

A GENERIC SEMI-IMPLICIT COUPLING METHODOLOGY FOR USE IN RELAP5-3D®

W. L. Weaver
INEEL

E. T. Tomlinson
D. L. Aumiller
Bettis

DE-AC11-98PN38206

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States, nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

BETTIS ATOMIC POWER LABORATORY

WEST MIFFLIN, PENNSYLVANIA 15122-0079

Operated for the U.S. Department of Energy
by Bechtel Bettis, Inc.

A GENERIC SEMI-IMPLICIT COUPLING METHODOLOGY
FOR USE IN RELAP5-3D

W. L. Weaver, E. T. Tomlinson and D. L. Aumiller

USDOE Contract No. DE-AC11-98PN38206

RECEIVED
JAN 11 2001
OSTI

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States, nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

BETTIS ATOMIC POWER LABORATORY

WEST MIFFLIN, PENNSYLVANIA 15122-0079

Operated for the U.S. Department of Energy
by Bechtel Bettis, Inc.

A Generic Semi-Implicit Coupling Methodology For Use In RELAP5-3D[®]

W. L. Weaver

Bechtel BWXT Idaho, LLC
Idaho National Engineering and Environmental Laboratory
P.O. Box 1625
2525 North Fremont Ave.
Idaho Falls, ID 83415

E. T. Tomlinson and D. L. Aumiller

Bechtel Bettis, Inc.
Bettis Atomic Power Laboratory
P.O. Box 79
West Mifflin, PA 15122-0079

Abstract

A generic semi-implicit coupling methodology has been developed and implemented in the RELAP5-3D[®] computer program. This methodology allows RELAP5-3D[®] to be used with other computer programs to perform integrated analyses of nuclear power reactor systems and related experimental facilities. The coupling methodology potentially allows different programs to be used to model different portions of the system. The programs are chosen based on their capability to model the phenomena that are important in the simulation in the various portions of the system being considered. The methodology was demonstrated using a test case in which the test geometry was divided into two parts each of which was solved as a RELAP5-3D[®] simulation. This test problem exercised all of the semi-implicit coupling features which were installed in RELAP5-3D[®]. The results of this verification test case show that the semi-implicit coupling methodology produces the same answer as the simulation of the test system as a single process.

1. Background

Computer programs have been developed to predict transient two-phase phenomena that are important for nuclear reactor safety assessments. Each of these programs, or family of programs, was developed to model particular aspects of the transient

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, make any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

**Portions of this document may be illegible
in electronic image products. Images are
produced from the best available original
document.**

with varying degrees of detail. System codes such as RELAP5-3D^{© 1} and TRAC-PF1/MOD1² are typically used to model the entire reactor plant including a coarsely noded model of the thermally limiting core locations. These system codes also have models for the major plant components, such as pumps, valves, accumulators and so forth.

The COBRA³ series of programs was developed for the detailed analysis of boiling in rod bundles. The COBRA programs use a three-field representation of two-phase flow, modelling the liquid film and droplets separately. Furthermore, the noding used in COBRA analyses is typically finer than is used in the system codes. A new class of thermal hydraulic programs is currently under development. These programs use extremely detailed models of two-phase flow and can be characterized as Computational Fluid Dynamics (CFD) type programs⁴. These CFD programs use a multi-field model of two-phase flow and explicitly includes turbulence models in the hydrodynamic solution. Currently, these programs are not appropriate for the analysis of an entire reactor system due to the prohibitive computational cost of the analysis. As a result, these detailed programs (COBRA and CFD) can only be used to analyze a portion of the reactor system and must be coupled to a system code, such as RELAP5-3D[©], to perform an integrated analysis of the entire system.

At the other end of the spectrum, the CONTAIN⁵ series of programs has been developed for the thermal-hydraulic analysis of containment systems. These programs usually are lumped parameter or empirical in nature and use a coarser noding to model expansive volumes.

Traditionally, the feedback effects among different programs have been approximated with user supplied boundary conditions. This process is cumbersome and may not fully capture the interdependence of the different phenomena. An example is the use of a containment program to calculate the back pressure required for a Loss-of-Coolant-Accident. In turn, the containment programs require the mass and energy flows calculated by the system code to determine the containment pressure response. Therefore, an iterative process is required to determine a consistent set of boundary conditions for each of the programs. A better methodology is to use an integrated code system which implicitly calculates the feedback effects among the constitutive programs.

The creation of these integrated systems has been performed previously using two separate paradigms. The first model integrates the solution matrices of the constitutive programs to provide a numerically stable solution. All of the implementations of this technique have used semi-implicit numerics. Previous implementations of this paradigm, COBRA/TRAC⁶ and COBRA/RELAP5⁷, have been very specific to their particular application and, therefore, are not amenable to direct extension to other programs. Another disadvantage of the COBRA/TRAC implementation is that once the source codes for TRAC-PD2 and COBRA were merged, it was impossible for the COBRA/TRAC program to stay current with the ongoing development of the TRAC and COBRA program series.

The second coupling paradigm allows a generic coupling of different programs. Previous implementations of this paradigm have all used explicit numerics which are less numerically stable than the numerics of the constitutive programs. In this methodology, boundary condition data are passed among the constitutive programs at the end of each time step. RELAP5 has been successfully coupled to both the CONTAIN⁸ and a CFD⁹ program using this technique. Both of these coupling efforts have used the PVM¹⁰ message passing software.

This paper discusses the development, implementation and testing of a coupling technique that provides the flexibility of the generic coupling paradigm and the numerical stability of the semi-implicit numerics. The following sections describe the stability implications of the coupling numerics as well as provide details of the implementation of this methodology in the RELAP5-3D[®] computer program.

2. Stability Considerations for Coupling Hydrodynamic Solutions

This section will discuss how the choice of a coupling technique can affect the numerical stability of the integrated code system. There are several criteria that need to be considered in the development of a hydrodynamic coupling paradigm. The most important criterion is that the methodology must conserve mass and energy. A desirable feature of the coupling algorithm is that the coupled code system should not be characterized by more restrictive stability limits than any of its constitutive programs.

At this point a brief description of time differencing schemes used in hydrodynamic computer programs and their associated stability limits is appropriate. The least stable method (i.e. requiring the smallest timestep size to achieve a stable solution) is referred to as fully explicit. In this technique, the only new time parameters that appear in the discretized equations are in the representation of the temporal derivative. Since sonic phenomena (i.e. pressure wave propagation and resultant velocities) are not treated implicitly in the spatial terms, this technique limits the timestep size to the sonic Courant limit. Application of fully explicit numerics results in impractical execution times for realistic problems due to this timestep restriction and none of the current two-phase safety programs employ this technique.

Two less restrictive numerical techniques which are currently used in safety programs are the semi-implicit¹¹ technique and variants of the SETS¹² method. The semi-implicit technique implicitly treats sonic phenomena such that the material Courant limit, and not the sonic Courant limit, is applicable for determining the maximum stable timestep size. In this technique, the convection terms are differenced using implicit velocities but explicit convected quantities such as void fraction and density. The SETS method is a two-step technique that uses the basic semi-implicit equation set with the addition of a stabilizing set of equations. The stabilizing equations propagate information concerning convected quantities such that the material Courant limit can be exceeded without introducing numerical

instabilities. One important characteristic of both the semi-implicit and SETS techniques is that the spatial coupling only involves one independent parameter.

Several programs have made use of fully implicit techniques. In this technique, the only old time parameters that appear in the discretized equations are in the representation of the temporal derivative. Like the SETS technique, the fully implicit method is not restricted by the material Courant limit. The primary disadvantage of the fully implicit technique is that the use of implicit convected quantities results in simultaneous spatial coupling of all independent variables.

