

# BENCHMARKING SIMULATIONS WITH CFD TO 1-D COUPLING

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## Abstract

CFD is being used more frequently to provide detailed information in a limited region of a reactor system. For such simulations, the boundary conditions from the balance of the reactor can be provided by thermal-hydraulics code such as CATHARE or RELAP5. Based on our experience, high quality results from such a linkage require some attention to the details at the connection surfaces between the coupled simulations. This paper provides a simple way of testing some coupling issues, and suggestions that may improve this class of reactor simulation.

## 1. INTRODUCTION

Reactor safety analysis is normally carried out using one-dimensional, area-averaged two-phase flow equations. Three-dimensional analysis has been available in some safety codes (e.g. and CATHARE[1] and TRAC[2] for many years. However, the 3-D tools have had a number of restrictions related to nodalization, field equations (usually Euler), and other aspects of physical modeling. The existing safety codes generally give good estimates of the system performance for a wide class of flow conditions. However, in some situations a detailed understanding of the flow may be required in a limited region of the system. In this case a 3-D Reynolds Averaged Navier-Stokes (RANS) code may be applied for the detailed analysis and the safety code used to provide boundary conditions reflecting feedback from the balance of the system.

Successful linkage will require care in both numerical and physical modeling. Impact of the transition between different spatial grids requires study. Differences in spatial difference methods may also have an impact. Most CFD codes use fully implicit time differencing, so coupling to a fully implicit 1-D code would be most direct. However, coupling to semi-implicit [3] or SETS [4] methods is also possible. The field equations in the two methods should at least match to the extent that conservation of mass and energy is possible, and better results can be expected if one equation of state is used. Where flow is from an Euler equation set to a CFD code, sources of turbulent kinetic energy will be needed at the junction. Consistency in wall friction modeling will also be needed, and care will be required in selection of velocity profiles for fluxes from an area averaged 1-D region to a resolved 3-D flow.

When benchmarking performance of coupled reactor safety and CFD codes, the temptation is to select problems with complex flow patterns, clearly requiring the power of CFD analysis. However, information about the coupling itself can be obscured by complex geometries and flow. Whenever we test a new or revised CFD code, one of the first things we do is to test against the Laufer's data [5] for fully developed pipe flow. We believe that a benchmark based upon his experiments is an excellent way to explore issues related to code coupling.

## 2. APPROACH

A simplified, code set has been developed to study code coupling. The 1-D portion of the calculation is handled by a package we have named FLOW1D. It solves the 1-D single-phase area-averaged flow equations (mass, momentum and energy conservation), and is a simple platform for studying the impact of various difference methods and coupling procedures. The momentum equation includes a frictional loss source term obtained from the correlation for fully developed pipe flow extracted from TRAC [2]. The energy equation includes a user-specified volumetric heating term. This code accurately reproduces the pressure drop versus Reynolds number behavior for both laminar and turbulent fully-developed pipe flows. The friction correlation does not correctly capture the friction factor variation for transitional flows.

The 3-D code employed is a multi-fluid code (NPHASE [6]) used only in the single phase mode. NPHASE is an “incompressible” pressure-based, cell-centered code that allows for density variation due to thermal effects. NPHASE correctly predicts the pressure drop behavior and velocity profiles observed by Laufer for  $Re = 500,000$  (based on pipe diameter and centerline velocity).

To properly simulate a fully developed pipe flow using a 3-D RANS code, one must apply physically consistent inflow and outflow boundary conditions to the 3-D code. For a stand-alone subsonic case, these might consist of specified velocity and temperature profiles at the inlet, and pressure extrapolation (or a suitable non-reflecting BC) at the inlet. At the pipe outlet the static pressure must be specified, while velocity and temperature would be extrapolated. For our first test case, the upstream boundary condition feeds the 1-D simulation, so upstream conditions for the 3-D RANS calculation are obtained from state conditions between the 1-D and 3-D difference equations. Velocity at the junction is generated by the 1-D code, using averaged pressures and other state information from the 3-D mesh. The 3-D analysis treats the 1-D velocity as an area average and imposes a radial velocity profile consistent with the Reynolds number (and the implied friction factor) from the upstream 1-D pipe flow. Fortunately, for single phase flow, there are some empirical, analytical expressions that permit the construction of a suitable inflow profile. Care must be taken to insure both the correct near-wall behavior and outer region behavior, while maintaining the correct mass flow. In addition, the definition of RANS turbulence quantities such as turbulence kinetic energy and dissipation rate requires a smooth velocity derivative normal to the wall.

