COUPLING RELAP5-3D[©] AND FLUENT TO ANALYZE A VERY HIGH TEMPERATURE REACTOR (VHTR) OUTLET PLENUM

A Thesis

by

NOLAN ALAN ANDERSON

Submitted to the Office of Graduate Studies of Texas A&M University in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

August 2006

Major Subject: Nuclear Engineering

COUPLING RELAP5-3D[©] AND FLUENT TO ANALYZE A VERY HIGH TEMPERATURE REACTOR (VHTR) OUTLET PLENUM

A Thesis

by

NOLAN ALAN ANDERSON

Submitted to the Office of Graduate Studies of Texas A&M University in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

Approved by:

Chair of Committee, Yassin Hassan Committee Members, William Marlow Kalyan Annamalai Head of Department, William Burchill

August 2006

Major Subject: Nuclear Engineering

ABSTRACT

Coupling RELAP5-3D[©] and Fluent to Analyze a Very High Temperature Reactor (VHTR) Outlet Plenum. (August 2006) Nolan Alan Anderson, B.S., Brigham Young University Chair of Advisory Committee: Dr. Yassin A. Hassan

The Very High Temperature Reactor (VHTR) system behavior should be predicted during normal operating conditions and during transient conditions. To predict the VHTR system behavior there is an urgent need for development, testing and validation of design tools to demonstrate the feasibility of the design concepts and guide the improvement of the plant components. One of the identified design issues for the gas-cooled reactor is the thermal mixing of the coolant exiting the core into the outlet plenum. Incomplete thermal mixing may give rise to thermal stresses in the downstream components. This analysis was performed by coupling a RELAP5-3D[©] VHTR model to a Fluent outlet plenum model. The RELAP5 VHTR model outlet conditions provide the inlet boundary conditions to the Fluent outlet plenum model. By coupling the two codes in this manner, the important three-dimensional flow effects in the outlet plenum are well modeled without having to model the entire reactor with a computationally expensive code such as Fluent. The two codes were successfully coupled. The values of pressure, mass flow rate and temperature across the coupled boundary showed only slight differences. The coupling tool used in this analysis can be applied to many

different cases requiring detailed three-dimensional modeling in a small portion of the domain.

ACKNOWLEDGEMENTS

I would like to thank my committee chair Dr. Yassin Hassan for his guidance and support. I would like to thank Richard Schultz at the Idaho National Lab for his unwavering support and help in completing this project. I would also like to thank Walter Weaver at the Idaho National Lab for his help in successfully coupling RELAP5-3D[©] and Fluent.

TABLE OF CONTENTS

	Page
ABSTRACT	iii
ACKNOWLEDGEMENTS	v
TABLE OF CONTENTS	vi
LIST OF FIGURES	vii
LIST OF TABLES	viii
1. INTRODUCTION	1
2. PROBLEM	6
 2.1. The RELAP5-3D VHTR Model 2.2. The Fluent Outlet Plenum Model 2.3. The PVM Executive Program 2.4. Sequence of Events in a Coupled Computation 	7 10 13 18
3. SOLUTIONS	23
3.1. The Steady-State Solution	23
4. CONCLUSIONS AND RECOMMENDATIONS	35
REFERENCES	38
APPENDIX A	40
APPENDIX B	55
VITA	72

LIST OF FIGURES

FIGUR	E	Page
1	VHTR Schematic	2
2	Cross-Sectional View of the VHTR Core	3
3	The RELAP5-3D [©] VHTR Core Model	8
4	Modified RELAP5-3D [©] VHTR Core Model	10
5	The Fluent Outlet Plenum Model	11
6	Schematic of a Coupled Computation	18
7	The Convergence of the RELAP5 Channel Pressures	23
8	Static Pressure Comparison in Channel 11	25
9	Mass Flow Rate Comparison in Channel 4	27
10	Mass Flow Rate Comparison in Channel 11	28
11	A One-Dimensional Discretized Mesh	30
12	Temperature Comparison in Channel 4	32
13	Temperature Pathlines in the Outlet Plenum	33
14	Temperature Contours in the Outlet Pipe	34
15	Pressure and Mass Flow Rate in Channel 11	36

LIST OF TABLES

TABL	E	Page
1	Initial Channel Pressure and Temperature at the Exit	. 9
2	Static Pressure Comparison across the Coupled Boundaries	. 24
3	Mass Flow Rate Comparison across the Coupled Boundaries	. 26
4	Temperature Comparison across the Coupled Boundaries	. 29

1. INTRODUCTION

The next generation nuclear plant is an advanced, next-generation nuclear reactor coupled to advanced electricity and hydrogen generation technology. As a result of the Generation IV International Forum (DOE, 2005) six candidates for the advanced nuclear reactor were chosen. One of the six candidates decided upon is the Very High Temperature Reactor (VHTR) system. The core configuration options for the high temperature ranges of the VHTR are the prismatic block or pebble bed designs.

The safety of the VHTR is based on its low power density, high heat capacity, and passive ability to remove heat from the reactor vessel without the need for active safety systems. The passive reactor vessel cooling system, which is located in the reactor building, should reliably remove all the decay heat released by the core in the event of an accident.

The VHTR system behavior should be predicted during normal and abnormal conditions. The plant accident scenario and the passive safety behavior should be accurately predicted. Small uncertainties in such passive safety behavior could have large effects on the resulting system characteristics. Due to these performance issues, there is an urgent need for development, testing and validation of design tools to demonstrate the feasibility of the design concepts and guide the improvement of the plant components.

This thesis follows the style of Progress in Nuclear Energy.

Design issues of the VHTR are dependent on the identification of key phenomena for various scenarios during normal and accident situations. This identification method is known as the Phenomenon Identification and Ranking Table (PIRT) which provides a good understanding of many of the safety characteristics of the design. Using the PIRT method, design issues have been identified and are currently being investigated (INL, et al., 2005).

One of the identified design issues for the gas cooled reactor of the prismatic block or pebble bed core is the thermal mixing of the coolant exiting the core into the outlet plenum. Variation in axial and radial power density as well as coolant flow rates in individual flow channels would give rise to non-uniform temperature entering the plenum. This phenomenon is called hot streaking. Nearly complete mixing would be necessary to prevent thermal stripping and hot spots in the plenum structure and the power conversion unit. The VHTR is seen in Fig. 1.



Fig. 1. VHTR schematic (GA, 2003). The location of the outlet plenum is indicated. The arrows show the flow direction.

The motivation of the current study is to determine if the outlet plenum structure or the downstream components such as turbines will be in danger of thermal damage as the helium coolant mixes in a prismatic core VHTR. The significant temperature variations of the gas would affect the thermodynamics and transport properties, as well as the buoyancy of the gas during loss-of-flow and loss-of-coolant scenarios and during reduced power operations.

Due to the symmetric nature of the VHTR outlet plenum and the reactor core, the analysis space size can be reduced. This was accomplished by dividing the outlet plenum and the core along a plane of symmetry; greatly reducing the required computation time of the analysis. A cross-sectional view of half of the VHTR prismatic core region is seen in Fig. 2.



Fig. 2. Cross-sectional view of the VHTR core (GA, 2003). The red prismatic regions represent the locations of the fission material. The white prismatic blocks represent the reflector regions.

In order to analyze this design issue, the computer codes RELAP5-3D[©] and Fluent were coupled. A Parallel Virtual Machine (PVM) executive program (Weaver, et

al., 2002a) which was designed to couple RELAP5-3D[©] to other codes was used to analyze the VHTR outlet plenum case. The object of this study is the development of this coupling executive program as a tool in analyzing the VHTR case and to allow its use for other Generation IV needs.

