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INCORPORATION OF COBRA-TF IN AN INTEGRATED CODE SYSTEM WITH RELAP5-3D USING SEMI-IMPLICIT COUPLING

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Abstract

The three-field COBRA-TF subchannel analysis program has been incorporated in an integrated code system using a semi-implicit coupling algorithm. The coupling scheme used in this work is numerically stable subject to the material Courant limit. The integrated code system is made possible by an Executive program that manages the execution of the coupled analysis. The basis for the coupling scheme, the interaction of between the Executive and COBRA-TF and the details regarding the unique features associated with the application of this technique to a three-field COBRA-TF program are presented. Finally, the results of a verification problem are presented.

Introduction

Individual thermal-hydraulic programs have always attempted to provide a balance between complexity/flexibility and run time that was appropriate for a particular class of problems. As a result two generic types of analysis programs have been developed, system codes and specialized component codes. System codes, such as the drift-flux based RETRAN program (Paulsen, 1996) the two-fluid RELAP5-3D (RELAP5-3D Development Team, 1999) and TRAC-PF1 (Schnurr, 1992) programs, have all of the features that are required to perform a complete analysis of the reactor plant. Specifically, system programs contain models for plant components such as pumps and valves, reactor kinetics models (either point or space-dependent) and control system models. The breadth of calculations addressed by these programs necessarily requires that some approximations be made to both maintain a level of consistency in the program and practical execution times. Therefore, they do not contain all of the specialized modeling that has been developed for certain applications. This specialized capability is usually embodied in standalone computer programs that are focussed on a particular physical system or set of phenomena. For example, the three-field COBRA-TF program was developed to model reflood heat transfer (Paik, 1985), the CONTAIN program (Murata et al., 1997) was developed to calculate the conditions in the reactor containment and multi-phase CFD programs (Antal, 2000 and Stosic and Stevanovic, 2002) were developed and applied to analyze problems of interest in nuclear engineering.

Ideally, an analyst should be able to exploit the advantages of the comprehensiveness of the system programs while, if appropriate, making use of the specialized analysis programs in various regions of a simulation. This need has led to the coupling of various computer programs to provide this capability. The best known example of this is the COBRA/TRAC program (Thurgood, 1983).

While the concept of coupling various computer programs is not new, previous attempts at coupled codes have been very specific in application or have been developed as academic exercises instead of fully-developed analysis tools. Recently, to alleviate these restrictions, the concept of an integrated code system has been investigated. There are two hallmarks of this concept: an Executive program that monitors and controls the analysis; and well-defined interfaces among the programs. Both features have been recently developed around the system program RELAP5-3D computer program. While the work described in this paper provides an analysis tool similar to the COBRA/RELAP work performed by Lee (1992), there are several important distinctions. The most important distinction is the generality of the coupling interfaces. In this integrated analysis system, RELAP need not know to which program it has been coupled. This is contrasted with the single use coupling effort described by Lee.

Many of the original coupling efforts (Martin, 1995 and Aumiller et al., 2001) used a simplistic explicit numerical technique. Aumiller described numerical instabilities that were caused by the explicit coupling algorithm. To eliminate the numerical instabilities associated with explicit numerics, Weaver et al. (2000) developed a generic semi-implicit coupling technique. Weaver provides a good discussion concerning the numerical stability issues related to thermal-hydraulic code coupling. A brief discussion of the methodology is presented later in this paper.

The most important features of the semi-implicit coupling methodology are its generality and its use of the Parallel Virtual Machine (PVM) software package (Geist, 1994) for communication among the programs. These features allow additional programs to be added to the integrated code system in a very straightforward manner. Additionally, by creating a generic and well-defined interface, it becomes easier to add additional programs to the integrated code system. To date, this semi-implicit coupling algorithm has been used to couple RELAP5-3D to the following programs: RELAP5-3D, a multiphase CFD program (Aumiller et al., 2002), the single-phase CFD program FLUENT (Weaver et al., 2002) and now COBRA-TF.

While the four-field multiphase CFD program described in Aumiller et al. (2002) provides a very mechanistic and detailed calculation of the two-phase flow, it is not yet feasible to analyze an entire reactor core during a large break loss-of-coolant accident (LBLOCA) using this tool. COBRA-TF has been chosen for inclusion in the integrated code system because it provides a three-field, subchannel analysis capability that was developed for reflood heat transfer and it provides the capability to model the entire reactor vessel from nozzle-to-nozzle including the reactor core.

Furthermore, since a message-passing paradigm is used, the development of all of the programs in the integrated system can proceed independently, provided the interfaces among the programs are maintained. This approach is contrasted with the “hard-wired” approach used in COBRA/TRAC and COBRA/RELAP where the programs are conjoined to form one new program. This approach makes code maintenance and development more difficult. This may partially explain why the COBRA/TRAC program has not kept current with the development of either the COBRA or TRAC programs.

The RELAP5-3D Executive (Weaver et al., 2002) is the enabling software for the integrated code system. It provides a framework into which different computer programs (kernels) can be placed to create a truly integrated analysis system. The Executive controls every aspect of the computation. It can be used to completely synchronize the execution of the different programs including such items as determining the success of a given time step and the appropriate time step sizes. Currently, the Executive provides for four different types of coupling: explicit thermal-hydraulic, explicit reactor kinetics, explicit control system and semi-implicit thermal-hydraulics. These four types have been developed to exploit fully the various aspects of the RELAP5-3D program.