For the proposed code coupling procedure, it is assumed that any transient simulation would be initiated from a steady flow condition. Therefore, the 3-D code should start from a converged steady flow simulation using the analytic inflow profile and the correct downstream pressure. If this were not done, a time-consuming iteration between the codes would be required until the 3-D domain solution converged. For simplicity the 3-D code was run in axisymmetric mode; however this is not a necessary restriction. The analytic inflow profile is interpolated onto the 3-D grid inflow plane by the 3-D code.

## 3. RESULTS

We have run two simple tests. The first demonstration case is a circular pipe flow with the geometric parameters given in Table 1 and the flow parameters for the adiabatic case in Table 2. The second case is a thermal transient case defined in Table 3. Computational parameters are defined in Table 4. In both instances we are testing a coupling method that is

basically explicit. During each time step the 1-D calculation is executed based on old time values from the 3-D, then the CFD calculation is advanced based upon the latest conditions from the 1-D. A consistent first-order spatial difference method is used in both regions.

Pipe geometry	
Cross-sectional area	0.4 m <sup>2</sup>
Radius	0.3568 m
Pipe length	
Pipe length (total)	15.28 m
Pipe length (1-D section)	6.0 m
Pipe length (3-D section)	9.28 m

**Table 1. Pipe flow specifications**

Velocity (average)	5.0 m/s
Fluid density (constant)	1000 kg/m <sup>3</sup>
Reynolds number -- Re(D)	4,149,000
Exit pressure (x = 15.28 m)	100,000 Pa

**Table 2. Flow parameters (adiabatic case)**

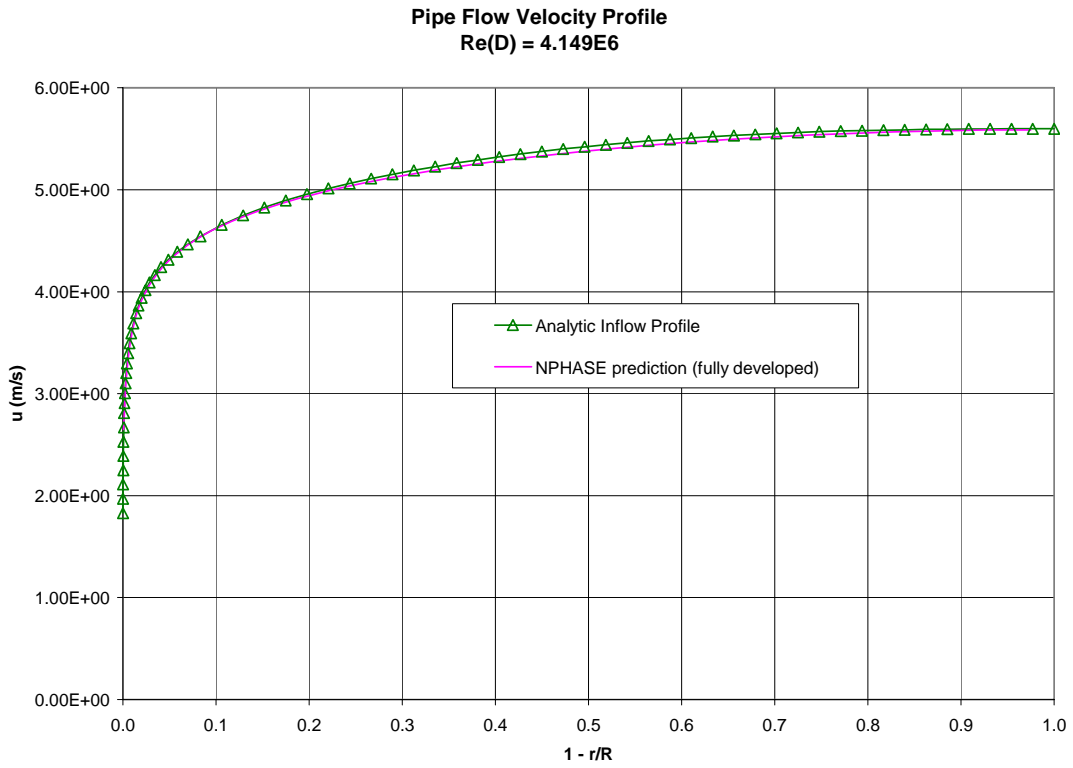
Velocity (average)	5.0 m/s
Fluid density (t = 0)	1000 kg/m <sup>3</sup>
Reynolds number -- Re(D), T=300 K	4,149,000
Exit pressure (x = 15.28 m)	100,000 Pa
Temperature (t = 0, all x)	300 K
Temperature (t = 0.05, x = 0)	350 K

