOSITE MATERIAL I=2                         (p)
< 5 >                                                            (q)
HOW MANY NODES IN COMPOSITE MATERIAL I=3                         (r)
< 5 >                                                            (s)
NODE NO.=1  MATERIAL TYPE=1  POSITION =.070   BACK SURF          (t)
NODE NO.=2  MATERIAL TYPE=1  POSITION =.068                      (u)
NODE NO.=3  MATERIAL TYPE=1  POSITION =.066                      (v)
NODE NO.=4  MATERIAL TYPE=1  POSITION =.064                      (w)
NODE NO.=5  MATERIAL TYPE=1  POSITION =.062                      (x)
NODE NO.=6  MATERIAL TYPE=1  POSITION =.060  INTERFACE           (y)
NODE NO.=7  MATERIAL TYPE=2  POSITION =.050                      (z)
NODE NO.=8  MATERIAL TYPE=2  POSITION =.040                      (aa)
NODE NO.=9  MATERIAL TYPE=2  POSITION =.030                      (bb)
NODE NO.=10 MATERIAL TYPE=2  POSITION =.020                      (cc)
NODE NO.=11 MATERIAL TYPE=2  POSITION =.010  INTERFACE           (dd)
NODE NO.=12 MATERIAL TYPE=3  POSITION =.008                      (ee)
NODE NO.=13 MATERIAL TYPE=3  POSITION =.006                      (ff)
NODE NO.=14 MATERIAL TYPE=3  POSITION =.004                      (gg)
NODE NO.=15 MATERIAL TYPE=3  POSITION =.002                      (hh)
NODE NO.=16 MATERIAL TYPE=3  POSITION =.0    FRONT SURF          (ii)

IS THE NODING SUITABLE (0=N 1=Y)                                 (jj)
<1>                                                              (kk)
```

```
INPUT HOW MANY NODAL TEMPS (<6) WILL BE SAVED                (11)
<4>                                                          (mm)
INPUT NODAL NUMBERS FOR SPATIAL LOCATIONS WHERE THE          (nn)
TEMPERATURE VS TIME DATA IS TO BE SAVED                      (oo)
<16,11,6,1>                                                  (pp)
```

Note that lines 19-47 and 12, a-pp correspond to box 8. Lines 8-47 (for single material slabs) and lines 8-12, a-pp (for composite slabs) are repeated for the number of user-specified surfaces.

The radiative parameters are now entered:

```
RADIATIVE INPUTS - CONFIGURATION FACTORS AND BEAM LENGTHS     (1)
BEAM LENGTHS IN UNITS OF M, CONFIGURATION FACTORS ARE         (2)
DIMENSIONLESS ( 0< FF < 1 )                                   (3)
SUM OF FFs FOR A SURFACE MUST TOTAL 1.0                       (4)
FF RECIPROCITY RELATIONS MUST BE SATISFIED                    (5)

ENTER BEAM LENGTH BETWEEN SFC 1 AND SFC 1                     (6)
<6>                                                           (7)
ENTER BEAM LENGTH BETWEEN SFC 1 AND SFC 2                     (8)
<12>                                                          (9)
ENTER BEAM LENGTH BETWEEN SFC 1 AND SFC 3                    (10)
<7>                                                          (11)
ENTER BEAM LENGTH BETWEEN SFC 2 AND SFC 1                    (12)
< 12 >                                                       (13)
ENTER BEAM LENGTH BETWEEN SFC 2 AND SFC 2                    (14)
< 10 >                                                       (15)
ENTER BEAM LENGTH BETWEEN SFC 2 AND SFC 3                    (16)
<5>                                                          (17)
ENTER BEAM LENGTH BETWEEN SFC 3 AND SFC 1                    (18)
<7>                                                          (19)
ENTER BEAM LENGTH BETWEEN SFC 3 AND SFC 2                    (20)
<5>                                                          (21)
ENTER BEAM LENGTH BETWEEN SFC 3 AND SFC 3                    (22)
<0>                                                          (23)

ENTER CONFIGURATION FACTOR FROM SFC 1 TO SFC 1               (24)
<.599833>                                                    (25)
ENTER CONFIGURATION FACTOR FROM SFC 1 TO SFC 2               (26)
```

```
<.4>                                                    (27)
ENTER CONFIGURATION FACTOR FROM SFC 1 TO SFC 3          (28)
<1.67E-4>                                               (29)
ENTER CONFIGURATION FACTOR FROM SFC 2 TO SFC 1          (30)
<.6>                                                    (31)
ENTER CONFIGURATION FACTOR FROM SFC 2 TO SFC 2          (32)
<.399625>                                               (33)
ENTER CONFIGURATION FACTOR FROM SFC 2 TO SFC 3          (34)
<3.75E-4>                                               (35)
ENTER CONFIGURATION FACTOR FROM SFC 3 TO SFC 1          (36)
<.4>                                                    (37)
ENTER CONFIGURATION FACTOR FROM SFC 3 TO SFC 2          (38)
<.6>                                                    (39)
ENTER CONFIGURATION FACTOR FROM SFC 3 TO SFC 3          (40)
<0>                                                     (41)

CONFIGURATION FACTOR RECIPROCITY CHECK                  (42)
```

If line 17 were entered as <9>, reciprocity would not hold between surfaces 2 and 3 for the beam lengths. The following error message is then printed:

```
BEAM LENGTHS BETWEEN SURFACES DO NOT MATCH               (a)
BL FROM 2 TO 3 EQUALS 9                                  (b)
BL FROM 3 TO 2 EQUALS 5                                  (c)
INPUT THE CORRECT BL FOR THESE SURFACES                  (d)
<5>                                                      (e)
```

Similarly, if line 27 were entered as <.3>, the sum of the configuration factors for surface 1 would not sum to unity. The following error message is then printed:

```
CONFIGURATION FACTORS FOR SURFACE 1 DID NOT
TOTAL TO 1.0 -- TRY AGAIN
```

Lines 24-29 would then be repeated so that the correct values for the configuration factors of surface 1 could be ente ed. If lines 37,39,41 were entered

as <.3>, <.5>, <.2> , reciprocity would not be satisfied between surfaces 2 and 3 and 1 and 3. The following error message is provided:

```
RECIPROCITY RELATIONS WERE NOT SATISFIED                          (a)
F FROM 1 TO 3 EQUALS 1.67E-4 AND AREA = 600.                      (b)
F FROM 3 TO 1 EQUALS .3 AND AREA = .25                            (c)

***** RESTART CONFIGURATION FACTOR INPUT *****                    (d)
CHECK ALL CONFIGURATION FACTORS TO INSURE THAT RECIPROCITY         (e)
HOLDS AND THAT Fs FOR A SURFACE TOTAL 1.0                         (f)
```

Lines 24-41 would then be repeated and the user would enter the correct configuration factors. Lines 1-42 correspond to box 9 in the flow chart.

The next section of the input data generation deals with the spray option:

```
DO YOU WANT SPRAYS? 1=YES 0=NO                                    (1)
<0>                                                               (2)
DO YOU WANT TO INCLUDE CONVECTIVE .....                           (3)
```

For the example problem 2 in Appendix D, where sprays are assumed operative, the following prompts must be answered.

```
DO YOU WANT SPRAYS? 1=YES 0=NO                                    (1)
<1>                                                               (2)
THE SPRAY MODEL USES A RUNGE KUTTA  OLVER TO INTEGRATE            (3)
THE FIRST ORDER ODE WHICH GOVERNS THE DROPLET EVAPORATION         (4)
OVER THE USER SPECIFIED FALL DISTANCE. THE SPRAY DROPLETS         (5)
ARE ASSUMED TO BE AT SATURATION. THE SPATIAL INCREMENT SHOULD     (6)
BE AROUND THE TOTAL FALL DISTANCE/100, AND FOR SOME CONDITONS     (7)
MIGHT NEED TO BE SMALLER FOR CONVERGENCE. BE SURE THAT THE        (8)
FALL DISTANCE IS EVENLY DIVISIBLE BY THE SPATIAL INCREMENT.       (9)
**** ENTER FALL DISTANCE (M) & SPATIAL INCREMENT (M) ****        (10)
<17,.10>                                                          (11)
ENTER FLOW RATE (GPM) AND NUMBER OF DROP SIZES (<4)               (12)
< 1000, 2 >                                                       (13)
ENTER FREQUENCY (FRACTION 0 < F < 1)                              (14)
AND DIAMETER (MICRONS) OF DROP SIZE 1                             (15)
< .5,400 >                                                        (16)
```

```
ENTER FREQUENCY                                          (17)
AND DIAMETER (MICRONS) OF DROP SIZE 2                    (18)
< .5,700 >                                               (19)
DO YOU WANT TO INCLUDE CONVECTIVE ....                   (20)
```

The lines 1-3 and 1-20 correspond to box 10 of the flow chart.

The user is now prompted to input the convective options (box 11)

```
DO YOU WANT TO INCLUDE CONVECTIVE HEAT TRANSFER?         (1)
1=YES 0=NO                                               (2)
<1>                                                      (3)

CONDENSATION MODEL DESCRIPTION                           (4)

TWO METHODS ARE AVAILABLE TO CALCULATE                   (5)
THE GAS/LIQUID INTERFACE TEMPERATURE                     (6)

IGIVE = 0:                                               (7)

QUASI-STEADY ASSUMPTION; THE INTERFACE TEMPERATURE IS    (8)
ITERATED UNTIL THE HEAT FLUX INCIDENT ON THE LIQUID FILM (9)
IS EQUAL TO THE FLUX ACROSS THE FILM AS CALCULATED USING (10)
NUSSELT FILM ANALYSIS. THIS METHOD MAY NOT CONVERGE FOR  (11)
LARGE MOLE FRACTIONS OF STEAM.                           (12)

IGIVE = 1:                                               (13)

THE INTERFACE TEMPERATURE IS SET EQUAL TO THE WALL       (14)
TEMPERATURE FOR THE STEAM PARTIAL PRESSURE. THIS OPTION  (15)
(IGIVE=1) DOES NOT REQUIRE ANY ITERATIVE CALCULATIONS    (16)
AND THUS RUNS CONSIDERABLY FASTER.                       (17)

 ***** INPUT IGIVE *****                                 (18)
<1> or <0>                                               (19)

FORCED CONVECTION CORRELATION DESCRIPTION                (20)

TWO OPTIONS ARE AVAILABLE TO COMPUTE THE FORCED          (21)
CONVECTION CORRELATION                                   (22)
```

```
ICHS = 0:                                                          (23)

REYNOLDS NUMBER CORRELATIONS: STEADY-STATE CORRELATIONS            (24)
FOR LAMINAR AND TURBULENT FLOW OVER A FLAT PLATE. THESE            (25)
MODELS REQUIRE THE INPUT OF A FREE STREAM GAS VELOCITY             (26)
WHICH IS CONSTANT FOR THE ANALYSIS.                                (27)

ICHS = 1:                                                          (28)

MEANS-ULRICH CORRELATION: A TRANSIENT FORCED CONVECTION            (29)
CORRELATION BASED ON A FOURIER NUMBER.                             (30)

***** INPUT ICHS *****                                            (31)
<1>                                                                (32)
ICE CONDENSER.....
```

Note that the same questions are asked for either choice of IGIVE. If the alternate convection option (Reynolds number) is selected, then the following additional prompt must be answered.

```
***** INPUT ICHS *****                                            (31)
<0>                                                                (32)
ENTER BULK VELOCITY; METERS PER SECOND                             (a)
ANALYSIS WILL ASSUME CONSTANT FREE STREAM VELOCITY                 (b)
THROUGHOUT CALCULATION                                             (c)
< .3 >                                                             (d)
ICE CONDENSER....                                                  (e)
```

Lines 1-33 and 31-e comprise box 11. Lines 4-19 comprise part (a) of box 11 and lines 20-32 and 31-e comprise part b of box 11. Lines 31, 32, a-e show that the print-out differs if the Reynolds number correlations are chosen instead of the Means-Ulrich correlation (lines 29-32). The print-out after line 19 is the same regardless of the condensation model chosen.

If the user does not wish to include convective heat transfer during the simulation, the output would be:

```
DO YOU WANT TO INCLUDE CONVECTIVE HEAT TRANSFER?                   (1)
```

```
1=YES 0=NO                                                    (2)
< 0 >                                                         (3)
ICE CONDENSER .....
```

Note that lines 4-32 or 31, 32, a-e are not printed out when convective heat transfer is not specified.

The user next can select the ice-condenser engineering model option or the containment leak option (box 12).

```
ICE CONDENSER (IC) REACTOR ENGINEERING OPTION                 (1)
OR LEAK TO ATMOSPHERE PROMPTS                                 (2)
***** YOU MAY CHOOSE EITHER OPTION OR NONE *****             (3)
IC REACTOR CALCULATION? 1=YES 0=NO                            (4)

FOR LOWER COMPARTMENT OF IC REACTOR CALCULATIONS ONLY         (5)
< 0 >                                                         (6)
DO YOU WANT TO SIMULATE LEAKS? (0=NO 1=YES)                   (7)
< 0 >                                                         (8)
```

Lines 1-8 represent box 12 of the flow chart. The ice-condenser engineering option and containment leak options have not been chosen. For example problem 3 in Appendix D which includes the ice-condenser engineering option, the following prompts must be answered.

```
IC REACTOR CALCULATION? 1=YES 0=NO                            (4)
FOR LOWER COMPARTMENT OF IC REACTOR CALCULATIONS ONLY         (a)
< 1 >                                                         (b)
ENTER VOLUME OF UPPER COMPARTMENT (M3)                        (c)
<10000>                                                       (d)
ENTER GAS TEMPERATURE IN UPPER COMPARTMENT (K)                (e)
<320>                                                         (f)
ENTER FAN RATING,CFM                                          (g)
<40000>                                                       (h)
ENTER FAN OPENING AREA (M**2)                                 (i)
<1.5>                                                         (j)
ENTER IC INLET AREA (M**2)                                    (k)
<2.0)                                                         (l)
ENTER THE TEMPERATURE OF THE GAS EXITTING THE ICE             (m)
```

```
CONDENSER - NO STEAM WILL BE ALLOWED OUT OF IC                    (n)
< 290 >                                                           (o)
ENTER THE MAX PRESSURE DIFFERENCE (ATM) AT WHICH THE              (p)
FAN OPERATION MAY BEGIN                                           (q)
< .005 >                                                          (r)
INPUT THE INITIAL ......                                          (s)
```

If the ice-condenser option were specified for the first deflagration of a multiple burn simulation, the upper compartment gas temperature must be specified. This temperature will change during the simulation. In generating additional data files in multiple burn sequences the following option is provided to allow the user to modify this temperature. Note that the last upper-compartment gas temperature would be written to file "FLOWS" from the previous deflagration analysis.

```
ENTER GAS TEMPERATURE (K) IN UPPER COMPARTMENT                    (e)
<320>                                                             (f)
** THE UPPER COMPARTMENT GAS TEMPERATURE MAY BE CHANGED
IF DESIRED **                                                     (f1)
CONSULT FINAL GAS TEMPERATURE IN "FLOWS" TO DECIDE IF             (f2)
PREVIOUSLY INPUT TEMPERATURE IS REASONABLE                        (f3)
*** DO YOU WANT TO MODIFY THE TEMP (0=N,1=Y)                      (f4)
<1>                                                               (f5)
ENTER THE UPDATED UPPER COMPARTMENT GAS TEMP IN K                 (f6)
<312.65>                                                          (f7)
ENTER FAN RATING,CFM                                              (g)
```

If the user would rather include the containment leak option, the output is presented below (as included in example problem 4 of Appendix D):

```
YOU MAY CHOOSE EITHER OPTION OR NONE                              (3)
IC REACTOR CALCULATION? 1=YES 0=NO                                (4)
FOR LOWER COMPARTMENT OF IC REACTOR CALCULATIONS ONLY             (5)
< 0 >                                                             (6)
DO YOU WANT TO SIMULATE LEAKS? (0=NO,1=YES)                       (7)
< 1 >                                                             (8)
ENTER LEAK AREA (M2), ENVIRONMENT PRESSURE (ATM), AND             (a)
TEMPERATURE (K)                                                   (b)
< .05, 1.0, 300. >                                                (c)
```

The user must now select information specified by box 13 of the flow chart: the time step, print interval, temperature change for time-step acceleration and maximum time step allowed.

```
INPUT THE INITIAL TIME STEP (SEC) FOR THE ANALYSIS.          (1)
WE RECOMMEND AN INITIAL STEP SIZE OF .01-.05 SEC             (2)
< .05 >                                                      (3)
IF DESIRED, YOU MAY ALLOW THE TIME STEP TO INCREASE          (4)
WHEN THE CHANGE IN GAS TEMPERATURE DURING A TIME STEP        (5)
IS LESS THAN "DTT", WHERE "DTT" IS SOME USER SPECIFIED       (6)
VALUE. THE USER MUST ALSO SPECIFY THE MAXIMUM TIME           (7)
ALLOWED. IT IS RECOMMENDED THAT THE MAXIMUM                  (8)
TIME STEP BE NO GREATER THAN 5.0 SEC FOR MOST                (9)
SIMULATIONS AND LESS IF LEAKS OR ICE CONDENSER              (10)
ENGINEERING OPTIONS ARE USED. IF YOU DO NOT WANT THE        (11)
TIME STEP TO CHANGE, INPUT DTT = 0. NOTE ALSO THAT IF       (12)
A LARGE DTT IS USED, YOU SHOULD SPECIFY A SMALL PRINT       (13)
INTERVAL SO THAT THE OUTPUT FILE WILL PROVIDE ENOUGH        (14)
DATA TO BE OF USE.                                          (15)

PRINT EVERY N-TH LINE, ENTER N                              (16)
<5>                                                         (17)
INPUT "DTT" FOR THE TIME STEP ACCELERATION.                 (18)
<2>                                                         (19)
INPUT MAXIMUM TIME STEP (S) ALLOWED                         (20)
<5>                                                         (21)
```

The user is now ready to enter the combustion data (box 14 of the flow chart). The first prompts provided are for the "base case" example problem. For this particular problem, note that water spray systems are inoperative.

```
**** COMBUSTION DATA CALCULATION SECTION ****                (1)

ENTER GAS CONSTITUENTS PRIOR TO COMBUSTION                  (2)
NOTE THAT THE SUM OF THESE MOLE FRACTIONS MUST TOTAL TO 1.0  (3)
H2 AND CO COMBUSTION ARE ACCOUNTED FOR IN THIS MODEL        (4)
CO2 IS INCLUDED AS A DILUENT IN THE COMBUSTION CALCULATION  (5)
THE RADIATION MODEL IN THE ALGORITHM INCLUDES ONLY STEAM    (6)
```

```
AND OMITS THE CO2 AND CO PARTICIPATING SPECIES                    (7)
FOR PROBLEMS IN WHICH EXPANSION OR GAS LEAKAGE IS ALLOWED,        (8)
THE H2 AND CO TO BE BURNED WILL REMAIN IN THE CONTAINMENT.        (9)
THE OTHER SPECIES MAY LEAVE THE VOLUME THRU THE DESIGNATED       (10)
PASSAGE AREA DURING AND FOLLOWING COMBUSTION.                    (11)

  ********** WARNING **********                                  (12)
IF THE INITIAL STEAM CONDITION IS GREATER THAN APPROXIMATELY     (13)
90 % SATURATED, THE CONDENSATION MODEL MIGHT  FAIL TO            (14)
CONVERGE. THIS APPLIES PRIMARILY TO SIMULATIONS WHERE THE        (15)
GAS AND WALL TEMPERATURES ARE LOW, -i.e. <350K .                 (16)

ENTER INITIAL GAS PRESSURE (ATM) & TEMPERATURE (K)               (17)
< 1.20,325 >                                                    (18)

**** ENTER H2,O2,H2O,N2,CO2,CO MOLE FRACTIONS *****              (19)
<.08, .29, .01, .62, 0, 0>                                      (20)
IS THE H2-AIR COMBUSTION TO BE COMPLETE (0=N,1=Y)               (21)
<0>                                                             (22)
WHAT IS THE COMPLETION PERCENTAGE (0<X<100)                     (23)
NOTE THAT THE UNBURNED H2 IS TREATED AS AN INERT SPECIES        (24)
WHICH SERVES ONLY AS A DILUENT IN THE COMBUSTION                (25)
CALCULATIONS. NOTE THAT CO-O2 COMBUSTION IS TO BE COMPLETE      (26)
< 85 >                                                          (27)

    ***** PRE-COMBUSTION CONDITIONS *****                       (28)

INITIAL GAS PRESSURE (ATM) = 1.20                               (29)
INITIAL GAS TEMPERATURE (DEG K) = 325.0                         (30)
INITIAL MOLE WT = 26.98                                         (31)
INITIAL GAS DENSITY (GM/CC) = 1.2113607E-03                     (32)
INITIAL COMPOSITION OF COMBUSTIBLE GAS                          (33)
  H2 = 6.8E-2    O2 = .29                                       (34)
  N2 = .62       INERT (UNBURNED HYDROGEN) = 1.2E-2             (35)
  CO2 = .00000    CO = .00000                                   (36)
  WATER VAPOR MOLE FRACTION = .01                               (37)
  ADDITIONAL MOLE OF H2O IN LIQUID = 0.                         (38)

  ***** AIC FINAL CONDITIONS *****                              (39)

FINAL PRESSURE (ATM) = 3.74                                     (40)
```

```
FINAL TEMPERATURE (DEG K) = 1048.63                              (41)
FINAL GAS MOLE WEIGHT = 27.9296                                  (42)
FINAL GAS DENSITY = 1.21136E-03                                  (43)
FINAL COMPOSITION MOLE FRACTIONS                                 (44)
  H2 = 2.3728E-11    O2 = .2650                                  (45)
  H2O = 8.0745E-02   N2 = .6418                                  (46)
  OH = 0.0           H = 1.6931E-14                              (47)
  O = 1.7276E-10     NO = 5.4748E-04                             (48)
  INERT(UNBURNED H2) = 1.2422E-2                                 (49)
  CO2 = 0.CO         CO = 0.00                                   (50)

IS THE FINAL TEMPERATURE SUITABLE? (0=N,1=Y)                     (51)
< 1 >                                                            (52)
```

Lines 1-27 are included in box 14 of the flow chart and lines 28-52 are part of box 15 (part b).

Three errors can occur during the inputting of the gas constituents (lines 4-20). First the mole fractions must sum to unity. If they do not, the following error message is printed (starting from line 20):

```
< .08,.2,.27,.47,0.,0.>                                          (20)

PRE-COMBUSTION MOLE FRACTIONS DID NOT SUM TO 1.0                 (a)
TRY INPUTTING THE MOLE FRACTIONS AGAIN                           (b)
```

After line b is printed, the user must re-enter all of the mole fractions.

Second, when beginning a simulation at low gas and wall temperatures, the user can specify too large of a steam mole fraction resulting in a supersaturated mixture (non-equilibrium case). The following error message is printed:

```
<.08,.2,.7,.020, 0,0>                                            (20)

INPUT INITIAL STEAM MOLE FRACTION IS TOO HIGH.                   (a)
THE SATURATION PRESSURE FOR THE INITIAL STEAM TEMPERATURE        (b)
INPUT IS .1322 ATM, WHICH IS LESS THAN THE INITIAL STEAM         (c)
PARTIAL PRESSURE. THUS, THE GAS IS SUPERSATURATED AND IS NOT     (d)
IN EQUILIBRIUM. TRY INPUTTING ALL MOLE FRACTIONS AGAIN.          (e)
```

Third, the AIC results may be suspect, if the quantity of steam and/or suspended liquid water is too large. During the AIC calculation, an energy balance term is computed. If this balance term is greater than 1.E-2, the accuracy of the results may be poor, and the following warning is printed:

```
 CO2 = 0.00        CO = 0.00                                          (50)

ENERGY BALANCE PARAMETER IS TOO LARGE -- INDICATES THAT THE          (a)
INITIAL CONDITIONS FOR COMBUSTION MAY BE NONPHYSICAL. IF YOU         (b)
ARE SATISFIED WITH THESE CONDITIONS, ANSWER THE NEXT QUESTION        (c)
AS A YES.                                                            (d)
****** THIS MESSAGE IS ONLY A WARNING ******                        (e)
```

Note that this message is only a warning and the the values can be used if they are acceptable to the user.

There are two additional permutations possible during this part of the combustion calculation which result only if the water-spray system has been previously prompted to be operative (box 10). If so, the following additional prompts (included in box 15a) must be answered.

