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A One-Dimensional Material Transfer Model for HECTR Version 1.5

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A One-Dimensional Material Transfer Model
for HECTR Version 1.5

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Abstract

HECTR (Hydrogen Event Containment Transient Response) is a lumped-parameter computer code developed for calculating the pressure-temperature response to combustion in a nuclear power plant containment building. The code uses a control-volume approach and subscale models to simulate the mass, momentum, and energy transfer occurring in the containment during a loss-of-coolant-accident (LOCA).

This document describes one-dimensional subscale models for mass and momentum transfer, and the modifications to the code required to implement them. Two problems were analyzed: the first corresponding to a standard problem studied with previous HECTR versions, the second to experiments. The performance of the revised code relative to previous HECTR versions is discussed as is the ability of the code to model the experiments.

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1 Introduction

In the event of a loss of coolant accident (LOCA) in a light water reactor (LWR), it has been shown [1, 2] that a significant amount of hydrogen (and carbon monoxide) may be produced which, if allowed to accumulate uncontrolled, could reach concentrations high enough to cause a threat of potential containment failure following combustion of the flammable gas. One solution to the problem of accumulation of flammable gases is the placement of igniters throughout the containment to burn hydrogen and carbon monoxide at low concentrations, thereby preventing the buildup to levels at which the possibility of containment failure may arise. In order to study the threat to the containment and the effectiveness of igniters for different accident scenarios and containment geometries, the Nuclear Regulatory Commission has sponsored a program at Sandia to investigate the response of containments to the combustion of flammable gasses. This investigation has resulted in a computer code to predict the response of the containment to gas-phase combustion. The code, Hydrogen Event Containment Transient Response (HECTR), has been released previously as Version 1.5.

HECTR Version 1.5 employs a finite difference method to solve the system of ordinary differential equations for the conservation of mass, momentum, and energy within a reactor containment (or other vessel) consisting of several compartments and the junctions between those compartments (through which mass, momentum, and energy may be exchanged). The HECTR Version 1.5 User's Manual [3] provides a detailed description of the various junction types that can be treated by HECTR. A linearized implicit formulation (backward Euler method) is used to solve the equations. Details are presented in the User's Manual. What is significant about the finite difference scheme used in HECTR is that the grid is set up so that each node represents a complete compartment or flow junction. Therefore, only average quantities within each compartment are calculated (hence, the description "control-volume"). Thus, not only are gradients of species concentration, temperature, and pressure within a compartment ignored, but the discrete regions of unburned material and combustion products in a burning compartment are averaged to yield a homogeneous environment. Although, in principle, there is no intrinsic limitation to using a finer mesh to resolve properties within a compartment, the original intent was for HECTR to be a portable, fast-running code, which imposes limitations on the mesh that make grids within a compartment impractical. The nodalization of each compartment (representing a control-volume) results in what can be thought of as a zero-dimensional representation of each compartment.

There is nothing inherently wrong with a control-volume solution technique provided it is able to resolve the details required by the user. The zero-dimensional treatment eliminates all geometric effects, and this is obviously unsuitable for combustion problems where, in addition to flame propagation between compartments, the flame moves within a compartment. Features that cannot be treated by the control-volume model are: convection of the proper material, either burned or unburned gas mixtures, through a flow junction; the effect of convecting fuel-rich gas into the region ahead of a flame; and any

manner of flame acceleration.

HECTR Version 1.5 addresses the limitations imposed by the control-volume treatment in two ways. For some phenomena the spatial coordinate is replaced by time. For example, to predict when a flame will propagate through a junction from a burning compartment to a neighboring one correctly, it is necessary to know the position of the flame front relative to the location of the junction. However, since HECTR Version 1.5 does not treat geometry within a compartment, this information is unavailable. This limitation in HECTR Version 1.5 is overcome by including a user-specified parameter for each junction that describes the fraction of the total burn *time* (calculated at ignition) that must pass before flame propagation can occur through the junction. This parameter replaces the spatial calculation of the flame position in a compartment with the temporal calculation of the time since ignition. A difficulty with this approach can be illustrated for the case of rectangular compartments with junctions at each end wall and a third junction in the middle of one side wall. If a flame ignites at either end wall, the entire burn time must pass before the flame passes through the far end, but if ignition occurs at the center junction, only half this time passes before a flame moves into a neighboring compartment.

The other approach that is taken to overcome the lack of geometry in the lumped-parameter treatment is to have subscale models (that do include system geometry) calculate geometry-independent average quantities which are then used in the finite difference equations. An example of this approach is seen in the calculation of the radiative heat transfer in a compartment. The steam in a compartment exchanges energy radiatively with the walls of the compartment, and there is radiative exchange between the compartment surfaces. A full geometric treatment would require a finite difference mesh in the interior of the compartment with the properties of the compartment surfaces providing the necessary boundary conditions. One could then solve the balance equations including radiative heat transfer in the energy equation to obtain the temperature and pressure in the compartment. In the control-volume method used in HECTR Version 1.5, the uniform temperature of the gas in the compartment together with an integrated form of the radiation equation are used to calculate the total radiative heat flux from the steam to the wall. This change in energy due to radiation is then applied in the differential equation for the time evolution of steam energy. Thus, the radiation model (which includes room geometry) produces a geometry-independent input for the linear equations derived for the control-volumes.

The use of geometry-dependent subscale models has previously been applied only to heat transfer mechanisms. In HECTR Version 1.8, we have extended this approach to include mass and momentum transfer processes as well. The space-time transformation method used to model combustion has been replaced with a one-dimensional model, and regions of burned or unburned material are tracked within a compartment to allow the convection of material with the proper composition through flow junctions.

2 Description of One-Dimensional Models

Although one-dimensional subscale heat transfer models were developed for HECTR Version 1.5, this approach had not previously been applied to the mass transfer mechanisms. The convection of material between compartments and combustion within a compartment were based on average gas compositions, and the motion of the flames treated by the space-time transformation described in Section 1. We felt that these simplifications greatly limited the ability of HECTR Version 1.5 to simulate containments with hydrogen combustion [4], so an attempt was made to introduce a one-dimensional model for combustion and mass transfer (the so-called "flame propagation model". This model has the capability to treat a moving flame front, and convect either unburned material or reaction products through flow junctions depending on the location of the junction relative to the flame fronts in a compartment. Also, the underlying philosophy behind the development of HECTR, that the code be fast and portable, was to be a consideration in constructing the modifications.

2.1 General Code Structure

These goals were accomplished in HECTR Version 1.8 by designing a one-dimensional flame model in which the flames divide a burning compartment into subvolumes each bounded by flame fronts or the compartment endwalls. The flames, then, behave as energy sources and mass shocks. That is, as the flame moves through the compartment, the composition of the gas undergoes a step change across the flame, analogous to the thermodynamic state of a gas across a pressure shock. The material in each subvolume consists of only the unreacted gas mixture or the reaction products depending on whether the subvolume is positioned ahead of or behind the bounding flame. The temperature and pressure in all subvolumes of a given compartment are assumed equal; therefore, the heat transfer calculations of Version 1.5 are unaffected by the flame propagation modifications in Version 1.8. Requiring uniform pressure throughout a compartment is equivalent to restricting the simulation to slow-moving flames. Figure 1 presents a simplified flowchart for HECTR Version 1.8. Comparing the flowchart to the one for Version 1.5 (HECTR Version 1.5 User's Manual [3] Figure A-1), the changes appear to be minimal – two additional checks on molar quantities after solution of the equations and an update of the flame position. This is a result of our deliberate attempt to retain the overall structure of Version 1.5 but with the addition of the new subscale models represented in the flow chart by the box labeled "CALCULATE EXPLICIT DERIVATIVE TERMS." The addition of the one-dimensional treatment greatly affects these explicit calculations which will now be discussed in detail.

Figure 1: Simplified Flow Chart for One-Dimensional Version of HECTR

Figure 1: Simplified Flow Chart for One-Dimensional Version of HECTR cont.

Figure 1: Simplified Flow Chart for One-Dimensional Version of HECTR cont.

Figure 1: Simplified Flow Chart for One-Dimensional Version of HECTR cont.

Figure 1: Simplified Flow Chart for One-Dimensional Version of HECTR cont.

Figure 2: Schematic of Burning Compartment

2.1.1 Mass, Energy, and Momentum Equations in a Burning Compartment

Figure 2 shows a schematic for a burning compartment with three flame fronts moving in the directions indicated by the arrows. The flames divide the compartment into four subvolumes, also referred to as subcompartments. Three flow junctions allow material to move into or out of the compartment changing the number of moles in the appropriate subvolume, and, of course, in the entire compartment. The balance equations for a compartment including the one-dimensional treatment are presented in Appendix A. Note that in addition to the variable $N_{i,j}$ (the number of moles of component j in compartment i) these equations include new composition variables for the subvolume mole numbers, $N_{i,j,k}$ (the number of moles of component j in the k th subvolume of compartment i). These values along with the size of subvolume k ($V_{i,k}$), are used in the balance equations to give the concentrations needed for the convection terms. The introduction of subvolume variables also introduces conservation equations for the subvolume quantities. These are

$$N_{i,j} = \sum_k N_{i,j,k} \quad (1)$$

$$V_i = \sum_k V_{i,k} \quad (2)$$

Subvolume variables are used exclusively for the terms on the right hand side of the balance equations with the exception of the enthalpies in Equation A-2 and pressure in

A-3 (if a compartment does not contain any flames, the subcompartment variables will be replaced in the balance equations with the corresponding compartment value; e.g., V_i for $V_{i,k}$). Due to our imposed constraint of constant temperature and pressure, the enthalpies are equal for every component in all the subvolumes, and a single value for $h_{i,j}$ can be used.