**Table 3. Flow parameters (thermal transient case)**

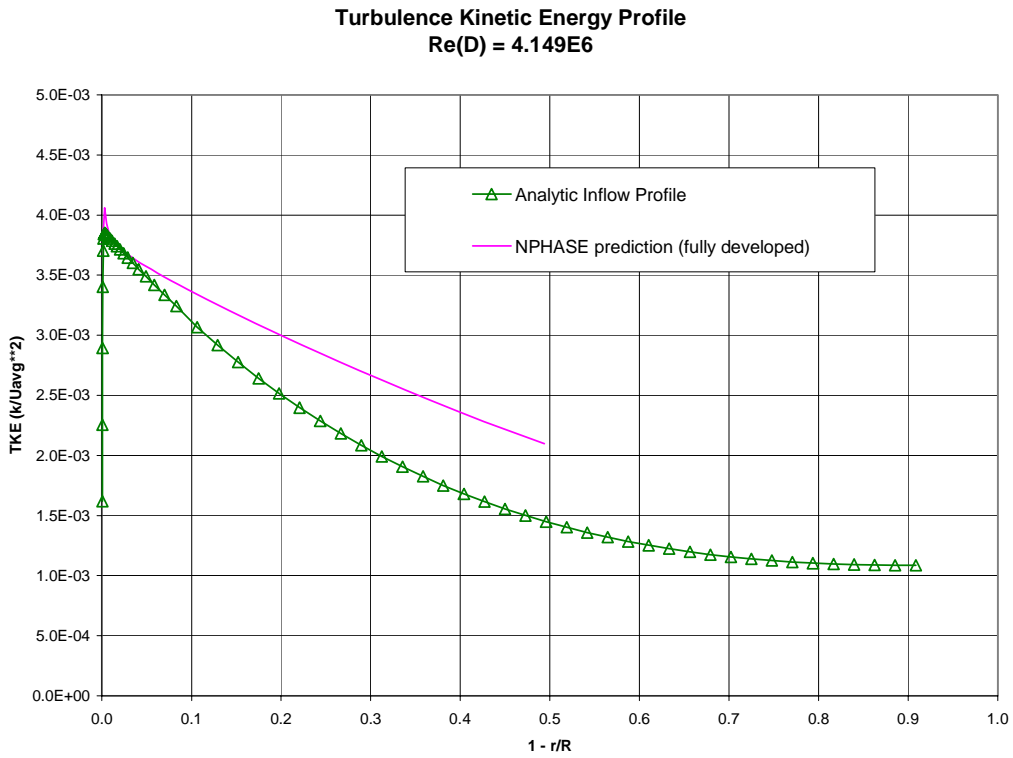
Computational parameters	1-D code	3-D code
No. of axial cells	12	20
Axial grid spacing	0.5 m	0.464 m
No. of radial cells	N/A	50
Radial grid spacing		
Wall – cell center	N/A	0.001 m (y+ = 74)
Centerline – cell center	N/A	0.025 m

**Table 4. Computational parameters**

The analytic radial velocity and turbulence profiles are shown in Figs. 1 and 2 along with comparisons to stand alone predictions from the 3-D code for a fully developed pipe flow case (L/D =130). The velocity profile is reproduced very well (Fig. 1), while the turbulence kinetic energy (Fig. 2) is relatively accurate compared to the RANS solution only near the wall. However, the analytic turbulence profiles (k and epsilon) are sufficient to maintain the correct pressure drop for this case. Future improvements in this area may be needed for high fidelity 3-D simulations where the core flow turbulence is more important.