```
WHAT IS THE COMPLETION PERCENTAGE (0<X<100)                          (23)
NOTE THAT THE UNBURNED H2 IS TREATED AS AN INERT SPECIES             (24)
WHICH SERVES ONLY AS A DILUENT IN THE COMBUSTION                     (25)
CALCULATIONS. NOTE THAT CO-O2 COMBUSTION IS TO BE COMPLETE           (26)
< 85 >                                                               (27)
DO YOU WANT TO MODEL SPRAYS ON DURING COMBUSTION? (0=N, 1=Y)         (a)
IF SO, THEN A COMBUSTION CALCULATION IS PERFORMED WHICH              (b)
INCLUDES SUSPENDED LIQUID WATER IN THE VOLUME OF                     (c)
GASES TO BE COMBUSTED IF YOU ANSWER YES,THIS                         (d)
MEANS THAT SPRAYS WERE ON BEFORE AND DURING COMBUSTION.              (e)
< 0 >                                                                (f)
```

By answering "no" to prompt a-e, the user has indicated that the spray systems are to be operative upon completion of the combustion process. By answering "yes", on the other hand, the user is indicating that the sprays are

on before and during combustion and that there is suspended water in the combustible gas due to sprays.

```
DO YOU WANT TO MODEL SPRAYS ON DURING COMBUSTION? (0=N,1=Y)     (a)
IF SO, THEN A COMBUSTION CALCULATION IS PERFORMED WHICH         (b)
INCLUDES SUSPENDED LIQUID WATER IN THE VOLUME OF                (c)
GASES TO BE COMBUSTED. IF YOU ANSWER YES,THIS                   (d)
MEANS THAT SPRAYS WERE ON BEFORE AND DURING COMBUSTION.         (e)
< 1 >                                                           (f)
THE TIME (MIN) IT TAKES AN AVERAGE DROP TO PASS THROUGH         (g)
THE FALL DISTANCE ASSUMING NO INITIAL VELOCITY IS 3.1E-2        (h)
COMPUTED VOLUMETRIC WATER ADDITION % = 2.349E-3                 (i)
IS THIS QUANTITY OF SUSPENDED WATER ACCEPTABLE (0=N,1=Y)        (j)
< 1 >                                                           (k)
```

If the suspended water percentage is not satisfactory, the user can answer "no" to prompt h and the following prompts must be answered

```
IS THIS QUANTITY OF SUSPENDED WATER ACCEPTABLE (0=N,1=Y)        (j)
< 0 >                                                           (k)
THE SPRAY MODEL USES A RUNGE KUTTA SOLVER TO INTEGRATE          (l)
THE FIRST ORDER ODE WHICH GOVERNS THE DROPLET EVAPORATION       (m)
OVER THE USER SPECIFIED FALL DISTANCE. THE SPRAY DROPLETS       (n)
ARE ASSUMED TO BE AT SATURATION. THE SPATIAL INCREMENT SHOULD   (o)
BE AROUND THE TOTAL FALL DISTANCE/100, AND FOR SOME CONDITONS,  (p)
MIGHT NEED TO BE SMALLER FOR CONVERGENCE. BE SURE THAT THE      (q)
FALL DISTANCE IS EVENLY DIVISIBLE BY THE SPATIAL INCREMENT.     (r)
**** ENTER FALL DISTANCE (M) & SPATIAL INCREMENT (M) ****       (s)
<17,.10>                                                        (t)
THE TIME (MIN) IT TAKES AN AVERAGE DROP TO PASS THROUGH         (u)
THE FALL DISTANCE ASSUMING NO INITIAL VELOCITY IS 3.1E-2        (v)
COMPUTED VOLUMETRIC WATER ADDITION % = 2.349E-3                 (w)
IS THIS QUANTITY OF SUSPENDED WATER ACCEPTABLE (0=N,1=Y)        (x)
< 1 >                                                           (z)
```

When the quantity of suspended water is acceptable, an AIC calculation is performed. Below are the results which were obtained for the second deflagration calculation of the sprays operative example (problem 2) given in Appendix D.

```
     ***** PRE-COMBUSTION CONDITIONS *****                          (28)

 INITIAL GAS PRESSURE (ATM) = 1.58                                  (29)
 INITIAL GAS TEMPERATURE (DEG K) = 351                              (30)
 INITIAL MOLE WT = 24.22                                            (31)
 INITIAL GAS DENSITY (GM/CC) = 1.325E-3                             (32)
 INITIAL COMPOSITION OF COMBUSTIBLE GAS                             (33)
   H2 = 6.8E-2     O2 = .20                                         (34)
   N2 = .47        INERT (UNBURNED HYDROGEN) = 1.2E-2               (35)
   CO2 = .00000    CO = .00000                                      (36)
   WATER VAPOR MOLE FRACTION = .25                                  (37)
   ADDITIONAL MOLE OF H2O IN LIQUID = 2.38E-2                       (38)

   ***** AIC FINAL CONDITIONS *****                                 (39)

 FINAL PRESSURE (ATM) = 4.36                                        (40)
 FINAL TEMPERATURE (DEG K) = 977.83                                 (41)
 FINAL GAS MOLE WEIGHT = 24.9                                       (42)
 FINAL GAS DENSITY = 1.347E-3                                       (43)
 FINAL COMPOSITION MOLE FRACTIONS                                   (44)
   H2 = 1.0213E-11   O2 = .1677                                     (45)
   H2O = .3453       N2 = .4748                                     (46)
   OH = 0.0          H = 2.042E-15                                  (47)
   O = 1.62E-11      NO = 1.748E-5                                  (48)
   INERT (UNBURNED H2) = 1.212E-2                                   (49)
   CO2 = 0.00        CO = 0.00                                      (50)

 IS THE FINAL GAS STATE SUITABLE? (0=N,1=Y)                         (51)
 < 1 >                                                              (52)
```

After the user decides that the final state and composition are reasonable, an additional AIC calculation is performed if the user has opted for suspended liquid in the combustible gas. In the latter calculation, the identical pre-combustion gas conditions are used (line 20) and the suspended liquid is omitted. The values computed during this calculation are written to NRCDAT and are used during the combustion simulation in SOLVER. During this simulation, the spray model is operative during and following combustion. The final gas state will thus be different from the AIC results obtained with suspended liquid included, although

these differences should be small. Typical results for the "dry" AIC calculation using the previously given initial pre-combustion conditions are provided below.

```
IF THE SAME QTY OF HYDROGEN WERE BURNED W/ SPRAYS OFF --      (53)
WE WOULD OBTAIN THE FOLLOWING AIC RESULTS                     (54)

    ***** PRE-COMBUSTION CONDITIONS *****                     (55)

INITIAL GAS PRESSURE (ATM) = 1.58                             (56)
INITIAL GAS TEMPERATURE (DEG K) = 351                         (57)
INITIAL MOLE WT = 24.22                                       (58)
INITIAL GAS DENSITY (GM/CC) = 1.3257E-3                       (59)
INITIAL COMPOSITION OF COMBUSTIBLE GAS                        (60)
  H2 = 6.8E-2          O2 = .20                               (61)
  N2 = .47             INERT (UNBURNED H2) = 1.2E-2           (62)
  CO2 = 0.00           CO = 0.00                              (63)
  WATER VAPOR MOLE FRACTION = .25                             (64)
 ADDITIONAL MOLE OF H2O IN LIQUID = 0.0                       (65)

  ***** AIC FINAL CONDITIONS *****                            (66)

FINAL PRESSURE (ATM) = 4.48                                   (67)
FINAL TEMPERATURE (DEG K) = 1030.37                           (68)
FINAL GAS MOLE WEIGHT = 25.072                                (69)
FINAL GAS DENSITY (GM/CC) = 1.3257E-3                         (70)
FINAL COMPOSITION MOLE FRACTIONS                              (71)
  H2 = 6.96E-11        O2 = .1718                             (72)
  H2O = .3292          N2 = .4865                             (73)
  OH = 0.00            H = 1.763E-14                          (74)
  O =8.022E-11         NO = 3.258E-5                          (75)
  INERT (UNBURNED H2) = 1.2422E-2                             (76)
  CO2 = 0.00           CO = 0.00                              (77)
```

An additional option is provided upon completion of the first AIC calculation. That is, the user is prompted about whether the final AIC results are suitable for the simulation to be performed. This option has been included to allow the user to be able to match the peak gas conditions of some other simulation. To do so, the user can alter the initial gas composition, the hydrogen:air combustion completeness, and,if sprays are operative during combustion, the quantity of

suspended water in the combustible gas. If the final AIC gas state is not suitable, the following prompts are printed:

```
IS THE FINAL GAS STATE SUITABLE? (1=Y,0=N)                          (51)
< 0 >                                                               (a)
REPEAT THE COMBUSTION CALCULATIONS                                  (b)

THE USER HAS OPTIONS TO MODIFY THE AIC STATE                        (c)
THE H2:AIR COMBUSTION COMPLETION MAY BE VARIED                      (d)
IF SPRAYS ARE OPERATIVE< THE QTY OF SUSPENDED                       (e)
LIQUID CAN BE MODIFIED BY CHANGING THE SPRAY FALL DISTANCE          (f)
THE GAS COMPOSITION PRIOR TO COMBUSTION MAY BE ALTERED              (g)
ANY COMBINATION OF THE ABOVE OPTIONS CAN BE                         (h)
USED IF THE USER STARTS BY CHANGING THE GAS COMPOSITION             (i)

CHANGE THE INITIAL CAS COMPOSITION (0=N,1=Y)?                       (j)
<1>                                                                 (k)
```

If the answer to prompt j is "yes", the user is returned to line 19 above and can modify the pre-combustion conditions to achieve the desired final combustion conditions. If the answer to prompt j is "no", then the following prompts are written if suspended water is to be included:

```
CHANGE THE INITIAL GAS COMPOSITION (0=N,1=Y)?                       (j)
<0>                                                                 (k)
CHANGE THE SUSPENDED LIQUID QTY (0=N,1=Y)?                          (l)
<1>                                                                 (m)
```

If the answer to prompt l is "yes", the user is returned to line l (following statement 27) above to modify the water droplet spray fall-time. If the answer is "no", or if the suspended liquid option is not applicable, then the following statement is written to the screen,

```
ONLY REMAINING OPTION IS TO MODIFY COMBUSTION COMPLETENESS          (n)
```

and the user is returned to line 23 above to modify the completeness percentage.

When the answer to prompt 51 is "yes", the AIC computed energy release is printed to the screen, concluding the AIC calculation segment of DATGEN. The remaining prompts for the combustion section depend upon whether the user wants to treat the combustion process as adiabatic or non-adiabatic (box 16). When heat transfer during combustion is specified, the adiabatic isochoric combustion energy is released over a period of time equal to the burn length divided by the flame speed such that the gas temperature increases nearly linearly. Heat transfer calculations are also performed in SOLVER during combustion. The gas temperature and pressure will increase but will not reach the AIC gas state because the gas is losing energy due to heat transfer while it is gaining energy due to combustion. When no heat transfer during combustion is specified, the adiabatic isochoric combustion energy is released instantaneously to the gas, and the final AIC gas state are used as the peak gas state following combustion. If heat transfer is to be included during combustion then the following prompts occur. Note that if the spray systems are operative during combustion or if the ice-condenser engineering option is specified "on", the combustion analysis must be non-adiabatic and lines 1-3 (below) are not printed to the screen. Prompting begins at line 4. Statements to these effects are provided in DATGEN, but are not shown below.

```
DO YOU WANT TO SIMULATE HEAT TRANSFER DURING                    (1)
COMBUSTION (1=YES, 0=NO)                                        (2)
< 1 >                                                           (3)
ENTER FLAME SPEED (M/S) AND BURN LENGTH (M)                     (4)
FLAME SPEED DATA ARE AVAILABLE FROM FITS AND VGES               (5)
< 5,15 >                                                        (6)
ENTER INITIAL ........
```

If the user wants to model an adiabatic combustion process, then:

```
DO YOU WANT TO SIMULATE HEAT TRANSFER DURING                    (1)
COMBUSTION (1=YES, 0=NO)                                        (2)
< 0 >                                                           (3)
ENTER INITIAL ........
```

The final information which the user must specify is the initial temperature for the surfaces and equipment (box 17). It is assumed that prior to the first combustion, the slabs are isothermal and in thermal equilibrium with each other.

```
ENTER INITIAL WALL TEMP (K) GREATER THAN 283                    (1)
NOTE THAT TWALL INITIAL MUST NOT BE EQUAL TO                    (2)
TGAS INITIAL. THE INITIAL GAS TEMPERATURE IS 325                (3)
< 324 >                                                         (4)
```

The input deck generation for the first deflagration of a multiple burn scenario is now complete. Two data files named NRCDAT and NRCDAT.NOD are provided for use in SOLVER. The final output prompts for this section are given below:

```
   **** INPUT DECK GENERATION COMPLETE ****                     (1)
TO RUN THIS INPUT, YOU MUST ASSIGN THIS FILE                    (2)
DESIGNATED AS "NRCDAT.DAT" TO "DATA" PRIOR                      (3)
TO RUNNING THE DRIVER PROGRAM.                                  (4)
IN ADDITION, DATA STORED IN "NRCDAT.NOD" MUST                   (5)
BE DESIGNATED AS "NODES" -- GOOD LUCK.                          (6)
```

C.3 SOLVER Execution

Upon completion of the input data generation, the procedure file RUN.BAT prints the following lines:

```
A> COPY A:NRCDAT B:DATA                                          (1)
          1 file(s) copied                                       (2)
A> COPY A:NRCDAT.NOD B:NODES                                     (3)
          1 file(s) copied                                       (4)
A>REM  THE FILES NRCDAT AND NRCDAT.NOD                           (5)
       ARE COPIED TO DRIVE B AND RENAMED DATA                    (6)
       AND NODES                                                 (7)
A>B:                                                             (8)
B>B: SOLVER.EXE                                                  (9)
```

Lines 1-6 indicate that NRCDAT and NRCDAT.NOD are copied to disk 2 in drive B and renamed DATA and NODES, respectively, to be used in SOLVER. Line 8 indicates that drive B becomes the default drive, and line 9 states that the PC is executing SOLVER.

The time, date, title of the simulation, and a summary of the data entered into DATGEN are printed to the screen as shown below for the base case described in the previous section. A nomenclature for these variables is provided in Appendix E.

```
EXAMPLE #1 -- MULTIPLE BURN SIMULATION -- BASE CASE - 1st BURN

 DATA SET GENERATED AT  12:00 PM  ON  14 MAR 84

** SIMULATION PARAMETERS: IBRN,IMUL,TIME,FTIME **
          1            1  0.0000000E+00   100.0000
**** GEOMETRY PARAMETERS: VOL,AREA,VDIA,INS ****
  5000.000       1000.000       17.00000              3
*** SURFACE I PARAMETERS: AREA,L,EMIS,IMAT ***
  600.0000       10.00000      0.8000000              1
**** MATERIAL PARAMETERS: ALPHA,K,THICK ****
 5.0000000E-07   1.000000      0.1000000
*** NUMBER OF NODES FOR SURFACE I ***          17
**** NO. OF NODAL LOCATIONS FOR WHICH TEMPS ARE SAVED ****
          5
*** NODE NUMBERS ASSOCIATED W/ STORED TEMPS ***
         17           12            7           5           1
```

```
*** SURFACE I PARAMETERS: AREA,L,EMIS,IMAT ***
  400.0000        7.000000        0.8500000                1
**** MATERIAL PARAMETERS: ALPHA,K,THICK ****
 9.9999997E-06    55.00000        5.0000001E-02
*** NUMBER OF NODES FOR SURFACE I ***           11
**** NO. OF NODAL LOCATIONS FOR WHICH TEMPS ARE SAVED ****
           3
*** NODE NUMBERS ASSOCIATED W/ STORED TEMPS ***
          11            6            1
*** SURFACE I PARAMETERS: AREA,L,EMIS,IMAT ***
 0.2500000       0.1500000       0.9000000                3
**** MATERIAL PARAMETERS: ALPHA,K,THICK ****
 9.9999997E-06    55.00000        9.9999998E-03
**** MATERIAL PARAMETERS: ALPHA,K,THICK ****
 4.9999999E-06    10.00000        5.0000001E-02
**** MATERIAL PARAMETERS: ALPHA,K,THICK ****
 1.9999999E-05    65.00000        9.9999998E-03
*** NUMBER OF NODES FOR SURFACE I ***           16
**** NO. OF NODAL LOCATIONS FOR WHICH TEMPS ARE SAVED ****
           4
*** NODE NUMBERS ASSOCIATED W/ STORED TEMPS ***
          16           11            6            1
**** BEAM LENGTHS ****
  6.000000        12.00000        7.000000        12.00000        10.00000
  5.000000        7.000000        5.000000       0.0000000E+00
**** CONFIGURATION FACTORS ****
 0.5998330       0.4000000       1.6700001E-04   0.6000000       0.3996250
 3.7500000E-04   0.4000000       0.6000000       0.0000000E+00
**** SPRAY CHOICE ****             0
**** CONVECTION CHOICE ****              1
**** CONDENSATION CHOICE ****              1
**** CONVECTION CORRELATION ****                  1
**** EXPANSION OPTION ****              0
**** LEAK OPTION ****             0
**** INITIAL TIME STEP ****  5.0000001E-02
**** PRINT INTERVAL ****              5
** MIN TEMP CHANGE FOR TIME STEP ACCEL. **    2.000000
** MAXIMUM TIME STEP ALLOWED **    5.000000
**** INITIAL PRE-COMBUSTION CONDITIONS ****
** P1,T1,H21,O21,H2O1,N21,CO21,CO1,ICOMPL,COMPL1,IH2OL **
  1.200000        325.0000        6.7999996E-02   0.2900000       9.9999998E-03
 0.6200000       0.0000000E+00   0.0000000E+00            0    85.00000
           0
**** AIC COMBUSTION DATA ****
** IBURN,TGO,PATM,TWINIT,(XF(I),I=1,6),TOTMOL,H2BRND,COBRND,EAICC **
           1    1048.633        3.740231        324.0000        0.6417945
 0.2649829       8.0745332E-02   0.0000000E+00   0.0000000E+00   1.2422360E-02
  224987.1        15299.12        0.0000000E+00   4.3898450E+09
**** BURN PARAMETERS: VBURN & LBURN ****
  3.000000        15.00000
```

```
**** GAS INITIALIZATION DATA ****
** PARAMETERS  MA,PGO,MAIR,MSTEAM,RHO **
  28.80873        0.3020062        5755.652        316.1626        1.214363
CHECK, DATA READ-IN COMPLETE
```

Once the data initialization is completed, the combustion and post-combustion heat transfer calculations are initiated. The time and gas temperature are periodically written to the screen (along with messages detailing the simulation progress) to indicate the current status of the calculation. A full listing of this progression is given below for the first deflagration of the base case generated in the previous section.