RELAP5-3D[©] is a systems analysis code. A systems analysis code gives an overview of the flow in an entire reactor system. In the VHTR outlet plenum case, RELAP5-3D[©] was primarily used to determine the pressure and temperature distribution within the core region. Hence, RELAP5-3D[©] provides boundary conditions to Fluent which actively change as the two codes communicate.

The flow geometry of the VHTR outlet plenum is very important to this analysis, and it must be well modeled to obtain an accurate result. The flow patterns inside the outlet plenum are complex, three-dimensional effects which RELAP5 cannot model well. For this reason, the Computational Fluid Dynamics (CFD) code Fluent was chosen to model the outlet plenum. A CFD code such as Fluent has the ability to model complex three-dimensional flow behavior. On the other hand, Fluent relies on a fine mesh to model the region of interest; consequently, even with fast modern computers, the region of a system that can be modeled is generally limited by practical computing times (Schultz, et al., 2003). For this reason, Fluent is only used to model a small portion of the VHTR system. By using Fluent to model a small portion of the VHTR system the computation times are greatly reduced. By modeling the VHTR system in this way, the strengths of both RELAP5-3D[©] and Fluent are exploited while their weaknesses are minimized.

RELAP5-3D[©] is used to solve the flow conditions exiting the reactor core at various radial positions. These exit conditions are then transferred to Fluent, where they are used as the inlet boundary conditions in the outlet plenum model. A time step is completed as Fluent sends information back to RELAP5-3D[©] which then solves for the exit conditions again and continues the process.

The executive program controls the communication between the two codes. Using this coupling tool drastically improves upon the stand-alone results produced by RELAP5-3D[©]. Because RELAP5-3D[©] has the proven ability to couple with Fluent (Schultz, et al., 2005) it is an ideal code to use for this study. By combining these two codes, the important aspects of the VHTR model in this analysis are well represented.

2. PROBLEM

One of the most significant aspects that must be addressed in the VHTR outlet plenum is the mixing of the hot exit gases from the reactor core.

Mixing refers to the degree to which coolant of differing temperatures entering a region mixes to produce a uniform temperature. Mixing is a three-dimensional phenomenon in the outlet plenum and a function of a number of variables. In the outlet plenum, mixing occurs between the bottom of the core and the turbine or immediate heat exchanger inlet during normal operation. A preliminary calculation of the temperature variation in the outlet plenum indicates that gas temperature variations could exceed 300° C. Although the specification for temperature variation at the immediate heat exchanger or turbine inlet has not been set, it is thought that the helium temperature variation must be less than $\pm 20^{\circ}$ C. It is likely that special design features will be required to ensure good mixing and minimal thermal streaking from the outlet plenum to the turbine inlet (Schultz, et al., 2005).

The use of the executive program to couple problems of this magnitude is in its beginning stages. For this reason, the program will first be used to obtain a steady-state solution between RELAP5-3D[©] and Fluent. This steady-state solution can be used later as the initial condition to a transient situation.

2.1. The RELAP5-3D[©] VHTR Model

RELAP5-3D[©] was created at the Idaho National Engineering and Environmental Laboratory to calculate the behavior of a reactor coolant system during transients and steady-state conditions. RELAP5-3D[©] is a systems analysis code, which is a code that can model the flow of an entire reactor system (RELAP5-3D[©], 2001). RELAP5-3D[©] can effectively model coolant flow across wide thermodynamic ranges and states. RELAP5 was originally developed to analyze the behavior of two-phase systems that could be modeled in one dimension. The need to analyze two-phase flow resulted in a simplification of the viscous stress terms and the use of empirical relationships. For this reason, RELAP5 is limited in its ability to produce widely accepted analyses of multi-dimensional flow behavior, and therefore would not be the ideal tool for modeling the outlet plenum (Schultz, et al., 2003).

RELAP5-3D[©] was chosen as the primary code in the coupling scheme because it provides the inlet conditions for the Fluent model. The RELAP5-3D[©] VHTR model used in this analysis was expanded from a three-channel core model (Bayless, 2003) into a nine-channel core model for this analysis. The reactor core portion of the model is divided into nine-channels that are nearly concentric. The inner and outer bypass flows of the core region are also modeled as channels in the core region. This VHTR model was used as the basis for the coupling analysis. Fig. 3 is a visual depiction of the core region of the VHTR model.



Fig. 3. The RELAP5-3D^{\circ} VHTR core model. Volumes 140 and 195 represent the inlet and outlet plenums respectively. Channels 2-10 show the nine-channel configuration used to model the core. Channels 1 and 11 represent the bypass flow in the inner and outer reflectors respectively. Flow direction is indicated by the arrows.

Each of the core channels (2-10) are divided vertically into seven hydrodynamic volumes. Therefore, the reactor core is modeled by a total of 63 hydrodynamic volumes. The inner and outer bypass channels are also modeled by seven hydrodynamic volumes.

The RELAP5-3D[©] Steady-State Solution

The RELAP5-3D^{$^{\circ}$} VHTR model was independently run to a steady-state solution. The values of pressure and temperature exiting each of the 11 flow channels were recorded to be used as boundary conditions. These extracted results were used in the Fluent model as the initial inlet boundary conditions, and in a modified RELAP5-3D^{$^{\circ}$} deck. The values of pressure and temperature at the exit of the 11 flow channels are tabulated in Table 1.

	Flow Channel	Pressure (MPa)	Temp (K)
	1	6.947	1117.2
	2	6.947	1311.0
	3	6.947	1373.0
	4	6.947	1338.2
	5	6.947	1197.9
	6	6.947	1097.9
	7	6.947	1047.6
	8	6.947	1110.5
	9	6.947	1112.8
	10	6.947	1113.4
_	11	6.947	886.2

 Table 1

 Initial channel pressure and temperature at the exit.

The Steady-State Coupling

After a steady-state solution of the RELAP5-3D[©] model was obtained, the VHTR model was modified to meet the demands of the coupling process. The multiple junction representing the exiting core flow and the outlet plenum branch (component 195) were removed. The outlet plenum branch was replaced by 11 time-dependent volumes. The time-dependent volumes were each connected to a distinct flow channel by a single junction directed toward the flow channel. The coupling procedure requires that information be sent to Fluent from a volume, in this case the exit volume of each of the 11 flow channels. Fluent will then send information back to RELAP5-3D[©] through the 11 single junctions connecting the flow channels to the time-dependent volumes. Fig. 4 shows the modifications that were made to the model. The time-dependent volumes are included solely to meet the geometric constraints of RELAP5. They do not interact in the coupled problem.



Fig. 4. Modified RELAP5-3D^{$^{\circ}$} VHTR core model. The outlet plenum was replaced by 11 time-dependent volumes, one for each of the 11 flow channels. The exit volume of each pipe section sends information to the Fluent model, and Fluent sends information back to RELAP5-3D^{$^{\circ}$} through the 11 single junctions (numbered 9 – 99) connected to the reactor outlet.

In preparation for the coupling, some of the control cards in the input deck of the RELAP5-3D^{$^{\circ}$} model had to be changed. The 2nd word of Card 100 had to be changed to transnt (transient) from stdy-st (steady-state). The time step size (Cards 200-299) had to be changed to match the time step used in the executive program input deck and the Fluent model.