The basis of any coupling methodology is that the problem is divided into multiple domains where each domain can be simulated by a different computer program, or by a different "instance" of any of the programs. Figure 1 shows a schematic of a simulation problem in which there are two connections between the two problem domains. In Figure 1, volume 1 is adjacent to and connected to volume I, and volume 2 is adjacent to and connected to volume II. The boundary volumes in one of the domains (i.e. 1 and 2) represent normal volumes in the interior of the other computational domain (i.e. I and II). Information about these volumes must be passed between the domains at the coupling boundary to achieve an integrated solution. Coupling methodologies for passing this information between programs can be developed based on any of the above numerical methods.

A schematic of a fully explicit coupling methodology is shown in Figure 2. The dashed arrows in Figure 2 indicate data flow between the domains. In this coupling methodology, pressures in the boundary volumes are held constant during each time step and are updated at the end of the time step. The constant boundary pressures cause the stability of the coupled systems to be limited by the sonic Courant condition. As proof of this restriction, an analysis using fully explicit coupling without regard to the sonic Courant limit was performed⁹ and, as expected, numerical oscillations were observed. This restriction makes fully explicit coupling impractical.

Neither SETS nor fully implicit based coupling techniques were considered because of problems associated with conservation of mass and energy. Neither the SETS nor fully implicit based coupling methodologies convect old-time quantities (i.e. density or energy). Therefore, to conserve mass and energy, intra-timestep iteration between the constitutive programs would be required to update convected quantities.

With the elimination of explicit, fully implicit and SETS based coupling algorithms, semi-implicit numerics were chosen for this application. There are two requirements for a successful implementation of a semi-implicit coupling algorithm. First, the semi-implicit methodology requires use of consistent, new-time velocities and pressures. Therefore, new-time velocities at the coupling junctions must depend on new-time pressures on each side of the coupling junction. Second, to conserve mass and energy, each program must convect the same quantities across the boundary. The next section describes the manner in which these requirements have been satisfied in the current work.

3. Description of Semi-Implicit Coupling Methodology

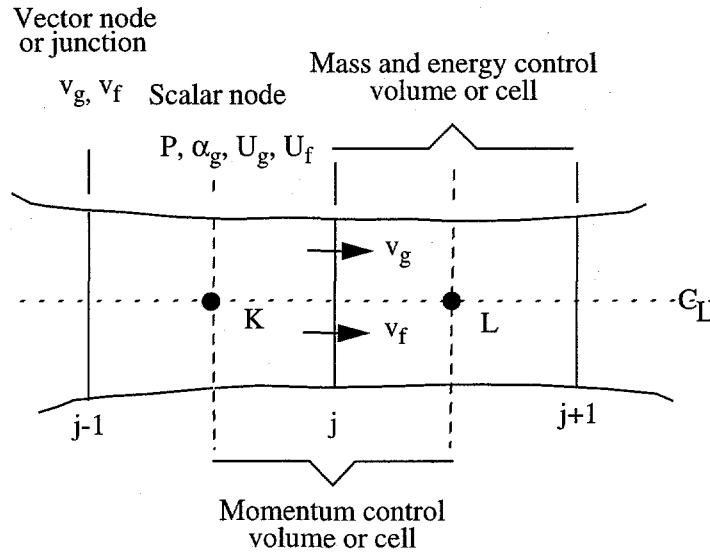
A master/slave approach is taken to meet both of the aforementioned requirements: consistent new-time velocities and conservation of mass and energy. Using this approach, both the master and slave processes have specific roles to ensure that all required information is provided. These roles are discussed in the next two subsections. When coupling multiple programs, RELAP5-3D[®] is most likely to be the master since it is a system code, while single component programs (i.e. CONTAIN and COBRA) are most likely to be slaves. In the work described in this paper, RELAP5-3D[®] can be used as the master process, the slave process or both.

The semi-implicit coupling algorithm is shown schematically in Figure 3. (Boundary volumes are needed in RELAP5-3D[®] only to satisfy the geometric constraints for input decks.) Dashed arrows in Figure 3 indicate data exchanges between master and slave processes. To satisfy the requirement of consistent new-time velocities and pressures, the changes in the pressures for all volumes in the master computational domain are represented as linear functions of the mass and energy flow rates in the coupling junctions. The coefficients in these linear relations are transmitted to the slave process for the coupling volumes in the master process. Using these coefficients, the slave process can simultaneously calculate the mass and energy flow rates across the coupling location and the change in the pressure of the coupled volume in the master process. These mass and energy flow rates are then transmitted back to the master process where they are used to compute the changes in pressure in a manner consistent with the slave process. In the current work, information is exchanged between the programs using the Parallel Virtual Machine (PVM) software¹⁰. PVM was chosen because of the authors' familiarity with its use, however, other equivalent message passing software could be substituted.

The approach described in this paper differs from a previous semi-implicit coupling of RELAP5/MOD3 to COBRA⁷. In that work the pressure gradient across the coupling junctions was used as the primary mechanism for implicitly transferring information between the programs. In that previous methodology, the momentum equations for the coupling junctions were solved by RELAP5/MOD3 (which is equivalent to the master process), whereas in the methodology described here, the momentum equations in the coupling junctions are solved by the slave process. This facilitates the coupling of RELAP5-3D[®] to slave processes that have more fluids and/or fields (e.g., COBRA has two liquid fields and CFD type can have multiple liquid and vapor fields). This methodology also facilitates having a finer nodalization in the slave process than in the master process. In this methodology, the master process only needs to know the total flow rates at the coupling location, not the finer details associated with the coupling location as calculated by the slave process. This reduces the amount of data that needs to be exchanged between the programs.

3.1 Implementation of Semi-Implicit Coupling for RELAP5-3D[©] as the Master Process

The description of the semi-implicit coupling algorithm begins with the derivation of the pressure equation for a single RELAP5-3D[©] computational volume. The schematic below is a representation of the staggered grid used in the RELAP5 family of programs.



The full set conservation equations for volume L may be written in matrix form as

$$\mathbf{A}\mathbf{x} = \mathbf{b} + g^1 v_{g,j+1}^{n+1} + g^2 v_{g,j}^{n+1} + f^1 v_{f,j+1}^{n+1} + f^2 v_{f,j}^{n+1} \quad (1)$$

where the matrix \mathbf{A} is a 5x5 matrix and the vectors on the right hand side each have five elements. Each row of matrix \mathbf{A} represents one of the volume conservation equations. In order, these conservation equations are: non-condensable gas mass, vapor energy, liquid energy, vapor mass and liquid mass. Definitions of the matrix elements can be found in Section 3.1 of Volume I of the RELAP5-3D[©] manual¹. Equation (1) assumes that there are two junctions attached to the volume. Multiplying both sides of this equation by the inverse of matrix \mathbf{A} , the last row of the resulting matrix equation becomes the pressure equation given by

$$\delta P^{n+1} = A_5^{-1} (b + g^1 v_{g,j+1}^{n+1} + g^2 v_{g,j}^{n+1} + f^1 v_{f,j+1}^{n+1} + f^2 v_{f,j}^{n+1}) \quad (2)$$

where δP^{n+1} is $(P^{n+1} - P^n)$ and A_5^{-1} represents the fifth row of the inverse of matrix \mathbf{A} . The pressure equations for each volume in the computational domain are assembled into a system matrix describing the change in the pressure in each volume in terms of the velocities in the junctions between the volumes. The velocities in each junction are then expressed in terms of the changes in the pressures in the volumes at either end of the junction using the momentum equations for the junctions as

$$v_{g,j}^{n+1} = \tilde{v}_{g,j}^n + \frac{dv_g}{d\Delta P} \Big|_j^n (\delta P_{K,j}^{n+1} - \delta P_{L,j}^{n+1}) \quad (3)$$

and

$$v_{f,j}^{n+1} = \tilde{v}_{f,j}^n + \frac{dv_f}{d\Delta P} \Big|_j^n (\delta P_{K,j}^{n+1} - \delta P_{L,j}^{n+1}). \quad (4)$$

These velocity equations are substituted in the right hand sides of the pressure equations [Equation (2)], and the unknown pressure changes are moved from the right hand side to the left hand side of the equations. The resulting matrix equation can then be solved for the changes in the pressures in the volumes in the system.