```
AIC CONDITIONS
GAS TEMP    AVE MW       CV       CP
  1048.633        27.93745        928.1377        1224.788


 INITIAL CONDITIONS
 GAS TEMP     AVE MW    CV1     MASS1    EAICC
  325.0000     26.98920     764.8541     6072.221    4.4005284E+09


 INITIATING COMBUSTION SIMULATION


 SIMULATION TIME (S) AND GAS TEMPERATURE (K)     0.0000000       325.000
 SIMULATION TIME (S) AND GAS TEMPERATURE (K)     1.0000001       469.515
 SIMULATION TIME (S) AND GAS TEMPERATURE (K)     1.9999992       613.405
 SIMULATION TIME (S) AND GAS TEMPERATURE (K)     2.9999983       756.109
 SIMULATION TIME (S) AND GAS TEMPERATURE (K)     3.9999974       897.137
 SIMULATION TIME (S) AND GAS TEMPERATURE (K)     5.0000000      1035.461
 SIMULATION TIME (S) AND GAS TEMPERATURE (K)     5.0000000      1035.461
 COMBUSTION SIMULATION COMPLETE
 SIMULATION TIME (S) AND GAS TEMPERATURE (K)     9.0499983       994.567
 SIMULATION TIME (S) AND GAS TEMPERATURE (K)    14.3999996       950.591
 SIMULATION TIME (S) AND GAS TEMPERATURE (K)    17.7000027       926.979
 SIMULATION TIME (S) AND GAS TEMPERATURE (K)    21.4500027       905.989
 SIMULATION TIME (S) AND GAS TEMPERATURE (K)    30.5000076       864.188
 SIMULATION TIME (S) AND GAS TEMPERATURE (K)    41.5999908       822.642
 SIMULATION TIME (S) AND GAS TEMPERATURE (K)    55.1000023       779.669
 SIMULATION TIME (S) AND GAS TEMPERATURE (K)    71.7500000       738.840
 SIMULATION TIME (S) AND GAS TEMPERATURE (K)    81.3999863       718.581
 SIMULATION TIME (S) AND GAS TEMPERATURE (K)    92.1499939       698.333
```

The first lines during the actual simulation execution show the gas heat-up during combustion. Note that the final AIC combustion temperature is not reached by the gas at the end of combustion; this is due to heat transfer and condensation on the containment walls during combustion. If no heat transfer during combustion is specified, the print out would start at the AIC temperature and would decrease with time.

Upon completion of the simulation, the following statements are written to the screen, to indicate which output files have been generated.

```
   RESTART INFORMATION FOR MULTIPLE BURN STUDIES

 INITIAL CONDITIONS FOR NEXT BURN ARE ON OLDDAT.DAT
 LATEST WALL TEMP. DISTRIBUTIONS ARE ON OLDWALT.DAT
 YOU MUST RE-RUN "NRCDATA" TO CREATE THE DATA DECK
 FOR THE NEXT BURN SEQUENCE. TO SPEED UP THIS DATA
 GENERATION, RENAME (OR ASSIGN) THE OLD DATA FILE
 "NRCDAT.DAT" TO "RESTART.DAT" AND THE PREVIOUSLY
 INPUT GEOMETRY AND CORRELATION PROMPTS WILL BE
 TAKEN FROM THE PRIOR DATA DECK. YOU WILL STILL BE
 ABLE TO CHANGE THE NECESSARY COMBUSTION PARAMETERS


          **** POST-COMBUSTION ANALYSIS COMPLETE ***

 DATA FOR GAS CONDITIONS AND SURFACE TEMPERATURES STORED IN "OUTPUT.DAT"
 DATA FOR TOTAL AND RADIATIVE FLUXES FOR EACH SURFACE ARE IN "FLUX.DAT"
 SPATIAL TEMPERATURE DISTRIBUTIONS ARE STORED IN "TEMPS*.DAT"
 IF REQUESTED DURING INPUT DECK GENERATION
```

If this simulation had been a single burn analysis, then the first set of messages given above would have been omitted, since several of the named output files are specific to multiple burn analyses (refer to Section 4 of the report). In addition, if either the leak or ice-condenser engineering option is specified, a message is provided indicating that the file "FLOWS" has been created. (This message is omitted from this presentation since the example does not include either option.)

C.4 RUN.BAT Post-Processing

After the execution of SOLVER is completed, the following procedural commands are performed using RUN.BAT:

```
B>A:                                                              (1)
A>COPY B:DATA A:RESTART                                           (2)
A>REM                                                             (3)
A>REM  FOR SINGLE OR MULTIPLE BURNS, A RESTART FILE IS            (4)
       ALWAYS READ ONTO THE DISK IN DRIVE A.                      (5)
A>REM  THE RESTART FILE GIVES THE USER THE OPTION TO:
       INTERACTIVELY                                              (6)
A>REM  1)START A NEW SINGLE OR MULTIPLE BURN WITH OLD             (7)
       SIMULATION PARAMETERS, OR 2)CONTINUE THE EXISTING          (8)
       MULTIPLE BURN.                                             (9)
A>PAUSE                                                           (10)
     Strike a key when ready ....                                 (11)
<return key>                                                      (12)
A>IF EXIST B:DBK GOTO ABC                                         (13)
A>COPY B:OLDDAT A:OLDDAT                                          (14)
A> COPY B: OLDWALL B:OLDWALT                                      (15)
A> IF EXIST B:DBK ERASE B:DBK                                     (16)
A> REM                                                            (17)
A> REM  TO CONTINUE A MULTIPLE BURN, OLDDAT MUST BE READ          (18)
        ONTO THE DISK IN DRIVE A AND                              (19)
A> REM  THE FINAL SLAB TEMPERATURES FROM THE FILE OLDWALL         (20)
        MUST BE STORED IN THE FILE OLDWALT ON DRIVE B             (21)
A>PAUSE                                                           (22)
     Strike a key when ready ...                                  (23)
<return key>                                                      (24)
A>REM                                                             (25)
A> REM THE EXECUTION OF SOLVER CREATES 4 TO 7 FILES:              (26)
       OUTPUT, FLUX, ENERGY, TEMPS1, TEMPS2, TEMPS3, FLOWS        (27)
A> REM NOTE THAT TEMPS1, TEMPS2, TEMPS3, AND FLOWS ARE            (28)
       OPTIONAL                                                   (29)
A>COPY B:OUTPUT A:                                                (30)
A>COPY B:FLUX A:                                                  (31)
A>COPY B:ENERGY A:                                                (32)
```

```
A>IF NOT EXIST B:TEMPS1 GOTO BCD                                    (33)
A>COPY B:TEMPS1 A:                                                  (34)
A>:BCD IF NOT EXIST B:TEMPS2 GOTO CDE                               (35)
A>COPY B:TEMPS2 A:                                                  (36)
A>:CDE IF NOT EXIST B:TEMPS3 GOTO DEF                               (37)
A>COPY B:TEMPS3 A:                                                  (38)
A>:DEF IF NOT EXIST B:FLOWS GOTO HIJ                                (39)
A>COPY B:FLOWS A:                                                   (40)
A>:HIJ REM  BEFORE MAKING ANOTHER RUN, THE FILES CREATED            (41)
       BY SOLVER MUST BE SAVED ON A SEPARATE DISK                   (42)
A>REM  THE OUTPUT FILES CREATED BY SOLVER ON DRIVE B                (43)
       HAVE BEEN COPIED TO DRIVE A                                  (44)
A>REM  REMOVE SOLVER FROM DRIVE B AND PLACE A FORMATTED             (45)
       DISK IN DRIVE B                                              (46)
A>PAUSE                                                             (47)
     Strike a key when ready ...                                    (48)
<carriage return>                                                   (49)
A>COPY OUTPUT B:REACB1.OUT                                          (50)
A>DEL OUTPUT                                                        (51)
A>COPY FLUX B:REACB1.FLX                                            (52)
A>DEL FLUX                                                          (53)
A>COPY ENERGY B:REACB1.NRG                                          (54)
A>DEL ENERGY                                                        (55)
A>IF NOT EXIST TEMPS1 GOTO EFG                                      (56)
A>COPY TEMPS1 B:REACB1.TS1                                          (57)
A>DEL TEMPS1                                                        (58)
A>IF NOT EXIST TEMPS2 GOTO FGH                                      (59)
A>COPY TEMPS2 B:REACB1.TS2                                          (60)
A>DEL TEMPS2                                                        (61)
A>IF NOT EXIST TEMPS3 GOTO GHI                                      (62)
A>COPY TEMPS3 B:REACB1.TS3                                          (63)
A>DEL TEMPS3                                                        (64)
A>IF NOT EXIST FLOWS GOTO IJK                                       (65)
A>COPY FLOWS B:REACB1.FLO                                           (66)
A>DEL FLOWS                                                         (67)
A>REM  THE OUTPUT FILES ARE NOW ON THE NEW DISK IN DRIVE B          (68)
       AND HAVE BEEN ERASED FROM DISK 1                             (69)
A>REM  THE OUTPUT FILES ON THE NEW DISK HAVE BEEN RENAMED           (70)
       AND CAN BE IDENTIFIED BY THEIR SUFFIXES                      (71)
A>REM  TO START ANY NEW BURN OR CONTINUE WITH THE EXISTING          (72)
       MULTIPLE BURN,                                               (73)
```

```
A>REM  REPLACE SOLVER IN DRIVE B AND ENTER                    (74)
       RUN DATGEN SOLVER FILNAM  OR                           (75)
       RUN DATFIL SOLVER FILNAM                               (76)
```

Lines 1-24 copy and/or rename files from drive B to drives A and B and explain why the file manipulations occur (lines 4-12, 17-24). The file manipulations allow a re-start of a new single burn or the first deflagration of a multiple burn sequence (line 2). It also allows for additional deflagration simulations in a multiple burn sequence (lines 14,15). The file DATA is renamed RESTART and is transferred to drive A to be accessed by DATGEN if needed for any interactive re-start option. OLDDAT contains the final gas conditions of the previous simulation and is placed in disk 1 so that DATGEN can access the values for the subsequent deflagration of a multiple burn sequence (line 14). OLDWALL is renamed OLDWALT and is left on disk 2 to be accessed by SOLVER for the next burn simulation of a multiple burn sequence (line 15). Line 13 checks to see if the file DBK has been created on disk 2 (drive B) and line 16 erases DBK if it exists on disk 2. DBK is only created for single burn simulations; therefore, lines 13 and 16 are disregarded for multiple burn analyses.

For single burn analyses, RUN.BAT does not print lines 14 and 15 since OLDDAT and OLDWALL are used only for multiple burn scenarios. Instead, line 13 transfers control to line 17. File DBK, created in SOLVER must be erased upon completion of the simulation (line 17). If it were not erased and the next simulation were part of a multiple burn sequence, the procedure file would treat the deflagration as a single burn because the file DBK would still exist in disk 1.

Lines 25-76 of the procedure file are the same for multiple or single burn analyses. Lines 26-40 copy all files created by SOLVER to disk 1 (drive A). Lines 30-32 copy the output files that are always created by SOLVER (OUTPUT, FLUX, ENERGY) to disk 1. Lines 33,35,37,and 39 check to see which optional file(s) (TEMPS1, TEMPS2, TEMPS3, or FLOWS) has/have been created during SOLVER execution. Lines 34,36,38,and 40 then transfer the optional file(s) that has/have been created onto disk 1.

Lines 41-76 of the procedure file transfer all SOLVER-generated output files from disk 1 to a new formatted disk (designated as disk 3) in drive B and erase the output files from disk 1. Lines 41-46 tell the user to replace the disk which contains SOLVER with disk 3.into Lines 50-55 copy the output files OUTPUT, FLUX, and ENERGY into disk 3 and delete these files from disk 1. Lines 56,59,62 and 65 check to see which of the optional files have been generated during SOLVER execution. If any of these files exist, then they are also copied to disk 3

and deleted from disk 1 (lines 57,58,60,61,63,64,66,67). Lines 68-71 tell the user that the output files have been transferred to disk 3.

Lines 72-76 tell the user how to begin another run of HYBER.

C.5 Output Files Obtained from SOLVER

The output files "OUTPUT","FLUX", and "TEMPS3" (for this simulation, these files would have been renamed "REACB1.OUT", "REACB1.FLX", and "REACB1.TS1") are provided in the following sub-sections for the "base case" data file generated in Section C.2. The file "ENERGY" is omitted since it is similar in form to "FLUX". Similarly, the files TEMPS1 and TEMPS2 are omitted in this presentation. Two input data files NRCDAT and NRCDAT.NOD are also listed in the first example of Appendix D and the summary results included there are plotted for the user's review of the results. Since a plotting package is not included in the algorithm, the user should familiarize him/herself with the output file tabulations included below.

C.5.1 OUTPUT File

The file output should be self-explanatory. If not, the user should refer to Section 4.2.1 for information on the abbreviations used in the headers.

```
EXAMPLE #1 -- MULTIPLE BURN SIMULATION -- BASE CASE - 1st BURN
   OUTPUT FILE -- T IN DEG K, P IN ATM, TIME IN SEC
                  CONDENSATION FLAG: T=CONDENSATION ON SURFACE, F=NONE
                  CONVECTION FLAG: B=NONE, F=FORCED, N=FREE CONV

    P1        T1        H21     H201     C021      C01   COMPL1  VPH2OL
 1.20000   325.00    0.068    0.010    0.000    0.000    85.00   0.000

TIME    PGAS     TGAS    FRACT    TS1      TS2      TS3       MFS      CONDF   CONVF
 0.00   1.200  325.000    0.0   324.00   324.00   324.00   0.01000  F F F   F F F
 0.25   1.331  361.171    0.0   324.02   324.00   324.01   0.01342  F F F   F F F
 0.50   1.462  397.316    0.0   324.08   324.01   324.03   0.01686  F F F   F F F
 0.75   1.592  433.432    0.0   324.20   324.03   324.06   0.02030  F F F   F F F
 1.00   1.722  469.515    0.0   324.37   324.06   324.10   0.02376  F F F   F F F
 1.25   1.851  505.559    0.0   324.61   324.10   324.16   0.02723  F F F   F F F
 1.50   1.979  541.560    0.0   324.92   324.15   324.22   0.03071  F F F   F F F
 1.75   2.107  577.511    0.0   325.32   324.21   324.30   0.03421  F F F   F F F
 2.00   2.234  613.405    0.0   325.82   324.28   324.40   0.03771  F F F   F F N
 2.25   2.360  649.234    0.0   326.43   324.37   324.53   0.04123  F F F   F F N
 2.50   2.486  684.990    0.0   327.17   324.47   324.67   0.04476  F F F   F F N
 2.75   2.611  720.661    0.0   328.05   324.59   324.84   0.04830  F F F   F F N
 3.00   2.735  756.109    0.0   329.08   324.74   325.04   0.05186  F T T   F F N
 3.25   2.858  791.567    0.0   330.30   324.92   325.28   0.05542  F T T   F F N
 3.50   2.981  826.901    0.0   331.71   325.13   325.55   0.05900  F T T   F F N
```

3.75	3.102	862.097	0.0	333.37	325.37	325.87	0.06259	F	T	T	N	F	N
4.00	3.222	897.137	0.0	335.28	325.65	326.24	0.06620	F	T	T	N	F	N
4.25	3.342	932.007	0.0	337.49	325.97	326.65	0.06981	F	T	T	N	F	N
4.50	3.460	966.695	0.0	340.00	326.32	327.11	0.07344	F	T	T	N	F	N
4.75	3.577	1001.186	0.0	342.85	326.72	327.63	0.07708	F	T	T	N	N	N
5.00	3.693	1035.461	0.0	346.06	327.16	328.20	0.08073	F	T	T	N	N	N
5.00	3.693	1035.461	0.0	346.06	327.16	328.20	0.08073	F	T	T	N	N	N
5.70	3.665	1027.707	0.0	359.26	328.93	330.34	0.08071	F	T	T	F	F	F
6.70	3.628	1017.376	0.0	374.73	330.54	331.99	0.08068	F	T	T	F	F	F
7.80	3.589	1006.458	0.0	388.66	331.77	333.42	0.08065	F	T	T	F	F	F
9.05	3.547	994.567	0.0	401.42	332.82	334.85	0.08063	F	T	T	F	F	F
10.30	3.506	983.185	0.0	411.68	333.65	336.15	0.08060	F	T	T	F	F	F
11.55	3.467	972.323	0.0	419.89	334.31	337.32	0.08058	F	T	T	F	F	F
12.90	3.429	961.554	0.0	426.22	334.76	338.32	0.08056	F	T	T	F	F	F
14.40	3.390	950.591	0.0	431.06	335.10	339.29	0.08054	F	T	T	F	F	F
15.95	3.352	940.133	0.0	434.51	335.35	340.20	0.08053	F	T	F	F	F	F
17.70	3.305	926.979	0.0	437.08	335.55	340.99	0.08051	F	T	F	F	F	F
19.45	3.269	916.839	0.0	438.82	335.70	341.77	0.08050	F	T	F	F	F	F
21.45	3.231	905.989	0.0	440.21	335.84	342.58	0.08049	F	T	F	F	F	F
23.45	3.194	895.820	0.0	441.13	335.94	343.31	0.08048	F	T	F	F	F	N
25.70	3.156	885.082	0.0	441.79	336.02	344.09	0.08047	F	T	F	F	F	N
28.00	3.119	874.778	0.0	442.14	336.08	344.83	0.08047	F	T	F	F	N	N
30.50	3.081	864.188	0.0	442.28	336.16	345.57	0.08046	F	T	F	F	N	N
33.05	3.045	853.935	0.0	442.27	336.23	346.26	0.08046	F	T	F	N	N	N
35.80	3.007	843.379	0.0	442.28	336.29	346.93	0.08045	F	T	F	N	N	N
38.60	2.971	833.124	0.0	442.25	336.34	347.56	0.08045	F	T	F	N	N	N
41.60	2.933	822.642	0.0	442.14	336.38	348.17	0.08045	F	T	F	N	N	N
44.70	2.896	812.320	0.0	441.94	336.41	348.73	0.08044	F	T	F	N	N	N
47.95	2.853	800.079	0.0	441.67	336.39	349.30	0.08044	F	F	F	N	N	N
51.40	2.817	789.981	0.0	441.27	336.28	349.81	0.08044	F	F	F	N	N	N
55.10	2.780	779.669	0.0	440.77	336.22	350.32	0.08044	F	F	F	N	N	N
58.95	2.744	769.461	0.0	440.18	336.18	350.78	0.08044	F	F	F	N	N	N
63.00	2.707	759.251	0.0	439.48	336.14	351.21	0.08044	F	F	F	N	N	N
67.25	2.671	749.072	0.0	438.69	336.11	351.61	0.08044	F	F	F	N	N	N
71.75	2.634	738.840	0.0	437.80	336.08	351.98	0.08044	F	F	F	N	N	N
76.45	2.598	728.703	0.0	436.84	336.05	352.32	0.08044	F	F	F	N	N	N
81.40	2.562	718.581	0.0	435.78	336.02	352.62	0.08044	F	F	F	N	N	N
86.60	2.526	708.508	0.0	434.66	336.00	352.88	0.08044	F	F	F	N	N	N
92.15	2.490	698.333	0.0	433.44	335.98	353.12	0.08044	F	F	F	N	N	N
98.00	2.454	688.197	0.0	432.15	335.97	353.32	0.08044	F	F	F	N	N	N
100.00	2.442	684.862	0.0	431.89	335.97	353.36	0.08044	F	F	F	N	N	N

C.5.2 FLUX File

The file output should be self-explanatory. If not, the user should refer to Section 4.2.2 for information on the abbreviations used in the headers.