2.1.2 Method of Solution

We have already stated that the implicit solution technique of HECTR Version 1.5 has been retained in Version 1.8. We now discuss the method of determining the value of the subcompartment variables. Inspection of the equations in Appendix A reveals that the variables are not included in the linear system of ordinary differential equations treated by the implicit solver. Including the subvolume variables in the linear system was considered, but the effect of including these additional unknowns in the solution scheme would essentially be to increase the number of compartments to the number of physical compartments plus the number of flames. This would lead to a much larger linear system for inversion if the number of flames in the containment became significant. Therefore, in order to reduce the additional computational cost, a mixed implicit-explicit scheme was developed. In this scheme, the variables for the compartment as a whole are calculated by the implicit technique used in the lumped-parameter versions of HECTR. The modification to the calculation of compartment variables comes in the calculation of the contribution from combustion and material transfer between compartments as described previously. Additionally, the moles and volume of each subcompartment are calculated from submodels to be described shortly, and integrated explicitly in time. Then, by applying Equations 1 and 2, the compartment variables can also be calculated from the explicit integration.

2.1.3 Time Step Control

The HECTR program considers two independent time steps; one associated with heat transfer mechanisms, the other with flow and mass transfer. The modifications to the code to incorporate the one-dimensional models affected only sections governed by the flow time step; therefore, the heat transfer time step sections were unaffected. However, modification to the flow time step control algorithms was required. In the limit of the flow time step going to zero, the moles of each component calculated by the implicit and explicit method would be equal, but for finite values of Δt , the two values will differ. A relative error check on the number of moles of each component in a compartment was included in the flow time step calculation. At the end of each time step, the numbers of moles of each component in the compartment as calculated by the two methods is compared and if the relative difference is above a specified threshold, *SUBTOL*, that time step calculation is discarded and the calculation repeated with a smaller time step until the difference is at an acceptable level. This procedure is carried out for the total

Chemistry	local
Flow Junctions	local
Leaks	local
Fans	local
Fan Coolers	local
Sources	homogeneous
Flashing	homogeneous
Sump Injection	homogeneous
Suppresion Pools	homogeneous
Sprays	homogeneous
Transfer to Walls	homogeneous
Subcooled Gas	homogeneous

Table 1: Mass Transfer Mechanisms

number of moles in the compartment as well (error limit *CMPTOL*). For the calculations discussed in this report, no time steps needed to be repeated because of differences between the explicitly and implicitly calculated values of mole numbers.

2.2 Physical Models

The first four terms in Equations A-1 and A-2 are for flow junction convection, and the remainder include other mass and energy transfer mechanisms. Some of these, such as chemical reactions and fans affect only the subvolumes in which they occur (for reactions, the two subvolumes bounded by the flame) and are referred to as "local". Others, such as sprays or evaporation, are homogeneous throughout a compartment. These homogeneous mechanisms are not affected by the creation of the subvolumes in the latest HECTR modification. Table 1 presents a list of the mechanisms affected by this update and whether they are local or homogeneous.

Of the four local mechanisms, the last three are affected only by changing the average gas composition in a compartment to the composition of material actually convected through a particular junction. The change to the chemistry model is more extensive, and will be described first.

Previously, the space-time transformation was discussed. With the one-dimensional model this artificial device is no longer needed. Now, a true flame propagation model can be included; albeit, only in one dimension. Furthermore, by use of modular programming further improvements over the current simple flame model can be included at a later date with only slight programming effort. In HECTR Version 1.5, at the start of ignition the duration of the burn and final mole fractions of combustible material are calculated. A burn rate is then calculated so that, after a time equal to the burn duration, the

concentration of combustibles reaches the final value. The final concentration of hydrogen and carbon monoxide can be specified by the user or calculated from default correlations; similarly, the burn time for a compartment can be specified by the user or left to be computed by the code. If the burn time is calculated in HECTR, it is equal to a burn length divided by a flame speed (again if not user-specified, flame speed is calculated in the code). The flame speed is a function of the combustible gas and diluent concentrations in a compartment at the time of ignition. The burn length, which *must* be user-specified, does not necessarily represent a physical dimension of the compartment, but may be some average length scale of the compartment adjusted to account for combustion phenomena (e.g., flame acceleration) that is not treated in the flame speed model.

Many of the terms in the control-volume calculation are no longer needed in HECTR Version 1.8; the meanings of others are modified. For example, it is unnecessary to calculate a burn time at ignition since the position of the flame and presence of a wall or a noncombustible mixture ahead of it are sufficient to determine the extinction of the flame.

2.2.1 Burn Model

The one-dimensional burn model consists of four parts: ignition, chemical kinetics, flame velocity, and extinction. Unlike the lumped-parameter treatment, the one-dimensional version of HECTR treats combustion through the use of "flame sheets." Figure 2 shows a compartment with three flame sheets. These sheets, which act to delineate regions of unburned and burned material, are created at ignition, move with a velocity determined by burn speed and flame speed correlations, and are removed at extinction of combustion. Each of the four parts of the combustion process will now be described in detail with the emphasis on the alterations caused by the one-dimensional treatment.

Ignition

The treatment of the ignition process in Version 1.8 is almost identical to that of previous HECTR versions, the description of which is included in the HECTR Version 1.5 Users Manual [3]. The only addition is to assign a position and identification number to the flame at the time of ignition. This is done in the subroutines *FLMSTR* and *BURN*. For flames propagating into a compartment through a flow path, the initial flame position is the location of that junction in the compartment. For spontaneous ignition due to high H_2 , CO , and O_2 levels, the default is for the flames to ignite in the center of the compartment. The spontaneous ignition location can be changed by specifying a value for *IGNLEN*, a NAMELIST variable for the fraction of the compartment length at which spontaneous ignition occurs.

Burn Velocity

The burn velocity, the rate at which the flame moves relative to the gas directly in front of the flame, reflects the reaction kinetics of combustion. In order to allow the most direct comparison of the effect of adding the one-dimensional models to earlier HECTR

versions, the burn velocity calculation, carried out in the subroutine *VFLAME*, was not altered. As in HECTR Version 1.5, the burn speed can be specified by the user (through specification of a burn time for a compartment which after division by the compartment length gives the burn speed) or calculated from default correlations contained in the code. The HECTR Version 1.5 correlations for burn velocity as a function of combustible and diluent concentration were used in HECTR Version 1.8. These correlations are derived from experimental data from the Variable Geometry Test Series (VGES) and the Fully Instrumented Test Series (FITS) facilities at Sandia National Laboratories [6, 7] and the Nevada Test Site (NTS) [8]. In the flame front model, however, there are modifications to how the burn speed correlations are applied. The most significant change is the use of the burn speed to model the physical movement of the flame as opposed to using the transformation to a burn time as was done previously. Also, the burn velocity is calculated at each flow time step based on the local composition ahead of the flame. This is a departure from previous HECTR treatments of combustion where the burn velocity was kept constant throughout a burn. Further, in a compartment with multiple flames, the burn velocity for each flame is calculated independently from the gas composition ahead of that particular flame.

It is assumed that as the flame sweeps out a volume of gas equal to $U_f(V_i/l_i)\Delta t$ in time Δt (where U_f is the burn speed, V_i is the volume of the compartment, l_i is the length of the compartment, and Δt is the time step) enough H_2 , and CO react to yield the correct final concentrations unless the reaction is oxygen-limited, with the production of reaction products in the proper stoichiometric ratio. The combustion of reactant and oxygen adds moles of inerts and combustion products and the volume swept out by the flame in time Δt to the subvolume behind the flame, while removing an equal volume and the material contained in that volume from the subvolume ahead of the flame. The gas concentration in the subcompartment ahead of the flame is unchanged by the chemical reaction.

Flame Velocity

So far, the only means of flame front movement discussed is that due to reaction of unburned material, and in a Lagrangian sense, this is the only way the flame moves. However, as mass can be produced at different rates in different compartment subvolumes, and flow junctions allow motion of gas into or out of a compartment, the gas within a compartment might be moving at some velocity. In that case, the convection speed of the flame from the local gas velocity must be added to the burn velocity of the flame due to kinetics. In a lumped-parameter treatment, however, the gas velocity within a compartment cannot be resolved. This limitation is overcome by utilizing the equation of state for the gas mixture in each subvolume to calculate that subcompartment's volume. The volume is calculated from the temperature and pressure for the entire compartment (which is also the value for each subvolume) along with the number of moles in each subvolume at the end of a time step. Thus, once the volume of each subcompartment is known, the position of the flames (that together with the fixed ends of the compartment are the bounding surfaces of the subvolumes, can be determined).

Extinction

In HECTR Version 1.5, extinction of combustion in a compartment occurs after a prescribed burn time that was calculated at ignition. In Version 1.8, use is made of the position of flames and geometric information provided by the user to determine extinction of each flame individually. There are three extinction mechanisms included in the latest modification. First, if the composition of the gas ahead of a flame is below the flammability threshold, that flame will extinguish and the material in the subvolume ahead of the flame will be combined with the material in the subcompartment behind the flame. If the subvolume lacking fuel or oxygen lies in the center of a compartment, three subvolumes will be combined. The second extinction mechanism is for a flame to burn into an end wall; that is, the burn velocity is such that the flame position will be at or ahead of a bounding wall at the end of the current time step. In this case, all the material ahead of the flame is consumed and the reaction products are added to the subvolume behind the flame. This mechanism can also be used when two flames burn into each other (again as for extinction in the center of a compartment, three subvolumes are combined into one). The final extinction mechanism is for the bulk flow to carry a flame into an end wall (usually one containing a flow junction) or another flame. As the burn velocity was such that combustible material remains ahead of the flame (or else the previous mechanism would have been invoked), this unburned material along with the combustion products are added to the subvolume ahead of the flame. These are the mechanisms for extinguishing single flames. Compartments are identified as burning or not burning as well. A compartment is burning as long as there are any flames present within it.