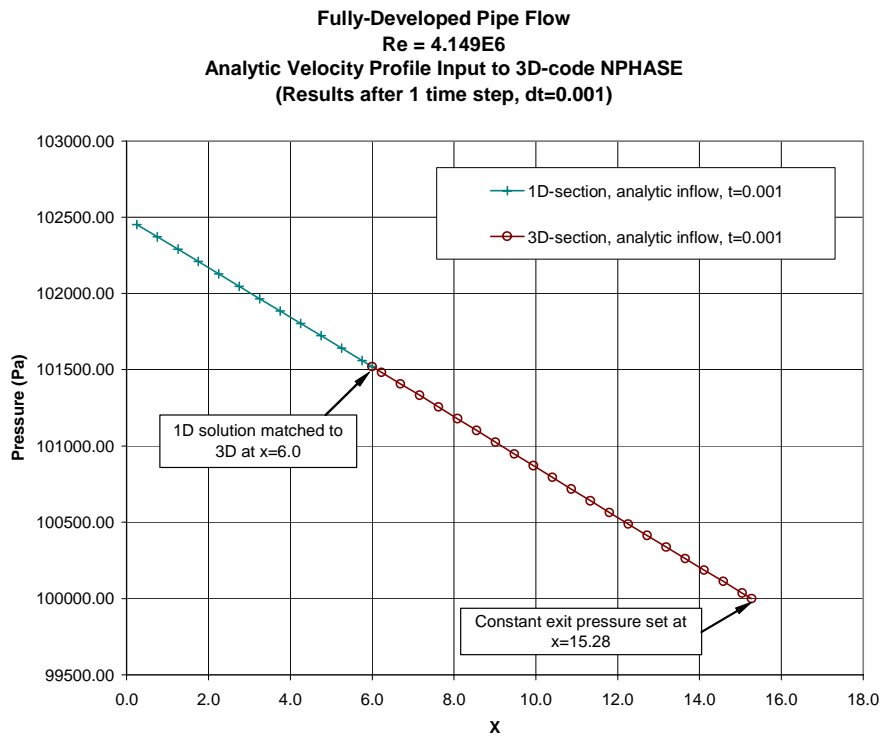
**Figure 1. Pipe Flow Velocity Profile Comparison.**



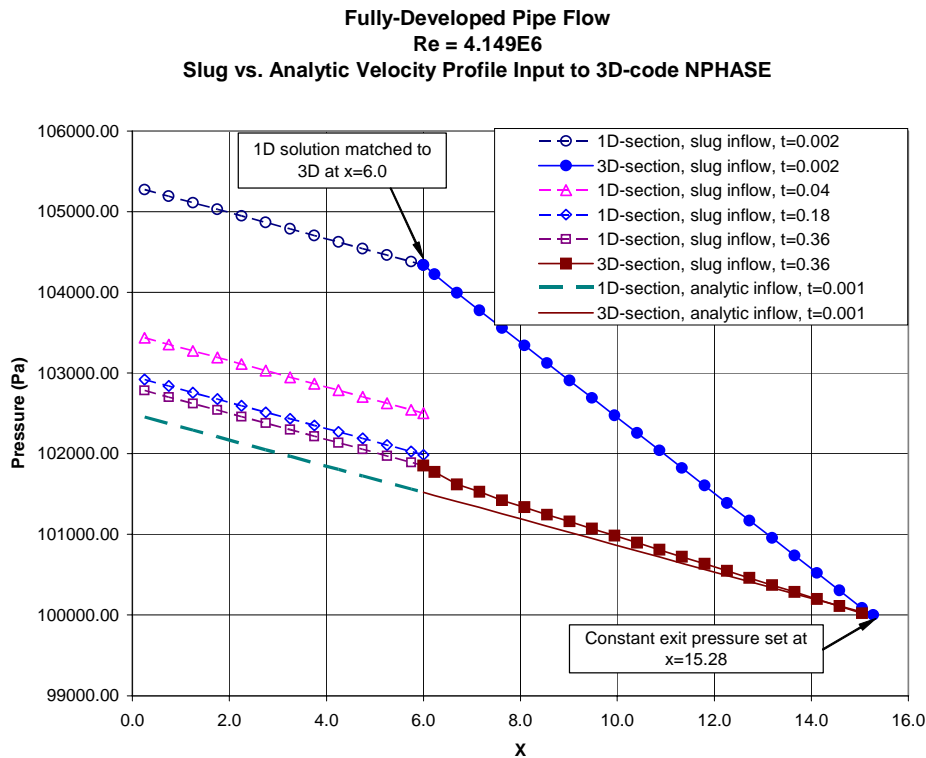
**Figure 2. Turbulence Kinetic Energy Profile Comparison**

The NPHASE code was run using a high-Reynolds number Launder-Spalding  $k$ -epsilon model along with a conventional wall-function formulation. Therefore, the near-wall viscous sublayer and buffer region are not resolved. This formulation gives very accurate skin friction predictions for fully-developed turbulent flows.