The semi-implicit coupling methodology modifies this procedure for the junctions representing the connections between the two systems. Suppose junction $j+1$ in Equation (2) represents a junction between a volume in the RELAP5-3D[®] computational domain and a slave process. The pressure equation for the volume in the RELAP5-3D[®] computational domain is modified by expressing the product of the g and f vectors and the vapor and liquid velocities in the coupling junction as

$$\frac{\Delta t^{n+1}}{V} \begin{bmatrix} a_{g,j+1}^{n+1} \\ u_{g,j+1}^{n+1} + P^n w_{g,j+1}^{n+1} \\ u_{f,j+1}^{n+1} + P^n w_{f,j+1}^{n+1} \\ m_{f,j+1}^{n+1} - m_{g,j+1}^{n+1} \\ m_{f,j+1}^{n+1} + m_{g,j+1}^{n+1} \end{bmatrix} \quad \text{where:} \quad (5)$$

$a_{g,j+1}^{n+1}$ = flow rate of non-condensable gas in junction $j+1$ (kg/s),

$u_{g,j+1}^{n+1}$ = flow rate of vapor internal energy in junction $j+1$ (J/s),

$w_{g,j+1}^{n+1}$ = volumetric flow rate of vapor in junction $j+1$ (m³/s),

$u_{f,n+1}^{n+1}$ = flow rate of liquid internal energy in junction $j+1$ (J/s),

$w_{f,j+1}^{n+1}$ = volumetric flow rate of liquid in junction $j+1$ (m³/s),

$m_{g,j+1}^{n+1}$ = mass flow rate of vapor in junction $j+1$ (kg/s), and

$m_{f,j+1}^{n+1}$ = mass flow rate of liquid in junction $j+1$ (kg/s).

Using Equation (5) for each coupling junction, the right hand side of the system matrix can be written in terms of the flow rates in the coupling junctions. The changes in the pressures in all of the volumes in the computational domain can then be

computed in terms of the flow rates in the coupling junctions as

$$\begin{aligned} \delta P_k^{n+1} = & a_k + \sum_{j=1}^{N_c} b_{k,j} a_{g,j}^{n+1} + \sum_{j=1}^{N_c} c_{k,j} u_{g,j}^{n+1} + \sum_{j=1}^{N_c} d_{k,j} u_{f,j}^{n+1} + \sum_{j=1}^{N_c} e_{k,j} m_{g,j}^{n+1} \\ & \sum_{j=1}^{N_c} f_{k,j} m_{f,j}^{n+1} + \sum_{j=1}^{N_c} g_{k,j} w_{g,j}^{n+1} + \sum_{j=1}^{N_c} h_{k,j} w_{f,j}^{n+1} \end{aligned} \quad (6)$$

where $k = 1, 2, \dots, N_v$, N_v is the number of volumes in the solution domain, and N_c is the number of coupling junctions. The coefficients a through h for the volumes in the RELAP5-3D[®] computational domain attached to the coupling junctions (volumes 1 and 2 in Figure 3) are then transmitted to the slave process. The slave process can then use coefficients a through h to calculate the interdependence of pressure and flow rates consistent with RELAP5-3D[®] solution strategy. This consistency is the key to the semi-implicit coupling methodology. When the mass, energy and volume flow rates in the coupling junctions have been received from the slave process, Equation (6) can be evaluated for the change in the pressure in each volume in the RELAP5-3D[®] system. Once the changes in the pressures in the volumes have been computed, the time advancement may be completed in the normal manner.

3.2 Implementation of Semi-Implicit Coupling for RELAP5-3D[®] as a Slave Process

In RELAP5-3D[®] as a slave process, the coupling boundary volume is represented by a special type of single volume component. In a slave process using the semi-implicit coupling methodology, the pressure equation for each coupling boundary volume has the form of Equation (6). The flow rates in these equations can be written in terms of the known donor properties in the coupling junctions and the unknown phasic velocities in the junctions as

$$\begin{aligned} \delta P_{cbv}^{n+1} = & a_{cbv} + \sum_{j=1}^{N_c} b_{cbv,j} (\dot{\alpha}_g^n \dot{\rho}_g^n \dot{X}_n^n) j \Delta t^{n+1} A_j v_{g,j}^{n+1} + \\ & \sum_{j=1}^{N_c} c_{cbv,j} (\dot{\alpha}_g^n \dot{\rho}_g^n \dot{U}_g^n) j \Delta t^{n+1} A_j v_{g,j}^{n+1} + \sum_{j=1}^{N_c} d_{cbv,j} (\dot{\alpha}_f^n \dot{\rho}_f^n \dot{U}_f^n) j \Delta t^{n+1} A_j v_{f,j}^{n+1} + \\ & \sum_{j=1}^{N_c} e_{cbv,j} (\dot{\alpha}_g^n \dot{\rho}_g^n) j \Delta t^{n+1} A_j v_{g,j}^{n+1} + \sum_{j=1}^{N_c} f_{cbv,j} (\dot{\alpha}_f^n \dot{\rho}_f^n) j \Delta t^{n+1} A_j v_{f,j}^{n+1} + \\ & \sum_{j=1}^{N_c} g_{cbv,j} (\dot{\alpha}_g^n) j \Delta t^{n+1} A_j v_{g,j}^{n+1} + \sum_{j=1}^{N_c} h_{cbv,j} (\dot{\alpha}_f^n) j \Delta t^{n+1} A_j v_{f,j}^{n+1} \end{aligned} \quad (7)$$

The velocities in the coupling junctions are expanded in the form of Equation (3) and Equation (4) to give

$$\begin{aligned}
 \delta P_{cbv}^{n+1} = & a_{cbv} + \sum_{j=1}^{N_c} b_{cbv,j} (\dot{\alpha}_g^n \dot{\rho}_g^n \dot{X}_n)_j \Delta t^{n+1} A_j \left[\tilde{v}_{g,j}^n + \frac{dv_g}{d\Delta P} \right]_j^n (\delta P_{K,j}^{n+1} - \delta P_{L,j}^{n+1}) + \\
 & \sum_{j=1}^{N_c} c_{cbv,j} (\dot{\alpha}_g^n \dot{\rho}_g^n \dot{U}_g)_j \Delta t^{n+1} A_j \left[\tilde{v}_{g,j}^n + \frac{dv_g}{d\Delta P} \right]_j^n (\delta P_{K,j}^{n+1} - \delta P_{L,j}^{n+1}) + \\
 & \sum_{j=1}^{N_c} d_{cbv,j} (\dot{\alpha}_f^n \dot{\rho}_f^n \dot{U}_f)_j \Delta t^{n+1} A_j \left[\tilde{v}_{f,j}^n + \frac{dv_f}{d\Delta P} \right]_j^n (\delta P_{K,j}^{n+1} - \delta P_{L,j}^{n+1}) + \\
 & \sum_{j=1}^{N_c} e_{cbv,j} (\dot{\alpha}_f^n \dot{\rho}_f^n)_j \Delta t^{n+1} A_j \left[\tilde{v}_{g,j}^n + \frac{dv_g}{d\Delta P} \right]_j^n (\delta P_{K,j}^{n+1} - \delta P_{L,j}^{n+1}) + \\
 & \sum_{j=1}^{N_c} f_{cbv,j} (\dot{\alpha}_f^n \dot{\rho}_f^n)_j \Delta t^{n+1} A_j \left[\tilde{v}_{f,j}^n + \frac{dv_f}{d\Delta P} \right]_j^n (\delta P_{K,j}^{n+1} - \delta P_{L,j}^{n+1}) + \\
 & \sum_{j=1}^{N_c} g_{cbv,j} (\dot{\alpha}_g^n)_j \Delta t^{n+1} A_j \left[\tilde{v}_{g,j}^n + \frac{dv_g}{d\Delta P} \right]_j^n (\delta P_{K,j}^{n+1} - \delta P_{L,j}^{n+1}) + \\
 & \sum_{j=1}^{N_c} h_{cbv,j} (\dot{\alpha}_f^n)_j \Delta t^{n+1} A_j \left[\tilde{v}_{f,j}^n + \frac{dv_f}{d\Delta P} \right]_j^n (\delta P_{K,j}^{n+1} - \delta P_{L,j}^{n+1})
 \end{aligned} \tag{8}$$