2.2. The Fluent Outlet Plenum Model

Fluent is a CFD code, which has the ability to model fluid flow in complex threedimensional geometry. A CFD code is a computational technology that enables the study of the dynamics of things that flow. Using CFD makes it possible to build a computational model that represents a system or device of study. Fluid flow physics and chemistry can then be applied to this virtual prototype, and the software will output a prediction of the fluid dynamics and the related physical phenomena. The CFD software will provide images and data which predict the performance of the design. CFD analysis makes it possible to virtually crawl inside a design to see how it performs (Fluent, 2006).

A model of the General Atomics VHTR outlet plenum was created at Fluent, Inc. (courtesy Fluent). It is anticipated that the Fluent model will successfully predict the flow field within the outlet plenum. The model consists of 704,947 cells, 2,175,124 faces and 767,064 nodes. To reduce the required computation time, the outlet plenum model is bisected by a line of symmetry. Applying a symmetry boundary condition to the outlet plenum model reduces the required computation time without altering the model itself. A graphic of the VHTR outlet plenum model created by Fluent can be seen in Fig. 5.



Fig. 5. The Fluent outlet plenum model. The black cylinders are the core support post positions, the blue areas are inlet flow faces, the grey areas are the wall boundary conditions, and the white area shows the location of the symmetry boundary condition.

Due to the complex three-dimensional geometry and the high temperature and velocity within the outlet plenum, model validation will be required in the future.

Validation work is currently being performed independently at the Idaho National Laboratory (INL). The Fluent model results are important to this study, because the outlet plenum presents significant design issues for the VHTR.

The Fluent Steady-State Solution

The flow inlet surfaces of the Fluent model were divided into 11 different flow boundaries to match the RELAP5-3D[©] VHTR model. This flow boundary division was performed by separating the flow inlet surfaces into 11 boundaries based on the flow area of the channels in the RELAP5-3D[©] model. The flow inlet boundaries must be set as pressure-inlet boundary conditions. This boundary condition requires a total pressure at the boundary. The outlet boundary condition must be a pressure-outlet boundary condition; this will require a static pressure. These requirements must be met in order to successfully couple RELAP5 and Fluent. The total pressures at each of the nine inlets were estimated using Eq. (1).

$$P_{tot,F} = P_{static,R} + \frac{1}{2}\rho_R V_R^2$$
(1)

Where $P_{tot,F}$ is the estimated total pressure to be used as the Fluent pressure-inlet boundary condition. $P_{static,R}$, ρ_R , and V_R represent the static pressure, density, and velocity respectively, from the RELAP5-3D[©] steady-state output. The resulting total pressures were applied as pressure-inlet boundary conditions for the 11 Fluent flow inlets. A steady-state solution for the outlet plenum was then obtained. The pressure at the outlet boundary was chosen such that the mass flow rate through the Fluent model was approximately equal to the mass flow rate in the RELAP5-3D[©] model. Obtaining steady-state solutions for the two codes greatly reduces the required computation time for the coupled problem, because the two models are already at convergence.

The Fluent model was executed to a first-order solution, because Fluent converges a first-order solution more quickly.

The Steady-State Coupling

To execute the coupled problem, a number of User Defined Functions (UDFs) must be read into the Fluent model. The UDFs are mandatory for Fluent to be capable of sending and receiving messages in the coupling process. The specific adjustments that must be made to the Fluent model in order to successfully couple the two codes can be found in the coupling manual in Appendix A.

2.3. The PVM Executive Program^{*}

Background

The coupling between RELAP5-3D[©] and the other code was accomplished using the PVM (Parallel Virtual Machine) message passing software developed at Oak Ridge

^{*} Sections 2.3 and 2.4 are reprinted with permission from "A PVM Executive Program For Use with RELAP5-3D[©]" by Weaver, W.L., Tomlinson, E.T., and Aumiller, D.L., 2002. ICONE10 Proceedings, paper number ICONE10-22678.

National Laboratory (Geist, et al., 1993). Data items are passed between the coupled codes in messages having unique message identifiers. In the original implementation of the PVM methodology, RELAP5-3D $^{\circ}$ could only be coupled to one other computer code. Other restrictions inherent in the original implementation of the PVM methodology in RELAP5-3D[©] include lack of coordination of the time step size to be used by the coupled codes, the inability to monitor the status of the two coupled codes, and lack of coordination in the printed and plotable output of the two coupled codes. Each code was required to choose its own time step size which forced the user to use a fixed time step size (i.e., fixed so that they would use the same time step size for semiimplicit coupling) or fixed simulation time intervals for explicit coupling (the explicit coupling algorithm exchanges data between coupled processes at fixed time intervals). The inability to monitor the status of the code also forced the user to choose a time step size in such a way that the time step advancements would always be successful so that no time step repeats or time step size reductions would be necessary. The user also had to configure the virtual machine by hand before executing the coupled calculation and the coupled codes had to be executed on the same computational node. The PVM executive program was developed to remove these restrictions and to make the PVM methodology used by RELAP5-3D[©] more versatile.

Design of the PVM Executive Program

The PVM executive program was designed to remove the restrictions of the original implementation of the PVM coupling methodology in RELAP5-3D[©]. It has five

major responsibilities. First, it must configure the virtual machine, starting the PVM daemon process on the computational nodes comprising the virtual machine. Second, it must start up the coupled processes on the several computational nodes. Third, it must tell each of the coupled processes what data to send to and what data to receive from the other processes. Fourth, it must manage the time advancements of the coupled codes, monitoring the status of the advancements and directing code backups and time step repeats as necessary. Fifth and lastly, it must coordinate the production of printed and plotable output between the coupled codes so that computational results are available from all of the coupled codes at the same simulation times during the computation.

The user supplies the information needed by the PVM executive program in an input file. The input file is divided into four sections (the input needed to accomplish fourth and fifth responsibilities are contained in the same section of the input file). The sections of the input file are delimited by reserved keywords. The first section of the input file is delimited by the keyword 'virtual'. The lines following this keyword contain the names of the computational nodes to be used in the virtual machine along with the location of the executable files to be used by that computational node and the location of the input files for the processes to be executed on that computational node (i.e., the working directory). Using this information, the PVM executive program builds a PVM hostfile for the virtual machine and starts the PVM daemon process on the several computational nodes.

The second section of the input file is delimited by the keyword 'processes' and specifies the processes (i.e., codes) to be executed on the several computational nodes. The names of the computational nodes contained in the first section of the input file become keywords in the second section of the input file. One or more coupled processes may be executed on each of the computational nodes. The specification of each coupled process contains a unique name for each process as well as any command line parameters that are to be passed to that process as it begins its execution (i.e., names of input files, output file, etc.). The names of the coupled processes are used to distinguish multiple instances of the same executable file being executed in the virtual machine. Finally each process is labeled as 'synchronous' or 'asynchronous'. These labels denote whether or not the time step size for the process is determined by the executive program. Synchronous processes, such as processes that are coupled semi-implicitly, need to use the same time step size for each advancement so their time step size is coordinated by the executive program. Asynchronous processes, such as processes coupled explicitly, need only exchange data at fixed intervals and it does not matter what size of time step they use to advance in time, only that they reach the same point in time to exchange data.

The third section of the input file is delimited by the keyword 'messages' and specified the data to be sent to and received from the other coupled processes. Each message uses the unique name of the sending and receiving process along with the specification of the data to be sent or received. The specification of messages occurs in pairs, one message specification for the process sending the data and the other specification for the process receiving the data. The data items to be sent by the sending process are specified in terms that the sending code can understand and vice-versa for the receiving code. This means that the same data item may be specified by a different identifier for the sending and receiving processes. For example, the sending code may refer to the liquid density using the code variable 'rhof' while the receiving code may refer to the liquid density by the code variable 'rholiq'. The data specifications are sent to the several coupled codes as they appear in the third section of the input file. It is the responsibility of the individual coupled codes to understand their data specification.