```
EXAMPLE #1 -- MULTIPLE BURN SIMULATION -- BASE CASE - 1st BURN
   SURFACE FLUXES -- FLUXES IN W/M2 AND TIME IN SEC

     P1         T1         H21       H2O1       CO21        CO1    COMPL1   VPH2OL
 1.20000    325.00      0.068      0.010      0.000      0.000     85.00    0.000

 TIME       HFRC1          HFR1          HFRC2          HFR2          HFRC3          HFR3
 0.00   0.9969E+01 -0.1633E+01  0.1071E+02 -0.1931E+01  0.9255E+01 -0.2087E+01
 0.25   0.3777E+03 -0.8419E+02  0.4058E+03 -0.9912E+02  0.3590E+03 -0.8515E+02
 0.50   0.7580E+03 -0.2210E+03  0.8148E+03 -0.2591E+03  0.7356E+03 -0.2242E+03
 0.75   0.1149E+04 -0.4263E+03  0.1236E+04 -0.4976E+03  0.1137E+04 -0.4347E+03
 1.00   0.1550E+04 -0.7166E+03  0.1669E+04 -0.8326E+03  0.1560E+04 -0.7344E+03
 1.25   0.1960E+04 -0.1110E+04  0.2111E+04 -0.1283E+04  0.2004E+04 -0.1143E+04
 1.50   0.2378E+04 -0.1625E+04  0.2563E+04 -0.1871E+04  0.2468E+04 -0.1682E+04
 1.75   0.2802E+04 -0.2283E+04  0.3023E+04 -0.2617E+04  0.2950E+04 -0.2375E+04
 2.00   0.3232E+04 -0.3102E+04  0.3490E+04 -0.3542E+04  0.3457E+04 -0.3242E+04
 2.25   0.3667E+04 -0.4102E+04  0.3964E+04 -0.4668E+04  0.4018E+04 -0.4304E+04
 2.50   0.4107E+04 -0.5312E+04  0.4443E+04 -0.6026E+04  0.4595E+04 -0.5593E+04
 2.75   0.4549E+04 -0.6759E+04  0.4928E+04 -0.7644E+04  0.5187E+04 -0.7140E+04
 3.00   0.4992E+04 -0.8317E+04  0.5460E+04 -0.1038E+05  0.5827E+04 -0.9061E+04
 3.25   0.5438E+04 -0.1029E+05  0.6018E+04 -0.1280E+05  0.6508E+04 -0.1125E+05
 3.50   0.5884E+04 -0.1257E+05  0.6577E+04 -0.1560E+05  0.7199E+04 -0.1379E+05
 3.75   0.6390E+04 -0.1520E+05  0.7137E+04 -0.1882E+05  0.7896E+04 -0.1673E+05
 4.00   0.6925E+04 -0.1820E+05  0.7697E+04 -0.2248E+05  0.8600E+04 -0.2010E+05
 4.25   0.7474E+04 -0.2144E+05  0.8267E+04 -0.2642E+05  0.9327E+04 -0.2374E+05
 4.50   0.8060E+04 -0.2503E+05  0.8860E+04 -0.3078E+05  0.1011E+05 -0.2779E+05
 4.75   0.8622E+04 -0.2901E+05  0.9448E+04 -0.3562E+05  0.1087E+05 -0.3229E+05
 5.00   0.9166E+04 -0.3340E+05  0.1012E+05 -0.4093E+05  0.1162E+05 -0.3726E+05
 5.00   0.9166E+04 -0.3340E+05  0.1012E+05 -0.4093E+05  0.1162E+05 -0.3726E+05
 5.70   0.2279E+05 -0.3233E+05  0.2508E+05 -0.3974E+05  0.2493E+05 -0.3616E+05
 6.70   0.2171E+05 -0.3093E+05  0.2432E+05 -0.3819E+05  0.2415E+05 -0.3473E+05
 7.80   0.2067E+05 -0.2950E+05  0.2356E+05 -0.3661E+05  0.2337E+05 -0.3327E+05
 9.05   0.1964E+05 -0.2799E+05  0.2278E+05 -0.3494E+05  0.2253E+05 -0.3174E+05
10.30   0.1873E+05 -0.2661E+05  0.2205E+05 -0.3339E+05  0.2174E+05 -0.3031E+05
11.55   0.1666E+05 -0.2534E+05  0.1988E+05 -0.3197E+05  0.1952E+05 -0.2899E+05
12.90   0.1399E+05 -0.2413E+05  0.1688E+05 -0.3059E+05  0.1651E+05 -0.2773E+05
14.40   0.1189E+05 -0.2295E+05  0.1448E+05 -0.2924E+05  0.1408E+05 -0.2648E+05
15.95   0.1029E+05 -0.2187E+05  0.1263E+05 -0.2799E+05  0.1221E+05 -0.2425E+05
17.70   0.8880E+04 -0.2059E+05  0.1098E+05 -0.2646E+05  0.1062E+05 -0.2291E+05
19.45   0.7844E+04 -0.1963E+05  0.9753E+04 -0.2533E+05  0.9436E+04 -0.2191E+05
21.45   0.6917E+04 -0.1865E+05  0.8645E+04 -0.2416E+05  0.8367E+04 -0.2087E+05
23.45   0.6180E+04 -0.1774E+05  0.7757E+04 -0.2307E+05  0.7724E+04 -0.1992E+05
25.70   0.5512E+04 -0.1680E+05  0.6947E+04 -0.2193E+05  0.7503E+04 -0.1891E+05
28.00   0.4957E+04 -0.1593E+05  0.6442E+04 -0.2088E+05  0.7293E+04 -0.1798E+05
30.50   0.4462E+04 -0.1507E+05  0.6242E+04 -0.1984E+05  0.7079E+04 -0.1707E+05
33.05   0.4247E+04 -0.1428E+05  0.6052E+04 -0.1886E+05  0.6874E+04 -0.1621E+05
35.80   0.4093E+04 -0.1349E+05  0.5861E+04 -0.1790E+05  0.6665E+04 -0.1536E+05
38.60   0.3947E+04 -0.1275E+05  0.5679E+04 -0.1700E+05  0.6465E+04 -0.1457E+05
41.60   0.3799E+04 -0.1203E+05  0.5496E+04 -0.1612E+05  0.6263E+04 -0.1380E+05
44.70   0.3657E+04 -0.1135E+05  0.5320E+04 -0.1528E+05  0.6066E+04 -0.1306E+05
47.95   0.3492E+04 -0.1075E+05  0.5113E+04 -0.1315E+05  0.5838E+04 -0.1258E+05
```

51	40	0.3359E+04	-0.1014E+05	0.4956E+04	-0.1247E+05	0.5650E+04	-0.1191E+05
55	10	0.3227E+04	-0.9534E+04	0.4797E+04	-0.1179E+05	0.5461E+04	-0.1124E+05
58	95	0.3099E+04	-0.8964E+04	0.4640E+04	-0.1115E+05	0.5276E+04	-0.1062E+05
63	00	0.2974E+04	-0.8419E+04	0.4485E+04	-0.1054E+05	0.5093E+04	-0.1002E+05
67	25	0.2852E+04	-0.7900E+04	0.4333E+04	-0.9955E+04	0.4914E+04	-0.9441E+04
71	75	0.2733E+04	-0.7402E+04	0.4181E+04	-0.9390E+04	0.4736E+04	-0.8888E+04
76	45	0.2617E+04	-0.6931E+04	0.4032E+04	-0.8854E+04	0.4562E+04	-0.8364E+04
81	40	0.2504E+04	-0.6483E+04	0.3885E+04	-0.8342E+04	0.4390E+04	-0.7863E+04
86	60	0.2394E+04	-0.6058E+04	0.3740E+04	-0.7853E+04	0.4222E+04	-0.7386E+04
92	15	0.2285E+04	-0.5650E+04	0.3596E+04	-0.7382E+04	0.4055E+04	-0.6926E+04
98	00	0.2179E+04	-0.5263E+04	0.3454E+04	-0.6933E+04	0.3891E+04	-0.6489E+04
100	0	0.2159E+04	-0.5188E+04	0.3426E+04	-0.6846E+04	0.3859E+04	-0.6405E+04

C.5.3 TEMPS3 File

Below are the nodal temperatures of the piece of equipment described in Sections C.1 and C.2 as a function of time. The node numbers are specified and the user must know this nodalization set-up as given in Section C.2 to be able to use these results. The file output should be self-explanatory. If not, the user should refer to Section 4.2.4 for information on the abbreviations used in the headers.

```
EXAMPLE #1 -- MULTIPLE BURN SIMULATION -- BASE CASE - 1st BURN
   NODAL TEMPERATURE VS TIME DATA FOR SURFACE 3
   TEMPERATURES IN DEG K AND TIME IN SEC
```

TIME	NODE 16 TW	NODE 11 TW	NODE 6 TW	NODE 1 TW
0.00	324.00	324.00	324.00	324.00
0.25	324.01	324.00	324.00	324.00
0.50	324.03	324.00	324.00	324.00
0.75	324.07	324.00	324.00	324.00
1.00	324.11	324.00	324.00	324.00
1.25	324.17	324.01	324.00	324.00
1.50	324.24	324.01	324.00	324.00
1.75	324.32	324.02	324.00	324.00
2.00	324.43	324.03	324.00	324.00
2.25	324.55	324.05	324.00	324.00
2.50	324.70	324.07	324.00	324.00
2.75	324.88	324.09	324.00	324.00
3.00	325.09	324.13	324.00	324.00
3.25	325.33	324.17	324.00	324.00
3.50	325.61	324.22	324.00	324.00
3.75	325.94	324.28	324.00	324.00
4.00	326.31	324.35	324.00	324.00
4.25	326.74	324.44	324.00	324.00
4.50	327.21	324.55	324.00	324.00
4.75	327.74	324.67	324.00	324.00
5.00	328.44	324.84	324.00	324.00
5.00	328.44	324.84	324.00	324.00
5.70	330.72	325.54	324.00	324.00
6.70	332.27	326.69	324.00	324.00
7.80	333.72	328.12	324.00	324.00
9.05	335.12	329.63	324.00	324.00
10.30	336.40	331.05	324.00	324.00
11.55	337.52	332.38	324.00	324.00
12.90	338.52	333.73	324.00	324.00
14.40	339.48	335.01	324.00	324.00

15.95	340.34	336.20	324.00	324.00
17.70	341.16	337.32	324.00	324.00
19.45	341.94	338.31	324.00	324.00
21.45	342.73	339.29	324.00	324.00
23.45	343.47	340.19	324.00	324.00
25.70	344.24	341.07	324.01	324.00
28.00	344.98	341.92	324.01	324.01
30.50	345.71	342.75	324.02	324.01
33.05	346.40	343.54	324.03	324.01
35.80	347.06	344.30	324.04	324.02
38.60	347.69	345.02	324.05	324.03
41.60	348.28	345.71	324.07	324.04
44.70	348.85	346.37	324.10	324.06
47.95	349.39	346.99	324.13	324.09
51.40	349.91	347.60	324.17	324.12
55.10	350.41	348.19	324.22	324.16
58.95	350.87	348.74	324.28	324.21
63.00	351.30	349.25	324.35	324.27
67.25	351.69	349.73	324.43	324.34
71.75	352.05	350.17	324.53	324.43
76.45	352.38	350.57	324.65	324.53
81.40	352.67	350.94	324.78	324.65
86.60	352.93	351.28	324.94	324.80
92.15	353.16	351.59	325.12	324.96
98.00	353.36	351.86	325.32	325.15
100.00	353.38	351.89	325.35	325.18

C.6 Re-start Options

The first deflagration simulation of a multiple deflagration scenario consisting of two burns has been provided in great detail in the previous sections. In this section, the interactive re-start option used to generate the second deflagration is described. In addition, a description of the interactive re-start option used to generate the first deflagration data files for the other three examples presented in Appendix D is given. Where appropriate, the use of these options in single burn simulation data file generation is also provided. Finally, a description of the re-start option by editing the data file, NRCDAT, for any deflagration simulation and any data file in Appendix D is also demonstrated.

C.6.1 Second Deflagration of a Multiple Burn Sequence

For the second deflagration of a muliple burn sequence, the prompts from DATGEN through the combustion parameters input section are as follows:

```
DATA INPUT GENERATOR FOR NRC ALGORITHM CODE                          (1)
WHAT IS THE TIME(INPUT CHARACTER STRING < 10)                        (2)
<12:10 >                                                            (3)
WHAT IS THE DATE(INPUT CHARACTER STRING < 10)                        (4)
< 14 MAR 84>                                                        (5)
INPUT ONE LINE DESCRIPTOR FOR DATA SET - 80 COL MAX                  (6)
<EXAMPLE #1 - MULTIPLE BURN SIMULATION -BASE CASE- 2nd BURN>         (7)
IS THIS PART OF A MULTIPLE BURN SIMULATION?                          (8)
1 = YES, 0 = NO                                                     (9)
< 1 >                                                               (10)
IS THIS THE FIRST PASS THROUGH THE INPUT GENERATOR                   (11)
FOR MULTIPLE BURN ANALYSES ( 0 = NO, 1 = YES )                       (12)
< 0 >                                                               (13)
PREVIOUS CALCULATION WAS STOPPED AT TIME = 100                       (14)
ENTER INITIAL TIME FOR THIS BURN, (S)                                (15)
< 100 >                                                             (16)
ENTER DURATION OF SIMULATION                                        (17)
< 200 >                                                             (18)

                                                                    (19)
```

```
FINAL GAS TEMPERATURE FROM PREVIOUS BURN = 684.8                    (20)
FINAL GAS PRESSURE FROM PREVioUS BURN = 2.443                       (21)
** NOTE THAT THE FINAL PRESSURES AND TEMPERATURES **                (22)
** SHOULD BE USED AS THE INITIAL CONDITIONS IN **                   (23)
**      MULTIPLE BURN SEQUENCES                  **                 (24)
GAS COMPOSITION FOLLOWING COMBUSTION IN PREVIOUS                    (25)
CALCULATION                                                         (26)
  XH2O = .081          XH2 = 1.2E-2                                 (27)
  XN2 = .642           XO2 = .265                                   (28)
  XCO2 = 0.00          XCO = 0.00                                   (29)

ENTER INITIAL GAS PRESSURE (ATM) & TEMPERATURE (K)                  (30)
< 2.44, 684.8 >                                                     (31)
                              .
                              .                                     (32)
                              .
**** ENTER H2,O2,H2O,N2,CO2,AND CO MOLE FRACTIONS ****              (33)
<.08,.24,.08,.60,0,0>                                               (34)
                              .
                              .                                     (35)
                              .
```

Lines 1-18 are part of boxes 1-3, 19a of the flow chart. Since the user has specified that this simulation is part of a multiple burn simulation, and further that this is not the first data generation of this sequence, then the previously generated geometry, heat transfer options, and engineering systems options are taken from file RESTART (line 19). Line 19 thus corresponds to boxes 6-13. Lines 20-29 correspond to box 23 and lines 30-34 to box 14. Boxes 15-18 are represented by line 35. Note that the information taken from RESTART (boxes 6-13) is echo-printed to the screen during the data generation so that the user is reminded of the parameters selected for the particular simulation being performed.

The information provided in lines 14 and 20-29 are obtained from the previously generated OLDDAT file. The user must enter mole fractions (line 34) to be used in the second deflagration. Since DATGEN and SOLVER do not account for hydrogen release or steam injection which can occur during the degraded core accident, any modifications to the gas composition are treated as step changes in the algorithm.

The final difference between the data generation prompts for a first and second and all subsequent deflagrations of a multiple burn simulation occurs in the specification of the initial surface temperatures. For all succeeding data generations following the first in a multiple burn sequence, initial wall temperatures (box 17) are not entered by the user. A dummy value for this temperature is written to NRCDAT but is not used during the data initialization in SOLVER. Instead, data written to file OLDWALL from the previous execution of SOLVER are used during the data initialization in SOLVER. Note also that the above prompting sequence would be repeated for all subsequent deflagration simulations of a multiple burn sequence following the first deflagration.

C.6.2 Restart Option for the First Burn of a Multiple Burn Scenario or for a Single Burn Simulation

The user can use a re-start option to simplify the input data file generation for a single or for the first deflagration of a multiple burn simulation. To use this option, the user must have previously created NRCDAT and NRCDAT.NOD files containing the appropriate geometry and radiative parameter data. Use of this option is demonstrated below for example problem 2 of Appendix D:

```
DATA INPUT GENERATOR FOR NRC ALGORITHM CODE                    (1)
WHAT IS THE TIME (INPUT CHARACTER STRING < 10)                 (2)
<2:00 PM>                                                      (3)
WHAT IS THE DATE (INPUT CHARACTER STRING < 10)                 (4)
<14 MAR 84>                                                    (5)
INPUT ONE LINE DESCRIPTOR FOR DATA SET - 80 COL MAX            (6)
<EXAMPLE #2 - MULTIPLE BURN SIMULATION -SPRAYS ON- 1st BURN>   (7)
IS THIS PART OF A MULTIPLE BURN SIMULATION?                    (8)
1 = YES  0 = NO                                                (9)
<1>                                                           (10)
IS THIS THE FIRST PASS THROUGH THE INPUT GENERATOR             (11)
FOR MULTIPLE ANALYSES ( 0=NO, 1=YES)                          (12)
< 1 >                                                         (13)
DO YOU WANT TO USE PREVIOUSLY GENERATED GEOMETRY              (14)
DATA DECKS AND CHANGE THE COMBUSTION CALC.                    (15)
(0=N, 1=Y)                                                    (16)
<1>                                                           (17)
ENTER INITIAL TIME FOR THIS BURN (S)                          (18)
< 0 >                                                         (19)
```

```
ENTER DURATION OF SIMULATION (S)                                    (20)
< 100 >                                                             (21)

                                                                    (22)

DO YOU WANT TO USE DIFFERENT CORRELATIONS OR CHANGE                 (23)
THE SPRAY, LEAK, OR EXPANSION OPTIONS OR CHANGE THE                 (24)
THE TIME STEP SIZE OR PRINT OUT ( 0=N, 1=Y )                        (25)
< 1 or 0 >                                                          (26)
```

The re-start option for a single burn simulation is identical to that of the first burn of a multiple burn simulation shown above except that line 10 is entered as "no". The following prompt, lines 11-13, is also omitted because of the negative response.

Lines 1-17 correspond to boxes 1-4 of the flow chart, and lines 18-21 correspond to box 20a. Line 22 corresponds to boxes 6-9. These inputs are obtained from file RESTART, the previously generated NRCDAT file and would be written to the screen for user review. The prompts of lines 23-25 (box 21) are provided so that previously chosen heat transfer, engineering systems options and time step and print out parameters (written in RESTART) can be used in the current simulation. If the user response to lines 23-25 is < 0 >, the prompts of boxes 10-13 are taken from RESTART, and the user will next answer prompts in the combustion section (box 14). If the user wishes to change any of the prompts of boxes 10-13, then all of the prompts for these sections must be answered. Note that in this re-start option, the prompts starting from the combustion section to the completion of the input file generation are identical to those of Section 3.2.

C.6.3 Re-start Option by editing the data file NRCDAT

The user can use the third re-start option by editing NRCDAT for any burn simulation. Unlike sections C.6.a and C.6.b, no interaction between DATGEN and the user is involved. After editing NRCDAT and placing it on disk 1 with the procedure file, the user may begin execution of the algorithm codes with line 1 below:

```
<RUN DATFIL SOLVER FILNAM>                                    (1)
A>REM DATGEN AND THE PROCEDURE FILE ARE IN DRIVE A            (2)
A>REM SOLVER IS IN DRIVE B                                    (3)
A>PAUSE STRIKE A KEY WHEN READY                               (4)
<carriage return>                                             (5)
A>IF DATFIL == DATFIL GOTO JKL                                (6)
A>:JKL COPY A:NRCDAT B:DATA                                   (7)
A>COPY A:NRCDAT.NOD B:NODES                                   (8)
A>REM THE FILES NRCDAT AND NRCDAT.NOD ARE COPIED TO           (9)
A>REM DRIVE B AND RENAMED DATA AND NODES                      (10)
B>                                                            (11)
B>SOLVER.EXE                                                  (12)
```

Line 6 checks to see if DATGEN is being used interactively with the user. Since "DATFIL" was entered in place of "DATGEN" in line 1, line 6 transfers execution to line 7, and DATGEN is not executed (see line 6, section C.2). Line 6 copies the edited version of NRCDAT from disk 1 to disk 2 to be used by SOLVER while it is executing. From line 7 on, the procedure file operates as described in section C.3.

This concludes the presentation of the detailed example and the presentation of the options available in the algorithm. The user should now review the example problems given in Appendix D and perform these or similar calculations (using these examples as reference cases) to become more familiar with the algorithm.

Appendix D. Sample Data Files and Results

D.1 Multiple Burn Simulation – Base Case

In this example, a degraded core accident is assumed to have occurred in the reactor geometry given in Appendix C. Hydrogen is released to the containment and the glow plug ignition system is operative resulting in two, 85% complete, 8% (by volume) hydrogen:air deflagrations which are assumed to occur within 100 seconds of each other. It is also assumed that there is no additional steam injection into containment prior to the second deflagration. In this particular example, the spray system in containment is inoperative, and the reactor geometry does not have any containment gas leakage. This reactor does not include ice condensers and fans. This example is termed the reactor "base case" and was described in detail in Appendix C.

Included in the following sub-sections are the user-generated data input files for this example and the file NRCDAT.NOD, generated in DATGEN. Specifics of these simulations are provided in the two NRCDAT files. In addition, plotted results are given for this example in D.1.4.

D.1.1 NRCDAT for the First Deflagration

```
12:00 PM        14 MAR 84
EXAMPLE #1 - MULTIPLE BURN SIMULATION - BASE CASE - 1st BURN
          1
          1
 0.0000000E+00   100.0000
  5000.000       1000.000        17.00000
          3
  600.0000       10.00000        0.8000000
          1
 5.0000000E-07   1.000000        0.1000000
         17
          5
```

```
        17          12          7          5          1
 400.0000    7.000000    0.8500000
         1
9.9999997E-06   55.00000    5.0000001E-02
        11
         3
        11          6          1
0.2500000   0.1500000   0.9000000
         3
9.9999997E-06   55.00000    9.9999998E-03
4.9999999E-06   10.00000    5.0000001E-02
1.9999999E-05   65.00000    9.9999998E-03
        16
         4
        16         11          6          1
 6.000000    12.00000    7.000000
 12.00000    10.00000    5.000000
 7.000000    5.000000    0.0000000E+00
0.5998330    0.4000000   1.6700001E-04
0.6000000    0.3996250   3.7500000E-04
0.4000000    0.6000000   0.0000000E+00
         0
         1
         1
         1
         0
         0
5.0000001E-02                    **********
         5
 2.000000
 5.000000
 1.200000    325.0000    6.7999996E-02   0.2900000    9.9999998E-03
0.6200000    0.0000000E+00   0.0000000E+00
         0   85.00000            0
         1   1048.633    3.740231    324.0000    0.6417945
0.2649829    8.0745332E-02   0.0000000E+00   0.0000000E+00   1.2422360E-02
 224987.1    15299.12    0.0000000E+00   4.3898450E+09
 3.000000    15.00000
 28.80873    0.3020062    5755.652    316.1626    1.214363
CHECK
```

D.1.2 NRCDAT for the Second Deflagration