2.2.2 Material Flows

The four remaining local material transfer mechanisms in Table 1 are similar, involving the convection of material between compartments. The exception to this is for leaks where the transfer is between a compartment and the external atmosphere, but for the purpose of this discussion, we will refer to the outside environment as a compartment and always refer to two compartments. The four mechanisms differ, however, in the submodels used to calculate the flowrate through each type of connection. These models are described in the HECTR Version 1.5 Users Manual and will not be described further here. The alterations in going from the control-volume approach of previous HECTR versions to the one-dimensional approach occur when there is flow between compartments of which at least one contains a flame. In that case, the position at which material enters or leaves the burning compartment is determined from input data on the fan, leak or flow junction and the corresponding subvolume identified. The subroutine *FLMLOC* performs this function. Then, for the case of flow out of a burning compartment, the composition of material that is transferred is that in the subvolume identified as containing the flow entrance and the moles of material flowing between compartments is removed from that subvolume alone. If the junction flow enters a burning compartment, all the material goes into the subvolume containing the junction exit and the composition is that determined

by the inlet conditions. So, for example, referring to Figure 2, if material is flowing out of the two junctions in subcompartment 1, the material leaving the subvolume and entering the outflow compartment would have the composition of subvolume 1 and mass determined from the appropriate flow connection model. If the flow is into subvolume 3, the composition of the material would be determined from the composition of the gas at the entrance to the connection, and only subcompartment variables for the third subvolume would be affected by the flow.

3 Input Description

In order to implement the one-dimensional models for combustion and flow junctions in HECTR Version 1.8, geometric data must be supplied by the user. This section will describe what additional information is required, and those cases where the meaning of an input variable has been altered from a lumped-parameter value to one which reflects the true geometry of the system. Appendix B lists the names of major variables added to the code for the one-dimensional implementation, and Appendix C gives an example of a typical input deck for Version 1.8 (in this case the one corresponding to the standard two-compartment problem described in the HECTR Version 1.5 Users Manual).

There are two types of input variables in the input file. The first is the usual data type where a value is read from a prescribed place in the input deck into a particular variable. For this type of input it is imperative that the order of the data be correct. The second type of input which can occur in either of two places in the input file is a NAMELIST type data statement. The format for this type of input is:

$$\text{varble}(i) = \text{value}.$$

where varble is the name of the variable receiving the value "value". If varble is an array and no value for the subscript i is included, all values in the array will be assigned "value". Otherwise, only the i^{th} element is assigned the value. NAMELIST variables can be placed in any order as long as they are placed in the proper section of the input; either in the initial NAMELIST input where the computing environment is defined, or at the end of the input file. The alterations to the input deck will now be described using the same format as the HECTR Version 1.5 Users Manual but not including sections left unaltered. For clarity, all input variables in a section with changes are presented.

3.1 Compartment Data

For i having values 1 to the total number of compartments:

$COMPID(i)$ [A] – A 72 – character or less compartment descriptor.

$Z(i)$ [R] – (m^3) Initial gas volume of compartment i .

$CHRLLEN(i)$ [R] – (m) Characteristic length for flame propagation for discrete burns.

$NSURFC(i)$ [I] – Number of heat – transfer surfaces in compartment i . This number may be 0.

$ISV(i)$ [I] – The number of the sump where water condensed from the atmosphere of compartment i due to subcooling is placed.

$ISSP(i)$ [I] – The number of the sump where the unevaporated spray drops that reach the floor of compartment i are placed.

$CMPLEN(i)$ [R] – The length of compartment i .

3.2 Containment Leakage Data

For i having values 1 to the total number of containment leaks:

NOL [I] – Compartment number where the leak or break is located.

$NTD(i)$ [I] – Number identifying temperature – dependent leakage curve to be used for this leak.

$NPD(i)$ [I] – Number identifying pressure – dependent leakage curve to be used for this leak.

$NCF(i)$ [I] – Containment failure flag.

$TPT(i)$ [R] – (seconds, Pascals or Kelvins) Containment failure criterion.

$AFL(i)$ [R] – (m^2) Containment failure area.

ZJI(i) [R] - (*m*) Elevation of leak or break.
FLI(i) [R] - Flow loss coefficient for leak or break.
LAI(i) [R] - (*1/m*) The flow length through the leak divided by an effective area.
OUTX(i) [R] - Location of leak in compartment.

3.3 Flow Junctions

For *n* having values 1 to the total number of flow junctions:

i [I] - Source compartment. If flow is positive, compartment supplying material.
j [I] - Receiving compartment. If flow is positive, compartment receiving material.
JTYPE(n) [I] - Junction type.
AI(n) [R] - (*m*²) Interconnection area.
FLOCO(n) [R] - Loss coefficient for flow between compartments *i* and *j*.
LA(n) [R] - (*1/m*) The flow length through the junction divided by an effective flow area.
RELATJ(n) [I] - Describes the spatial relationship of compartment *i* to compartment *j* for burn propagation.
ZJUN(n) [R] - Junction elevation.
INTOX(n) [I] - Location of junction *n* in compartment *j*.
OUTX(n) [I] - Location of junction *n* in compartment *i*.

3.4 Fan Data

For n having values 1 to the total number of fans.

<i>TSETF</i>	[R]	– (Kelvin) Temperature set point for automatic activation of the fans. This quantity is used when the fans are in AUTO mode otherwise, this value is ignored.
<i>PSETF</i>	[R]	– (Pascals) Pressure set point for automatic activation of the fans. This quantity is used when the fans are in AUTO mode.
<i>DELAYF</i>	[R]	– (seconds) Time delay for fan activation in AUTO mode. The fans are turned on at a time DELAYF after either TSETF or PSETF is exceeded anywhere in the containment.
<i>TFRUN</i>	[R]	– (seconds) Length of time that the fans will remain on. If the fans should run indefinitely, enter a large number.
<i>i</i>	[I]	– Source compartment.
<i>j</i>	[I]	– Receiving compartment.
<i>FANVFR(n)</i>	[R]	– (m^3/sec) Volumetric flow rate of the fan. Positive values are for steady flow rates, negative values give the maximum rate with the actual rate determined by a head curve.
<i>DPFMAX(n)</i>	[P]	– (Pascals) Maximum pressure difference under which the fan can operate.
<i>ETA(n)</i>	[R]	– Fan efficiency.
<i>RELATF(n)</i>	[I]	– Describes the spatial relationship of compartment i to compartment j for burn propagation through the fans.
<i>FANIN(n)</i>	[R]	– The location of the fan in compartment i .
<i>FANOUT(n)</i>	[R]	– The location of the fan in compartment j .

3.5 Fan Cooler Data

For ij having values 1 to the total number of fan coolers.

<i>PSETFC</i>	[<i>R</i>]	— (Pascals) Pressure set point for switching into LOCA mode of fan cooler operation.
<i>DELAYFC</i>	[<i>R</i>]	— (seconds) Time delay for switching to LOCA mode after PSETFC is exceeded anywhere in the containment.
<i>TFCRUN</i>	[<i>R</i>]	— (seconds) Length of time that the fan cooler will run after being turned on.
<i>NCROWS</i>	[<i>I</i>]	— Number of rows of coils in a coil unit.
<i>NCIRC</i>	[<i>I</i>]	— Number of circuits in a coil unit.
<i>VP</i>	[<i>R</i>]	— (m) Vertical pitch of coils.
<i>HP</i>	[<i>R</i>]	— (m) Horizontal pitch of coils.
<i>CID</i>	[<i>R</i>]	— (m) Coil inner diameter.
<i>COILL</i>	[<i>R</i>]	— (m) Coil length.
<i>HFG</i>	[<i>R</i>]	— ($K - m^2/Watt$) Heat transfer fouling factor for gas flow side of coils.
<i>HFW</i>	[<i>R</i>]	— ($K - m^2/Watt$) Heat transfer fouling factor for coolant side of coils.
<i>CONDCM</i>	[<i>R</i>]	— ($Watts/m - K$) Thermal conductivity of coils.
<i>XK</i>	[<i>R</i>]	— ($Watts/m - K$) Thermal conductivity of fins.
<i>DELT</i>	[<i>R</i>]	— (m) Thickness of fins.
<i>ITBEL</i>	[<i>I</i>]	— Indicates relative location of fan and coils.

Enter data for fan cooler assemblies that operate both in normal and LOCA mode (assemblies that operate only in LOCA mode are input in the following section).

FRMFC(*ij*) [*I*] - Compartment that assembly draws from.
QDTRN(*ij*) [*R*] - (Watts) Rated capacity in normal mode.
QDTRL(*ij*) [*R*] - (Watts) Rated capacity in LOCA mode.
QFANN(*ij*) [*R*] - (m³/sec) Rated fan flow rate in normal mode.
QFQNL(*ij*) [*R*] - (m³/sec) Rated fan flow rate in LOCA mode.
NFCU(*ij*) [*I*] - Total number of coil units in this assembly.
FCIN(*ij*) [*R*] - Location of the fan cooler in compartment FRMFC.