The last section of the input file is delimited using the keyword 'timesteps'. This section of the input file contains data for one of more simulation intervals during the coupled computation. The data for each interval are the end time for the simulation interval, the maximum and minimum time step sizes for the simulation interval, the print, plot, restart write, and explicit coupling frequencies for that interval along with other control information for that interval.

A schematic of a typical coupled computation is shown in Fig. 6. In this coupled computation, two instances of RELAP5-3D^{$^{\circ}$} are coupled semi-implicitly to model the coolant systems in a reactor power plant, one of the instances of RELAP5-3D^{$^{\circ}$} is coupled to a code that performs a reactor power computation using a nodal neutron kinetics methodology, and the other instance of RELAP5-3D^{$^{\circ}$} is coupled explicitly to a containment analysis code. The data flows between the several coupled codes as well as between the coupled codes and the executive program is also shown in Fig. 6. What Fig. 6 does not shown is that each of the processes might be executing on a different computational node and that the communication between the processes would be carried

over a network. Also not shown is that the computational nodes might be different computer architectures from different vendors, i.e., a mix of different types of UNIX workstations and PCs.



Fig. 6. Schematic of a coupled computation.

2.4. Sequence of Events in a Coupled Computation

A coupled computation can be divided into two phases, that are the input and initialization phase of the computation and the transient simulation phase of the coupled computation.

Input and Initialization Phase

The PVM executive program is executed by the user in a manner appropriate for the users operating system specifying the input file and the output file for the executive program as command line parameters (default input and output files are also defined). The executive program reads the first section of its input file, constructs a PVM hostfile, and starts the PVM daemon process on the several computational nodes in the virtual machine. Then the executive program spawns the several coupled processes on the one or more computational nodes. The coupled processes that are spawned read their respective input files, process the data contained in their input files and then listen to receive messages from the executive process. After the executive process has spawned all of the coupled processes, it sends messages to each of the spawned processes containing the data specifications for messages to send to and receive from the other coupled processes. Each spawned process proceeds with its own input and initialization after the coupling data specifications have been received from the executive process. The executive process listens to receive a message from each process describing its initialization status and its run status. Each coupled code sends its initialization status to the executive program at the end of its initialization process. This initialization status may be zero (initialization successful) or one (errors during input and initialization). They also sent the executive program their run status, where zero denotes no transient to be executed because of input or initialization errors or because this run was for input checking only, or one, ready for transient simulation. The coupled computation is terminated if any of the coupled processes return an initialization error or returns a zero

run status. The executive program determines the global initialization and run status and broadcasts this status to all of the coupled processes.

Transient Computation Phase

Assuming that the initialization was successful for all of the coupled processes and that the run status indicated that all coupled processes are ready to perform a transient simulation, the executive program broadcasts an initial set of output control times. This message specifies the next simulation times for the production of printed output, printing of RELAP5-3D[©] minor edit variables, generation of plot data, writing of restart data and the next time explicit coupling data transfers are to be performed. The PVM executive program assumes that each code will produce its own initial printed output, plot data, and restart data automatically. The executive program then coordinates the initial exchange of any explicit coupling data between asynchronously coupled processes. When more than two codes are coupled explicitly, the data exchanges between the codes needs to be coordinated by the executive program. The data exchange paradigm used in the PVM coupled computation is that all messages received will be followed by an acknowledgement returned to the sender. The sending process waits to receive an acknowledgement before sending the next message. If all of the codes were to send all of their messages and then listen to receive all of their messages, there would be a deadlock condition because all processes would be sending and no processes would be listening for acknowledgements. The executive program broadcasts the PVM identifiers of each of the explicitly coupled processes to all of the explicitly coupled processes one

20

at a time. The process named in the broadcast message sends its data and all of the other explicitly coupled process listen to receive the messages sent by the process named by the executive process. This works like the old telephone party line where each of the explicitly coupled processes must wait its turn to talk on the party line. Each explicitly process receives permission to send its data in its turn. This process of coordinating the exchange of explicit coupling data occurs each time the simulation time reaches the time for an explicit exchange of data.

Once any initial explicit coupling data is exchanged, time step advancements may begin. The executive program listens to receive a time step size from each of the synchronously coupled processes. Each synchronically coupled code determines the time step size that it wants to use and sends it to the PVM executive. The executive program receives the several time step sizes, determines a global time step size as the minimum of the time step sizes received from the synchronously coupled processes and broadcasts the global time step size back to the synchronously coupled processes. This message also contains updated edit, print, and plot times so that output may be produced each time step rather than at predetermined intervals. Output every time step is useful in debugging and this capability existed previously in RELAP5-3D[©]. After the synchronously coupled processes receive the global time step size from the executive program, they proceed with the time step advancement, performing any communication needed with the other coupled processes during the advancement. At the end of the advancement, just before the point of no return, each of the synchronously coupled processes sends its advancement status to the PVM executive program. The point of no return is that point

21

in the computations sequence after which no backup may be performed in order to fix any errors that occurred during the advancement. The executive program listens to receive the advancement status from all of the synchronously coupled processes, determines the global advancement status, and broadcasts the global advancement status to the synchronously coupled processes. Assuming that no errors have occurred during the advancement, the coupled codes and the executive program proceed to the next time step advancement. Time step advancements are performed until the end time for the simulation is reached. The executive program assumes that all of the coupled processes will terminate automatically when the end time is reached. The executive program waits for the coupled code to finish, and then shuts down the virtual machine. (For more information on the semi-implicit coupling scheme, see Weaver, et al., 2002b.)

3. SOLUTIONS

3.1. The Steady-State Solution

The steady-state solution for the coupling problem was obtained by using a time step size of 2.0E-4 sec for a total of 30 iterations to 6.0E-3 sec. The problem was then restarted with a time step size of 1.0E-4 sec and run an additional 5 iterations to 6.5E-3 sec. The total run time to reach the steady-state results was about 30 hours. The results of the RELAP5 static pressures at the 11 coupling boundaries are displayed below.





Fig. 7. The convergence of the RELAP5 channel pressures. The pressures from the 11 coupling boundaries are approaching a single converged value.

The RELAP5 outlet pressures from each of the 11 coupling boundaries are approaching a single value. This result indicates that the coupling is successfully approaching a converged solution. As the steady-state problem is continued indefinitely, the converged results for the VHTR problem will continue to improve.

The coupling program requires that the values of static pressure, mass flow rate and temperature be equivalent across the coupling boundaries. These three variables will be addressed in turn.

The Boundary Static Pressures

The tabulated results of static pressure across the coupled boundaries can be seen

in Table 2.

Table 2

p				
Static Pressure (Pa)				
Channel	RELAP5	Fluent	Difference	% Difference
1	6953920	6954169	249	0.0036%
2	6953960	6953943	17	0.0002%
3	6953750	6954090	340	0.0049%
4	6953210	6953409	199	0.0029%
5	6952800	6953088	288	0.0041%
6	6952980	6953111	131	0.0019%
7	6953480	6953102	378	0.0054%
8	6953210	6953102	108	0.0016%
9	6953120	6952960	160	0.0023%
10	6952670	6952198	472	0.0068%
11	6953590	6952407	1183	0.0170%
Average	6953335	6953234	101	0.0015%
Std. Dev.	439	636		

Static pressure comparison across the coupled boundaries.