```
12:10 PM        14 MAR 84
EXAMPLE #1 - MULTIPLE BURN SIMULATION - BASE CASE - 2nd BURN
          1
          0
 100.0000         200.0000
 5000.000         1000.000         17.00000
          3
 600.0000         10.00000         0.8000000
          1
5.0000000E--07    1.000000         0.1000000
         17
          5
         17          12           7            5            1
 400.0000         7.000000         0.8500000
          1
9.9999997E--06    55.00000         5.0000001E--02
         11
          3
         11          6            1
0.2500000         0.1500000        0.9000000
          3
9.9999997E--06    55.00000         9.9999998E--03
4.9999999E--06    10.00000         5.0000001E--02
1.9999999E--05    65.00000         9.9999998E--03
         16
          4
         16          11           6            1
 6.000000         12.00000         7.000000
 12.00000         10.00000         5.000000
 7.000000         5.000000         0.0000000E+00
0.5998330         0.4000000        1.6700001E--04
0.6000000         0.3996250        3.7500000E--04
0.4000000         0.6000000        0.0000000E+00
          0
          1
          1
```

```
          1
          0
          0
5.0000001E-02
          5
  2.000000
  5.000000
  2.440000        684.8000        6.7999996E-02   0.2400000       7.9999998E-02
 0.6000000        0.0000000E+00   0.0000000E+00
          0   85.00000                0
          1   1340.820        4.615033        500.0000        0.6208785
 0.2130093        0.1532036       0.0000000E+00   0.0000000E+00   1.2422355E-02
  217113.0        14763.67        0.0000000E+00   4.3801303E+09
  5.000000        15.00000
  28.61796        0.7070398       5082.549        578.8837        1.132287
CHECK
```

D.1.3 NRCDAT.NOD for All Examples of Appendix D

```
0.25000E-01 0.18182E-03 0.72727E-04 0.31250E+03 0.25000E+01 0.40000E+00
0.10000E+01 0.10000E+01 0.10000E+01 0.62500E+03 0.50000E+01 0.80000E+00
0.10000E+01 0.10000E+01 0.10000E+01 0.62500E+03 0.50000E+01 0.80000E+00
0.10000E+01 0.10000E+01 0.10000E+01 0.62500E+03 0.50000E+01 0.80000E+00
0.10000E+01 0.10000E+01 0.10000E+01 0.62500E+03 0.50000E+01 0.80000E+00
0.10000E+01 0.10000E+01 0.36364E-01 0.62500E+03 0.50000E+01 0.11273E+01
0.50000E+01 0.10000E+01 0.10000E+01 0.37500E+03 0.50000E+01 0.40000E+02
0.10000E+01 0.10000E+01 0.10000E+01 0.25000E+02 0.50000E+01 0.40000E+02
0.10000E+01 0.10000E+01 0.10000E+01 0.25000E+02 0.50000E+01 0.40000E+02
0.10000E+01 0.10000E+01 0.10000E+01 0.25000E+02 0.50000E+01 0.40000E+02
0.10000E+01 0.18182E-03 0.32500E+02 0.25000E+02 0.25000E+01 0.26500E+02
0.10000E+01 0.00000E+00 0.10000E+01 0.25000E+02 0.00000E+00 0.40000E+00
0.10000E+01 0.00000E+00 0.10000E+01 0.25000E+02 0.00000E+00 0.40000E+00
0.10000E+01 0.00000E+00 0.10000E+01 0.25000E+02 0.00000E+00 0.40000E+00
0.10000E+01 0.00000E+00 0.10000E+01 0.25000E+02 0.00000E+00 0.40000E+00
0.10000E+01 0.00000E+00 0.61538E-04 0.25000E+02 0.00000E+00 0.20000E+00
0.50000E-02 0.00000E+00 0.00000E+00 0.12500E+02 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
```

REPEAT THE ABOVE LINE 80 TIMES TO COMPLETE THIS FILE

D.1.4 Plotted Results for Example #1

Summary results for the gas pressure, temperature, and steam mole fraction and for the concrete and equipment surface temperatures as a function of time are presented in the following figures for example #1. Temperature distributions at specified locations within the concrete and equipment composite slabs are also provided.

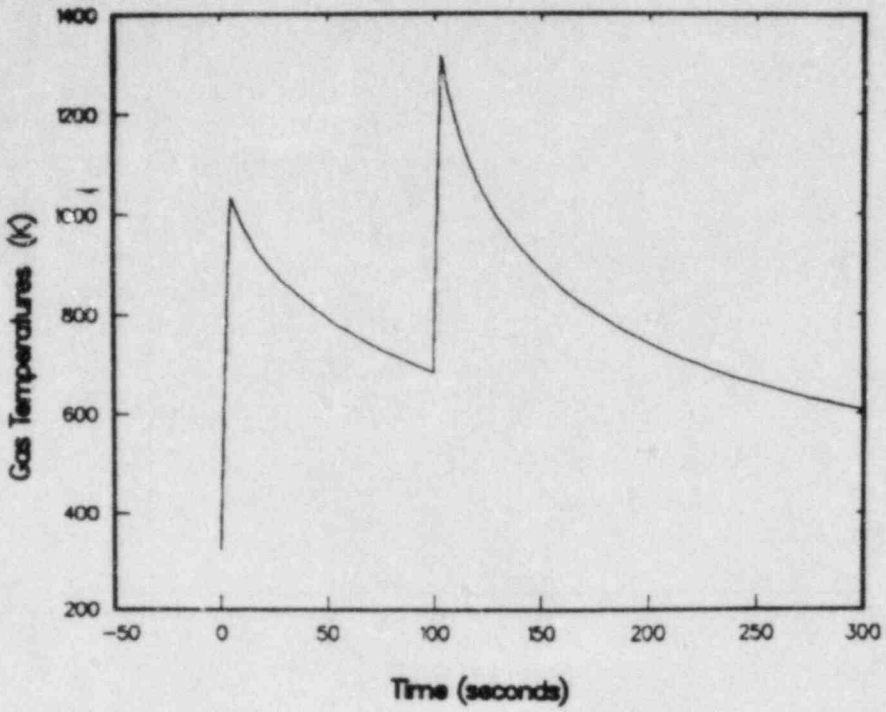

Figure 8. Gas temperature for example #1.

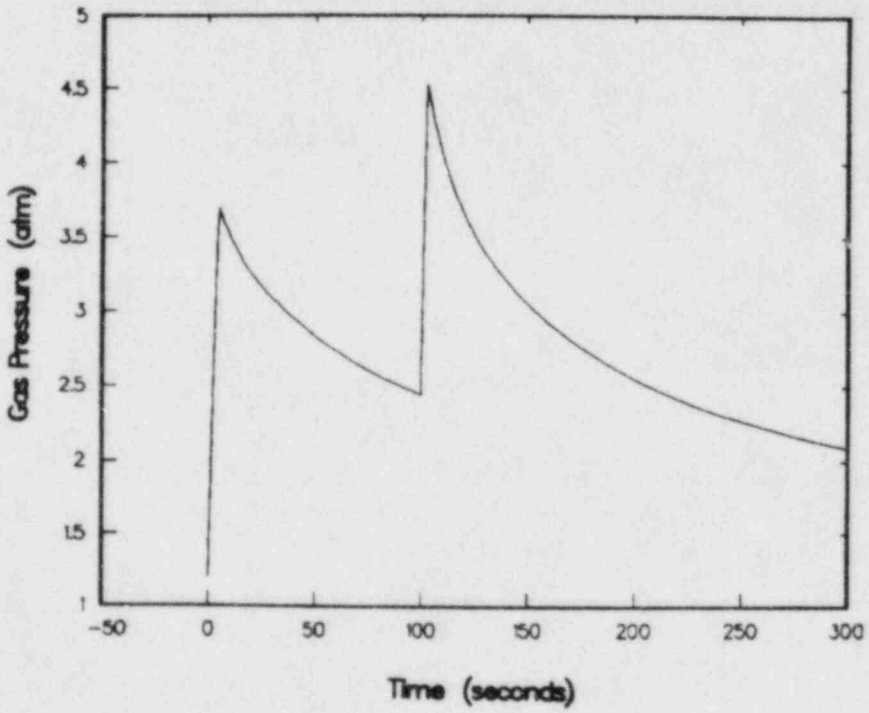

Figure 9. Gas pressure for example #1.

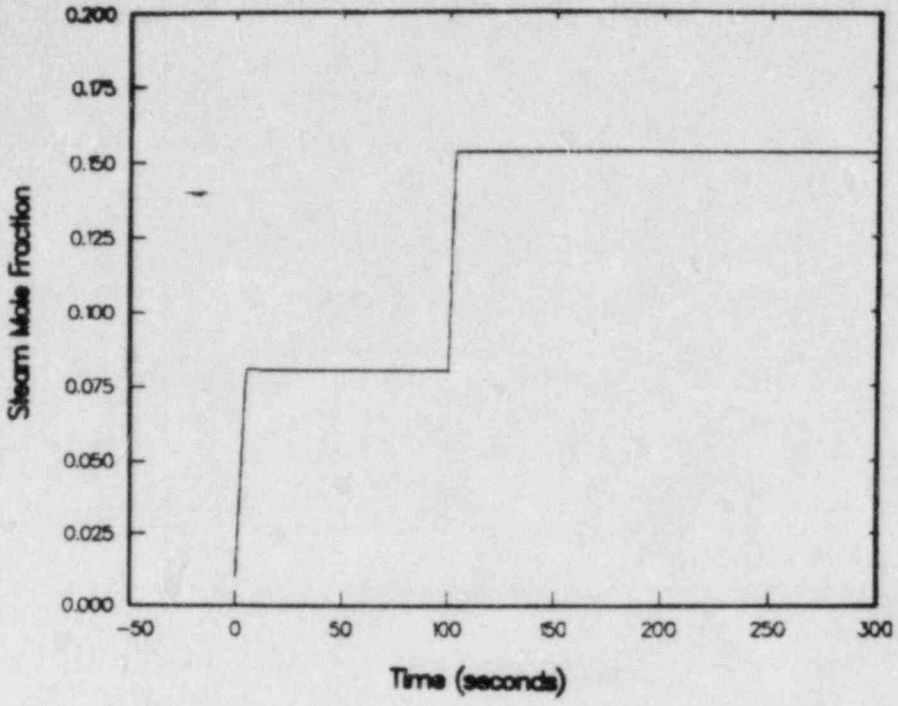

Figure 10. Steam mole fraction for example #1.

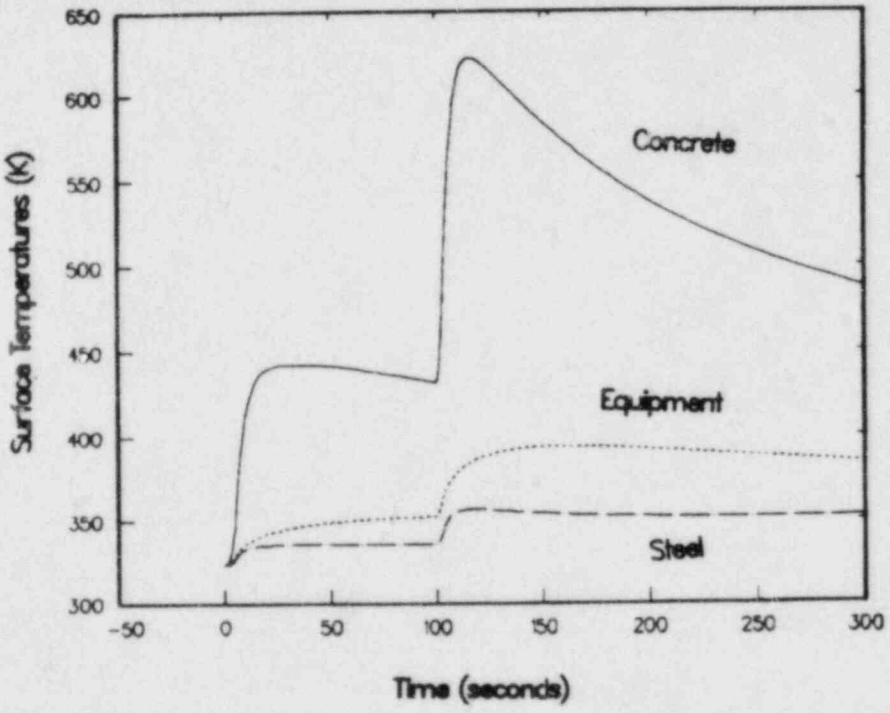

Figure 11. Containment and equipment surface temperatures for example #1.

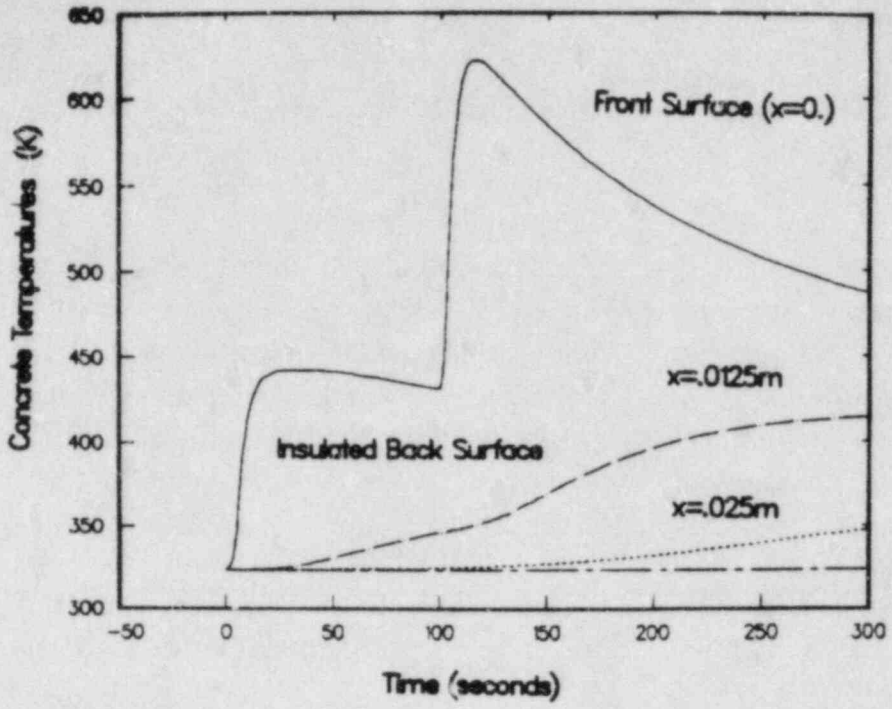

Figure 12. Concrete containment wall thermal response for example #1.

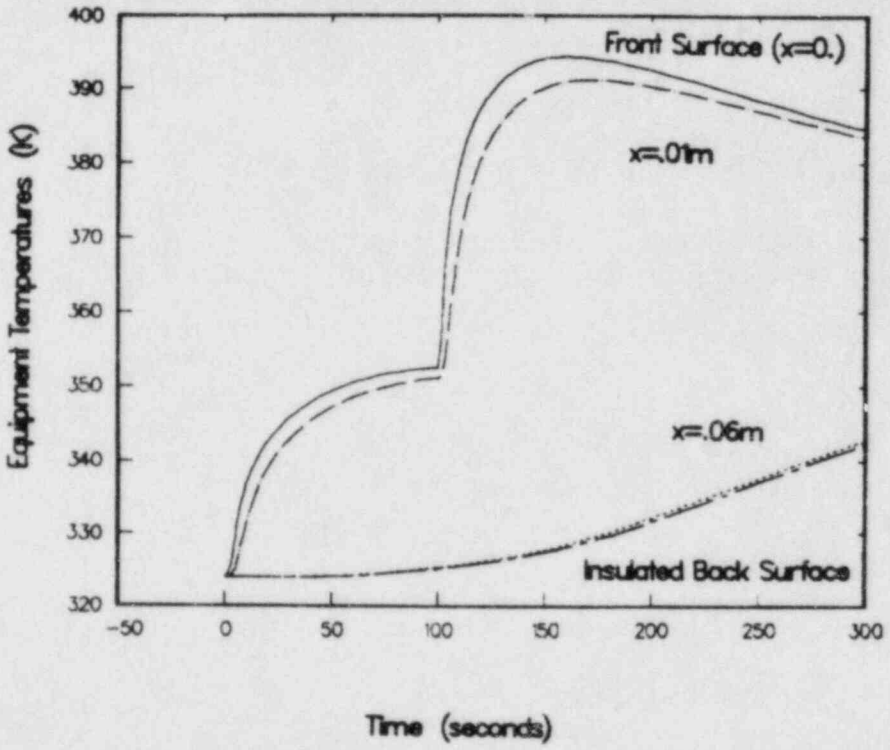

Figure 13. Equipment thermal response for example #1.

D.2 Multiple Burn Simulation with Spray Systems Operative

In this example, a degraded core accident is assumed to have occurred in the reactor geometry given in Appendix C. Hydrogen is released to the containment and the glow plug ignition system is operative resulting in two, 85% complete, 8% (by volume) hydrogen–air deflagrations which are assumed to occur within 100 seconds of each other. It is also assumed that there is no additional steam injection into containment prior to the second deflagration. In this particular example, the spray system in containment is operative following completion of the first deflagration. Particulars associated with the water-spray model have been provided in the example of C.2. The reactor geometry does not have any containment gas leakage and does not include ice condensers and fans.

Included in the following sub-sections are the user-generated data input files for this example. The file NRCDAT.NOD needed for execution of these data files is given in D.1.3. Specifics of these simulations are provided in the two NRCDAT files. In addition, plotted results are given for this example in D.2.3.

D.2.1 NRCDAT for the First Deflagration

```
2:00 PM          14 MAR 84
EXAMPLE #2 - MULTIPLE BURN SIMULATION - SPRAYS ON - 1st BURN
           1
           1
0.0000000E+00    100.0000
 5000.000        1000.000        17.00000
           3
 600.0000        10.00000        0.8000000
           1
5.0000000E-07    1.000000        0.1000000
          17
           5
          17          12           7           5           1
 400.0000        7.000000        0.8500000
           1
9.9999997E-06    55.00000        5.0000001E-02
          11
           3
          11           6           1
```

```
 0.2500000       0.1500000       0.9000000
         3
9.9999997E-06    55.00000        0.9999998E-03
4.9999999E-06    10.00000        5.0000001E-02
1.9999999E-05    65.00000        9.9999998E-03
        16
         4
        16          11           6           1
 6.000000        12.00000        7.000000
 12.00000        10.00000        5.000000
 7.000000        5.000000        0.0000000E+00
0.5998330        0.4000000       1.6700001E-04
0.6000000        0.3996250       3.7500000E-04
0.4000000        0.6000000       0.0000000E+00
         1
 17.00000        0.1000000
 1000.000                2
0.5000000         400.0000
0.5000000         700.0000
         1
         1
         1
         0
         0
5.0000001E-02
         5
 2.000000
 5.000000
 1.200000         325.0000       6.7999996E-02  0.2900000       9.9999998E-03
0.6200000       0.0000000E+00   0.0000000E+00
         0   85.00000                 0
         1   1048.633        3.740231        324.0000        0.6417945
0.2649829       8.0745332E-02   0.0000000E+00  0.0000000E+00   1.2422360E-02
 224987.1        15299.12       0.0000000E+00  4.3898450E+09
 3.000000        15.00000
 28.80873        0.3020062       5755.652        316.1626        1.214363
CHECK
```

D.2.2 NRCDAT for the Second Deflagration

```
2:15 PM          14 MAR 84
EXAMPLE #2 - MULTIPLE BURN SIMULATION - SPRAYS ON - 2nd BURN
          1
          0
  100.0000         200.0000
  5000.000         1000.000         17.00000
          3
  600.0000         10.00000         0.8000000
          1
5.0000000E-07      1.000000         0.1000000
         17
          5
         17           12               7              5              1
  400.0000         7.000000         0.8500000
          1
9.9999997E-06      55.00000         5.0000001E-02
         11
          3
         11            6               1
0.2500000          0.1500000        0.9000000
          3
9.9999997E-06      55.00000         9.9999998E-03
4.9999999E-06      10.00000         5.0000001E-02
1.9999999E-05      65.00000         9.9999998E-03
         16
          4
         16           11               6              1
  6.000000         12.00000         7.000000
  12.00000         10.00000         5.000000
  7.000000         5.000000         0.0000000E+00
0.5998330          0.4000000        1.6700001E-04
0.6000000          0.3996250        3.7500000E-04
0.4000000          0.6000000        0.0000000E+00
          1
  17.00000         0.1000000
  1000.000                  2
0.5000000          400.0000
```