Data for fan cooler assemblies that operate only in LOCA mode.

FRMFC(*ij*) [*I*] - Compartment that assembly draws from.
QDTRL(*ij*) [*R*] - (Watts) Rated capacity in LOCA mode.
QFQNL(*ij*) [*R*] - (m³/sec) Rated fan flow rate in LOCA mode.
NFCU(*ij*) [*I*] - Total number of coil units in this
 assembly.
FCIN(*ij*) [*R*] - Location of the fan cooler in compartment FRMFC.

3.6 NAMELIST Input

These variables are specified (in any order) only when the default variables are to be overridden. Only the new NAMELIST variables or ones whose meaning has been altered are described here.

- CMPTOL* [R] — The error limit on the difference between the total number of moles in a compartment as calculated by the implicit and explicit calculations.
- FLMEPS* [R] — (m) The initial separation of two flames created by an ignition in the center of a compartment.
- KPROPF* [R] — Maximum distance between a flame and the center of a fan intake for propagation of the flame through the fan
- KPROPJ* [R] — Maximum distance between a flame and the center of a flow junction intake for propagation of the flame through the flow junction
- SUBTOL* [R] — The error limit on the difference between the number of moles of a component in a compartment as calculated by the implicit and explicit calculations.

4 Example Calculations

This section presents two example calculations. These calculations were performed to assess the performance of HECTR Version 1.8 once the one-dimensional submodels for mass and momentum had been included. One simulation is for comparison to previous control-volume calculations. For this purpose, the "Simple Two Compartment Problem-Case 1" from the HECTR Version 1.5 Users Manual [3] was chosen. This problem uses many of the HECTR submodels, and so is a good test of the ability of the code to model the interaction of the various processes, while retaining a simple geometry. The second problem corresponds to an experimental test in a vented cylinder. The experiments were performed by Cummings, Torczynski, and Benedick [5]. The geometry of the experiments also consists of two compartments (the test vessel and the atmosphere), but in contrast to the previous example, this case is dominated by the combustion process and few of the other mass transfer models are employed. These two problems could not validate all the submodels affected by the change to the one-dimensional treatment, and for this purpose, additional calculations were performed isolating the submodel involved. The results of these tests will not be reported here as they served only to confirm the behavior of the particular submodels.

4.1 Simple Two-Compartment Calculation

The simple two-compartment problem is based on a geometry in which a concrete-lined compartment (compartment 2, volume=3534 m³, l=20 m) lies beneath a much larger steel lined one (compartment 1, volume=10603 m³, l=25 m). There is a two-way flow junction between the compartments with the positive flow direction chosen for flow from the lower to upper compartment. There is a steady hydrogen source in the lower compartment and ignition occurs in the center of the compartment when the minimum concentrations for spontaneous ignition are exceeded. The system includes sprays and fans which operate automatically when a temperature or pressure set point is passed. The fans direct gas from the lower to the upper compartment with the intake and outlet both located 10 m from the end of the respective compartment. The flow junction always enters the upper compartment 18 m from the end wall, but the location of the junction in the lower compartment, *OUTX*, was varied to assess the effect of its position on the calculated temperature and pressure rise. The full input for this calculation is presented for reference in Appendix C.

The results of the calculations are presented in Appendix E.1. Figures E.1-E.3 give the temperature, pressure, and mole fractions as calculated by HECTR Version 1.5 for reference. The remaining plots in Appendix E.1 present the same results for calculations using the one-dimensional submodels with several vent locations. The results clearly show the occurrence of two distinct burns during the simulation. Figures 3-4 show the effect of vent location on the maximum temperature and pressure rise, respectively, compared to

Figure 3: Maximum Temperature as a Function of Vent Location

the constant value calculated by HECTR Version 1.5. They also display the effect of vent location on the maximum temperature and pressure rise. One cause (but not the only one) of the variation in the maximum rise is that as the position of the vent moves from the wall, $OUTX = 0$, toward the center of the compartment, $OUTX = 10$, combustion products rather than fuel-rich gas are vented to the upper compartment for a greater fraction of the burn time. As a result, more fuel remains in the lower compartment, and higher maximum temperatures and pressures are observed. This effect could not be seen in the lumped-parameter model as a mixture of fuel and reaction products will always be vented. The upper compartment does not ignite in this simulation, but if flame propagation through the junction were possible, the time for propagation would be affected by the vent location as well.

The location of the vent does more than affect the maximum temperature and pressure rise in Compartment 1. The length of time over which the burn occurs is also affected. With the vent ahead of the flame, as is always the case with $OUTX=0$, the bulk flow is in the same direction as the burn. This causes the flame velocity to exceed the burn speed. As a result, short burn times (1.984, 2.765 s) are calculated for $OUTX=0$. With the vent behind the flame, the bulk velocity opposes the burn speed and so the flame velocity is less than the burn velocity. For the calculation with $OUTX=9$, long burn times (2.408, 2.815 s) are predicted. This effect couples with the previously discussed convection effects to further increase the temperature and pressure rise as the vent moves closer to the compartment center. As there is a constant homogeneous source of hydrogen,

Figure 4: Maximum Pressure as a Function of Vent Location

a longer burn time also means that there is more fuel available for combustion adding to the increase in temperature and pressure rise.

The relative strength of the two burns also varies with vent location. In the one-dimensional calculation, the strength (as measured by the maximum temperature during the burn) of the first burn approaches that of the stronger second burn as the vent moves closer to the center of the compartment. For the case of $OUTX=9$, the first burn is stronger. In HECTR Version 1.5, the combustion process is determined by the conditions at ignition and the two burns behave almost identically. In the one-dimensional calculation, however, the combustion process is determined by the instantaneous conditions at each time step and can vary throughout a burn. This is what causes the variation in magnitude of the temperature and pressure rise between the two burns for the different vent locations. As the previous discussions showed for the coupling of burn time and hydrogen source, there is not always a simple correlation between vent location and a single mechanism to explain the combined effects of mass transfer (sources, fuel convected from a compartment), momentum transfer (flame versus burn velocity), and energy transfer. Mechanisms interact in complex ways to control the temperature and pressure rise in a compartment during a burn. It can be said, though, that significant geometric effects can be expected in complex systems depending on vent locations.

It has been our intention in making these modifications to maintain the computational speed of HECTR when including the geometric effects. Table 2 presents the results of

	Comp. 1		Comp. 2		
	T_{max} (K)	P_{max} (kPa)	T_{max} (K)	P_{max} (kPa)	Run Time (s)
Vers. 1.5	379	156	1138	156	18.36
$OUTX=0$	354	143	980	143	18.53
$OUTX=3$	360	145	1053	145	18.35
$OUTX=6$	371	151	1156	151	22.67
$OUTX=9$	397	165	1323	165	26.09

Table 2: Simple Two-Compartment Problem Results

our one-dimensional model and those from Version 1.5 for the maximum temperature and pressure in each compartment and the total cpu time for the simulation. One can see that for this problem the run time was very modest, less than 30 s on a VAX 8600 for even the longest calculation. Even though the run time increase for the $OUTX=9$ calculation was nearly 50%, the increase dropped sharply as the vent moved away from the center of the compartment.

4.2 Cylindrical Combustion Vessel Calculation

In order to study the acceleration of flames in hydrogen-air mixtures, Cummings, Torczynski, and Benedick [5] performed experiments in a vented container. Briefly, the system consisted of a cylindrical tank vented at one end to the atmosphere. The vessel contained a flammable hydrogen-air mixture. The mixture was ignited at the closed end of the tank, and the flame allowed to propagate through the tank to the open end. The vessel was 4.27 m (14 ft.) in length and 1.22 m (4 ft.) in diameter. Most of the experiments were performed on systems demonstrating flame acceleration – a feature which is not included in the HECTR combustion model. One series that was suitable for comparison with HECTR calculations was a test set performed in the vented tank with no obstacles. Experiments were conducted at hydrogen concentrations of 15% and 30%, both of which were simulated by the one-dimensional version of HECTR. The 15% experiments showed no flame acceleration behavior; however, there was some degree of acceleration for the 30% mixture. Figure 5 presents a schematic of the experimental apparatus with instrumentation.

Two geometries were used to model the experimental vessel. In the first, the geometry of the tank as modeled was identical to the experimental system. The compartment length was 4.27 m and the area, 1.17 m². The flow junction was a two-way connection with area 1.169 m² located at the end of the tank. The atmosphere was modeled as a second compartment with volume one thousand times larger than the vessel. There were no sprays, fans or other features included in HECTR operating for this simulation. A pure nitrogen-oxygen atmosphere was used for the large compartment but this choice was irrelevant to the calculation as no material flowed from the atmosphere into the vessel and the size of the second compartment made ignition there impossible. The second

- THERMOCOUPLES (TCs)
- PCB PRESSURE GAUGES
- IGNITER
- ▽ KULITE PRESSURE GAUGE
- ⌘ MIXING FAN AT GAS INLET

Figure 5: Schematic diagram of experimental tank

% H_2	Experimental			2-Comp. Model			5-Comp. Model		
	T_m (K)	P_m (kPa)	t_b	T_m (K)	P_m (kPa)	t_b	T_m (K)	P_m (kPa)	t_b
15	-	110	0.5	1000	115	0.168	1332	118	0.170
30	-	151	0.04	1533	138	0.081	2536	156	0.095

Table 3: Vented Cylinder Results

model represented the test vessel as four equally sized compartments connected by two-way flow junctions with area equal to the area of the tank. This five-compartment model was added to see if a nonphysical representation of the system improved or decreased the ability of the code to predict the experimental results. It was thought that the addition of extra compartments might reduce any limitations imposed by the requirement of uniform temperature and pressure in a compartment.