Each of the static pressure values should be equivalent, because all of the boundaries share the same elevation in the outlet plenum. The difference between the

averages of the results of the two codes across the coupling boundaries is only about 100 Pa. The standard deviation between each of the individual flow channels is small as well in comparison to the magnitude of the static pressures.

The largest difference is found in channel 11, the outer reflector. In Fig. 7 it is seen that the pressure in channel 11 exhibits the largest oscillation as the pressures approach convergence. Fig. 8 shows the comparison of the convergence in the two codes for the static pressure in the outer reflector as time advances in the executive program. The fluctuation in the static pressure in channel 11 causes the observed difference across the boundary.





Fig. 8. Static pressure comparison in channel 11. The RELAP5 results show a rapid change, which Fluent is following.

The Boundary Mass Flow Rates

The tabulated results of mass flow rate across the coupled boundaries can be seen in Table 3.

	Mass Flow Rate (kg/s)				
Channel	RELAP5	Fluent	Difference	% Difference	
1	1.336	0.856	0.480	43.80%	
2	5.201	5.345	0.144	2.73%	
3	9.747	10.234	0.487	4.87%	
4	9.961	10.127	0.166	1.65%	
5	19.307	19.517	0.210	1.08%	
6	59.267	59.597	0.330	0.56%	
7	7.715	7.598	0.117	1.53%	
8	14.442	14.489	0.047	0.32%	
9	14.283	14.29	0.007	0.05%	
10	19.56	19.513	0.047	0.24%	
11	17.608	17.291	0.317	1.82%	

 Table 3

 Mass flow rate comparison across the coupled boundaries.

The large percent difference in mass flow rate observed in channel 1 is primarily due to the small amount of mass flowing through it. The mass flow rate difference across the boundary is on the same order as some of the other boundaries. The small mass flow rate however, makes the percent difference very large. Some of the difference in mass flow rate can be attributed to the fact that the helium density used by RELAP5 and Fluent are not identical. The helium density used by Fluent is interpolated from a table of density versus temperature. The values used by RELAP5 are both pressure and temperature dependent and are therefore different to the values used by Fluent. This density difference accounts for some of the difference across the boundaries.

A side-by-side comparison plot of the mass flow rate in channel 4 between RELAP5 and Fluent is seen in Fig. 9.



Mass Flow Rate in Channel 4

Fig. 9. Mass flow rate comparison in channel 4. This figure is indicative of the other flow channels. The mass flow rates in the 11 different channels are converging.

The RELAP5 mass flow rate results show that the fluctuation is decreasing in nearly all of the channels and are approaching a constant value. The mass flow rate through channel 11 is the exception, because the mass flow rate is increasing in this channel. Although the mass flow rate in channel 11 has not completely steadied out, it was observed that the RELAP5 and Fluent results closely match, indicating that the executive coupling program is successfully coupling the boundary. The mass flow rate through channel 11 is displayed in Fig. 10.



Fig. 10. Mass flow rate comparison in channel 11. The Fluent results are only reported at t = 0, 0.006 and 0.0065 sec.

The figure shows that the Fluent results are following the changing mass flow rate in RELAP5. The mass flow rate through this channel will level off as the executive program continues to iterate.

The Boundary Temperatures

The boundary temperatures converge very slowly. The tabulated results across the coupled boundaries can be seen in Table 4.

Mass Flow Rate in Channel 11
Temperature (K)				
Channel	RELAP5	Fluent	Difference	% Difference
1	1080.5	1101.5	21	1.92%
2	1304.7	1290.9	13.8	1.06%
3	1371.4	1350.7	20.7	1.52%
4	1338.6	1330.1	8.5	0.64%
5	1198.1	1198.4	0.3	0.03%
6	1097.8	1099.1	1.3	0.12%
7	1049.6	1054	4.4	0.42%
8	1100.7	1099.3	1.4	0.13%
9	1112.8	1110	2.8	0.25%
10	1113.2	1090	23.2	2.11%
11	897.6	910.3	12.7	1.40%

Table 4Temperature comparison across the coupled boundaries.

There are significant temperature differences across the coupled boundary in some of the flow channels. The temperature, pressure and mass flow rate are dependent on one another. This dependency means that an observed change in one of these variables will affect the others. There is interdependence between the different flow channels as well. As changes occur in one of the channels, the other channels will be affected. This greatly complicated reaching convergence between the two codes.

The temperature values across some of the boundaries are relatively large. The Fluent results for temperature have exhibited a resistance to change. This can partially be explained by the way in which Fluent determines the degree of convergence. The degree of convergence of a problem is determined by the scaled residuals of the model. The Fluent residuals are a measure of how well the current solution satisfies the discrete form of the governing equations (Cornell University, 2002). To explain the residuals, a figure showing a one-dimensional discretized mesh is provided.



Fig. 11. A one-dimensional discretized mesh.

In Fig. 11 ϕ is the value of a general variable at the three different points (i.e. points *P*, nb,1 and nb,2), *a_P* is the center coefficient and *a*_{nb} are the coefficients for the neighboring cells. The conservation equation of a discretized mesh for a general variable ϕ can be written as:

$$a_P \phi_P = \sum_{\rm nb} a_{\rm nb} \phi_{\rm nb} + b \tag{2}$$

In this equation, b is the contribution of the constant part of the source term and of the boundary conditions.

The scaled residual used by Fluent (R^{ϕ}) to solve for the convergence of the problem is provided by the following equation.

$$R^{\phi} = \frac{\sum_{cellsP} \left| \sum_{nb} a_{nb} \phi_{nb} + b - a_{P} \phi_{P} \right|}{\sum_{cellsP} \left| a_{P} \phi_{P} \right|}$$
(3)

Here, the imbalance in Eq. (2) is summed over all the computational nodes P and is then scaled by a factor representing the flow rate of the general variable, ϕ through the domain (Fluent, 2003).

As the Fluent case approaches convergence, the value of the scaled residual will decrease. This is because the imbalance in the numerator of Eq. (3) is decreasing. The scaling factor (the denominator) used in Eq. (3) is summed over all of the computational nodes P in the domain. This fact indicates that if the majority of the cells in the computational domain have reached convergence, the unconverged cells will have little effect on the value of the residuals. The fact that there are over 700,000 cells in the computational domain will make it less likely that convergence is reached in the entire domain. Fluent does not allow the prioritization of the convergence of a specific domain, thus some of the unconverged cells near the coupled boundaries are overlooked.

The comparison plots of temperature at the coupled boundaries do show however that RELAP5 and Fluent are approaching a converged solution. An example of the convergence of temperature between RELAP5 and Fluent is shown in Fig. 12.



Fig. 12. Temperature comparison in channel 4. The temperature is converging between the two codes. Note: the Fluent results were only reported at t = 0, 0.006 and 0.0065 sec.

The comparison plots for pressure, temperature and mass flow rate for each of the 11 coupled boundaries can be seen in Appendix B.

Mixing in the Outlet Plenum

The helium temperature leaving the outlet plenum must be well distributed to avoid damage to the downstream components. Fig. 13 gives an indication of the degree to which the outlet gases are mixing. The results presented here are first-order solutions to the Fluent outlet plenum model.



Fig. 13. Temperature pathlines in the outlet plenum.

In Fig. 13 the pathlines are colored by temperature. The higher temperatures exist in the areas where the pathlines are red. The lower temperatures exist in the areas where the pathlines are blue. The temperature of the helium as it exits the outlet pipe appears to be nearly uniform from the temperature pathlines.