The following two sections describe the two basic types of changes that were required to implement COBRA-TF into the integrated analysis system. The first type of change that was required to integrate the semi-implicit coupling capability into COBRA-TF. The second type of change that was required to alter COBRA-TF to function in the integrated analysis environment where the Executive determines the success criterion for the time step, the time step size and the edit frequencies. Implementation details for each class of changes are presented in the following sections.

Mathematical Changes to COBRA-TF

Weaver et al. (2001) provides a complete description of the semi-implicit coupling algorithm. The following is a brief synopsis of the methodology.

A coupled system performs a domain decomposition of the complete problem to allow each program to solve a piece of the problem. This is shown schematically in Figure 1. The advantage of the semi-implicit coupling technique is that it is numerically stable for larger time steps than the simpler explicit coupling schemes. The numerical instability of the explicit coupling algorithm was shown in Aumiller et al. (2001) and requires time steps with lengths on the order of the inverse sonic velocity.

The use of implicit velocities and pressures in the discretized conservation equations in the semi-implicit numerical method (Weaver et al., 2001) provides numerical stability for time step sizes smaller than the material Courant limit. One advantage of this method is that a single matrix containing only new-time pressures can be developed. This matrix contains the effect of all of the new-time variables. This feature is the key to the semi-implicit coupling algorithm.

Using the nomenclature of Weaver et al. (2001), RELAP5-3D will be the master process and

COBRA-TF will be the slave process in this system. The semi-implicit coupling methodology modifies the solution procedure in RELAP5-3D for the junctions representing the connections between the two systems. The pressure equation for the volume attached to the coupling location in the RELAP5-3D computational domain is modified by retaining the mass, energy, volume and non-condensable gas flow rates as unknowns. By retaining these terms, the changes in the pressures in all of the volumes in the computational domain can be computed in terms of the flow rates in the coupling junctions as:

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

where n_g, u_g, u_l, m_g, m_l, w_g and w_l represent the flow rate of non-condensable gas and the phasic flow rates of energy, mass and volume at the coupling locations and N_c is the number of coupling junctions. The coefficients **a** through **h** for the volumes attached to the coupling junctions in the RELAP5-3D computational domain (volumes 1 and 2 in Figure 1) are transmitted to COBRA-TF. COBRA-TF then uses coefficients **a** through **h** to calculate the interdependence of pressure and flow rates at the coupling plane consistent with the RELAP5-3D solution strategy. This consistency is the key to the semi-implicit coupling methodology. When the mass, energy, volume and non-condensable flow rates in the coupling junctions have been received from COBRA-TF, Equation (1) 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 in RELAP5-3D may be completed in the normal manner.

As stated previously, the role of the COBRA-TF in this coupling algorithm is to calculate the phasic flow rates of mass, energy, volume and gaseous non-condensable gas across the coupling plane. (For the remainder of this paper, the phrase “net phasic flow rate” will refer to the net phasic flow rates of mass, energy, volume and the mass flow rate of a non-condensable gas). Using COBRA-TF to calculate the net phasic flow rates across the coupling plane instead of calculating volume conditions has a significant advantage: the ability to interface easily between the two-field RELAP5-3D and three-field COBRA-TF computer programs. Using this approach, COBRA-TF can use its three momentum equations to determine the three phasic mass flow rates and then combine the liquid and droplet fields using the following relationship:

$$\text{Net Liquid Flow} = A\,(V_{film}\varphi_{film} + V_{drop}\varphi_{drop}) \quad (2)$$

where A is the flow area, V is the velocity and φ is the convected quantity (e.g., macroscopic density for the mass equation). There would be no corresponding way to split the two momentum equations solved by RELAP5-3D into the proper three fields required at the boundary condition. Therefore, the choice of coupling variables has significant implications in the implementation of the semi-implicit coupling algorithm in COBRA-TF. Note that the technique used to integrate the liquid and droplet fields allows COBRA-TF to calculate counter-current phasic flows (i.e., a falling liquid film and rising liquid drops) at the coupling plane and determine the proper net phasic flow rates.

The semi-implicit coupling in COBRA-TF is implemented as a new boundary condition type. This is a special type of pressure boundary condition, where the pressure is determined by Equation (1). It needs to be stated that the new-time pressure in each of the coupled boundary cells depends on the new-time flow rates across all of the coupling planes. The result is an implicit relationship between the pressures in the all of the coupled cells and all of the interior computational cells attached to any of the coupling planes. As an example, consider the simple one-dimensional COBRA-TF problem shown in Figure 2.

This problem consists of four COBRA-TF volumes with coupled junctions attached to the first and last node. The structure of the pressure matrix for this problem is:

$$\begin{bmatrix} x & x & 0 & 0 & x & 0 \\ x & x & x & 0 & 0 & 0 \\ 0 & x & x & x & 0 & 0 \\ 0 & 0 & x & x & 0 & x \\ x & 0 & 0 & x & x & x \\ x & 0 & 0 & x & x & x \end{bmatrix} \begin{bmatrix} \delta P_1 \\ \delta P_2 \\ \delta P_3 \\ \delta P_4 \\ \delta P_{CPL_1} \\ \delta P_{CPL_2} \end{bmatrix} = \begin{bmatrix} x \\ x \\ x \\ x \\ x \\ x \end{bmatrix} \quad (3)$$

This matrix structure has several undesirable conditions. First it is asymmetric in structure; the consequence of this is that an entire class of linear solvers cannot be used in the solution of this problem. Second, the fullness of the last two rows in the matrix makes iterative domain decomposition techniques, such as the default COBRA-TF solver, less attractive. The nature of these domain decomposition methods is that their convergence behavior is dominated by the error in the interface between the domains. Unfortunately for the structure of the COBRA-TF pressure matrix, the error in the solution could accumulate in the coupled cells and flow rates. To overcome this condition, a generic direct solver has been implemented in COBRA-TF. This choice represents a trade-off in computer run time for accuracy in the coupled calculations. To accommodate the new direct solver, a new pressure matrix storage structure was required. The correct implementation of the new solver was verified by comparing the results of uncoupled calculations using both the previous solver and the new direct solver. All of these tests confirmed that the new solver has been correctly implemented.