The terms are then collected to give

$$\delta P_{cbv}^{n+1} = A_{cbv} + \sum_{j=1}^{N_c} B_{cbv,j} (\delta P_{K,j}^{n+1} - \delta P_{L,j}^{n+1}) \tag{9}$$

where

$$\begin{aligned}
 A_{cbv} = & a_{cbv} + \sum_{j=1}^{N_c} b_{cbv,j} (\dot{\alpha}_g^n \dot{\rho}_g^n \dot{X}_n^n)_j \Delta t^{n+1} A_j \tilde{v}_{g,j}^n + \\
 & \sum_{j=1}^{N_c} c_{cbv,j} (\dot{\alpha}_g^n \dot{\rho}_g^n \dot{u}_g^n)_j \Delta t^{n+1} A_j \tilde{v}_{g,j}^n + \sum_{j=1}^{N_c} d_{cbv,j} (\dot{\alpha}_f^n \dot{\rho}_f^n \dot{u}_f^n)_j \Delta t^{n+1} A_j \tilde{v}_{f,j}^n + \\
 & \sum_{j=1}^{N_c} e_{cbv,j} (\dot{\alpha}_g^n \dot{\rho}_g^n)_j \Delta t^{n+1} A_j \tilde{v}_{g,j}^n + \sum_{j=1}^{N_c} f_{cbv,j} (\dot{\alpha}_f^n \dot{\rho}_f^n)_j \Delta t^{n+1} A_j \tilde{v}_{f,j}^n + \\
 & \sum_{j=1}^{N_c} g_{cbv,j} (\dot{\alpha}_g^n)_j \Delta t^{n+1} A_j \tilde{v}_{g,j}^n + \sum_{j=1}^{N_c} h_{cbv,j} (\dot{\alpha}_f^n)_j \Delta t^{n+1} A_j \tilde{v}_{f,j}^n
 \end{aligned} \tag{10}$$

and

$$\begin{aligned}
 B_{cbv,j} = & b_{cbv,j} (\dot{\alpha}_g^n \dot{\rho}_g^n \dot{X}_n^n)_j \Delta t^{n+1} A_j \frac{dv_g}{d\Delta P} \Big|_j^n + c_{cbv,j} (\dot{\alpha}_g^n \dot{\rho}_g^n \dot{U}_g^n)_j \Delta t^{n+1} A_j \frac{dv_g}{d\Delta P} \Big|_j^n + \\
 & d_{cbv,j} (\dot{\alpha}_f^n \dot{\rho}_f^n \dot{U}_f^n)_j \Delta t^{n+1} A_j \frac{dv_f}{d\Delta P} \Big|_j^n + e_{cbv,j} (\dot{\alpha}_g^n \dot{\rho}_g^n)_j \Delta t^{n+1} A_j \frac{dv_g}{d\Delta P} \Big|_j^n + \\
 & f_{cbv,j} (\dot{\alpha}_f^n \dot{\rho}_f^n)_j \Delta t^{n+1} A_j \frac{dv_f}{d\Delta P} \Big|_j^n + g_{cbtdv,j} (\dot{\alpha}_g^n)_j \Delta t^{n+1} A_j \frac{dv_g}{d\Delta P} \Big|_j^n + \\
 & h_{cbv,j} (\dot{\alpha}_f^n)_j \Delta t^{n+1} A_j \frac{dv_f}{d\Delta P} \Big|_j^n
 \end{aligned} \tag{11}$$

Equation (9) defines new matrix elements that must be added to the rows of the pressure matrix representing the coupling boundary volumes in the slave process. Once the extra matrix elements have been added to the pressure matrix, the changes in the pressures in the volumes in the slave process can be computed along with the velocities in the junctions. The mass flow rates in the coupling junction can then be computed and sent to the master process completing the semi-implicit computational cycle.

In addition to passing the hydrodynamic quantities described above, the surface temperature of any heat structure attached to a coupled volume in the slave process is required for the calculation of the wall viscosity effects (e.g., Sieder-Tate drag correlation). To account for this effect, a heat structure is attached to the volume in the slave process and its surface temperature is provided by the master process. Since the conduction solution for the heat structure in the coupling volume has already been performed in the master process, it is bypassed in the slave process.

4. Restrictions and Assumptions

The following list describes the current restrictions and assumptions used in the implementation of the semi-implicit coupling:

- RELAP5-3D[©] may be coupled to only one instance of any program.
- At present, each of the constitutive programs must use the same time steps. A code backup cannot be handled so that velocity flip/flop and water packing logic are disabled in RELAP5-3D[©] in a coupled run.
- Multiple coupling junctions may not be connected to any single volume.
- The equation of state (EOS) model for water and steam in the coupled program will most likely be different than the steam table methodology in RELAP5-3D[©]. With this in mind, the coupling variables were chosen to conserve mass and energy. The effect of the different EOS methodologies is that saturated fluid leaving one solution domain may appear in the other solution domain as either subcooled or superheated fluid having a different temperature in the receiving domain from its temperature in the sending domain.

5. Verification Testing of Semi-Implicit Coupling Algorithm

A single test case was developed to verify the implementation of the semi-implicit coupling algorithm. This test case uses RELAP5-3D[©] as the master process coupled to RELAP5-3D[©] as the slave process. There are two versions of the test case. In the first version of the test case the entire system is simulated as a single process without the use of the semi-implicit coupling. The second version of the test case divides the test system into two parts which are simulated as a coupled problem using the semi-implicit coupling methodology. Figure 4 and Figure 5 are schematics of the single process problem and coupled problem, respectively.

The test case is based on Run 15 of the Christensen sub-cooled boiling experiments¹⁴. The model was modified to include a parallel flow path for purposes of testing the coupling methodology and used hydraulic resistances to remove the characteristic oscillations. The test section is modelled by a single heated pipe component and the bypass is modelled by an unheated pipe component. The two parallel flow paths are connected to common single volumes at the top and bottom of the test section. These volumes are in turn connected to time dependent volumes. These time dependent volumes impose a pressure gradient on the system. To provide a transient problem, the pressure linearly increases between 0 and 2 seconds and the problem is unheated for the first 5 seconds and then the power is linearly increased to its maximum value at 10 seconds. This system is simulated by RELAP5-3D[©] as a single system to provide a baseline for comparison with the coupled simulation.

The coupled simulation is constructed from two input decks. The first input deck contains the upper and lower common volumes, the time dependent volumes, the bypass channel and the upper and lower portions of the test section. The center ten volumes of the test section were removed and moved to the second input deck along with the heat structures attached to these volumes. Coupling volumes and coupling junctions were added to each input deck as appropriate. Dotted lines in the schematic of the coupled problem, Figure 5, indicate data exchanges between the coupling volumes and coupling junctions in the two instances of RELAP5-3D[®]. Boundary volumes in the master system are shown with dotted outlines because they do not contribute boundary conditions to the solution but are required by the input checker in RELAP5-3D[®].

Both the coupled and stand alone calculations require 4880 timesteps for the 60 second transient. Typical results from the two simulations are shown in Figure 6 through Figure 8. Figure 6 shows the flow rates in the upper coupling junction (single junction 115 in Figure 5). The corresponding junction in the uncoupled simulation is pipe junction 115. The solid line is the result from the uncoupled solution, and the circles represent the results from the slave process of the coupled solution (every 250th point is plotted). The pressures in the lower coupling volume are shown in Figure 7. As in the previous figure, the solid line represents the results from the simulation as a single process, and the circles represent the results of the slave process of the coupled simulation. Excellent agreement between the results of the simulation as a single process and the simulation as a coupled process is shown in these two figures.