The test cases were run with a specified constant downstream pressure at  $x = 15.05$  m. The predicted axial pressure (area averaged in 3D) variation after one time step ( $dt = 0.001$  s) is shown in Fig. 3 for the case with the analytic inflow profile. It can be seen that a smooth transition occurs between the 1-D and 3-D sections (at  $x = 6.0$ ), and the correct pressure gradient is maintained. However, Fig. 4 shows the behavior if a slug-flow (uniform) velocity profile is supplied as the 3-D inlet condition (intermediate 3-D solutions are omitted for clarity). A significant transient is observed. The converged solution (at  $t = 0.36$  s) maintains the wrong pressure drop and has a slope discontinuity at the 3-D inflow. This is equivalent to an abrupt pipe-entrance effect since the 3-D simulation sees the slug inflow velocity rather than a fully-developed velocity profile. Also, the 3-D axial grid spacing is relatively large as resolution of the entrance-like behavior was not intended. Therefore, it is necessary to specify a proper 3-D inflow velocity profile to maintain the consistency of the coupled solution.



**Figure 3. Pressure Distribution in Pipe with Analytic Inflow Profile**

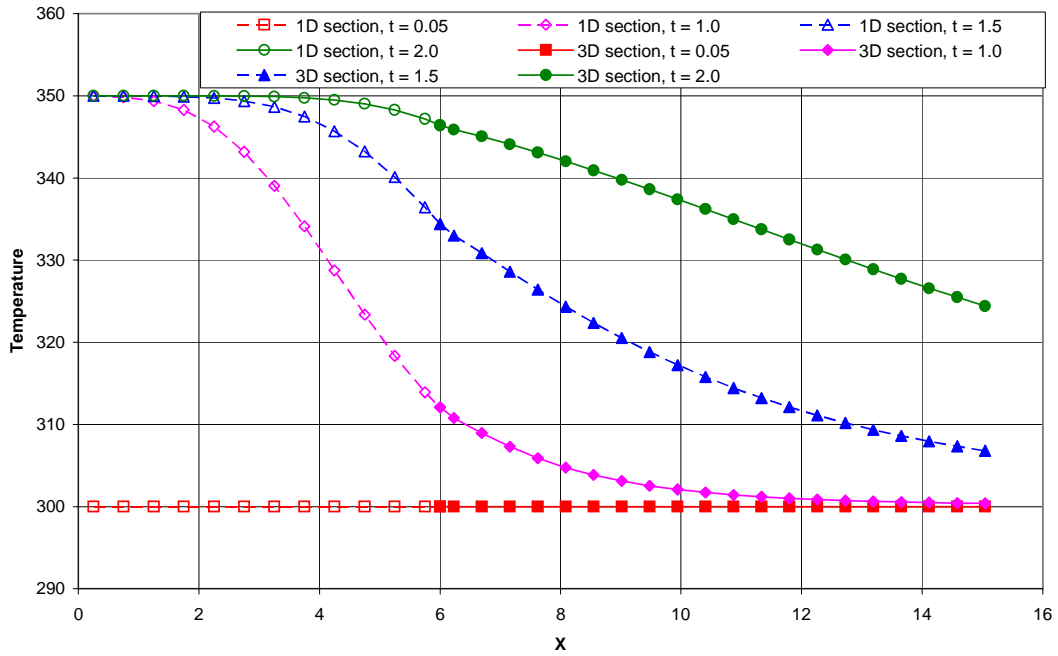


**Figure 4. Comparison of Pressure Distribution in Pipe with Slug and Analytic Inflow Profiles**

In the second demonstration case, the pipe inlet temperature was abruptly increased at  $t=0.05$  with the analytic velocity profile. For slug flow input to the 3D code, the thermal transient was started after the initial pressure transient relaxed to a steady state ( $t = 0.36$  s in Fig. 4). Therefore temperature was abruptly increased at  $t = 0.41$  s. The results for these cases are shown in Figures 5 and 6, respectively. In the 3D section an adiabatic wall boundary condition is applied, hence the enthalpy (and temperature in this case) is constant in the radial direction in the absence of viscous dissipation. Thus the thermal wave is one-dimension here. The temperature distribution versus axial location is shown at several times during the transient. The 3D code inlet temperature is passed from the 1D code as a Dirichlet boundary condition. It can be seen (Figure 5) that a slight discontinuity is evident in the slope at the matching location ( $x = 6$ ) between the 1D and 3D computations. This can be corrected through a more implicit coupling procedure between the 1D and 3D codes. This discontinuity is much more severe in the case with slug flow input to the 3D computation (Fig. 6).