Next, one time step in the coupled calculation will be examined. At the beginning of each time step, RELAP5-3D passes the old-time volume parameters (pressure, void fraction, phasic densities, phasic internal energies and non-condensable quality) to COBRA-TF. Using these conditions, the COBRA-TF uses upwind differencing to determine the convected quantities across the boundary (void fraction, phasic densities, phasic internal energies, phasic velocities and non-condensable quality). At this point in the solution scheme, the convected quantities are fixed for the time step. Using these convected quantities, RELAP5-3D creates the pressure matrix as described above and transmits coefficients **a** through **h** to COBRA-TF. COBRA-TF then uses these coefficients to generate and solve the pressure matrix, shown schematically in Equation (3). The new-time coupled phasic flow rates are determined based on the new-time pressures. These are then returned to RELAP5-3D, which then uses them to calculate the new-time pressures in the coupling volumes. These pressures are then used in the back-substitution process to calculate the remaining RELAP5-3D new-time variables. This completes one time step and the process is repeated for the next time step.

In addition to collapsing the fields at the coupling plane to determine the net phasic flow rates, the coupling algorithm must also create data to translate from the two-field volume conditions represented by the RELAP5-3D program to the three-field representation used by COBRA-TF. In the current implementation, a function has been used to determine the fraction of liquid that is in the dispersed form. The same technique has been used in this application as previously described in the work to couple RELAP5-3D to a multiphase CFD computer program (Aumiller et al., 2001). The function is shown in Figure 3. The choice of parameters for the transition point is based on the following assumptions, a bubbly flow regime will exist for all void fractions less than 40% and a thin liquid film could coexist with droplets if any liquid is present. It should be noted that these parameters and this technique is not considered to be optimal for all situations and current work is ongoing to define a more mechanistic approach to split a two-field representation into three or four-fields.

The semi-implicit coupling algorithm could be implemented as a master process for any number of system codes. However, the implementation into RELAP5-3D is easier since it uses a “single-shot” linearization technique. By only linearizing the conservation equations once per time step, the coupling coefficients remain fixed during the course of the time step. If the conservation equations are linearized more than once per time step, new coupling coefficients would be calculated at each iteration in the master process and the slave process (COBRA-TF in this application) would need to recalculate the flow field for each new set of coupling coefficients.

An additional task that has to be performed when integrating separate thermal-hydraulic codes is to ensure that the fluid properties are consistent between the codes. RELAP5-3D uses a unique reference point to determine the effective enthalpy of formation for non-condensable gases. Previously, COBRA-TF allowed the user to change the enthalpy of formation via input. To prevent input errors related to inconsistent enthalpies of formation, the RELAP5-3D technique has been coded into COBRA-TF and the input values are no longer used. To provide the maximum degree of consistency between COBRA-TF and RELAP5-3D, the RELAP5-3D based bi-cubic spline water properties will be included into COBRA-TF.

Administrative Changes to COBRA-TF

The inclusion of synchronous coupling in COBRA-TF requires many changes to its time step control logic.

Specifically, COBRA-TF must be able to do the following:

- reach a common point in each time step where the success or failure of the time step can be determined
- communicate the time step success to the Executive
- receive the global time step success from the Executive
- if required, repeat the time step based on the received success flag
- transmit its requested time step size to the Executive
- receive and use the time step size as determined by the Executive
- receive and use the edit frequencies from the Executive
- receive error flags from the Executive and gracefully terminate the coupled processes

All of these changes have been implemented in COBRA-TF and have been verified through the use of many different sample problems.

Verification of RELAP5-3D/COBRA-TF Coupling

A test case was developed to verify the implementation of the semi-implicit coupling algorithm between COBRA-TF and RELAP5-3D. As previously stated, in the RELAP5-3D/COBRA-TF coupling, RELAP5-3D must be the master and COBRA-TF the slave. Weaver et al. (2001) and Aumiller et al. (2001) have previously verified the RELAP5-3D implementation of the semi-implicit coupling algorithm. This study uses a similar problem and master RELAP5-3D input. Since the RELAP5-3D implementation is known to work, this section will concentrate on the implementation details for COBRA-TF.

The test case divides the test system into two parts that are simulated as a coupled problem using the semi-implicit coupling methodology. Figure 4 is a schematic coupled problem. The first input file, for the RELAP5-3D domain, contains the upper and lower common volumes, the time dependent volumes, the bypass channel and the lower and upper portions of the test section. The middle ten volumes of the test section were removed and moved to the COBRA-TF domain. Coupling volumes and coupling junctions were added to each input file as appropriate. Dotted lines in Figure 4 indicate data exchange between the coupling volumes and coupling junctions. 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. The nodalization in the COBRA-TF portion is consistent with the RELAP5-3D domain.