It is necessary to obtain a better indication of the temperature distribution in the outlet pipe. The contours of temperature as the helium enters, at the mid-point and at the exit of the outlet pipe are seen in Fig. 14.



Fig. 14. Temperature contours in the outlet pipe. The three contour plots represent the entrance, the midpoint and exit of the outlet pipe. The pipe is 1.565 m long.

The temperature range of the outlet gases as they first enter the outlet pipe section is about $\pm 44^{\circ}$ C. Fig. 14 shows that the gas temperature variation in the outlet pipe is decreasing as it flows through the pipe. The temperature variation as the helium gas exits the outlet pipe is $\pm 32^{\circ}$ C. Thus over the total pipe length of 1.565 m, the temperature variation has decreased by 12°C

4. CONCLUSIONS AND RECOMMENDATIONS

There is a need to develop computational tools which can demonstrate the feasibility of the design concepts and guide the improvement of plant components. The coupling executive program can successfully couple RELAP5-3D[©] and Fluent in analysis of the outlet plenum of the VHTR. The fact that there are 11 RELAP5 flow channels venting into the Fluent outlet plenum made it difficult to find a balanced solution. The problem results will not be greatly improved upon by increasing the run time.

The static pressures in the outlet plenum are converging to a single value. There is some large fluctuation in channel 11 that can be slightly reduced by running the problem longer. Channel 11 has an increasing mass flow rate as well. Fig. 15 is a comparison plot of the pressure and mass flow rate in channel 11.

As the pressure in channel 11 increases, the mass flow rate responds by increasing as well. A decrease in the pressure in channel 11 causes a slight decrease in mass flow rate. As the pressure in channel 11 stabilizes, so will the mass flow rate. Thus to improve the flow conditions in this channel, the problem will need to be run for a longer period of time.



Pressure and Mass Flow Rate in Channel 11

Fig. 15. Pressure and mass flow rate in channel 11.

It may be necessary to achieve a better match of the helium density across the coupled boundary. This will be difficult because Fluent uses a density profile which is only temperature dependent and RELAP5 uses a density which is both pressure and temperature dependent. By improving the density correlation across the boundary, the difference in mass flow rate can be reduced.

The large computational domain adversely affects the convergence at some points in the domain. It may be possible to improve the convergence at the Fluent boundaries by decreasing the residual value, and thus forcing Fluent to arrive at a better convergence in the boundary regions. The recommendation can also be made to Fluent to make it possible to prioritize the convergence in specific domains. The preliminary Fluent calculations show that the temperature of the helium exiting the outlet plenum is not within the $\pm 20^{\circ}$ C limit. First and foremost, a higher order Fluent solution method will be used. If similar results are obtained, the outlet pipe of the plenum can be lengthened. By lengthening the pipe, the temperature will have a greater distance over which it can equilibrate. If necessary, a geometry feature which induces the helium mixing may be added to the model.

The coupling problem currently requires long run times. To simulate a transient there is a need to speed up the computation. The small time step sizes that are used to obtain a solution will require over 100,000 iterations to simulate a slow transient.

This coupling tool can successfully be applied to many problems which require that the three-dimensional effects of a specific area be well modeled.

REFERENCES

- Bayless, P. D., (2003). VHTR Thermal-Hydraulic Scoping Analyses Using RELAP5-3D/ATHENA, Proceedings of Conference, pp. 312-319, GLOBAL 2003, New Orleans, LA, 16-20 November 2003, American Nuclear Society.
- Cornell University, (2002). Fluent Tutorials, Cornell University Course web sites, http://instruct1.cit.cornell.edu/courses/fluent/plate/step5.htm, accessed February 2006.
- Department of Energy (DOE), (2005). Generation IV Nuclear Energy Systems web site, http://gen-iv.ne.doe.gov, accessed January 2006.
- Fluent, (2003). Fluent 6.1 Users Guide, vol. 3, Fluent Inc., Lebanon, NH (pp. 70-71, Chapter 24).
- Fluent, (2006). Fluent web site, http://www.fluent.com/solutions/whatcfd.htm, accessed January to February 2006.
- General Atomics (GA), (2003). GT-MHR Reactor System Design, American Nuclear Society Gas Reactor Technology Course presented by Dr. A. Shenoy, June 5-6.
- Geist, A., Beguelin, A., Dongarra, J., Weicheng, J., Manchek, R., Sunderman, V., (1993). PVM (Parallel Virtual Machine) User's Guide and Reference Manual, Oak Ridge National Laboratory, ORNL/TM-12187.
- Idaho National Laboratory (INL), Oak Ridge National Laboratory (ORNL), Argonne National Laboratory (ANL), (2005), Next Generation Nuclear Plant Research and Development Program Plan, January, pg 64.
- RELAP5-3D[©], (2001). RELAP5-3D Code Manual, vol. I, Idaho National Engineering and Environmental Laboratory, INEEL-EXT-98-00834, Revision 1.3a.
- Schultz, R.R., Riemke, R.A., Davis, C.B., Nurnberg, G., (2003). Comparison: RELAP5-3D[©] Systems Analysis Code and Fluent CFD Code Momentum Equation Formulations, Proceedings of Conference, pp. 1-9, ICONE11-36585, Tokyo, Japan, 20-23 April 2003, American Society of Mechanical Engineers.
- Schultz, R.R., Weaver, W.L., Johnson, R.W., Schowalter, D.G., Basu, N., (2005). Evaluating Fluid Behavior in Advanced Reactor Systems Using Coupled Computational Fluid Dynamics and Systems Analysis Tools, Proceedings of

Conference, pp. 1-11, ICONE13-50723, Beijing, China, 16-20 May, 2005, American Society of Mechanical Engineers.

- Weaver, W.L., Tomlinson, E.T., Aumiller, D.L., (2002a). A PVM Executive Program for Use with RELAP5-3D[©], Proceedings of Conference, pp. 1-5, ICONE10-22678, Arlington, VA, 14-18 April, 2002, American Society of Mechanical Engineers.
- Weaver, W.L., Tomlinson, E.T., Aumiller, D.L., (2002b). A Generic Semi-Implicit Coupling Methodology for Use in RELAP5-3D[©], Nuclear Engineering and Design 211, 13-26.

APPENDIX A THE COUPLING MANUAL

RELAP5-3D[©] Setup

After a steady-state solution of the RELAP5-3D[©] model has been reached, modifications must be made to the model in preparation of coupling to Fluent. The physical domain which Fluent is used to model must be removed from the RELAP5 model. After removing the portion of the domain that Fluent will be used to model, each coupling boundary must be represented by a time-dependent volume and a single junction directed into the RELAP5 domain. This scheme is represented in Fig. A1.



Fig. A1. Changes made to the RELAP5 model in preparation for the coupling process.

The coupling requires that information be sent from a RELAP5 volume element to Fluent. Fluent will send information back to RELAP5-3D[©] through the single junction connected to the time-dependent volume. Without these model changes, the coupling will not be successful.

Some of the control cards in the input deck of the RELAP5-3D^{$^{\odot}$} model need to be changed as well. The 2nd word of Card 100 has to be changed to transnt (transient) from stdy-st (steady-state). The timestep size (Cards 200-299) has to be changed to match the timestep used in the executive program input deck and the Fluent model.

Fluent setup

The Fluent model is run to convergence with the boundary conditions set to a pressure-inlet boundary condition at the inlet(s) and a pressure-outlet boundary condition at the outlet(s). The values of pressure and temperature used in these boundary conditions come from the output produced by the RELAP5-3D[©] model.