Figure 8 shows the inner surface temperatures for the heat structure connected to the lower coupling volume. This temperature is computed in the master process and sent to the slave process. The temperature is plotted for the slave process. The agreement between the two simulations shows that the correct temperature is being computed by the master process and that it is being transferred to the slave process correctly. Figure 8 also shows the centerline temperature of the heat structure connected to the lower coupling volume. This temperature is computed by the master process but is not transferred to the slave process. The figure shows that the outer surface temperature in the slave process remains at its initial value. Since the heat conduction solution is not computed for heat structures connected to coupling volumes in the slave process, the figure shows the expected result. It verifies that the heat conduction solution is bypassed for heat structures connected to coupling volumes in the slave process as designed.

The previous figures present a qualitative assessment of the coupling algorithm; a quantitative assessment was performed. Figure 9 presents the relative errors for the same mass flow and pressure predictions at the same locations as in Figure 6 and Figure 7. This figure shows that relative error is almost accurate to machine precision for the first several timesteps, and the error slowly increases with number of timesteps and reaches an acceptable steady value. It should be noted that exact agreement between the two solutions is not expected because of roundoff error in the inversion of the system matrices. The system matrices are of different sizes in the

two solutions where the single process solves the system as a single large matrix and the coupled solution solves two solution matrices of smaller sizes. Similar agreement between the results of the simulation as a single process and as a coupled process can be shown for conditions in all of the volumes and junctions in the test system.

The results shown in this section show that the methodology has been correctly implemented in RELAP5-3D[®]. This test exercised all of the options described in this paper including: use of RELAP5-3D[®] as the master process, use of RELAP5-3D[®] as the slave process, and the correct wall viscosity effects for coupling volumes that have associated heat structures.

6. Summary

The paper describes the development, implementation and testing of a generic, semi-implicit coupling methodology for use with RELAP5-3D[®]. This methodology permits coupling of the hydrodynamic solution of various computer programs in a manner that conserves mass and energy and is also numerically stable subject to the material Courant limit. The feasibility of this methodology was demonstrated by performing a calculation where RELAP5-3D[®] was coupled to itself. This problem demonstrated that RELAP5-3D[®] can be executed as either a master or slave process.

References

- 1 RELAP5-3D Code Manuals, Volumes I, II, IV, and V," Idaho National Engineering and Environmental Laboratory, INEEL-EXT-98-00834, Revision 1.1b, 1999.
- 2 "TRAC-PF1/MOD1: An Advanced Best-Estimate Computer Program for Pressurized Water Reactor Thermal-Hydraulic Analysis," LA-10157-MS, NUREG/CR-3858, Los Alamos National Laboratory, 1986.
- 3 "Analysis of FLECHT SEASET 163-Rod Blocked Bundle Data Using COBRA-TF," NUREG/CR-4166. U. S. Nuclear Regulatory Commission, 1985.
- 4 J. Zhou and M. Z. Podowski," Modeling and Analysis of Hydrodynamic Instabilities in Two-Phase Flow using a Two-Fluid Model," Proceedings of the 1999 NURETH Conference (available from American Nuclear Society), San Francisco, 1999.
- 5 K. K. Murata et al., "User's Manual for CONTAIN 1.1, A Computer Code for Severe Nuclear Reactor Accident Containment Analysis," NUREG/CR-5026 (SAND-87-2309), 1989.
- 6 M. J. Thurgood et al., "COBRA/TRAC - A Thermal Hydraulics Code for Transient Analysis of Nuclear Reactor Vessels and Primary Coolant Systems," NUREG/CR-3046 (Vol. 2), U. S. Nuclear Regulatory Commission, 1983.

- 7 S. Y. Lee et al., "COBRA/RELAP5: A Merger Version of the COBRA-TF and RELAP5/MOD3 Codes," Nuclear Technology, Vol 99, pp. 177-187, 1992.
- 8 R. P. Martin, "RELAP5/MOD3 Code Coupling Model," Nuclear Safety, Vol. 36, No. 2, pp. 290-299, 1995.
- 9 D. L. Aumiller, E. T. Tomlinson and R. C. Bauer, "A Coupled RELAP5-3D/CFD Methodology with Proof-of-Principle Calculation," available as B-T-3268 from DOE Office of Scientific and Technical Information, 2000.
- 10 A. Geist et. al., "PVM (Parallel Virtual Machine) User's Guide and Reference Manual," Oak Ridge National Laboratory, ORNL/TM-12187, 1993.
- 11 D. R. Liles and W. H. Reed, "A Semi-Implicit Method for Two-Phase Fluid Dynamics," Journal of Computational Physics, Vol 26, pp. 390-407, 1978.
- 12 J. H. Mahaffy, "A Stability-Enhancing Two-Step Method for Fluid Flow Calculations," Journal of Computational Physics, Vol 46, pp. 329-341, 1982.
- 13 "RELAP5/MOD3 Code Manuals," NUREG/CR-5535, Idaho National Engineering and Environmental Laboratory, 1990.
- 14 H. Christensen, "Power-to-Void Transfer Functions," ANL-6385, AEC Research and Development Report, 1961.