The geometry for the test case is based on Run 15 of the Christensen (1961) subcooled boiling experiments. Unlike the experiments, the input model includes a parallel flow path for purposes of testing the coupling methodology and uses hydraulic resistance to remove the characteristic oscillations. The problem is unheated. To provide a transient problem, the void fraction is ramped from 0.0 to 0.2 and back to 0.0. Furthermore, to test the ability of the coupling to account for the presence of non-condensable gas properly, the air content is ramped 0 to 20% by mass and back to 0%. The transient boundary conditions are shown in Figure 5.

The essence of the semi-implicit coupling methodology is that the two different programs must use the same relationship between new-time flow rates and pressures. Therefore, the new-time pressure predictions between the master and slave processes for the coupling volumes must be compared. For the coupling to function properly, both codes must calculate the same pressure associated with the coupling volume that is part of the RELAP5-3D problem domain. While implementing the methodology, these numbers were often compared and were shown to be correct to machine precision. Figure 6 shows the results of a comparison of the pressure in the lower coupling volume. For the coupled problem, the RELAP5-3D and COBRA-TF solutions are identical to the precision printed in the data files.

Figure 7 shows the predicted mass flow rates at both of the coupling planes. Since there are no mass sources or sinks in the COBRA-TF problem and the total mass flow rate is the same at both coupling planes during the plateau regions, it can be concluded that the coupled code conserves mass. One of the important implementation issues is the correct integration over the number of fields and over the flow area to determine the correct net phasic flow rates. During the time in which the large vapor slug passes through the system, the void fraction is large enough such that liquid drops exist at the coupling plane. The coupling algorithm properly handled this situation.

In addition to conservation of total mass, other parameters are important to determine that the coupling has been correctly implemented. These other parameters are conservation of total and phasic energies, conservation of phasic masses and conservation of mass for the non-condensable gas. Figures 8 and 9 show the plots for conservation of total energy and non-condensable gas mass. As expected, the response at the top plane is delayed relative to the bottom plane. The other plots have been omitted for brevity.

At the present time, the coupling between COBRA-TF and RELAP5-3D does not conserve momentum. The momentum source associated with the flow in the COBRA-TF domain has not yet been implemented. This is not a problem for plant problems because the momentum associated with the loop flow is typically assumed to be dissipated in the vessel by the presence of the downcomer.

This test problem, when combined with all of the other RELAP5-3D/COBRA-TF test problems has shown the proper interaction between COBRA-TF and the Executive. Specifically, the ability of the Executive to perform the following tasks with respect to COBRA-TF have been verified:

- Force a repeated time step
- Determine the proper time step size
- Determine the appropriate edit frequencies
- Terminate at the end of the problem

Conclusions

COBRA-TF, a three-dimensional, three-field subchannel analysis program has been correctly implemented into an integrated code system. COBRA-TF was chosen for inclusion to take advantage of its advanced capabilities for performing reflood heat transfer calculations and its ability to model the entire reactor vessel. The integrated code system is controlled by an Executive program and uses the RELAP5-3D program to provide the required system code capabilities. The results of a sample problem were used to verify the proper implementation of the semi-implicit coupling algorithm and the interactions between COBRA-TF and the Executive.

References

Antal, S. P., Podawski, M. Z., and Lahey Jr., R. T., 2000, "A contribution to Mechanistic Multidimensional Modeling of Annular Flows," Proceedings of 34th National Heat Transfer Conference, Pittsburgh, PA.

Aumiller, D. L., Tomlinson, E. T., Bauer, R. C., 2001, "A Coupled RELAP5-3D/CFD Methodology with a Proof-of-Principle Calculation," Nuclear Engineering and Design, 205, pp. 83-90.

Aumiller, D. L., Tomlinson, E. T., and W. L. Weaver, 2002, "An Integrated RELAP5-3D and Multiphase CFD Code System Utilizing the Semi-Implicit Coupling Technique," Nuclear Engineering and Design, 216, pp. 77-87

Christensen, H., 1961, "Power-to-Void Transfer Functions," ANL-6385, AEC Research and Development Report.

Geist, A., et al., 1994. "PVM3 User's Guide and Reference" ORNL/TM–12187, Oak Ridge National Laboratory.

Lee, S. Y., Jeong, J. J., and Kim, S-H, "COBRA/RELAP: A Merged Version of the COBRA-TF and RELAP/MOD3 Codes," Nuclear Technology, 99, pp. 177-187.

Liles, D. R., Reed W. H., 1978. "A Semi-Implicit Method for Two-Phase Fluid Dynamics," Journal of Comp. Phys. 26, 390-407.

Martin, R. P., 1995. "RELAP5/MOD3 Code Coupling Model," Nuclear Safety, 36, pp. 290-299.

Murata, K. K. et al., 1997, "Code Manual for CONTAIN 2.0: A Computer Program for Nuclear Reactor Containment Analysis," NUREG/CR-6535.

Paik, C., Hochreiter, L., Kelly, J., Kohrt, R., 1985, "Analysis of FLECHT-SEASET 163 - Rod Blocked Bundle Data Using COBRA-TF," NUREG/CR-4166.

Paulsen, M., et al., 1996, "RETRAN-3D A Program for Transient Thermal-Hydraulic Analysis of Complex Fluid Systems," EPRI NP-7450.

RELAP5-3D Development Team, 1999, "RELAP5-3D Code Manuals, Volumes I, II, IV, and V," Idaho National Engineering and Environmental Laboratory, INEEL- EXT-98-00834, Revision 1.1b.

Schnurr, N. M. et al., 1992, "TRAC-PF1/MOD2 Code Manual - User's Guide," NUREG/CR-5673.

Stosic, Z. V. and V. D. Stevanovic, 2002, "Multiphasing CFD," Proceedings of ICONE-10, Arlington VA, April 2002.