After convergence of the Fluent model has been reached, the solver must be set for the transient run. This is performed by opening the solver via Define/Models/Solver. Here the time field should be set to unsteady.

The User Defined Functions (UDFs) which allow Fluent to communicate with RELAP5 must be read into Fluent. To do this, open Define/User-Defined/Functions /Compiled and select the following functions:

- pvm_adjust
- pvm_init

- pvm_test_init
- pvm_execute_at_end
- pvm_pin_bc
- pvm_pout_bc
- pvm_temp_bc

Next, proceed to Define/User-Defined/Function Hooks. Here, the Adjust Function is set to pvm_adjust and the Execute At End Function is set to pvm_execute_at_end.

The Boundary Conditions panel is opened with Define/Boundary Conditions. Select one of the coupling boundaries and click Set. Two options are available here:

- If the coupling boundary is a pressure-inlet, click on the arrow to the right of Gauge Total Pressure and select pvm_pin_bc. The arrow to the right of Total Temperature must also be selected and set to pvm_temp_bc.
- If the coupling boundary is a pressure-outlet, click on the arrow to the right of Gauge Static Pressure and select pvm_pout_bc. The arrow to the right of Total Temperature must also be selected and set to pvm_temp_bc.

For the first iteration, the boundary condition values are given by the file fluent_bc.in. After the first iteration, the boundary condition values come directly from the RELAP5-3D[©] model.

A UDF which saves the case and data files at a prescribed frequency must be read into Fluent via Solve/Execute Commands. Add a one (1) to the defined command box. In the command field type (save_case_data). Select the small box under the "On" field (so that it is illuminated) at the left side. The saving frequency must be indicated in two locations, in the "Every" field and in the timestep control for the executive program. Select Time Step under the "When" field. Fluent is now ready to be coupled.

The Coupling Process – master: RELAP5-3D[©], slave: Fluent

To couple the two codes, the following user-modified files are needed:

- RELAP5-3D[©] input file (i.e. relap.i) a converged steady-state input file.
- Fluent converged case and data files:
 - \circ i.e. fluent.cas
 - o i.e. fluent.dat
- fluent_bc.in The Fluent boundary conditions are set for the first timestep.
- fluent_cntrl.in Fluent solver designation, and the enthalpy of the fluid being used at the problem pressure and a temperature of 298.15 K. This is a required conversion between RELAP5-3D[©] and Fluent.
- Fluent configuration file (i.e. fluent.in) Reads in the Fluent case and data files and Fluent setup and configured for a run.
- Executive program input file (i.e. executive.i) The configuration of the executive program and arrangement of the coupling communication.

The following files are needed for the coupling process to function successfully:

• UDF libraries – User Defined Functions for Fluent

- pvmexec.x The executable of the executive program
- pvmcatchout.x writing the output
- fluent_scheme.scm saves a Fluent case and data file at the user-indicated frequency

The setup of the coupling process was arranged by Walt Weaver at INL. The current coupling configuration is used with Fluent 6.1.22 and RELAP5-3D[©].

Execution Line for PVM coupling process: pvmexec.x -i executive.i -o arbitrarily named output file (i.e. executive.p)

fluent_bc.in

1st card - Number of junctions to be coupled (N)

N cards follow (will vary slightly for a Fluent pressure-inlet and pressure-outlet)

For a pressure-inlet (All units SI unless otherwise specified)

W1 - Fluent zone id number (found in Fluent Define/Boundary Conditions)

W2 - Total pressure (Pa)

W3 - Temperature (K)

For a pressure-outlet (All units SI unless otherwise specified)

W1 - Fluent zone id number (found in Fluent Define/Boundary Conditions)

W2 - Static pressure (Pa)

W3 - Temperature (K)

fluent_cntrl.in

1st card - solver set and UDF update cycle

W1 - assign an integer: either 0 or 1. A value of 0 indicates that Fluent will use the segregated solver. A value of 1 indicates that Fluent will use the coupled solver.

W2 - UDF update cycle number (integer). This value indicates the frequency at which the boundary conditions are updated per iteration.

2nd card - Coupling under-relaxation factor and the fluid enthalpy at problem pressure and a temperature of 298.15 K.

W1 - Under-relaxation factor for the coupling problem.

W2 - The fluid enthalpy at problem pressure and a temperature of 298.15

K. This is a necessary conversion between RELAP5-3D[©] and Fluent.

Fluent configuration file (fluent.in)

1st card - read the Fluent case file

W1 - rc

W2 - Fluent case file name (i.e. fluent.cas)

2nd card - read the Fluent data file

W1 - rd

W2 - Fluent data file name (i.e. fluent.dat)

3rd card - load the file designed to save a Fluent case and data file at a userdefined frequency.

W1 - (load 'fluent_scheme.scm)

4th card - call UDF pvm_init

W1 - define/user-defined/execute-on-demand

W2 - "pvm_init"

Optional cards - report surface average values of field variable of interest.

W1 - report/surface-avg

W2 - words from 2 to M are the zone-surface id numbers of the surfaces

of interest (may be different than the boundary condition zone id

numbers).

Note: zone-surface id numbers can be located in Fluent by going to

Surfaces/Manage. After clicking on the surface of interest, the id

number will be displayed.

WM+1 - ()

WM+2 - name of field variable of interest (i.e. Pressure, Temperature,

etc.)

5th card - Set the timestep

W1 - solve/set/timestep

W2 - timestep size (must match the RELAP5-3D[©] and the executive program timestep size)

6th card - Setup the Fluent iteration.

W1 - solve/dual-time-iterate

W2 - number of iterative steps taken between the coupled codes.

W3 - maximum number of iterations taken by Fluent after having received information from RELAP5-3D[©].

7th card - exit card

W1 - exit

Executive program input file (executive.i)

<u>virtual cards</u>

1st card - virtual declaration

W1 - virtual

2nd card - working directory and export directory

- W1 computational node name
- W2 wd=(working directory)
- W3 ep=(executables directory)

 3^{rd} and 4^{th} cards - writing output files

processes cards

1st card - processes declaration

W1 - processes

2nd card - computational node name

W1 - computational node name

 3^{rd} card - RELAP5- $3D^{\odot}$ execution line

W1 - primary (This title is what the master program will be called in the operation)

W2 - synchronous (semi-implicitly coupled programs must be run

synchronously)

W3 - RELAP5-3D[©] execution line, i.e. relap5.x -i relap.i -o relap.p -r relap.r

(executable, input file, output file, and restart file)

4th card - writing the output of the RELAP execution

W1 - primary writes W2 - RELAP5-3D[©] output file name will write banner and iteration steps RELAP5-3D[©] takes (i.e. relap.out)

5th card - Fluent initialization line

W1 - core (This title is what the slave program will be called in the operation)

W2 - synchronous (semi-implicitly coupled programs must be run synchronously)

W3 - Fluent startup path (must run in batch mode)

usr/local/Fluent.Inc/bin/fluent 3ddp -r6.1.22 -g -i

W4 - The Fluent configuration file name (i.e. fluent.in)

6th card - writing the output of the Fluent execution

W1 - core writes

W2 - Fluent output file name (i.e. fluent.out)

<u>messages cards</u>

1st card - messages declaration

W1 - messages

2nd card - declaration of solution method (semi-implicit)

W1 - semi-implicit

3rd card - data sent from RELAP5-3D[©] to Fluent

W1 - primary sends core

W2 - name of RELAP5-3D[©] connecting component (must be a volume,

i.e. single volume, pipe, etc.)