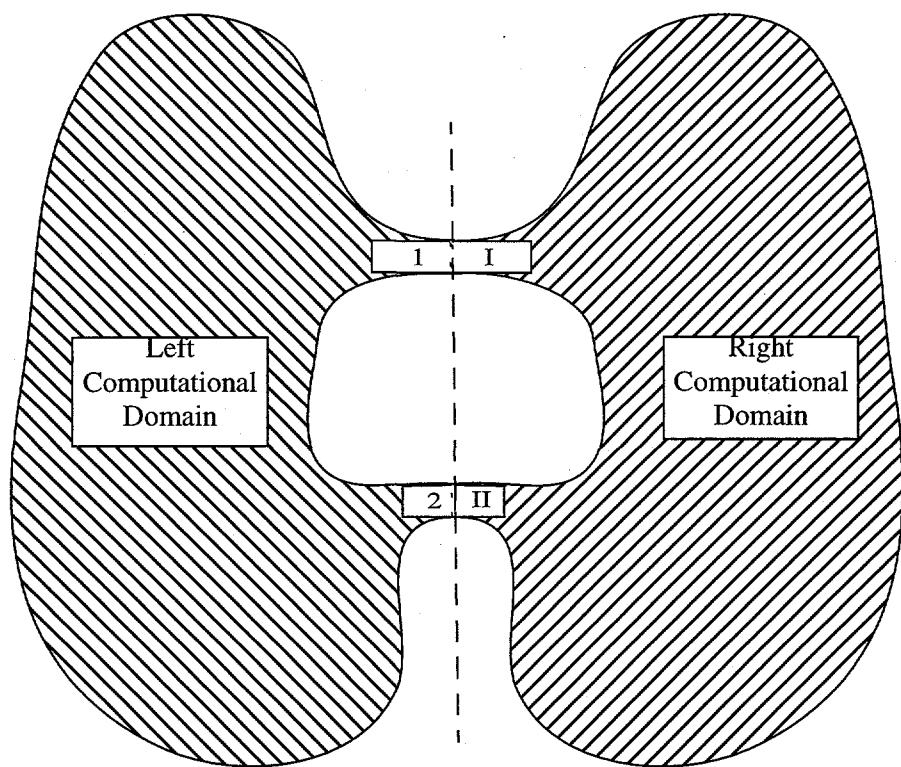


Figure 1 Schematic of Coupled Problem Solution Domain

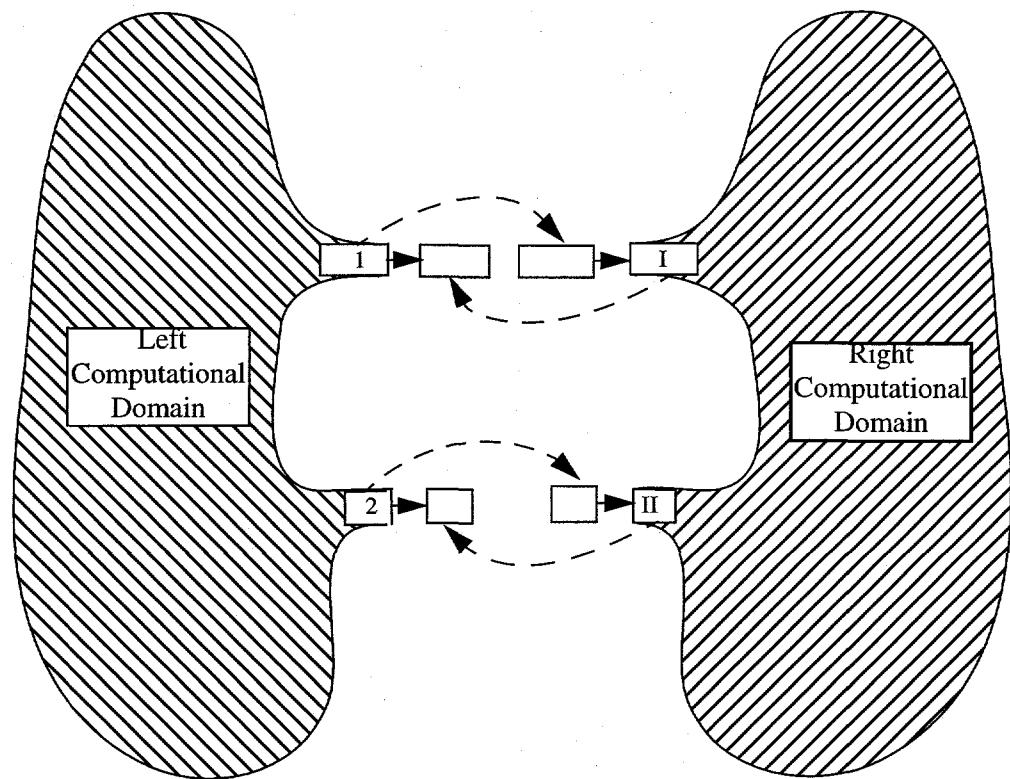


Figure 2 Schematic of Explicit Coupling Methodology

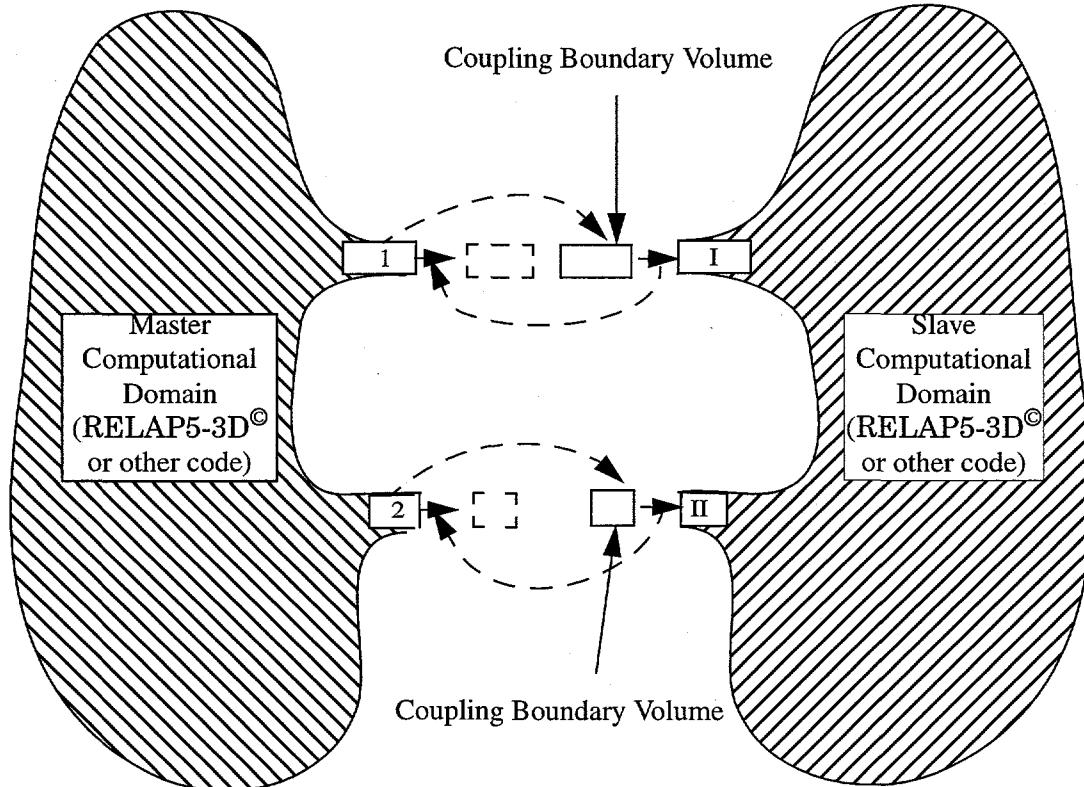


Figure 3 Schematic of Semi-Implicit Coupling methodology

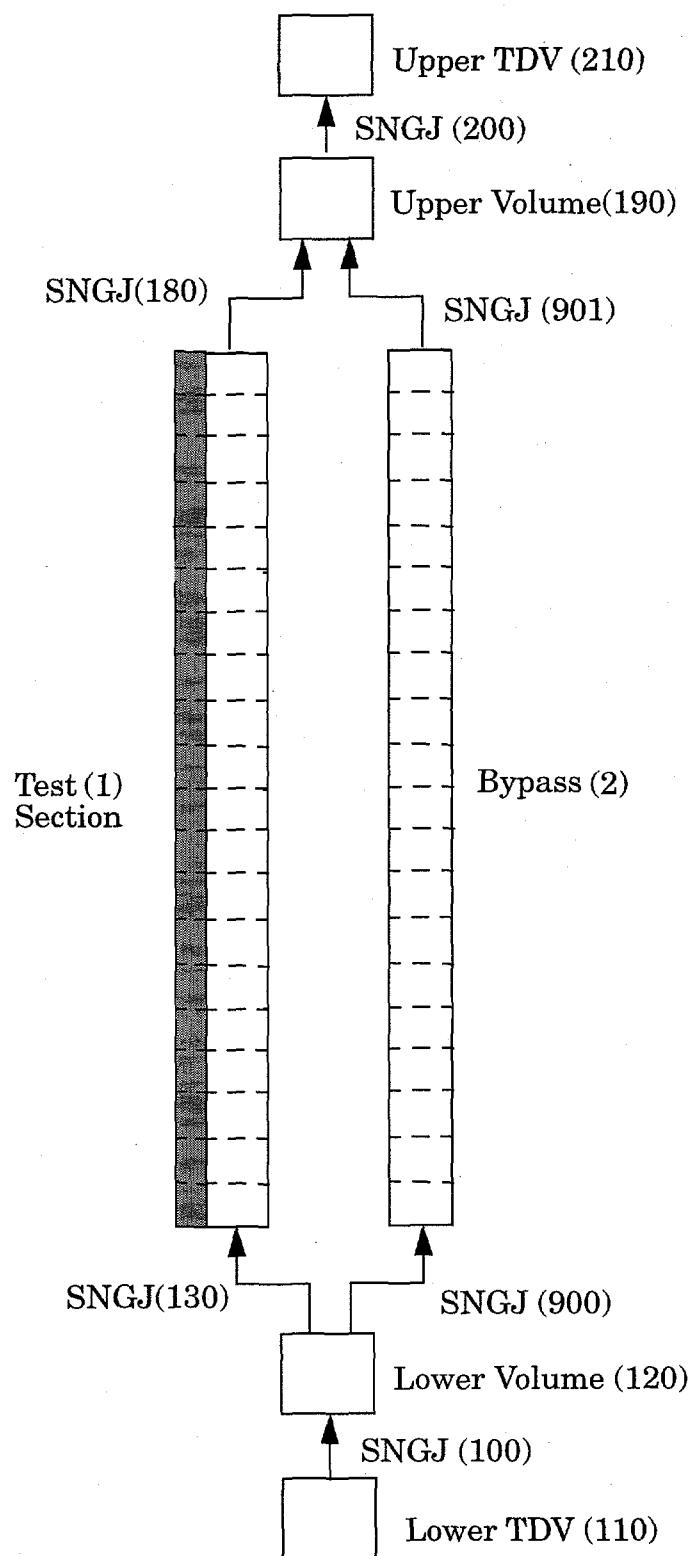


Figure 4 Schematic of Single System Representation of the Modified Christensen Experiment