Thurgood, M. J., Kelly, J. M., Guidotti, T. E., Kohrt, R. J., Crowell, K. R., 1983. "COBRA/TRAC – A Thermal Hydraulics Code for Transient Analysis of Nuclear Reactor Vessels and Primary Coolant Systems," NUREG/CR- 3046.

Weaver, W. L., Tomlinson, E. T., Aumiller, D. L., 2001, "A Generic Semi-Implicit Coupling Methodology For Use In RELAP5-3D©," Nuclear Engineering and Design, 211, pp. 13-26.

Weaver, W. L., Tomlinson, E. T., Aumiller, D. L., 2002, "A PVM Executive Program for Use with RELAP5-3D," Proceedings of ICONE-10, Arlington VA, April 2002.

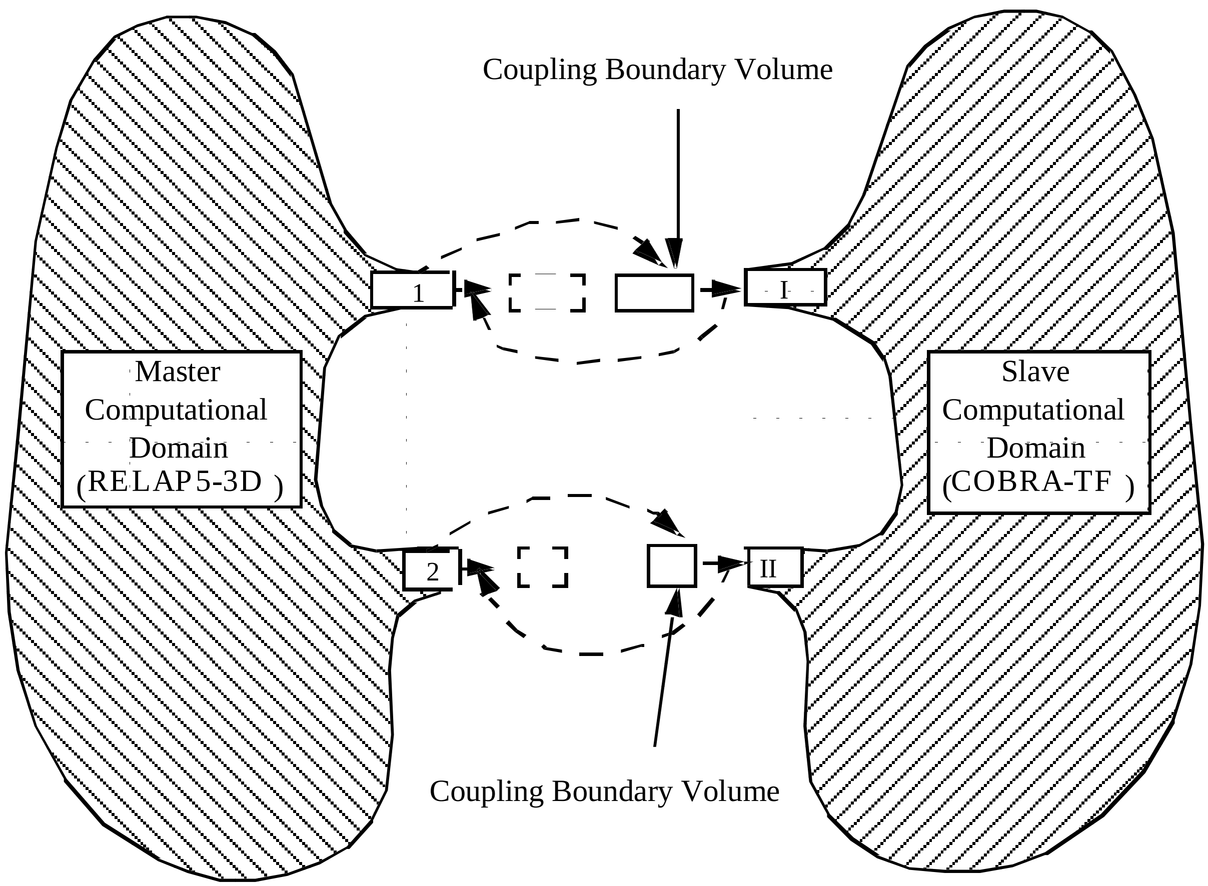

Figure 1: Solution Domains for Semi-Implicit Coupling

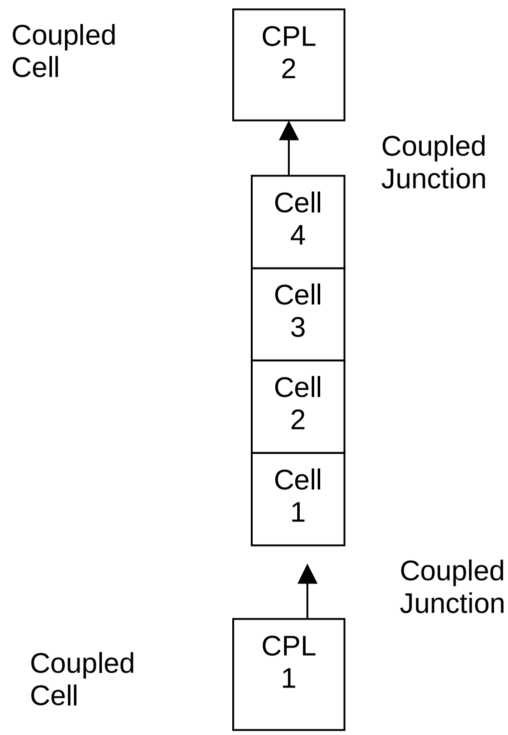