The results of the calculations are summarized in Table 3 for the maximum temperature and pressure in the vessel and the duration of the burn. The detailed plots of temperature and pressure vs. time for each compartment are included in Appendix E.2. The effect of adding the extra compartments increased the maximum calculated temperature and pressure but had only a weak effect on the total burn time. Though not shown in the table, the time to reach the maximum pressure was not affected by increasing the number of compartments, but the time to reach the maximum temperature was delayed in the five-compartment calculation. Neither of the calculations agree particularly well with the experimental observations. The difference ranges from an overprediction of 80% for the pressure rise in the 15% hydrogen test calculated with the five-compartment model, to a 25% underprediction in the 30% hydrogen test using the two-compartment model. The better agreement for the five-compartment model compared to the two-compartment calculation in the 30% test is a result of the overprediction of the temperature and pressure when using the five-compartment geometry correcting for flame acceleration effects present in the experiment but not treated in HECTR. As flame acceleration is not included in the HECTR submodels, this fortuitous agreement should not be taken to validate the use of the nonphysical five-compartment model. Rather, the better agreement of the two-compartment model in the case where no acceleration takes place indicates that physical representations of a system work better with the one-dimensional version of the code and future work should be devoted to improving the flame models.

5 Conclusions

The two problems simulated have shown the ability of HECTR Version 1.8 to incorporate one-dimensional submodels in the mass and momentum conservation equations. The solution of the simple two-compartment test problem further reveals the ability of the one-dimensional version to reproduce geometry-dependent effects which either required including geometric information in the input file (such as the time for flames to propagate between compartments), or could not be resolved by the lumped-parameter code at all (e.g., the effect of vent location on flame speed and burn time). HECTR Version 1.8 can now be applied to actual containment geometries for likely accident scenarios. Furthermore, the user will be able to model the containment with compartments which correspond closely to those in the physical containment.

The comparison of calculated results with experimental data revealed that even with the addition of the one-dimensional submodels, the results are only as good as the flame model in the code. The vented cylinder system places an extreme burden on the flame model to give precise results as there are no other mechanisms present to mitigate errors from this one submodel. This situation is one for which HECTR was never intended. The intent behind developing this code was to produce a systems code that could simulate the gross features of what takes place during the very complicated scenario of a loss-of-coolant accident.

The results of the comparison between the vented cylinder experiments and the HECTR calculations for the two input geometries (two- and five-compartment) has shown that the inclusion of a one-dimensional mass and momentum treatment greatly reduces model geometry as a source of error in the simulation. The treatment of combustion appears to be the limiting submodel. Therefore, additional improvement in the flame model will increase the predictive capability of the code, and future work should focus on developing a more accurate flame submodel. Although there are no plans to continue developmental work on HECTR at the present time, the conclusions drawn from the addition of the flame-sheet model can be applied to other reactor codes such as CONTAIN.

6 References

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Appendix A Conservation Equations

Conservation of Molar Content:

$$\begin{aligned}
 \frac{dN_{i,j}}{dt} = & - \sum_l \left(\frac{N_{i,j,k}}{V_{i,k}} \right) F_l \quad (F_l > 0) - \sum_l \left(\frac{N_{m,j,p}}{V_{m,p}} \right) F_l \quad (F_l < 0) - \sum_q \left(\frac{N_{i,j,k}}{V_{i,k}} \right) F_{lk,q} \quad (F_{lk,q} > 0) - \sum_q F_{lk,q} \left(\frac{N}{V} \right)_{j, \text{env}} \quad (F_{lk,q} < 0) \\
 & + \left(\frac{dN_{i,j}}{dt} \right)_{\text{chem.}} + \left(\frac{dN_{i,j}}{dt} \right)_{\text{fans}} + \left(\frac{dN_{i,j}}{dt} \right)_{\text{fan cool.}} + \left(\frac{dN_{i,j}}{dt} \right)_{\text{SP.}} \\
 & + \left(\frac{dN_{i,H_2O}}{dt} \right)_{\text{a.}} + \left(\frac{dN_{i,j}}{dt} \right)_{\text{ext. source}} + \left(\frac{dN_{i,H_2O}}{dt} \right)_{\text{evap., cond.}} \quad (\text{A.1})
 \end{aligned}$$

Conservation of Energy:

$$\begin{aligned}
 \frac{dE_i}{dt} = & - \sum_{j=1}^{N_{\text{gases}}} \left[- \sum_l \left(\frac{N_{i,j,k}}{V_{i,k}} \right) F_l h_{i,j} \quad (F_l > 0) - \sum_l \left(\frac{N_{m,j,p}}{V_{m,p}} \right) F_l h_{m,j} \quad (F_l < 0) - \sum_q \left(\frac{N_{i,j,k}}{V_{i,k}} \right) F_{lk,q} h_{i,j} \quad (F_{lk,q} > 0) \right. \\
 & \left. - \sum_q F_{lk,q} \left(\frac{Nh}{V} \right)_{j, \text{env}} \quad (F_{lk,q} < 0) + \left(\frac{dN_{i,j}}{dt} \right)_{\text{ext. source}} h_{j, \text{source}} \right] + \left(\frac{dN_{i,H_2O}}{dt} \right)_{\text{a.}} h_{\text{a}} \\
 & + \left(\frac{dN_{i,H_2O}}{dt} \right)_{\text{evap., cond.}} h_{i,H_2O} + \left(\frac{dE_i}{dt} \right)_{\text{fans}} + \left(\frac{dE_i}{dt} \right)_{\text{fan cool.}} \\
 & + \left(\frac{dE_i}{dt} \right)_{\text{SP.}} - \left(\frac{dQ}{dt} \right)_{\text{rad. conv.}} - \left(\frac{dQ}{dt} \right)_{\text{sprays}} \quad (\text{A.2})
 \end{aligned}$$

Conservation of Momentum:

$$\frac{dF_l}{dt} = \frac{2}{(\rho_i + \rho_k)(L/a)_l} \left\{ (P_i - P_k) + g[\rho_i(z_i - z_l) + \rho_k(z_l - z_k)] - \frac{K_l(\rho_i + \rho_k)F_l|F_l|}{4A_l^2} \right\} \quad (\text{A.3})$$

$$\frac{dF_{lk,q}}{dt} = \frac{2}{(\rho_i + \rho_{\text{env}})(L/a)_q} \left\{ (P_i - P_{\text{env}}) + g[\rho_i(z_i - z_q) + \rho_{\text{env}}z_q] - \frac{K_q(\rho_i + \rho_{\text{env}})F_{lk,q}|F_{lk,q}|}{4A_q^2} \right\} \quad (\text{A.4})$$

Equation of State:

$$P_i = \frac{ZN_{i,H_2O}RT_i}{V_i} + \sum_{j=2}^{N_{\text{gases}}} \frac{N_{ij}RT_i}{V_i} \quad (\text{A.5})$$

where

$V_{i,k}$ = volume of subvolume k in compartment i (m^3).

$\left(\frac{N}{V}\right)_{j,\text{env}}$ = moles per unit volume of gas species j in the environment (moles/ m^3).

$\left(\frac{dN_{i,j}}{dt}\right)_{\text{ext. source}}$ = rate of addition of species j into compartment i from an external source (moles/s).

$\left(\frac{dN_{i,j}}{dt}\right)_{\text{chem.}}$ = chemical molar rate of change of species j due to combustion (moles/s).

- $\left(\frac{dN_{i,H_2O}}{dt}\right)_{\text{evap., cond.}}$ = positive or negative rate of change of atmospheric water vapor due to evaporation from or condensation on surfaces and spray droplets (moles/s).
- $\left(\frac{dN_{i,j}}{dt}\right)_{\text{fans}}$ = rate of addition of gas species j into compartment i due to intercompartment fans (moles/s).
- $\left(\frac{dN_{i,j}}{dt}\right)_{\text{fan cool.}}$ = rate of addition of gas species j into compartment i due to fan cooler (moles/s).
- $\left(\frac{dN_{i,H_2O}}{dt}\right)_{\text{fl.}}$ = rate of addition of steam to compartment i due to sump boiling (moles/s).
- $\left(\frac{dN_{i,j}}{dt}\right)_{\text{SP.}}$ = rate of addition of gas due to flow through the suppression pool (moles/s).
- $h_{i,j}$ = enthalpy of the j^{th} gas evaluated at the temperature in the i^{th} compartment (J/mole).
- $h_{j,\text{env.}}$ = enthalpy of gas species j in the environment (J/mole).
- h_{fl} = saturated vapor enthalpy at saturated sump temperature (J/mole).
- $h_{j,\text{source}}$ = enthalpy of the j^{th} gas evaluated at the source temperature (J/mole).
- $\left(\frac{dQ}{dt}\right)_{\text{sprays}}$ = rate of heat transfer from the gas to the spray droplets (W).
- $\left(\frac{dQ}{dt}\right)_{\text{rad. conv.}}$ = sum of the rates of radiative and convective heat transfer from the gas (W).