```
0.5000000          700.0000
         1
         1
         1
         0
         0
5.0000001E-02
         5
 2.000000
 5.000000
 1.563000          350.2000          6.7999996E-02  0.2000000          0.2400000
0.4800000          0.0000000E+00     0.0000000E+00
         0  85.00000                        1
 17.00000          0.1000000
         1  1031.445          4.446990          500.0000          0.4968778
0.1718260          0.3188406          0.0000000E+00  0.0000000E+00  1.2422360E-02
 271958.4          18493.17           0.0000000E+00  5.4982303E+09
 5.000000          15.00000
 28.54276          1.417881           5107.689       1509.078       1.323353
CHECK
```

D.2.3 Plotted Results for Example #2

Summary results for the gas pressure, temperature, and steam mole fraction and for the concrete and equipment surface temperatures as a function of time are presented in the following figures for example #2. Temperature distributions at specified locations within the concrete and equipment composite slabs are also provided.

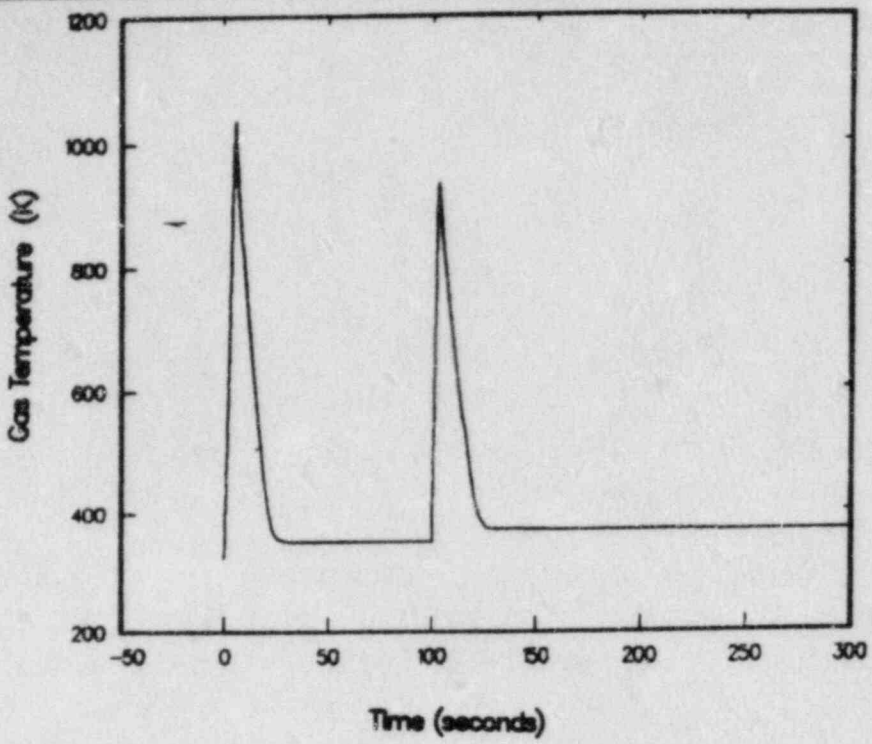

Figure 14. Gas temperature for example #2.

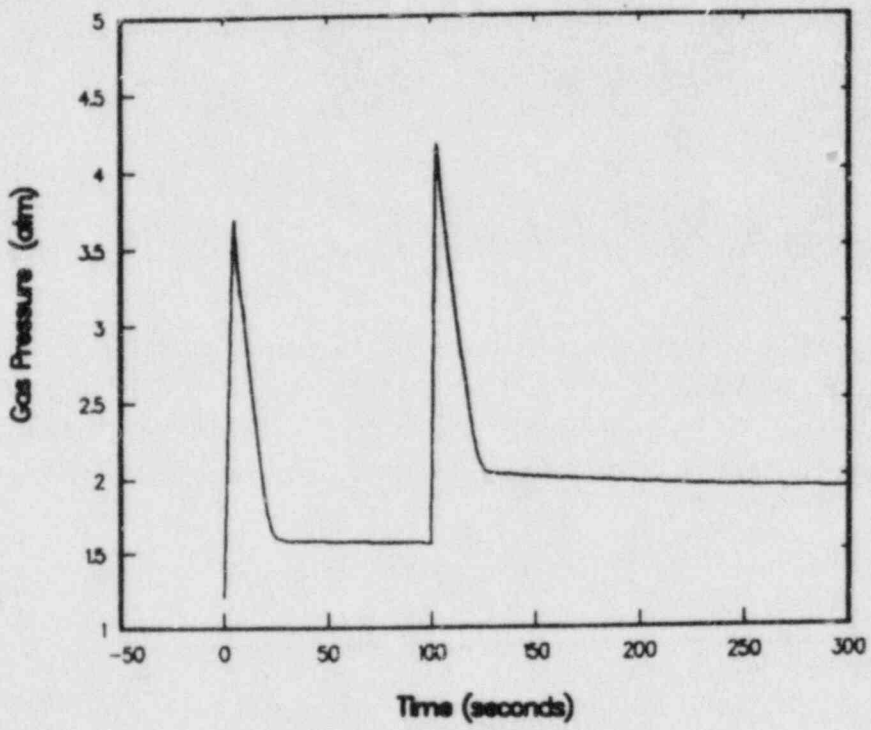

Figure 15. Gas pressure for example #2.

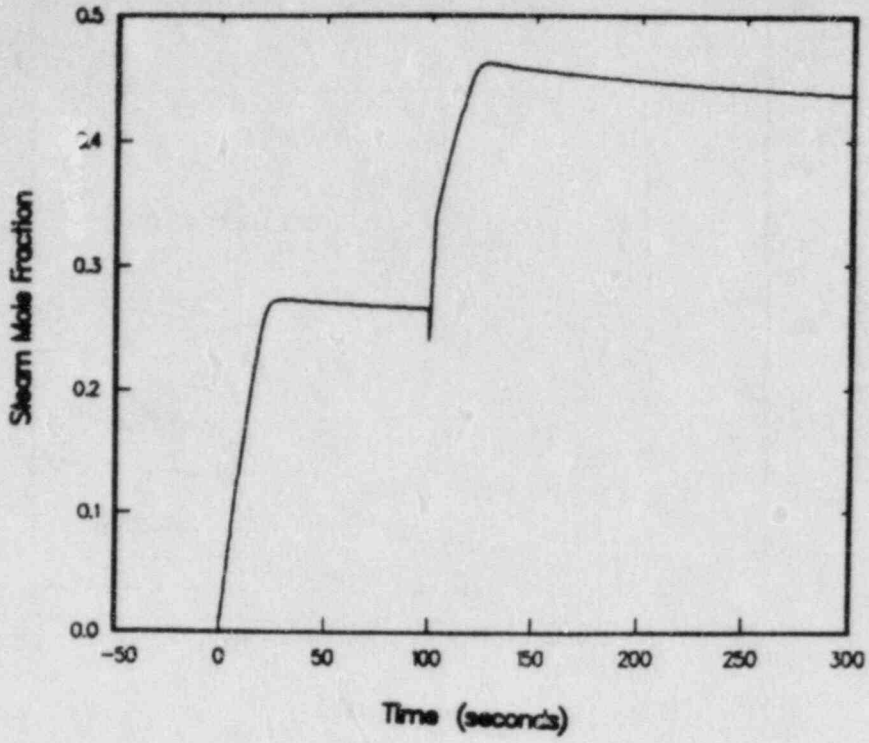

Figure 16. Steam mole fraction for example #2.

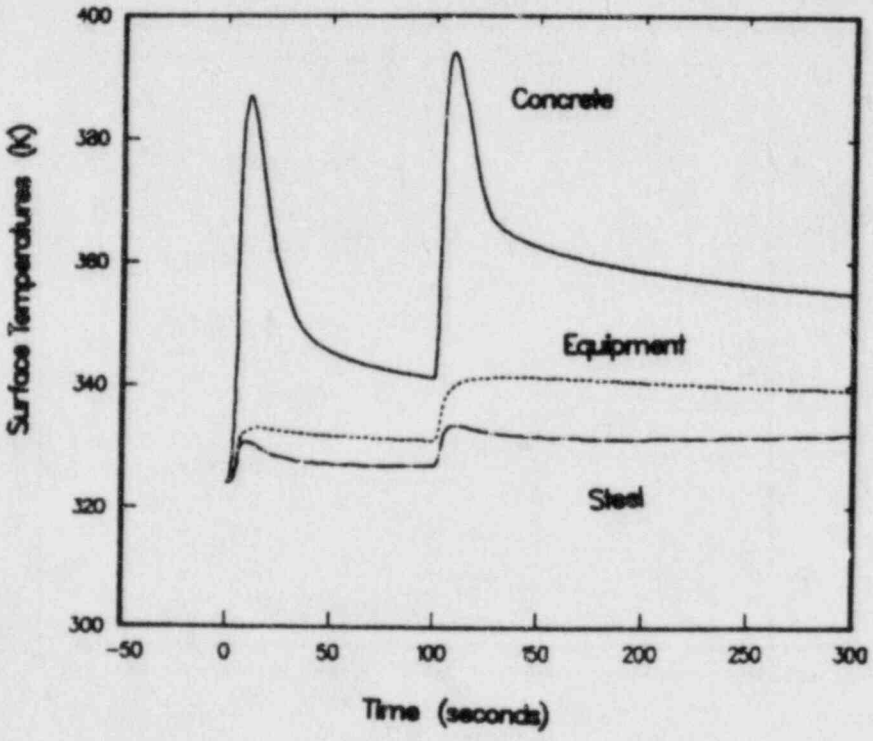

Figure 17. Containment and equipment surface temperatures for example #2.

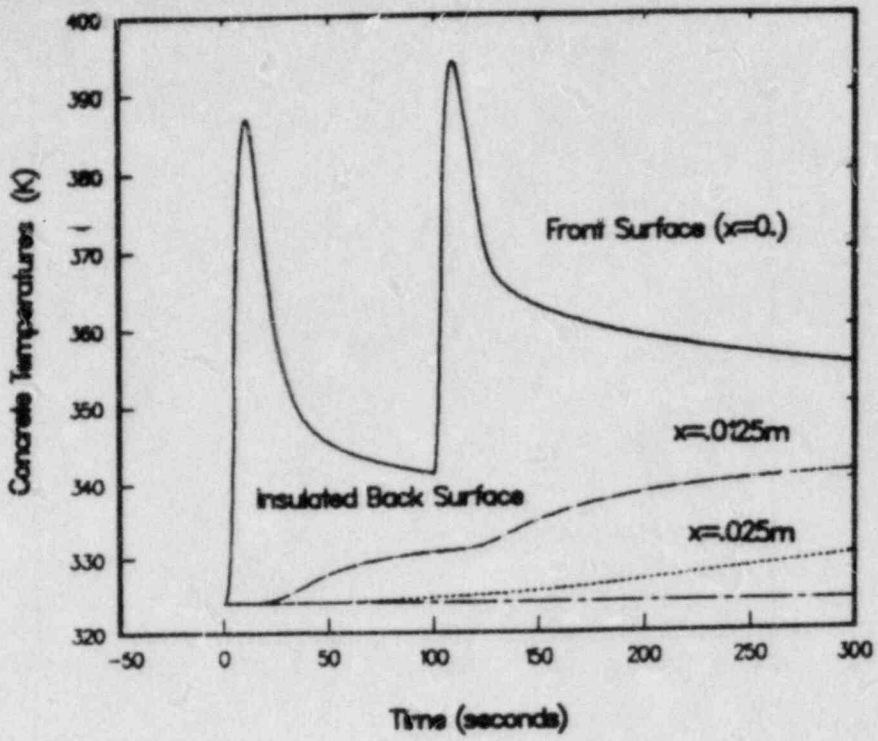

Figure 18. Concrete containment wall thermal response for example #2.

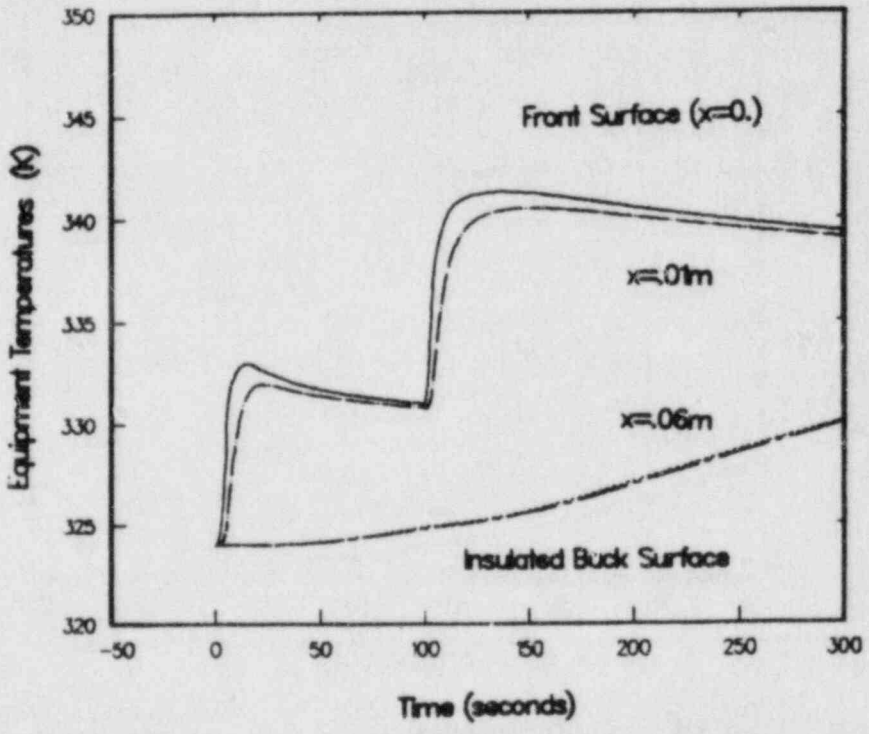

Figure 19. Equipment thermal response for example #2.

D.3 Multiple Burn Simulation Which Includes Ice-Condenser Engineering Model

In this example, a degraded core accident is assumed to have occurred in the reactor geometry given in Appendix C. Hydrogen is released to the containment and the glow plug ignition system is operative resulting in two, 85% complete, 8% (by volume) hydrogen–air deflagrations which are assumed to occur within 100 seconds of each other. It is also assumed that there is no additional steam injection into containment prior to the second deflagration. In this particular example, the spray system in containment is inoperative, and the reactor geometry does not have any containment gas leakage. This reactor includes ice condensers and fans. The upper compartment is assumed to have a volume of 10000 m^3. Other particulars associated with the engineering model have been provided in the example of C.2.

Included in the following sub-sections are the user-generated data input files for this example. The file NRCDAT.NOD needed for execution of these data files is given in D.1.3. Specifics of these simulations are provided in the two NRCDAT files. In addition, plotted results are given for this example in D.3.3.

D.3.1 NRCDAT for the First Deflagration

```
3:00 PM          14 MAR 84
EXAMPLE #3 - MULTIPLE BURN SIMULATION - ICE CONDENSER - 1st BURN
         1
         1
0.0000000E+00   100.0000
 5000.000       1000.000        17.00000
         3
 600.0000       10.00000        0.8000000
         1
5.0000000E-07   1.000000        0.1000000
        17
         5
        17          12          7           5           1
 400.0000       7.000000        0.8500000
         1
9.9999997E-06   55.00000        5.0000001E-02
        11
```

```
          3
         11          6          1
 0.2500000  0.1500000  0.9000000
          3
 9.9999997E-06  55.00000  9.9999998E-03
 4.9999999E-06  10.00000  5.0000001E-02
 1.9999999E-05  65.00000  9.9999998E-03
         16
          4
         16         11          6          1
  6.000000  12.00000  7.000000
  12.00000  10.00000  5.000000
  7.000000  5.000000  0.0000000E+00
 0.5998330  0.4000000  1.6700001E-04
 0.6000000  0.3996250  3.7500000E-04
 0.4000000  0.6000000  0.0000000E+00
          0
          1
          1
          1
          1
  10000.00
  320.0000
  40000.00
  1.500000
  2.000000
  290.0000
 4.9999999E-03
          0
 5.0000001E-02
         11
  1.000000
 0.5000000
  1.200000  325.0000  6.7999996E-02  0.2900000  9.9999998E-03
 0.6200000  0.0000000E+00  0.0000000E+00
          0  85.00000  0
          1  1048.633  3.740231  324.0000  0.6417945
 0.2649829  8.0745332E-02  0.0000000E+00  0.0000000E+00  1.2422360E-02
  224987.1  15299.12  0.0000000E+00  4.3898450E+09
  3.000000  15.00000
  28.80873  0.3020062  5755.652  316.1626  1.214363
CHECK
```

D.3.2 NRCDAT for the Second Deflagration

```
3:15 PM        14 MAR 84
EXAMPLE #3 - MULTIPLE BURN SIMULATION  - ICE CONDENSER - 2nd BURN

         1
         0
 100.0000        200.0000
 5000.000        1000.000        17.00000
         3
 600.0000        10.00000        0.8000000
         1
5.0000000E-07    1.000000        0.1000000
        17
         5
        17          12           7          5          1
 400.0000        7.000000        0.8500000
         1
9.9999997E-06    55.00000        5.0000001E-02
        11
         3
        11          6           1
0.2500000       0.1500000       0.9000000
         3
9.9999997E-06    55.00000        9.9999998E-03
4.9999999E-06    10.00000        5.0000001E-02
1.9999999E-05    65.00000        9.9999998E-03
        16
         4
        16          11          6          1
 6.000000        12.00000        7.000000
 12.00000        10.00000        5.000000
 7.000000        5.000000        0.0000000E+00
0.5998330       0.4000000       1.6700001E-04
0.6000000       0.3996250       3.7500000E-04
0.4000000       0.6000000       0.0000000E+00
         0
         1
         1
         1
         1
 10000.00
 312.6500
 40000.00
 1.500000
 2.000000
```