Figure 2: Simple One-Dimensional Test Problem for COBRA-TF

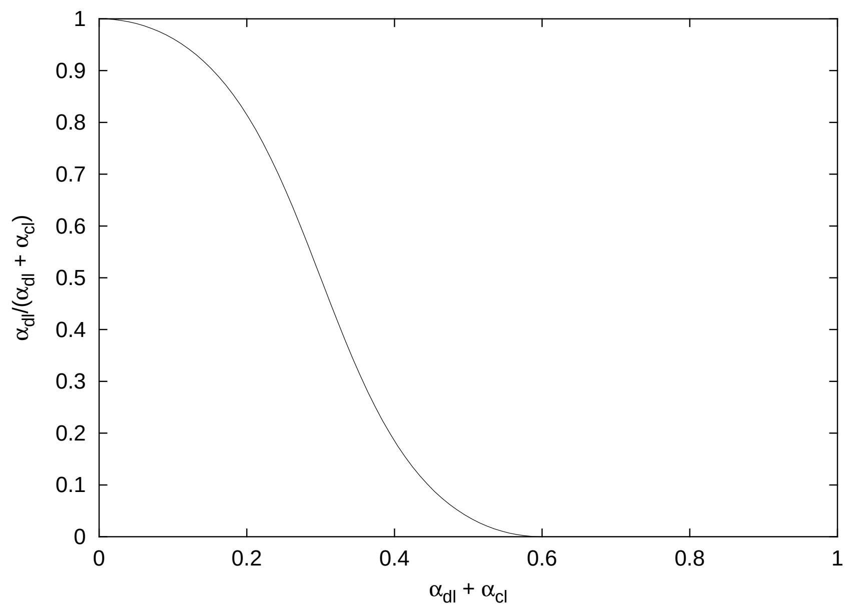

Figure 3: Schematic of the Function Used to Split the Liquid Field

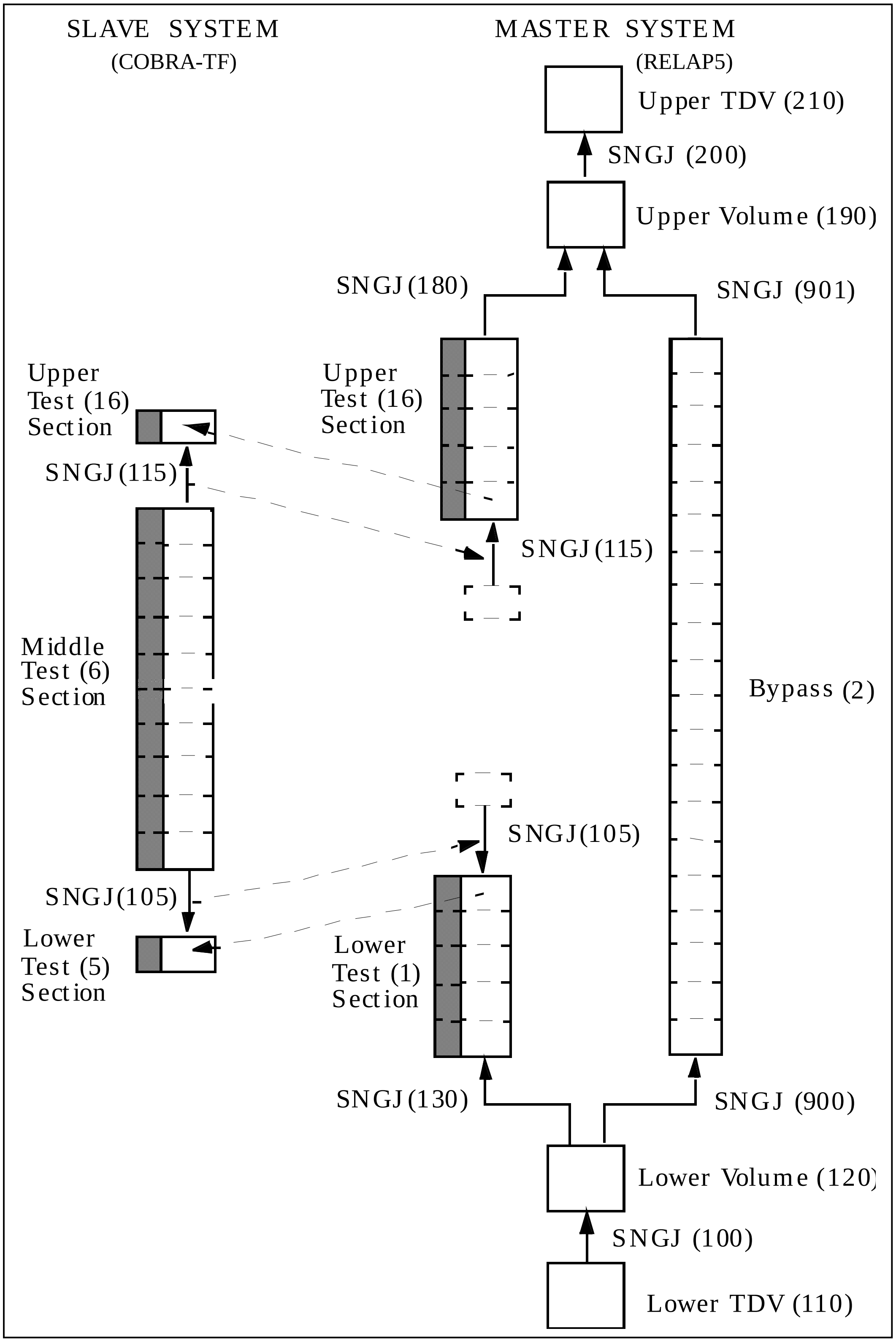

Figure 4: Schematic of Verification Problem

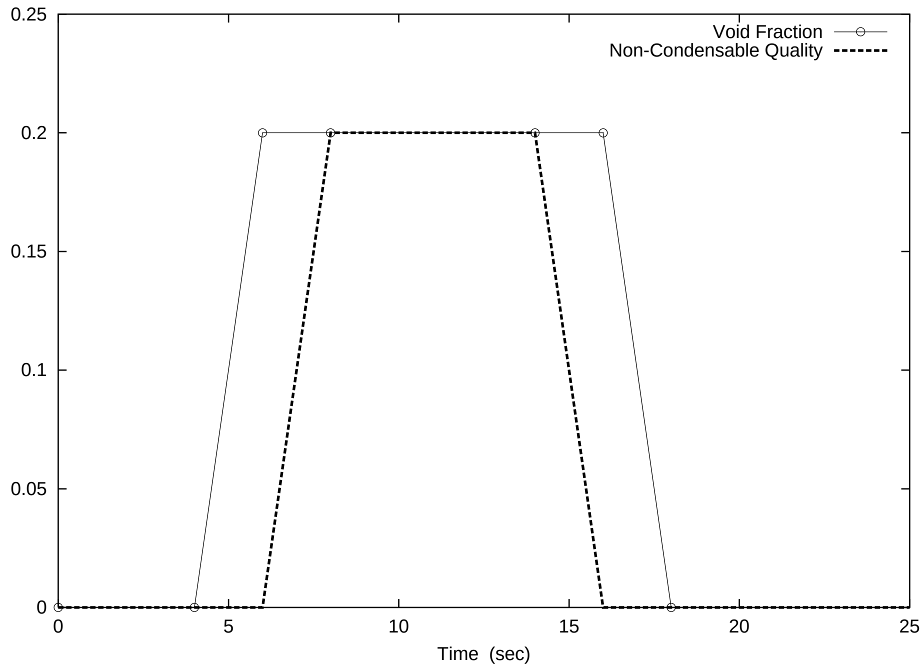

Figure 5: Transient Boundary Conditions Used for Verification Testing