- $\left(\frac{dE_i}{dt}\right)_{\text{fans}}$ = energy addition to compartment i due to intercompartment fans (W).
- $\left(\frac{dE_i}{dt}\right)_{\text{fan cool.}}$ = energy addition to compartment i due to fan cooler (W).
- $\left(\frac{dE_i}{dt}\right)_{\text{SP.}}$ = energy addition to compartment i due to gas flow through suppression pool (W).
- ρ_i = gas density in compartment i (kg/m^3).
- ρ_{env} = gas density in the environment (kg/m^3).
- $(L/a)_l, (L/a)_q$ = ratio of effective gas inertial length to effective gas flow area for the l^{th} junction or q^{th} leak (m^{-1}).
- P_i = pressure in compartment i (Pa).
- P_{env} = pressure in the environment (Pa).
- g = acceleration due to gravity (m/s^2).
- z_i = elevation of compartment i (m).
- z_l = elevation of flow junction l (m).
- z_q = elevation of leak q (m).
- K_l = loss coefficient due to flow through the l^{th} junction.
- K_q = loss coefficient due to flow through the q^{th} leak.
- A_l = interconnection area of the l^{th} junction (m^2).

A_q = interconnection area of the qth leak (m^2).

Z = compressibility factor for steam.

R = universal gas constant (J/mole-K).

T_i = gas temperature in compartment i (K).

Appendix B Subroutine Call Tree

```

HECTR--LOOK
!
+-NAMLST--NUMBER
!
!         +-GET--NUMBER
!         !
!         !         +-UPCASE
!         !         !
!         !         +-LENGTH
!         !
!         +-LENGTH
!
+-ZEROUT
!
+-INPUT1--NUMSTR
!
!         +-GET--NUMBER
!         !
!         !         +-UPCASE
!         !         !
!         !         +-LENGTH
!         !
+-INPUT2--LOOK
!
!         +-GET--NUMBER
!         !
!         !         +-UPCASE
!         !         !
!         !         +-LENGTH
!         !
+-CHECK
!
+-INITAL--LOOK
!
!         +-IMARCH--GET--NUMBER
!         !
!         !         +-UPCASE
!         !         !
!         !         +-LENGTH
!         !
!         +-IEXTSC--GET--NUMBER
!         !
!         !         +-UPCASE
!         !         !
!         !         +-LENGTH
!         !
!         +-RAIH2O
!         !
!         +-RAICO
!         !
!         +-RAICO2
!         !
!         +-NODES
!         !
!         +-SPJUN
!         !
!         +-ZZZ
!         !
!         +-PROP--LOOK
!

```

```

!           +-CLEAK--KABOOM
!
+-START
!
+-IMARCH--GET-+-NUMBER
!           !
!           +-UPCASE
!           !
!           +-LENGTH
!
+-IEXTSC--GET-+-NUMBER
!           !
!           +-UPCASE
!           !
!           +-LENGTH
!
+-INIOUT
!
+-RAIH2O
!
+-RAICO
!
+-RAICO2
!
+-BOOM--KABOOM
!
+-FZERO
!
+-RADHTO--INTERP
!           !
!           +-RADH2O
!           !
!           +-RADHT1
!           !
!           +-RADCO
!           !
!           +-RADCO2
!           !
!           +-RADHT2-+-ARANG--SEARCH
!           !           !
!           !           +-PLFRA
!           !
!           +-INDEXX
!           !
!           +-SGEFA
!           !
!           +-SGESL
!
+-CONVCT--INTERP
!           !
!           +-LOOK
!           !
!           +-INDEXX
!           !
!           +-ZZZ
!
+-MELTHT--LOOK
!
+-SPHE
!
+-SPRAY-+-SPRAY1
!           !

```

```

!      +-LOOK
!      +-ZZZ
!      +-DERKF
!
+-FLMLOC
!
+-FRCTFL
!
+-FCOOL-+-LOOK
!      +-FILMC--LOOK
!      +-BESJ
!
+-OUTPTH-+-OUTH
!      +-OUTA
!
+-CONTRL-+-LOOK
!      +-OUTPTF--OUTF
!      +-CONADJ
!      +-NEFEQN-+-INTERP
!          +-LOOK
!          +-INDEXX
!          +-MARCHI
!          +-EXTNSC--LOOK
!          +-FCFAN--FLMLOC
!          +-SUMPUP-+-LOOK
!              +-INTERP
!              +-INDEXX
!              +-SPHE
!              +-SPOOL-+-LEVCHK
!                  +-SGECO
!                  +-SGESL
!
!          +-FAN-+-INTERP
!              +-INDEXX
!              +-FLMLOC
!              +-FRCTFL
!
+-BURN-+-FLMSTR
!

```

```

!      !      !      +-IGNTST--FLMLOC
!      !      !      !      +-FLMSTR
!      !      !      !      +-CLCVL
!      !      !      !      +-FLMVEL--VFLAME
!      !      !      !      !      +-IGNLOC--IGNTST--FLMLOC
!      !      !      !      !      !      +-FLMSTR
!      !      !      !      +-UNBRNF
!      !      !      !      +-RBURN
!      !      !      +-FLMLOC
!      !      !      +-FRCTFL
!      !      +-JACOB--FLMLOC
!      !      !      +-FRCTFL
!      !      +-SOLVE--SCALE--ISAMAX
!      !      !      !      +-SSCAL
!      !      !      +-HSGECO--SDOT
!      !      !      !      +-SASUM
!      !      !      !      +-HSGEFA--ISAMAX
!      !      !      !      !      +-SSCAL
!      !      !      !      !      +-SAXPY
!      !      !      !      +-SSCAL
!      !      !      !      +-SAXPY
!      !      !      +-HSGEFA--ISAMAX
!      !      !      !      +-SSCAL
!      !      !      !      +-SAXPY
!      !      !      +-HSGESL--SAXPY
!      !      +-FLMLOC
!      !      +-ZZZ
!      !      +-SUBC--LOOK
!      !      !      +-ZZZ
!      !      +-FRCTFL
!      !      +-IGNLOC--IGNTST--FLMLOC
!      !      !

```

```

!           !           +-FLMSTR
!           !
!           +-PROP--LOOK
!           !
!           +-FZERO
!           !
!           +-CLEAK--KABOOM
!
+-EXTNSC--LOOK
!
+-TWALL--TRIDAG
!
+-DUMP

```


Appendix C Major Variables Added in HECTR Version 1.8

Internal Variables:

ADDRAT(I,J) - the total rate at which moles of species I are added to compartment J through mechanisms considered to be homogeneous throughout the compartment.

ADDNUM(I) - the number of moles of steam gained or lost from the gas in compartment I due to evaporation or condensation from walls.

AREAXS(I) - the cross-sectional area of compartment I.

FLMORD(I,J) - a pointer array giving the index of the Ith flame encountered with increasing distance from $x = 0$ in compartment J.

IGNLEN(I) - the fraction of the total length of compartment I (CMPLN(I)) at which spontaneous ignition occur.

INDIST(I) - the position in compartment I at which material is entering.

NFLAME(I) - the total number of flames in compartment I.

OUTDST(I) - the position in compartment I at which material is leaving.

SUBMLS(I,J) - the total number of moles in SUBVOL(I,J).

SUBN(I,J,K) - the number of moles of species I in SUBVOL(J,K).

SUBVOL(I,J) - the volume of the Ith subsection of compartment J.

TSUBN(I,J,K) - similar to SUBN(I,J,K) but used as a holding variable to update the moles in SUBVOL(J,K) after a combustion subject to confirmation by a mass balance throughout compartment K.

VL(I,J) - the linear velocity of the Ith flame in compartment J.

VQ(I,J) - the volumetric velocity of the Ith flame in compartment J.

XF(I,J) - the location of the Ith flame in compartment J.

XIGN(I,J) - the location of the ignition of the Ith flame in compartment J.

Input Variables:

CMPLN(I) - the length chosen to model the extent of compartment I. Specified as last entry in compartment data section of input.

CMPTOL - the error limit on the difference between the total number of moles in a compartment containing at least one flame as calculated by the implicit solver and as calculated from the sum of the moles in all subvolumes.

FANIN(I) - the location of fan I in the compartment identified as FRMFAN(I). Specified in fan data section after RELATF.

FANOUT(I) - the location of fan I in the compartment identified as TOFAN(I). Given after FANIN.

FCIN(I) - the location of the inlet to fan cooler I in the compartment identified as FRMFC(I). Specified after NFCU in fan cooler section of input.

FCOUT(I) - the location of the outlet from fan cooler I in the compartment identified as TOFC(I). Specified after JSMPNR in fan cooler section of input.

FLMEPS - the initial separation of the two flame fronts created by an ignition in the center of a compartment. Given in NAMLST section of input.

INTOX(I) - location of junction I in compartment identified as TOCOMP(I). Given after ZJUN in flow junction section of input.

OUTX(I) - location of junction I in compartment identified as FRMCMP(I). Input after INTOX in flow junction section and after LAI in leak.

SUBTOL - the error limit on the difference between the number of moles of each species in a compartment containing at least one flame as calculated by the implicit solver and as calculated from the sum of the moles of the component in all subvolumes. section.

Program Units:

CLCVL - calculates the volume bounded by two flames or a wall and a flame.

FLMLOC - identifies the subvolume containing a given junction in a burning compartment.

FLMSTR - gives the identifying number and order in a compartment to a newly ignited flame.

FLMVEL - calculates the velocity of a flame front.

FRCTFL - calculates the composition of the gas flowing through a flow junction, fan, or fan cooler.

PRPFLM - calculates the new position of a flame front after a time step has been accepted.

Appendix D Example Input Decks for HECTR Version 1.8

Appendix D.1 Simple Two-Compartment Problem

The following is the input deck used for the calculations corresponding to the simple two-compartment problem.