```
 290.0000
4.9999999E-03
           0
5.0000001E-02
          11
 1.000000
0.5000000
 1.258000          439.3000          6.7999996E-02  0.2600000          3.9999999E-02
0.6200000          0.0000000E+00     0.0000000E+00
           0    85.00000                    0
           1    1140.137          3.153942          500.0000          0.6417627
0.2338951          0.1118009         0.0000000E+00  0.0000000E+00     1.2422358E-02
 174493.4          11865.55          0.0000000E+00  3.4615020E+09
 5.000000          15.00000
 28.69505          0.3523134         4296.093       339.5157          0.9271217
CHECK
```

D.3.3 Plotted Results for Example #3

Summary results for the lower compartment gas pressure, temperature, and steam mole fraction and for the concrete and equipment surface temperatures as a function of time are presented in the following figures for example #3. In addition, the gas pressure and temperature in the upper compartment of the reactor are provided for comparison. Temperature distributions at specified locations within the concrete and equipment composite slabs are also provided.

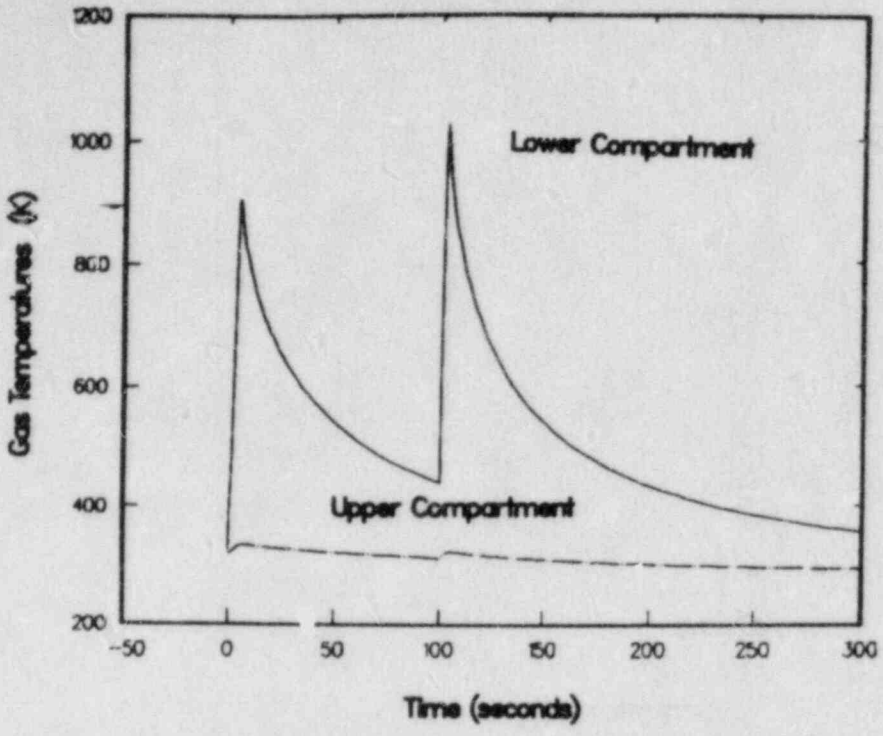

Figure 20. Gas temperature for example #3.

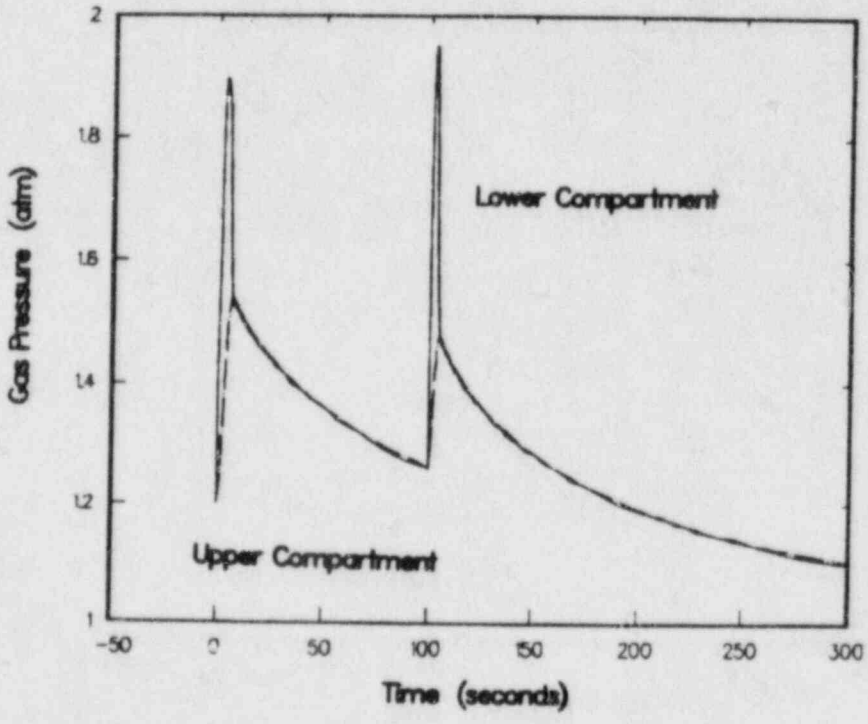

Figure 21. Gas pressure for example #3.

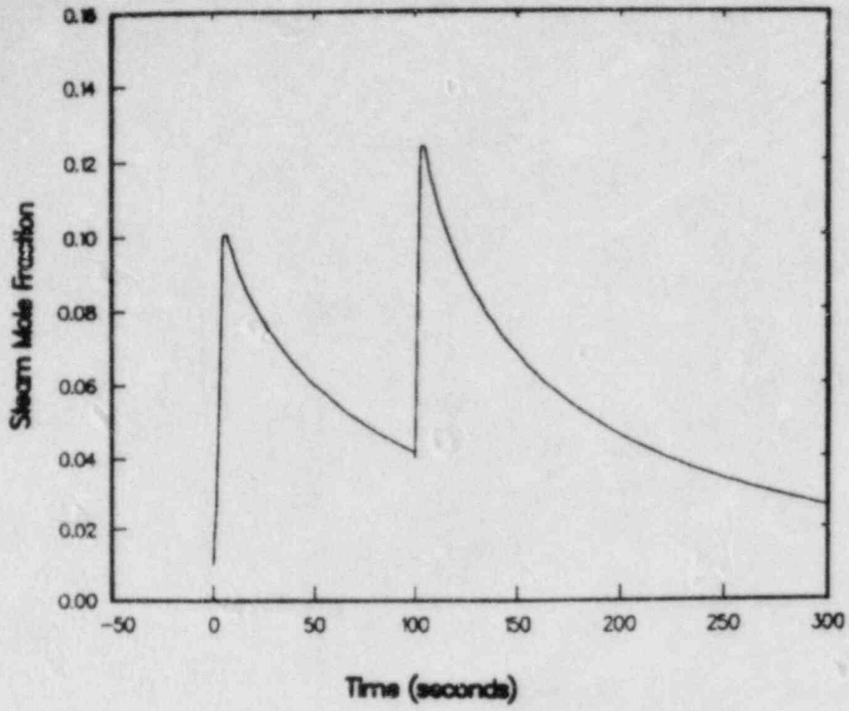

Figure 22. Steam mole fraction for example #3.

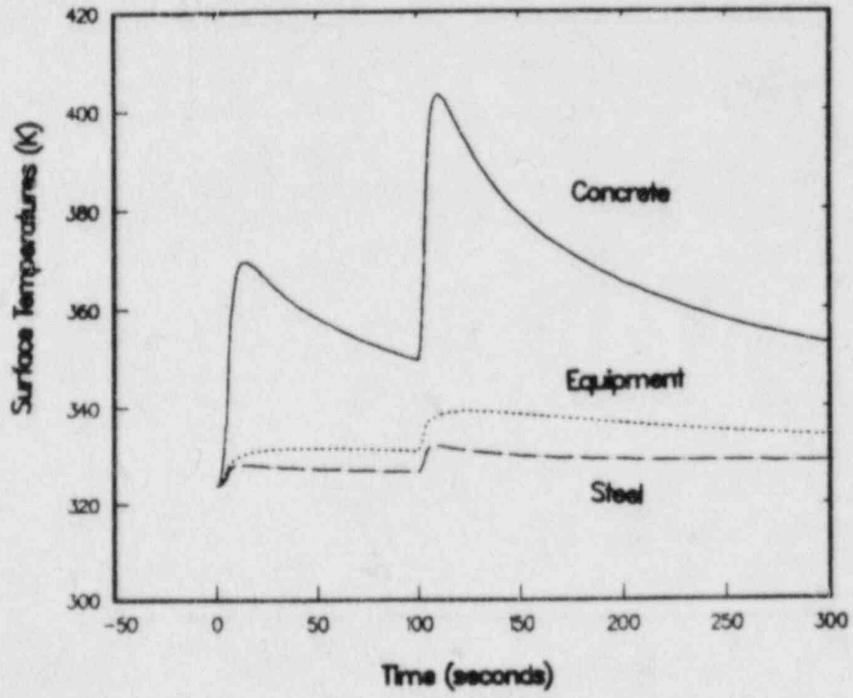

Figure 23. Containment and equipment surface temperatures for example #3.

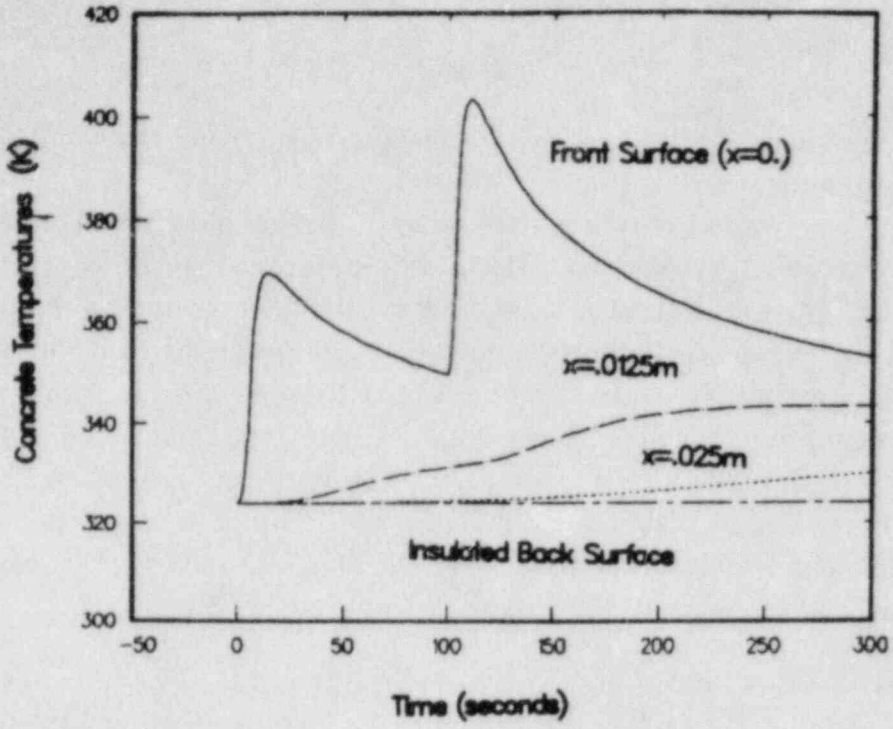

Figure 24. Concrete containment wall thermal response for example #3.

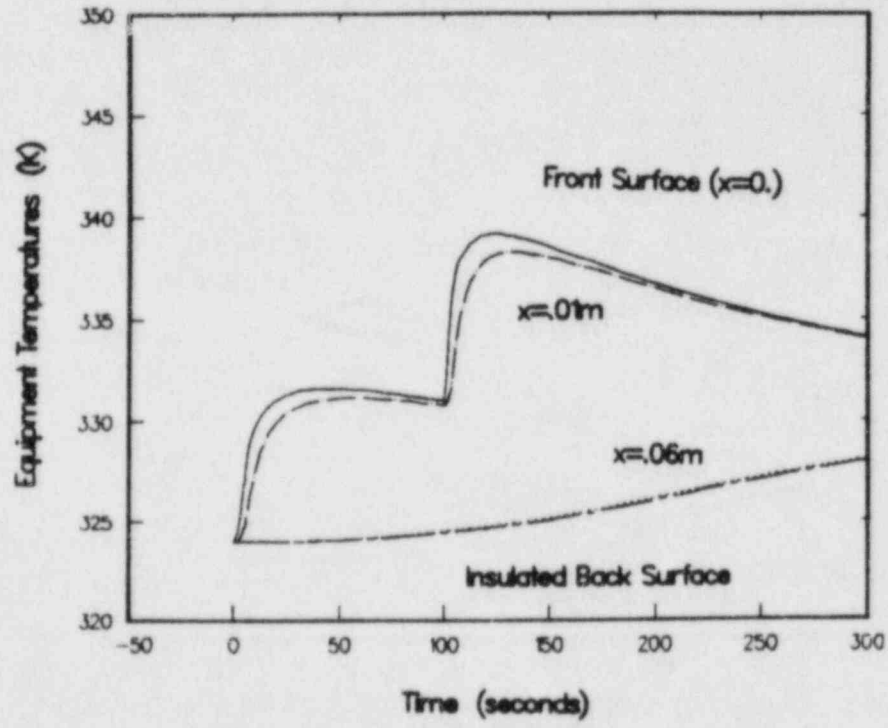

Figure 25. Equipment thermal response for example #3.

D.4 Multiple Burn Simulation with Gas Leakage from the Containment

In this example, a degraded core accident is assumed to have occurred in the reactor geometry given in Appendix C. Hydrogen is released to the containment and the glow plug ignition system is operative resulting in two, 85% complete, 8% (by volume) hydrogen–air deflagrations which are assumed to occur within 100 seconds of each other. It is also assumed that there is no additional steam injection into containment prior to the second deflagration. In this example, the spray system in containment is inoperative, and the reactor does not include ice condensers and fans. The reactor geometry has a containment penetration of 0.1 m^2 through which gas leakage can occur. Other particulars associated with the engineering model have been provided in the example of C.2.

Included in the following sub-sections are the user-generated data input files for this example. The file NRCDAT.NOD needed for execution of these data files is given in D.1.3. Specifics of these simulations are provided in the two NRCDAT files. In addition, plotted results are given for this example in D.4.3.

D.4.1 NRCDAT for the First Deflagration

```
4:00 PM          14 MAR 84
EXAMPLE #4 - MULTIPLE BURN SIMULATION - CONTAINMENT LEAK - 1st BURN

           1
           1
0.0000000E+00    100.0000
 5000.000         1000.000         17.00000
           3
 600.0000         10.00000         0.8000000
           1
5.0000000E-07     1.000000         0.1000000
          17
           5
          17           12            7            5            1
 400.0000         7.000000         0.8500000
           1
9.9999997E-06     55.00000         5.0000001E-02
          11
           3
          11            6            1
```

```
0.2500000       0.1500000       0.9000000
          3
9.9999997E-06    55.00000       9.9999998E-03
4.9999999E-06    10.00000       5.0000001E-02
1.9999999E-05    65.00000       9.9999998E-03
         16
          4
         16          11           6           1
 6.000000        12.00000        7.000000
 12.00000        10.00000        5.000000
 7.000000        5.000000        0.0000000E+00
0.5998330        0.4000000       1.6700001E-04
0.6000000        0.3996250       3.7500000E-04
0.4000000        0.6000000       0.0000000E+00
          0
          1
          1
          1
          0
          1
5.0000001E-02    1.000000        300.0000
5.0000001E-02
         11
 1.000000
 1.000000
 1.200000        325.0000        6.7999996E-02   0.2900000       9.9999998E-03
0.6200000        0.0000000E+00   0.0000000E+00
          0   85.00000                 0
          1   1048.633        3.740231        324.0000        0.6417945
0.2649829        8.0745332E-02   0.0000000E+00   0.0000000E+00   1.2422360E-02
 224987.1        15299.12        0.0000000E+00   4.3898450E+09
 3.000000        15.00000
 28.80873        0.3020062       5755.652        316.1626        1.214363
CHECK
```

D.4.2 NRCDAT for the Second Deflagration

```
4:10 PM          14 MAR 84
EXAMPLE #4 - MULTIPLE BURN SIMULATION - CONTAINMENT LEAK - 2nd BURN

          1
          0
  100.0000          200.0000
  5000.000          1000.000          17.00000
          3
  600.0000          10.00000          0.8000000
          1
 5.0000000E-07      1.000000          0.1000000
         17
          5
         17          12          7          5          1
  400.0000          7.000000          0.8500000
          1
 9.9999997E-06      55.00000          5.0000001E-02
         11
          3
         11           6          1
 0.2500000          0.1500000         0.9000000
          3
 9.9999997E-06      55.00000          9.9999998E-03
 4.9999999E-06      10.00000          5.0000001E-02
 1.9999999E-05      65.00000          9.9999998E-03
         16
          4
         16          11          6          1
  6.000000          12.00000          7.000000
  12.00000          10.00000          5.000000
  7.000000          5.000000          0.0000000E+00
 0.5998330          0.4000000         1.6700001E-04
 0.6000000          0.3996250         3.7500000E-04
 0.4000000          0.6000000         0.0000000E+00
          0
          1
```

```
          1
          1
          0
          1
 5.0000001E-02    1.000000        300.0000
 5.0000001E-02
         11
  1.000000
  1.000000
  1.548000        616.7000        6.7999996E-02   0.2500000       7.9999998E-02
 0.5900000        0.0000000E+00   0.0000000E+00
          0   85.00000                0
          1   1281.348        3.107003        500.0000        0.6106007
 0.2234362        0.1532061       0.0000000E+00   0.0000000E+00   1.2422354E-02
  152952.5        10400.77        0.0000000E+00   3.0769838E+09
  5.000000        15.00000
  28.67204        0.4760118       3587.325        407.8202        0.7990291
CHECK
```

D.4.3 Plotted Results for Example #4

Summary results for the reactor containment gas pressure, temperature, and steam mole fraction and for the concrete and equipment surface temperatures as a function of time are presented in the following figures for example #4. In addition, the environment pressure and temperature are included for comparison. Temperature distributions at specified locations within the concrete and equipment composite slabs are also provided.

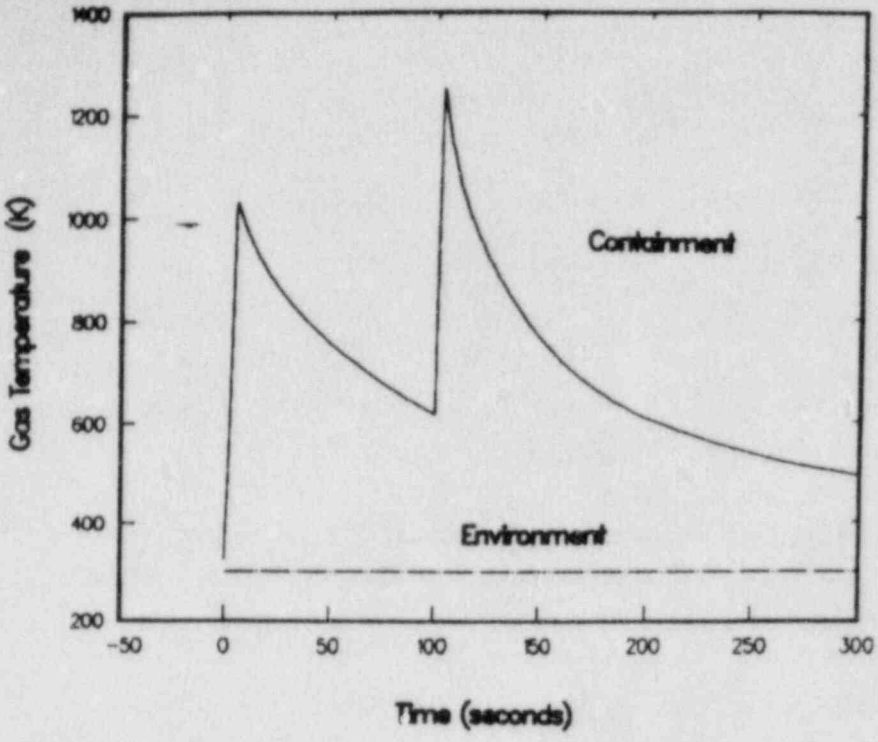

Figure 26. Gas temperature for example #4.

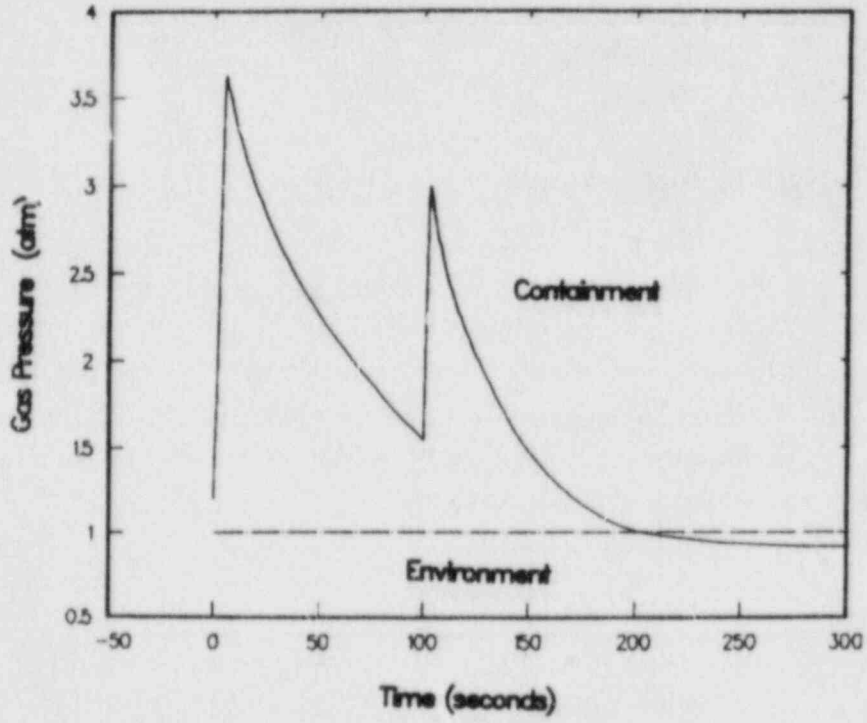

Figure 27. Gas pressure for example #4.

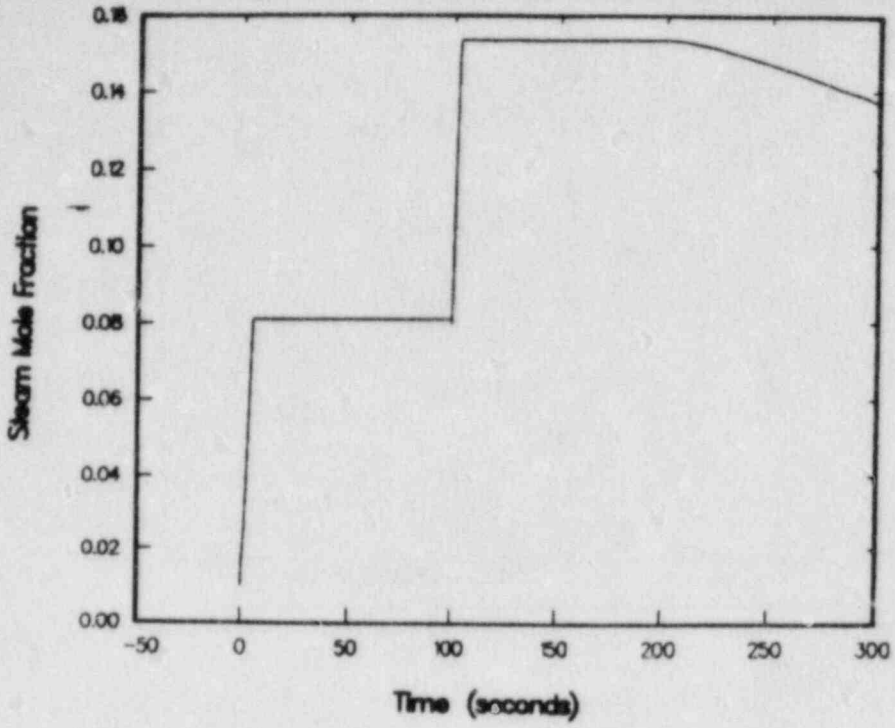

Figure 28. Steam mole fraction for example #4.

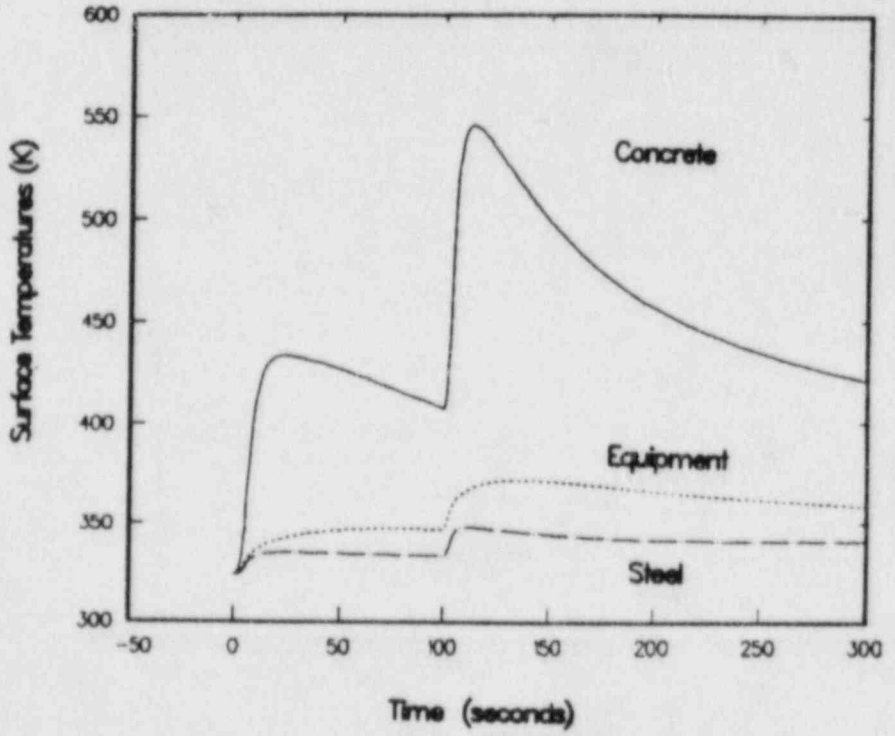

Figure 29. Containment and equipment surface temperatures for example #4.

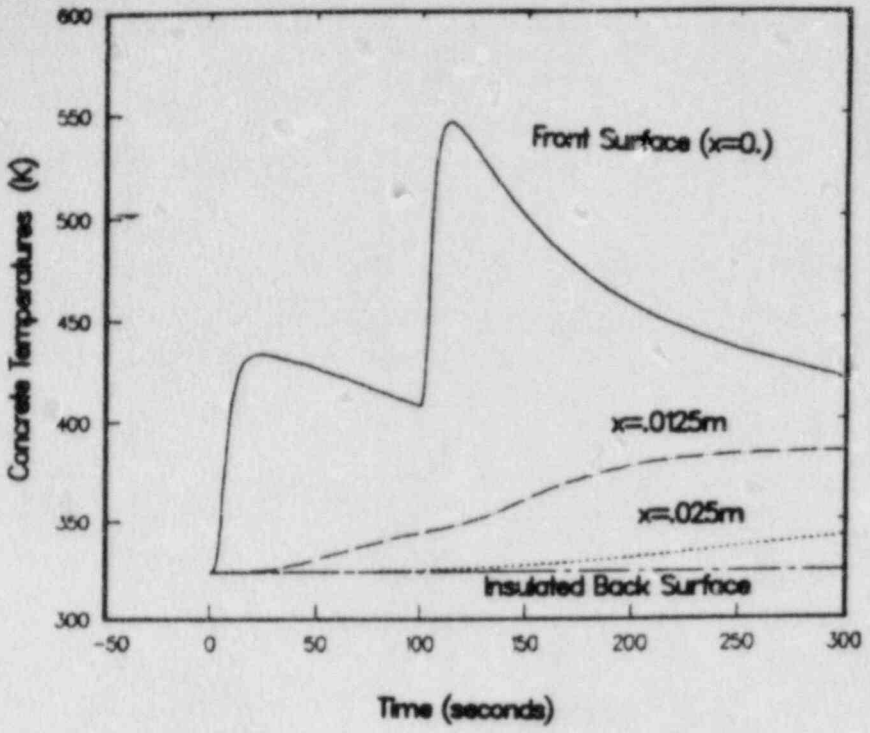

Figure 30. Concrete containment wall thermal response for example #4.

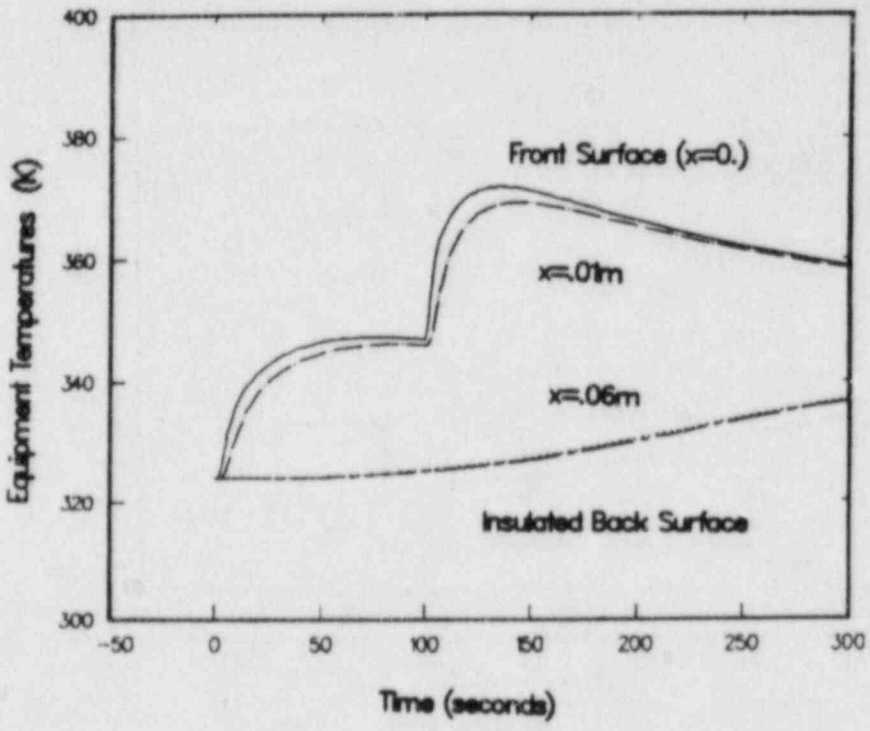

Figure 31. Equipment thermal response for example #4.

Appendix E. Nomenclature for Data Initialization in SOLVER

A nomenclature is provided to define the variables which are echo-printed to the screen during the data initialization in SOLVER. Also included are the units used in HYBER (those variables without units are dimensionless).

AIC	Inlet area of ice condenser	$[m^2]$
ALPHA(I,II)	Thermal diffusivity of surface I and composite material II	$[m^2/s]$
AOUT	Leak area	$[m^2]$
AFAN	Fan opening area	$[m^2]$
AREA	Total containment surface area	$[m^2]$
AREA(I)	Surface area of suface I	$[m^2]$
CO1	Initial carbon monoxide mole fraction	
CO21	Initial carbon dioxide mole fraction	
COBRND	Number of moles of carbon monoxide burned	[*moles*]
COMPL1	Percent combustion completion	
DIAM(I)	Diameter of water spray droplet i	[*microns*]
EAICC	Adiabatic isochoric combustion energy	$[J]$
EMIS(I)	Emissivity of surface I	
FANCFM	Fan rating	$[ft^3/min]$
FREQ(I)	Frequency of water spray droplet i	
FTIME	Time duration of current simulation	$[s]$
H21	Initial hydrogen mole fraction	
H2O1	Initial steam mole fraction	
H2MBRND	Number of moles of hydrogen that are burned	[*moles*]
IBRN	Multiple burn simulation? 1=yes, 0=no	
IBURN	Heat transfer during combustion? 1=yes, 0=no	
ICOMP	Is the ice-condenser engineering model to be operative? 1=yes, 0=no	
ICOMPL	Is combustion complete? 1=yes, 0=no	
INDS	Number of drop sizes	
ISPRAY	Are water spray systems operative? 1=yes, 0=no	

IH2OL	Is suspended water to be included in combustion calculation? 1=yes, 0=no	
IMAT(I)	Number of materials comprising slab i	
IMUL	Is this the first pass through the data generator for a multiple burn? 1=yes, 0=no	
INS	Number of surfaces	
K(I,II)	Thermal conductivity of surface I and composite II	$[W/(m-K)]$
LBURN	Burn length	$[m]$
L(I)	Characteristic length of surface I	$[m]$
MA	Air molecular weight	$[gm/mole]$
MAIR	Mass of air in gas	$[kg]$
MSTEAM	Mass of steam in gas	$[kg]$
MW	Molecular weight	$[kg/mole]$
N21	Initial nitrogen mole fractior	
O21	Initial oxygen mole fraction	
P1	Initial gas pressure	$[atm]$
PATM	Gas pressure	$[atm]$
PINF	Pressure outside containment	$[atm]$
PGO	Steam partial pressure	$[atm]$
PTOL	Pressure differential for fan operation	$[atm]$
SPINC	Spatial increment for water spray calculation	$[m]$
SPFLO	Water spray total flow rate	$[gal/min]$
T1	Initial gas temperature	$[K]$
TEMPIC	Temperature of gas exitting the ice condenser	$[K]$
TEMPU	Initial gas temperature in upper compartment of ice-condenser nuclear reactor	$[K]$
TIME	Initial time for current simulation	$[s]$
TGO	Gas temperature	$[K]$
THIK(I,II)	Thickness of composite material II from surface I	$[m]$
TINF	Temperature outside containment	$[K]$
TOTMOL	Total number of moles of gas	$[moles]$
TWINIT	Initial temperature of each slab	$[K]$
VOL	Containment volum	$[m^3]$
VOLU	Upper compartment volume of ice-condenser reactor	$[m^3]$
VDIA	Effective containment diameter	$[m]$
XF(I)	Mole fraction of gas species I	
ZTOT	Total water spray fall distance	$[m]$

Appendix F. Procedure Files for Executing HYBER

F.1 RUN.BAT Procedure File

RUN.BAT is a procedure file which performs all computer file assignments necessary for executing the algorithm on an IBM Personal Computer. The procedure file performs appropriate file assignments needed in performing the different types of analyses. The computer listing is given below.