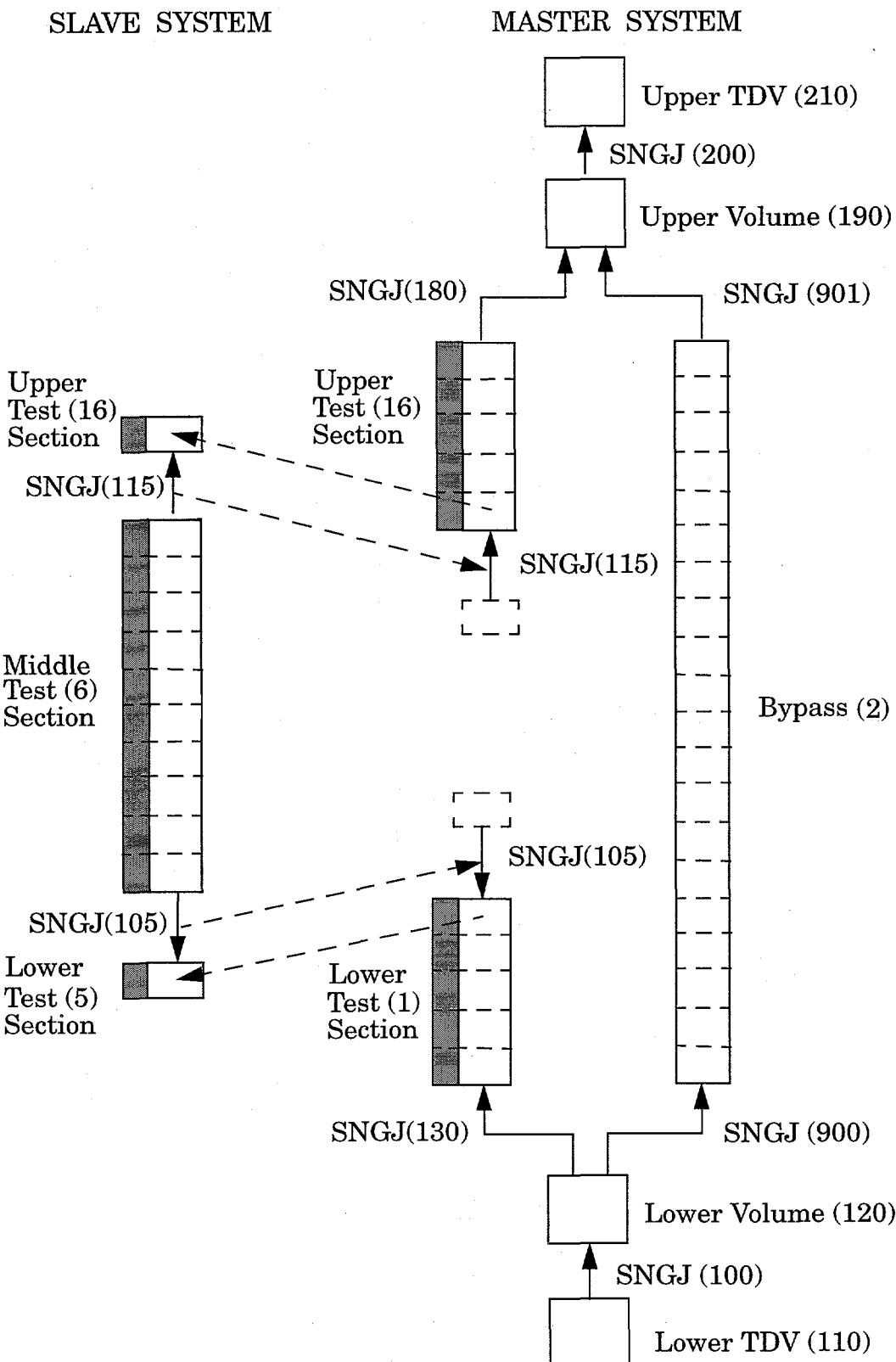


Figure 5 Schematic of the Coupled Representation of the Modified Christensen Experiment