(S)IMPLE TWO-COMPARTMENT PROBLEM\$

THIS IS THE SITUATION OF TWO COMPARTMENTS, ONE STACKED ABOVE THE OTHER.

THE UPPER COMPARTMENT IS ABOUT THREE TIMES LARGER THAN THE LOWER COMPARTMENT.

```

2          ! Number of compartments
!
! Compartment Data
!
UPPER COMPARTMENT
10603.     ! Volume (m**3)
10.        ! Elevation (m)
15.        ! Flame propagation length (m)
1          ! Number of surfaces
1          ! Water generated from subcooling goes into sump 1
1          ! Any spray carryover will go directly into sump 1
25.0       ! Compartment length
LOWER COMPARTMENT
3534.      ! Volume (m**3)
0.         ! Elevation (m)
15.        ! Flame propagation length (m)
2          ! Number of surfaces
1          ! Water generated from subcooling goes into sump 1
1          ! Any spray carryover will go directly into sump 1
20.0       ! Compartment length
!
! Sump Data
!
1          ! Sump number
  
```

```

11000.    ! Capacity (m**3)
0         ! Sump overflow disappears from the system
$ END OF SUMPS
!
! Surface Data
!
UPPER COMPARTMENT STEEL
2         ! Surface type (lumped mass)
1.53E5    ! Mass (kg)
2121.     ! Area (m**2)
15.       ! Convective length (m)
460.5     ! Specific heat (J/kg-K)
.7        ! Emissivity
1         ! Any wall condensation will go directly into sump 1
LOWER COMPARTMENT CONCRETE
1         ! Surface type (slab)
1.        ! Mass (kg) - ignored for slabs
471.      ! Area (m**2)
5.        ! Convective length (m)
879.      ! Specific heat (J/kg-K)
.9        ! Emissivity
1         ! Any wall condensation will go directly into sump 1
! Layer information
1         ! Number of layers in slab
.762      ! Thickness of layer 1 (m)
5.5E-7    ! Thermal diffusivity of layer 1 (m**2/s)
1.385     ! Thermal conductivity of layer 1 (W/m-K)
! Slab mesh spacing control variables and back surface condition
0 0.      ! Let mesh spacing be chosen automatically
0.        ! Backside convective heat transfer coefficient (indicates an
           ! insulated back surface)
0.        ! Environmental temperature (indicates an insulated back surface)
LOWER COMPARTMENT POOL (SUMP)
3         ! Surface type (pool)
1000.     ! Mass (kg)
707.      ! Area (m**2)
15.       ! Convective length (m)
1.        ! Specific heat (J/kg-K) - ignored for pools
.94       ! Emissivity
1         ! This is the surface of sump number 1
!
$ NO CONTAINMENT LEAKAGE
!
! Flow Junction Data

```

```

!
2 1      ! Positive flow is from compartment 2 to compartment 1
1        ! Junction type (2-way flow)
300.     ! Interconnection area (m**2)
1.2      ! Flow coefficient
.015     ! Ratio of the flow length to the flow area (1/m)
1        ! Flow from compartment 2 to 1 is in the upward direction
5.       ! Junction elevation (m)
18.0     ! Location of junction in compartment 1
3.0      ! Location of junction in compartment 2
$ END OF FLOW JUNCTIONS
$ NO ICE CONDENSER INPUT
$ NO SUPPRESSION POOL INPUT
!
! Fan Data
!
350. 202650. ! Temperature (K) and pressure (Pa) setpoints
18.        ! Time delay (s)
1.0E+06    ! Time that the fans remain on (s)
1 2        ! Fan blows from compartment 1 into compartment 2
50.        ! Constant volumetric flow rate (m**3/s)
1013.25    ! Shutoff head (Pa)
1.         ! Efficiency
-1         ! Flow from compartment 1 to 2 is in the downward direction
10.0       ! Location of fan
10.0       ! Location of fan
$ END OF FAN CONNECTIONS
$ USE DEFAULT HEAD CURVE
$ NO FAN COOLER
!
! Radiative Heat Transfer Data
!
! Beam lengths (m)
13.5 15. 15.
12. 12.
1.
! View factors
.667 .094 .239
.154 .423
.001
!
! Spray Data
!
1          ! Number of compartments with spray sources

```

```

! Loop on compartments with spray sources
1          ! Compartment where spray originates
330.37     ! Spray inlet temperature (K)
.5         ! Spray flow rate (m**3/s)
2          ! Number of drop sizes
.95 309.   ! Frequency and diameter (um) of drops of the first drop size
.05 810.   ! Frequency and diameter (um) of drops of the second drop size
!
1 2 .02     ! Spray carryover of .02 from compartment 1 into compartment 2
$ END OF SPRAY CARRYOVER DESCRIPTION
1 15.       ! Compartment and the spray fall height (m) in it
2 15.
$ END OF SPRAY FALL HEIGHTS
350. 202650. ! Temperature (K) and pressure (Pa) setpoints
5.         ! Time delay (s)
1.0E+06    ! Time that the sprays remain on (s)
10.        ! Time spent in spray injection phase (s)
587.       ! Rated spray heat exchanger mass flow rate (kg/s)
3.74E+06   ! Rated spray heat exchanger effectiveness (W/K)
301.5      ! Spray heat exchanger secondary side inlet temperature (K)
755.       ! Spray heat exchanger secondary side mass flow rate (kg/s)
1          ! Draw water from sump 1 when sprays are in recirculation mode
!
$ END OF HEAT EXCHANGERS
60.0       !Simulation time (s)
!
! Compartment Data
!
300.       ! Initial temperature of the upper compartment (K)
3400.      ! Initial partial pressure of steam (Pa)
77000.     ! Initial partial pressure of nitrogen (Pa)
21000.     ! Initial partial pressure of oxygen (Pa)
0.0        ! Initial partial pressure of hydrogen (Pa)
.3         ! Convective gas velocity (m/s)
!
300.       ! Initial temperature of the lower compartment (K)
3400.      ! Initial partial pressure of steam (Pa)
77000.     ! Initial partial pressure of nitrogen (Pa)
21000.     ! Initial partial pressure of oxygen (Pa)
0.         ! Initial partial pressure of hydrogen (Pa)
.3         ! Convective gas velocity (m/s)
!
! Source Terms
!

```



```

2          ! Number of compartments
!
! Compartment Data
!
LEFT COMPARTMENT
4.99       ! Volume (m**3)
0.         ! Elevation (m)
4.27       ! Flame propagation length (m)
1          ! Number of surfaces
0          ! Water generated from subcooling leaves system
0          ! Any spray carryover will leave the system
4.27       ! Compartment length (m)
RIGHT COMPARTMENT
5000.      ! Volume (m**3)
0.         ! Elevation (m)
2000.0     ! Flame propagation length (m)
0          ! Number of surfaces
0          ! Water generated from subcooling leaves system
0          ! Any spray carryover will leave the system
2000.0     ! Compartment length (m)
!
$ NO SUMPS
!
! Surface Data
!
UPPER COMPARTMENT STEEL
1          ! Surface type (lumped mass)
216.00     ! Mass (kg)
16.366     ! Area (m**2)
2.5        ! Convective length (m)
460.5      ! Specific heat (J/kg-K)
.7         ! Emissivity
0          ! Any wall condensation will leave the system
1          ! surface is not a lumped mass
0.152      ! Thickness of steel layer
0.390E-5   ! Thermal diffusivity polished type 304 stainless steel
16.2       ! Thermal conductivity
0          ! Default spacing
0          ! Default distribution
0          ! Insulated back side
0.0        ! Insulated back side temperature
!
$ NO CONTAINMENT LEAKAGE

```



```

!
! Flow Junction Data
!
1 2      ! Positive flow is from compartment 1 to compartment 2
1        ! Junction type (2-way flow)
1.169    ! Interconnection area (m**2)
1.0      ! Flow coefficient
0.50     ! Ratio of the flow length to the flow area (1/m)
0        ! Flow from compartment 2 to 1 is in the sideways direction
0.       ! Junction elevation (m)
0.0      ! Location of junction in compartment 2
4.27     ! Location of junction in compartment 1
$ END OF FLOW JUNCTIONS
$ NO ICE CONDENSER INPUT
$ NO SUPPRESSION POOL INPUT
$ NO FAN
$ NO FAN COOLER
!
! RADIATION DATA
1.22 !beam length
1.0  !view factor
!
0  ! NO SPRAY
$ NO HEAT EXCHANGERS
!
20.      ! Simulation time (s)
!
! Compartment Data
!
300.     ! Initial temperature of the small compartment (K)
0.       ! Initial partial pressure of steam (Pa)
58586.96 ! Initial partial pressure of nitrogen (Pa)
15978.26 ! Initial partial pressure of oxygen (Pa)
31956.52 ! Initial partial pressure of hydrogen (Pa)
.3       ! Convective gas velocity (m/s)
!
300.     ! Initial temperature of the large compartment (K)
0.       ! Initial partial pressure of steam (Pa)
83695.65 ! Initial partial pressure of nitrogen (Pa)
22826.09 ! Initial partial pressure of oxygen (Pa)
0.       ! Initial partial pressure of hydrogen (Pa)
.3       ! Convective gas velocity (m/s)
!
! Source Terms

```

```

!
$ END OF STEAM SOURCES
$ END OF NITROGEN SOURCES
$ END OF OXYGEN SOURCES
$ END OF HYDROGEN SOURCES
$ NO WATER IS TO BE REMOVED FROM SUMPS
$ NO EXTERNAL ENERGY SOURCE
$ NO CONTINUOUS BURNING
$ NO TRIP
$ NO TABLE
!
300.0   ! Surface Temperature (K)
!
! Namelist Type Input
!
IGNLEN=0.00
XHMNDT=0.40
KPROPJ=0.01
$ END OF NAMLST INPUT