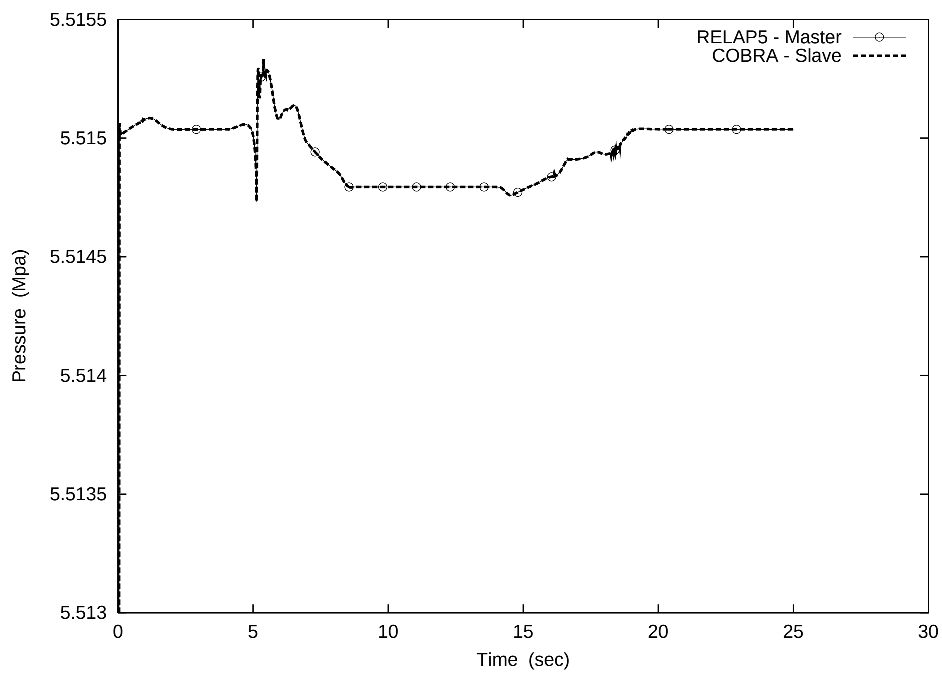

Figure 6: Comparison of RELAP5-3D and COBRA-TF Calculated Pressures

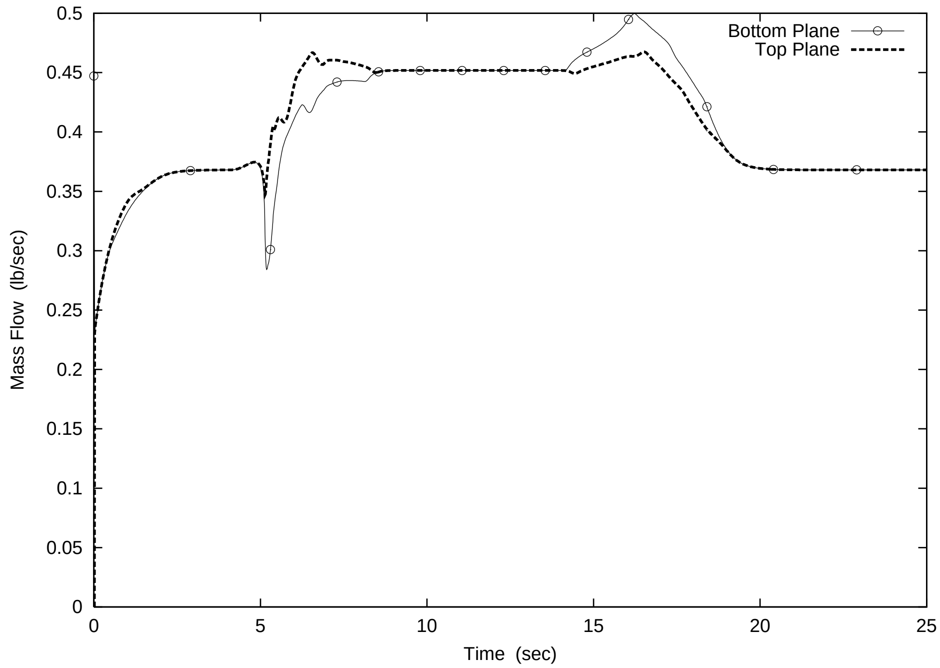

Figure 7: Conservation of Total Mass

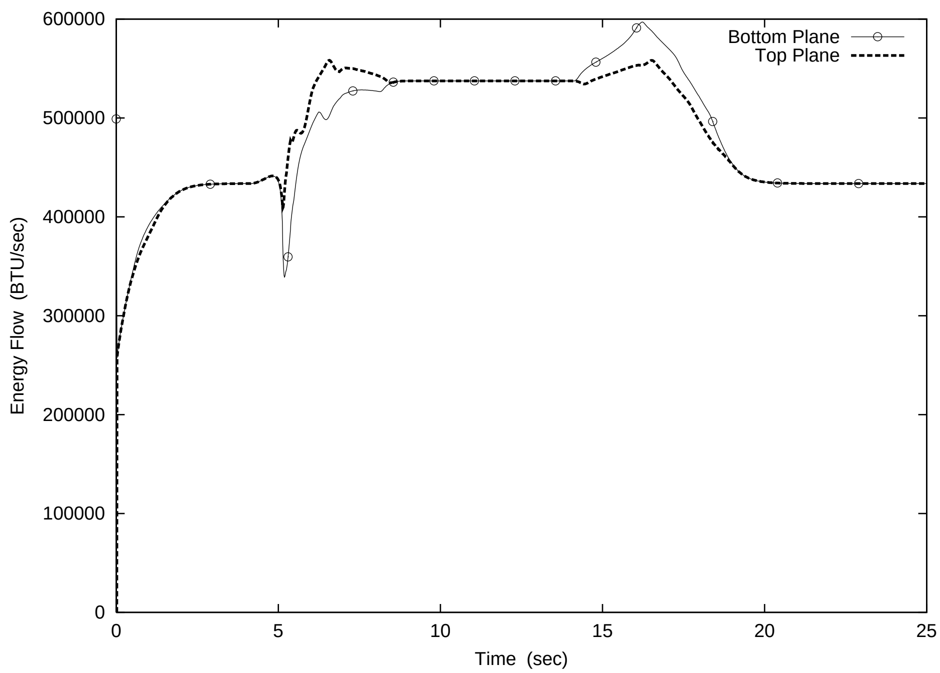

Figure 8: Conservation of Total Energy

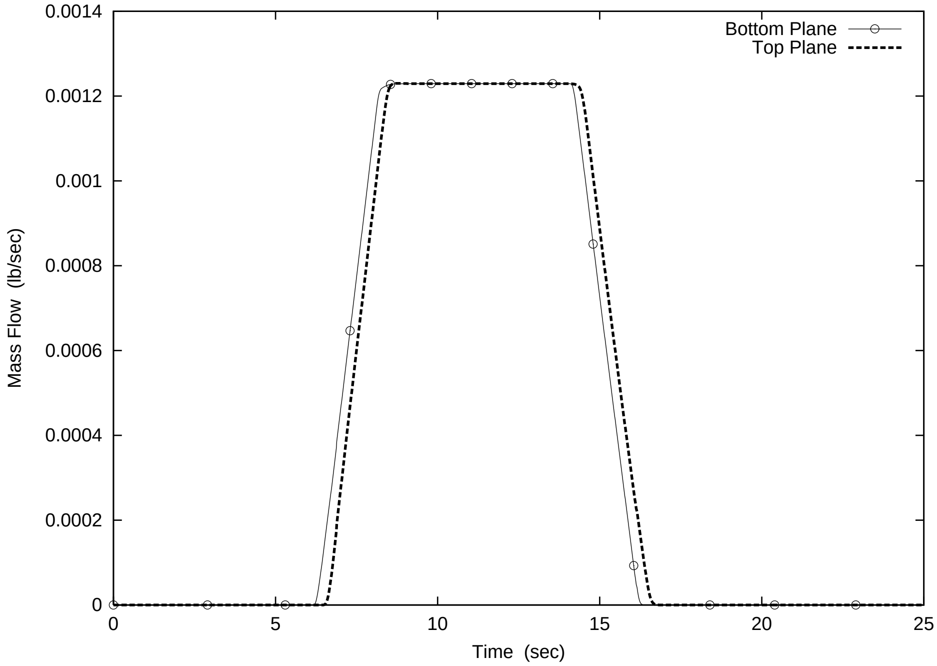

Figure 9: Conservation of Non-Condensable Gas Mass