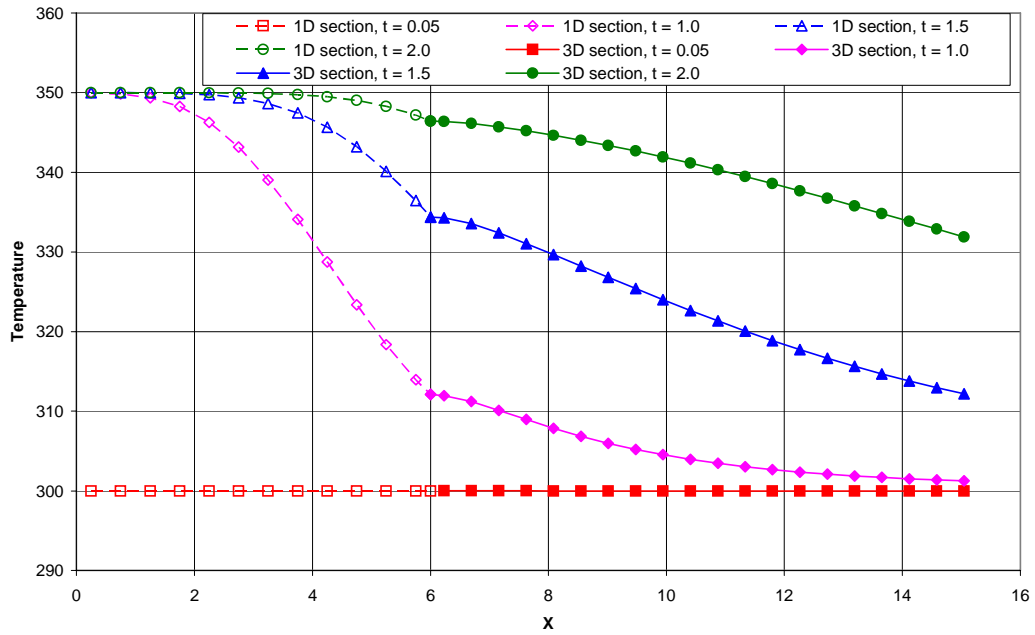
Figures 5 and 6 emphasize the importance of a good assumption of flow distribution across the surface separating the 1-D region from the 3-D CFD region. For single phase flow, a standard distribution worked well. For two-phase flow, the problem is much more complex. As a minimum, cross-channel distributions of two-velocities and void fraction will be needed. This may require a large number of full CFD calculations to develop a range of profiles for fully developed flow, consistent with geometry and flow conditions expected in the coupled calculation

**Thermal Transient  
Analytic Inflow Profile to 3D Code**



**Figure 5. Thermal transient with Analytic Inflow Velocity Profile**

**Thermal Transient  
Slug Inflow to 3D Code**



**Figure 6. Thermal transient with Uniform Inflow Velocity Profile.**

#### 4. CONCLUSIONS AND RECOMMENDATIONS

Results presented here reflect a limited amount of effort available to study the issue of benchmarking. Within the context of Laufer's experiments, we would suggest both the problem presented here and one in which flow is from the 3-D to the 1-D region, to provide a controlled study of coupling effects. Within this context several key aspects of the coupling problem can be carefully studied:

1. Interaction of spatial and temporal difference methods in the two regions;
2. Implicitness of the coupling between the regions;
3. Significance of consistent wall terms and state equations;
4. Distribution of mean 1-D variables over the connecting surface for use by the 3D calculation; and
5. Averaging methods to extract 3-D information for use by the 1-D calculation.

With basic understanding of coupling accomplished, more ambitious benchmarks may also be attempted. Results of the University of Maryland boron dilution tests [7] provide one obvious option. CFD could be used to model the vessel, and a systems code used for the balance of the experiment. However, results should be viewed with caution. Macian and Mahaffy [8] performed a 3-D simulation of a similar experiment [9] using an Euler based code (no turbulence). Results matched quite well with a relatively coarse mesh, provided correct azimuthal splitting of the flow was obtained as it entered the downcomer. We suggest focusing attention of such a benchmark on the ability to model spreading of the inlet liquid jet as it impacts the downcomer wall.

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