```

Appendix D.2.2 Five-Compartment Model

(F)IVE-COMPARTMENT PROBLEM\$

THIS IS THE CASE CORRESPONDING TO THE CUMMINGS-TORCZYNSKI TESTS
 THE RIGHT COMPARTMENT IS ABOUT THOUSAND TIMES LARGER THAN THE LEFT COMPARTMENT.

```

5           ! Number of compartments
!
! Compartment Data
!
LEFT COMPARTMENT 1
1.248      ! Volume (m**3)
0.         ! Elevation (m)
1.068      ! Flame propagation length (m)
0          ! Number of surfaces
0          ! Water generated from subcooling goes into sump 1
0          ! Any spray carryover will go directly into sump 1

```

```

1.068      ! Compartment length (m)
LEFT COMPARTMENT 2
1.248      ! Volume (m**3)
0.         ! Elevation (m)
1.068      ! Flame propagation length (m)
0          ! Number of surfaces
0          ! Water generated from subcooling goes into sump 1
0          ! Any spray carryover will go directly into sump 1
1.068      ! Compartment length (m)
LEFT COMPARTMENT 3
1.248      ! Volume (m**3)
0.         ! Elevation (m)
1.068      ! Flame propagation length (m)
0          ! Number of surfaces
0          ! Water generated from subcooling goes into sump 1
0          ! Any spray carryover will go directly into sump 1
1.068      ! Compartment length (m)
LEFT COMPARTMENT 4
1.248      ! Volume (m**3)
0.         ! Elevation (m)
1.068      ! Flame propagation length (m)
0          ! Number of surfaces
0          ! Water generated from subcooling goes into sump 1
0          ! Any spray carryover will go directly into sump 1
1.068      ! Compartment length (m)
RIGHT COMPARTMENT
5000.      ! Volume (m**3)
0.         ! Elevation (m)
200.0      ! Flame propagation length (m)
0          ! Number of surfaces
0          ! Water generated from subcooling goes into sump 1
0          ! Any spray carryover will go directly into sump 1
200.0      ! Compartment length (m)
!
$ NO SUMPS
!
! NO SURFACE
!
!
$ NO CONTAINMENT LEAKAGE
!
! Flow Junction Data
!
1 2        ! Positive flow is from compartment 1 to compartment 2

```

```

1      ! Junction type (2-way flow)
1.169  ! Interconnection area (m**2)
3.5    ! Flow coefficient
0.15625 ! Ratio of the flow length to the flow area (1/m)
0      ! Flow from compartment 1 to 2 is in the horizontal direction
0.     ! Junction elevation (m)
0.0    ! Location of junction in compartment 2
1.068  ! Location of junction in compartment 1
!
2 3    ! Positive flow is from compartment 2 to compartment 3
1      ! Junction type (2-way flow)
1.169  ! Interconnection area (m**2)
3.5    ! Flow coefficient
0.15625 ! Ratio of the flow length to the flow area (1/m)
0      ! Flow from compartment 2 to 3 is in the horizontal direction
0.     ! Junction elevation (m)
0.0    ! Location of junction in compartment 3
1.068  ! Location of junction in compartment 2
!
3 4    ! Positive flow is from compartment 3 to compartment 4
1      ! Junction type (2-way flow)
1.169  ! Interconnection area (m**2)
3.5    ! Flow coefficient
0.15625 ! Ratio of the flow length to the flow area (1/m)
0      ! Flow from compartment 3 to 4 is in the horizontal direction
0.     ! Junction elevation (m)
0.0    ! Location of junction in compartment 4
1.068  ! Location of junction in compartment 3
!
4 5    ! Positive flow is from compartment 4 to compartment 5
1      ! Junction type (2-way flow)
1.169  ! Interconnection area (m**2)
3.5    ! Flow coefficient
0.15625 ! Ratio of the flow length to the flow area (1/m)
0      ! Flow from compartment 4 to 5 is in the horizontal direction
0.     ! Junction elevation (m)
0.0    ! Location of junction in compartment 5
1.068  ! Location of junction in compartment 4
$ END OF FLOW JUNCTIONS
$ NO ICE CONDENSER INPUT
$ NO SUPPRESSION POOL INPUT
$ NO FAN
$ NO FAN COOLER
!
```

```

! NO RADIATIVE HEAT TRANSFER
!
O ! NO SPRAY
$ NO HEAT EXCHANGERS
!
10.      ! Simulation time (s)
!
! Compartment Data
!
300.      ! Initial temperature of the small compartment (K)
0.        ! Initial partial pressure of steam (Pa)
58586.96 ! Initial partial pressure of nitrogen (Pa)
15978.26 ! Initial partial pressure of oxygen (Pa)
31956.52 ! Initial partial pressure of hydrogen (Pa)
.3        ! Convective gas velocity (m/s)
!
300.      ! Initial temperature of the small compartment (K)
0.        ! Initial partial pressure of steam (Pa)
58586.96 ! Initial partial pressure of nitrogen (Pa)
15978.26 ! Initial partial pressure of oxygen (Pa)
31956.52 ! Initial partial pressure of hydrogen (Pa)
.3        ! Convective gas velocity (m/s)
!
300.      ! Initial temperature of the small compartment (K)
0.        ! Initial partial pressure of steam (Pa)
58586.96 ! Initial partial pressure of nitrogen (Pa)
15978.26 ! Initial partial pressure of oxygen (Pa)
31956.52 ! Initial partial pressure of hydrogen (Pa)
.3        ! Convective gas velocity (m/s)
!
300.      ! Initial temperature of the small compartment (K)
0.        ! Initial partial pressure of steam (Pa)
58586.96 ! Initial partial pressure of nitrogen (Pa)
15978.26 ! Initial partial pressure of oxygen (Pa)
31956.52 ! Initial partial pressure of hydrogen (Pa)
.3        ! Convective gas velocity (m/s)
!
300.      ! Initial temperature of the large compartment (K)
0.        ! Initial partial pressure of steam (Pa)
83695.65 ! Initial partial pressure of nitrogen (Pa)
22826.09 ! Initial partial pressure of oxygen (Pa)
0.        ! Initial partial pressure of hydrogen (Pa)
.3        ! Convective gas velocity (m/s)
!

```

```

! Source Terms
!
$ END OF STEAM SOURCES
$ END OF NITROGEN SOURCES
$ END OF OXYGEN SOURCES
$ END OF HYDROGEN SOURCES
$ NO WATER IS TO BE REMOVED FROM SUMPS
$ NO EXTERNAL ENERGY SOURCE
$ NO CONTINUOUS BURNING
$ NO TRIP
$ NO TABLE
!
! NO Surface Temperatures (K)
!
!
! Namelist Type Input
!
XHMNIG=1.0
XHMNIG(1)=0.07
IGNLEN=0.0
XHMNDT=0.40
KPROPJ=0.01
$ END OF NAMLIST INPUT

```

Appendix E Numerical Results

Appendix E.1 Simple Two-Compartment Test Problem

Figure E.1: Temperature for Two-Compartment Problem, version 1.5

Figure E.2: Pressure for Two-Compartment Problem, version 1.5

Simple two compartment problem
Compartment 1

Simple two compartment problem
Compartment 2

Figure E.3: Mole Fractions for Two-Compartment Problem, version 1.5

Simple two compartment problem
Compartment 1

Simple two compartment problem
Compartment 2

Figure E.4: Temperature for Two-Compartment Problem, OUTX=0

Simple two compartment problem
Compartment 1

Simple two compartment problem
Compartment 2

Figure E.5: Pressure for Two-Compartment Problem, OUTX=0

Simple two compartment problem
Compartment 1

Simple two compartment problem
Compartment 2

Figure E.6: Mole Fractions for Two-Compartment Problem, OUTX=0

Figure E.7: Temperature for Two-Compartment Problem, OUTX=3

Figure E.8: Pressure for Two-Compartment Problem, OUTX=3

Figure E.9: Mole Fractions for Two-Compartment Problem, OUTX=3

Figure E.10: Temperature for Two-Compartment Problem, OUTX=6

Figure E.11: Pressure for Two-Compartment Problem, OUTX=6

Figure E.12: Mole Fractions for Two-Compartment Problem, OUTX=6

Figure E.13: Temperature for Two-Compartment Problem, OUTX=9

Figure E.14: Pressure for Two-Compartment Problem, OUTX=9

Simple two compartment problem
Compartment 1

Simple two compartment problem
Compartment 2

Figure E.15: Mole Fractions for Two-Compartment Problem, OUTX=9

Appendix E.2 Cylindrical Tank Results

Figure E.16: Temperature for Cylindrical Tank Problem, 15% H_2 , 2-comp. model

Figure E.17: Pressure for Cylindrical Tank Problem 15% H_2 , 2-comp. model

Figure E.18: Temperature for Cylindrical Tank Problem, 30% H_2 , 2-comp. model

Figure E.19: Pressure for Cylindrical Tank Problem 30% H_2 , 2-comp. model

Figure E.20: Temperature for Cylindrical Tank Problem, 15% H₂, 5-comp. model

Figure E.21: Pressure for Cylindrical Tank Problem 15% H₂, 5-comp. model

Figure E.22: Temperature for Cylindrical Tank Problem, 30% H₂, 5-comp. model

Figure E.23: Pressure for Cylindrical Tank Problem 30% H₂, 5-comp. model

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