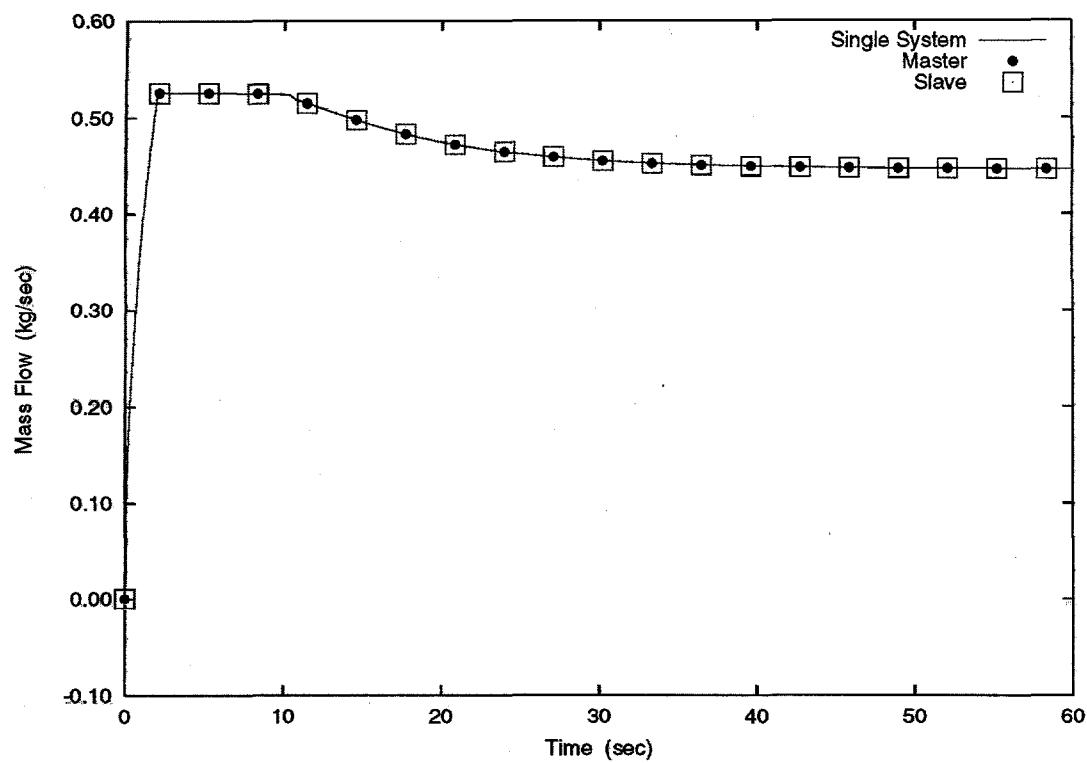


Figure 6 Comparison of Total Mass Flow at Upper Coupling Junction

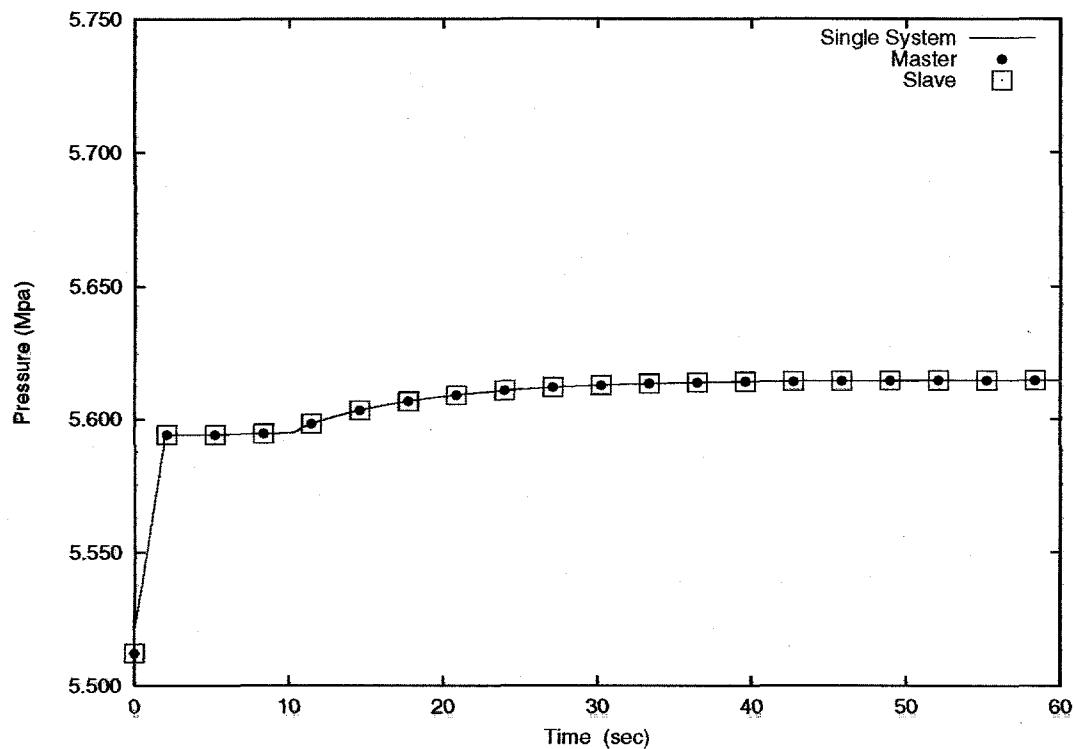


Figure 7 Comparison of Pressure in the Lower Coupling Volume

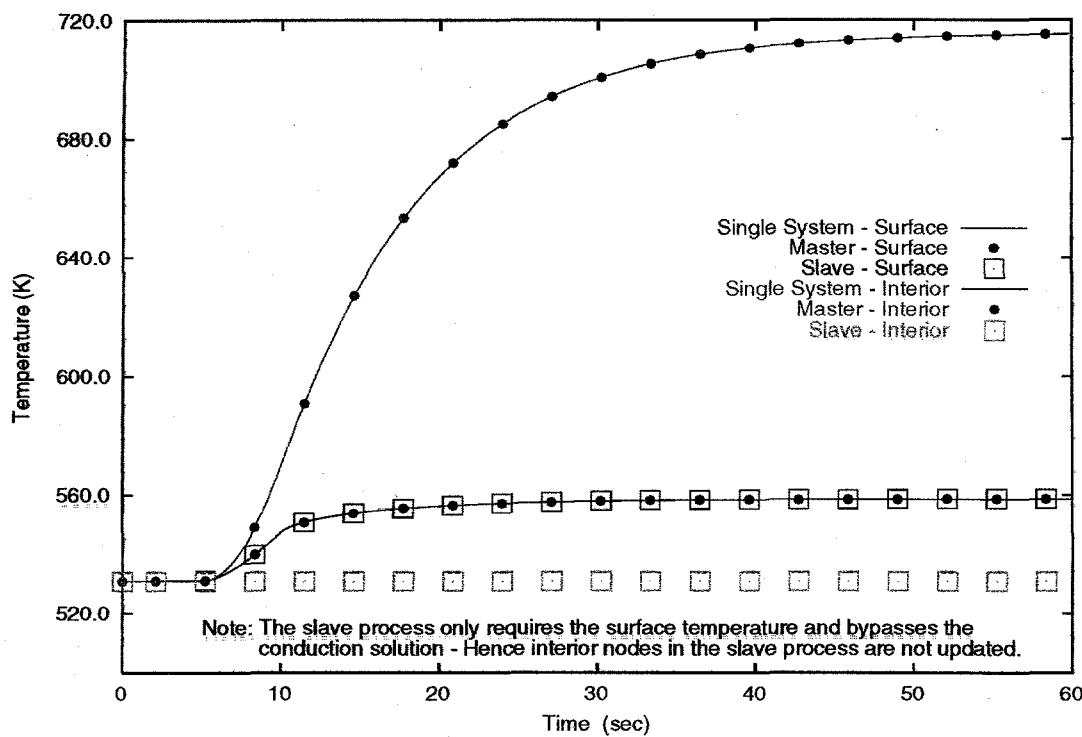


Figure 8 Comparison of Temperatures for the Heat Structure in the Lower Coupling Volume

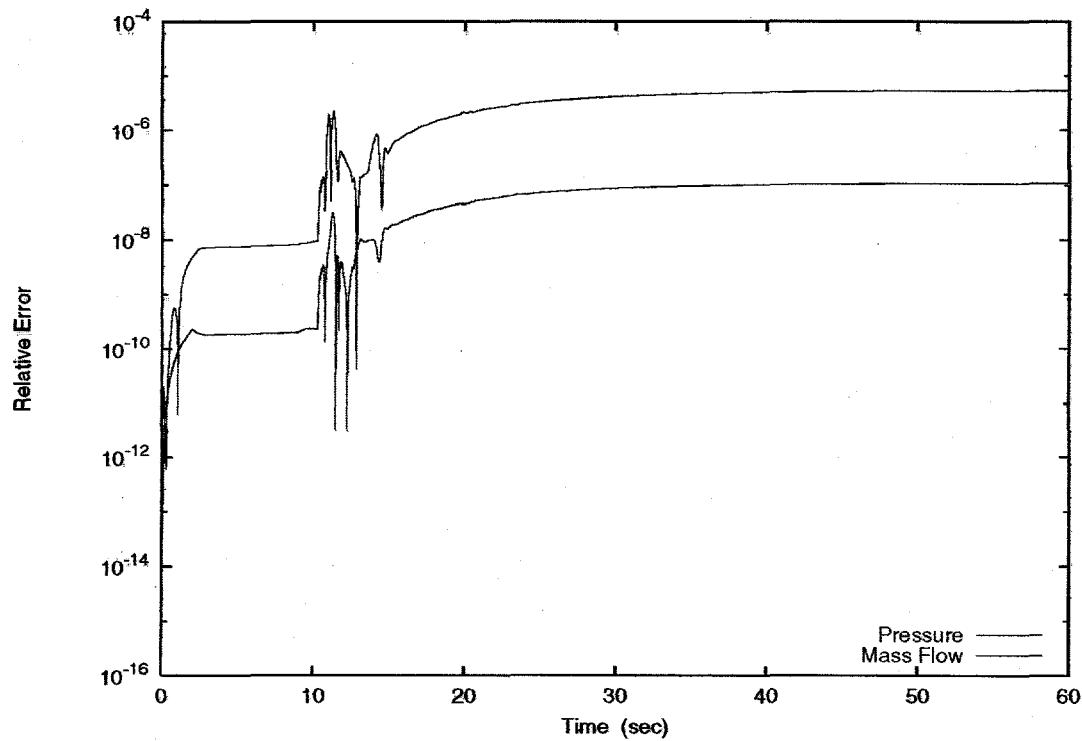


Figure 9 Relative Error in Predicted Mass Flow and Pressure