```
A:
REM    THE PROCEDURE FILE AND DATGEN ARE IN DRIVE A
REM    SOLVER IS IN DRIVE B
PAUSE
IF %1 == DATFIL GOTO JKL
A:%1.EXE
:JKL
COPY A:NRCDAT B:DATA
COPY A:NRCDAT.NOD B:NODES
REM    THE FILES NRCDAT AND NRCDAT.NOD ARE COPIED TO
REM    DRIVE B AND RENAMED DATA AND NODES
B:
B:%2.EXE
A:
COPY B:DATA A:RESTART
REM
REM    FOR SINGLE OR MULTIPLE BURNS, A RESTART FILE IS ALWAYS
REM    READ ONTO THE DISK IN DRIVE A.
REM    THE RESTART FILE GIVES THE USER THE OPTION TO
REM    INTERACTIVELY:
REM    1)START A NEW SINGLE OR MULTIPLE BURN WITH OLD
REM      SIMULATION PARAMETERS, OR
REM    2)CONTINUE THE EXISTING MULTIPLE BURN
PAUSE
IF EXIST B:DBK GOTO ABC
COPY B:OLDDAT A:OLDDAT
COPY B:OLDWALL B:OLDWALT
:ABC
IF EXIST B:DBK ERASE B:DBK
REM
REM     TO CONTINUE A MULTIPLE BURN, OLDDAT MUST BE READ
REM     ONTO THE DISK IN DRIVE A  AND
REM     THE FINAL SLAB TEMPERATURES FROM THE FILE OLDWALL
REM     MUST BE STORED IN THE FILE OLDWALT ON DRIVE B
PAUSE
REM
REM     FOR ANY BURN, THE EXECUTION OF SOLVER CREATES
REM     4 TO 7 FILES:
```

```
REM     OUTPUT, FLUX, ENERGY, TEMPS1, TEMPS2, TEMPS3, FLOWS
REM     NOTE THAT TEMPS1, TEMPS2, TEMPS3, FLOWS ARE OPTIONAL
COPY B:OUTPUT A:
COPY B:FLUX A:
COPY B:ENERGY A:
IF NOT EXIST B:TEMPS1 GOTO BCD
COPY B:TEMPS1 A:
:BCD
IF NOT EXIST B:TEMPS2 GOTO CDE
COPY B:TEMPS2 A:
:CDE
IF NOT EXIST B:TEMPS3 GOTO DEF
COPY B:TEMPS3 A:
:DEF
IF NOT EXIST B:FLOWS GOTO HIJ
COPY B:FLOWS A:
:HIJ
REM     BEFORE MAKING ANOTHER RUN, THE FILES CREATED BY
REM     SOLVER MUST BE SAVED ON A SEPARATE DISK.
REM     THE OUTPUT FILES CREATED BY SOLVER ON DRIVE B
REM     HAVE BEEN COPIED TO DRIVE A.
REM     REMOVE SOLVER FROM DRIVE B AND PLACE A FORMATTED
REM     DISK IN DRIVE B
PAUSE
COPY OUTPUT B:%3.OUT
DEL OUTPUT
COPY FLUX B:%3.FLX
DEL FLUX
COPY ENERGY B:%3.NRG
DEL ENERGY
IF NOT EXIST TEMPS1 GOTO EFG
COPY TEMPS1 B:%3.TS1
DEL TEMPS1
:EFG
IF NOT EXIST TEMPS2 GOTO FGH
COPY TEMPS2 B:%3.TS2
DEL TEMPS2
:FGH
IF NOT EXIST TEMPS3 GOTO GHI
COPY TEMPS3 B:%3.TS3
DEL TEMPS3
:GHI
IF NOT EXIST FLOWS GOTO IJK
COPY FLOWS B:%3.FLO
DEL FLOWS
:IJK
REM     THE OUTPUT FILES ARE NOW ON THE NEW DISK IN
REM     DRIVE B AND HAVE BEEN ERASED FROM DISK 1.
REM     THE OUTPUT FILES ON THE NEW DISK HAVE BEEN
REM     RENAMED AND CAN BE IDENTIFIED BY THEIR SUFFIXES
REM     TO START ANY NEW BURN OR CONTINUE WITH THE
REM     EXISTING MULTIPLE BURN, REPLACE SOLVER IN
REM     DRIVE B AND ENTER:
REM     RUN DATGEN SOLVER casename  OR
REM     RUN DATFIL SOLVER casename
```

F.2 RUNALG.COM

RUNALG.COM is a procedure file which performs all computer file assignments necessary for executing the algorithm on a VAX 11/780 computer. The procedure file provides interactive prompts to the user in order to set up appropriate file assignments needed in performing the different types of analyses. The computer listing is given below.

```
$!!
$!!    RUNALG IS DESIGNED TO OPERATE THE ALGORITHM COMPUTER
$!!    CODES ON THE VAX 11/780 COMPUTER FOR ALL OPTIONS INCLUDING:
$!!
$!!       SINGLE BURN WITH FULL DATA INPUT REQUIRED
$!!       SINGLE BURN USING PREVIOUSLY GENERATED GEOMETRY
$!!       MULTIPLE BURN SEQUENCES - 1ST BURN WITH FULL DATA
$!!              INPUT REQUIRED
$!!       MULTIPLE BURN SEQUENCES - 1ST BURN USING RESTART
$!!              OPTION TO INPUT GEOMETRY PREVIOUSLY CREATED
$!!       MULTIPLE BURN SEQUENCES - USING RESTART OPTION
$!!              AND USING PREVIOUSLY GENERATED GEOMETRY
$!!       SINGLE AND MULTIPLE BURN OPTIONS WHERE DATA FILES HAVE
$!!              BEEN PREVIOUSLY GENERATED (EXECUTE ONLY SOLVER)
$!!
$!!
$ ASSIGN TT: SYS$INPUT
$!!
$!!   DUMMYS USED FOR SELECTING OPTIONS IN SOLVER
$!!
$ ASK1=0
$ ASK2=0
$ ASK3=0
$ ASK4=0
$ ASK5=0
$ ASK6=0
$ ASK7=0
$ ASK8=0
$ ASK9=0
$ ASK10=0
$!!
$!!   PROMPTS TO DETERMINE TYPE OF ANALYSIS TO BE RUN
$!!
$ WRITE SYS$OUTPUT "1=YES, 0=NO FOR ALL PROMPTS"
$ INQUIRE ASK1 "DO YOU NEED TO GENERATE THE DATA FILES?"
$ INQUIRE ASK2 "IS THIS PART OF A MULTIPLE BURN CALCULATION?"
$ IF ASK2.EQ.1 THEN -
  INQUIRE ASK3 "IS THIS THE FIRST BURN OF THE SEQUENCE?"
$!!
$!!    TEST TO DETERMINE IF DATA FILES NEED TO BE GENERATED
$!!
```

```
$ IF ASK1.EQ.1 THEN GOTO LOOP1
$!!
$!!     DATA FILES GENERATED PREVIOUSLY
$!!
$ ASK4=1
$ ASK5=ASK2+ASK3
$ INQUIRE NAME "ENTER FILE NAME FOR DATA FILES *.DAT, *.NOD, "
$ WRITE SYS$OUTPUT "THIS WILL ALSO BE THE NAME FOR ALL RESULTS"
$ ASSIGN 'NAME'.DAT DATA
$ ASSIGN 'NAME'.NOD NODES
$ IF ASK5.EQ.10 THEN INQUIRE NAMEO "ENTER FILE NAME FOR FILE *.TLD"
$ IF ASK5.EQ.10 THEN ASSIGN 'NAMEO'.TLD OLDWALT
$ GOTO LOOP3
$!!
$ LOOP1:
$!!
$ IF ASK3.EQ.0 THEN ASK4=1
$ IF ASK3.EQ.1 THEN -
  INQUIRE ASK4 "DO YOU WANT TO USE A PRIOR GENERATED GEOMETRY"
$ IF ASK2.EQ.0 THEN -
  INQUIRE ASK4 "DO YOU WANT TO USE A PRIOR GENERATED GEOMETRY"
$!!
$ ASK5=ASK2+ASK3
$!!
$!!     TEST TO DETERMINE IF RESTART OPTION TO BE USED
$!!
$ IF ASK4.EQ.0 THEN GOTO LOOP2
$!!
$!!     INPUT OLD FILE DATA NEEDED FOR RESTART
$!!
$ INQUIRE NAMEO "ENTER OLD FILE NAME"
$ ASSIGN 'NAMEO'.DAT RESTART
$ COPY 'NAMEO'.NOD NRCDAT.NOD
$ IF ASK5.EQ.10 THEN ASSIGN 'NAMEO'.OLD OLDDAT
$!!
$!! ********* RUN DATA DECK GENERATOR *********
$!!
$ LOOP2:
$!!
$ RUN DATGEN
$ IF ASK4.EQ.1 THEN DEASSIGN RESTART
$ IF ASK5.EQ.10 THEN DEASSIGN OLDDAT
$ IF ASK5.EQ.10 THEN ASSIGN 'NAMEO'.TLD OLDWALT
$!!
$!!      INPUT NEW FILE NAME FOR CASE TO BE RUN
$!!
$ INQUIRE NAME "ENTER NEW FILE NAME"
$!!
$!!     ASSIGN NECESSARY DATA FILES FOR RUNNING SOLVER
$!!
$ RENAME NRCDAT.DAT 'NAME'.DAT
$ RENAME NRCDAT.NOD 'NAME'.NOD
$ ASSIGN 'NAME'.NOD NODES
$ ASSIGN 'NAME'.DAT DATA
$!!
```

```
$!! ** DETERMINE WHETHER NODAL TEMP FILES SAVED FOR SURFACES **
$!!
$ LOOP3:
$!!
$ WRITE SYS$OUTPUT "INDICATE IF NODAL TEMPERATURES ARE SAVED"
$ WRITE SYS$OUTPUT "IF THE SURFACE IS NOT INCLUDED ANSWER NO=0"
$ INQUIRE ASK6 "ARE NODAL TEMPS SAVED FOR SURFACE 1?"
$ INQUIRE ASK7 "ARE NODAL TEMPS SAVED FOR SURFACE 2?"
$ INQUIRE ASK8 "ARE NODAL TEMPS SAVED FOR SURFACE 3?"
$!!
$!!  **** DETERMINE WHETHER ANALYSIS INCLUDES ICE CONDENSER MODEL ****

$!!
$ INQUIRE ASK9 "IS THE ICE CONDENSER OR LEAK MODEL OPERATIVE?"
$!!
$!!    ******** RUN DRIVER PROGRAM SOLVER *********
$!!
$ RUN SOLVER
$!!
$!!    DEASSIGN FILES FOLLOWING ANALYSIS
$!!
$ DEASSIGN DATA
$ DEASSIGN NODES
$ IF ASK5.EQ.10 THEN DEASSIGN OLDWALT
$!!
$!!   RENAME OUTPUT AND STORE IN FILES FOR LATER USE
$!!
$ SET NOVERIFY
$ RENAME OUTPUT.DAT 'NAME'.OUT
$ RENAME ENERGY.DAT 'NAME'.NRG
$ RENAME FLUX.DAT 'NAME'.FLX
$ IF ASK2.EQ.1 THEN RENAME OLDDAT.DAT 'NAME'.OLD
$ IF ASK2.EQ.1 THEN RENAME OLDWALL.DAT 'NAME'.TLD
$ IF ASK6.EQ.1 THEN RENAME TEMPS1.DAT 'NAME'.TS1
$ IF ASK7.EQ.1 THEN RENAME TEMPS2.DAT 'NAME'.TS2
$ IF ASK8.EQ.1 THEN RENAME TEMPS3.DAT 'NAME'.TS3
$ IF ASK9.EQ.1 THEN RENAME FLOWS.DAT 'NAME'.FLO
$!!
$!!   SIMULATION RESULTS PRINT-OUT OPTION
$!!
$ INQUIRE ASK10 "DO YOU WANT TO PRINT OUT THE HYBER RESULTS?"
$ IF ASK10.EQ.0 THEN GOTO LOOP4
$!!
$ PRINT 'NAME'.DAT,'NAME'.OUT,'NAME'.FLX,'NAME'.NRG
$ IF ASK2.EQ.1 THEN PRINT 'NAME'.OLD
$ IF ASK6.EQ.1 THEN PRINT 'NAME'.TS1
$ IF ASK7.EQ.1 THEN PRINT 'NAME'.TS2
$ IF ASK8.EQ.1 THEN PRINT 'NAME'.TS3
$ IF ASK9.EQ.1 THEN PRINT 'NAME'.FLO
$!!
$ LOOP4:
$ EXIT
```

Appendix G. Computer Programs DATGEN and SOLVER

Computer listings of DATGEN and SOLVER are provided on microfiche in an attached envelope. These codes are set up to execute on the IBM Personal Computer.

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13. ABSTRACT (200 words or less)

The users guide for the Hydrogen Burn Survival algorithm, HYBER, is provided in this report. HYBER (Hydrogen Burn - Equipment Response) is comprised of two self-contained computer programs, DATGEN and SOLVER. These computer codes may be used to estimate the thermal response of safety-related equipment exposed to hydrogen combustion in nuclear reactor containments. The state and composition gases are obtained by modeling single or multiple deflagrations in mixtures of hydrogen, steam, carbon monoxide, and air.

This users manual describes the interactive generation of the input data files using DATGEN and discusses the execution of SOLVER. Special usage of the algorithm on IBM Personal Computer (PC) and IBM compatible computer systems is also described. Illustrative examples, including the input data files, are provided to demonstrate some of the capabilities of the algorithm.

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