W3 - volume number of RELAP5-3D[©] coupling component (if using a pipe section broken into five volumes, must designate either 1 or 5 as the volume to be coupled to Fluent)

W4 - W2 and W3 are repeated until N (the number of RELAP5-3D[©] to Fluent coupling connections) is reached.

4th card - maximum amount of time RELAP5-3D[©] will wait for information to arrive from Fluent. This assures that the program will shut itself down if it is unable to continue.

W1 - primary awaits core

W2 - maximum amount of time that primary will wait for core in seconds.

 5^{th} card - data received from Fluent to RELAP5-3D $^{\odot}$

W1 - primary receives core
W2 - name of RELAP5-3D[©] connecting junction (must be a single junction)
W3 - 0
W4 - W2 and W3 repeated until N (the number of RELAP5-3D[©] to Fluent coupling junctions) is reached.

 6^{th} card - data sent from Fluent to RELAP5-3D[©]

W1 - core sends primary

W2 - zone

W3 - Fluent boundary condition zone id number (**The order of these words** is critical. The boundaries will be coupled such that the first boundary condition zone presented here will correspond to the first connecting junction presented in the 4th card above.)

Note: boundary condition id numbers can be located in Fluent by going to Define/Boundary Conditions. Click on the boundary of interest, and the id number will be displayed.

W4 - W2 and W3 are repeated until N (the number of RELAP5-3D[©] to Fluent coupling junctions) is reached. **(Be sure to present these cards in the proper order.)**

7th card - maximum amount of time Fluent will wait for information to arrive from RELAP5-3D[©]. This assures that the program will shut itself down if it is unable to continue.

- W1 core awaits primary
- W2 maximum amount of time that core will wait for primary in seconds.

 8^{th} card - data received from RELAP5-3D[©] to Fluent

- W1 core receives primary
- W2 zone

W3 - Fluent boundary condition zone id number (**The order of these words** is critical. The boundaries will be coupled such that the first boundary

condition zone presented here will correspond to the first connecting volume presented in the 2nd card above.)

W4 - words from 4 to N are repetitions of W2 and W3 until N (the number of RELAP to Fluent coupling boundaries) is reached. (Be sure to present these cards in the proper order.)

timesteps cards

1st card - timesteps declaration

W1 - timesteps

2nd card - timestep control

- W1 end time step (sec)
- W2 minimum time step
- W3 maximum time step
- W4 control option
- W5 minor edit and time frequency
- W6 major edit frequency
- W7 restart frequency (this field will also save a Fluent case and data file
- at the indicated frequency)
- W8 explicit coupling frequency (for semi-implicit coupling use 0)

Example files:

Assume two coupling boundaries a pressure-inlet and a pressure-outlet. File names in **bold**.

fluent_bc.in

Tot. Pres. Temp.
 Stat. Pres. Temp.

fluent_cntrl.in

0 3 0.5 h(P, T = 298.15 K)

fluent.in (Fluent read in case and data files, and configure)

```
rc fluent.cas
rd fluent.dat
(load 'fluent_scheme.scm)
Define/user-defined/execute-on-demand "pvm_init"
report/surface-avg 3 4 () pressure
report/surface-avg 3 4 () temperature
solve/set/timestep timestep size
solve/dual-time-iterate 10 1000
report/surface-avg 3 4 () pressure
report/surface-avg 3 4 () temperature
exit
```

```
executive.i (Executive program input file)
```

virtual

computational node wd=/working directory path ep=/executables directory path

processes

computational node primary synchronous relap5.x -i relap.i -o relap.p -r relap.r primary writes relap.out core synchronous fluent startup path -g -i fluent.in core writes fluent.out

messages

semi-implicit

primary sends core *alphanumeric name of the RELAP volume to be coupled to Fluent* **RELAP volume number** *alphanumeric name of the RELAP volume to be coupled to Fluent* **RELAP volume number**

primary awaits core *amount of time RELAP will wait for information to be* sent from Fluent

primary receives core *alphanumeric name of the RELAP single junction to be coupled to Fluent* 0 *alphanumeric name of the RELAP single junction to be coupled to Fluent* 0 core sends primary zone *Fluent boundary condition zone id number to be coupled* zone *Fluent boundary condition zone id number to be coupled*

core awaits primary *amount of time Fluent will wait for information to be* sent from RELAP

core receives primary zone *Fluent boundary condition zone id number to be coupled* zone *Fluent boundary condition zone id number to be coupled*

timesteps

end time *minimum time step* maximum time step *control option* minor edit and time frequency *major edit frequency* restart frequency 0

APPENDIX B

THE COUPLED BOUNDARIES COMPARISON PLOTS*

Pressures



Static Pressure in Channel 1

Fig. B1. The static pressure in channel 1.





Fig. B2. The static pressure in channel 2.

Static Pressure in Channel 3



Fig. B3. The static pressure in channel 3.

Static Pressure in Channel 4



Fig. B4. The static pressure in channel 4.

Static Pressure in Channel 5



Fig. B5. The static pressure in channel 5.





Fig. B6. The static pressure in channel 6.

Static Pressure in Channel 7



Fig. B7. The static pressure in channel 7.



Static Pressure in Channel 8

Fig. B8. The static pressure in channel 8.

Static Pressure in Channel 9



Fig. B9. The static pressure in channel 9.





Fig. B10. The static pressure in channel 10.

Static Pressure in Channel 11



Fig. B11. The static pressure in channel 11.

Mass Flow Rate



Mass Flow Rate in Channel 1

Fig. B12. The mass flow rate in channel 1.

Mass Flow Rate in Channel 2



Fig. B13. The mass flow rate in channel 2.



Fig. B14. The mass flow rate in channel 3.

Mass Flow Rate in Channel 4



Fig. B15. The mass flow rate in channel 4.





Fig. B16. The mass flow rate in channel 5.

Mass Flow Rate in Channel 6



Fig. B17. The mass flow rate in channel 6.

Mass Flow Rate in Channel 7



Fig. B18. The mass flow rate in channel 7.

Mass Flow Rate in Channel 8



Fig. B19. The mass flow rate in channel 8.




Fig. B20. The mass flow rate in channel 9.

Mass Flow Rate in Channel 10



Fig. B21. The mass flow rate in channel 10.



Mass Flow Rate in Channel 11

Fig. B22. The mass flow rate in channel 11.



Temperature in Channel 1



Fig. B23. The helium temperature in channel 1.



Fig. B24. The helium temperature in channel 2.

Temperature in Channel 3



Fig. B25. The helium temperature in channel 3.





Fig. B26. The helium temperature in channel 4.

Temperature in Channel 5



Fig. B27. The helium temperature in channel 5.





Fig. B28. The helium temperature in channel 6.

Temperature in Channel 7



Fig. B29. The helium temperature in channel 7.





Fig. B30. The helium temperature in channel 8.

Temperature in Channel 9



Fig. B31. The helium temperature in channel 9.



Fig. B32. The helium temperature in channel 10.

Temperature in Channel 11



Fig. B33. The helium temperature in channel 11.

VITA

Nolan Alan Anderson received his Associate of Science degree from Pima Community College in 2000 and his Bachelor of Science degree in mechanical engineering from Brigham Young University in 2003. He is currently performing research at the Idaho National Lab in Idaho Falls, ID. Future contact can be made by email at nolan.anderson@gmail.com or by mail forwarded through the Department of Nuclear Engineering, c/o Dr. Yassin Hassan, Texas A&M University, College Station, TX 77843-3133.