RANS CFD SIMULATIONS FOR CASL THM USING DREKAR::CFD

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Abstract. This brief report describes work directed towards completion of the Thermal Hydraulics Methods (THM) Level 3 Milestone THM.CFD.P5.02 for the Consortium for Advanced Simulation of Light Water Reactors (CASL) Nuclear Hub effort. The focus of this milestone was to deliver validated results from the Sandia Drekar CFD simulation code for Reynolds Averaged Navier-Stokes (RANS) turbulent models for the CASL Benchmark Test Cases #1 and #2. This milestone is a continuation of the THM Level 3 Milestone THM.CFD.P5.01 completed June 30, 2012.
1 INTRODUCTION

Full scale system level simulations of high Reynolds number flows in PWR reactors with coupled neutronics and conjugate heat transfer remain a very computationally challenging problem. Even solving the turbulent flow alone in a geometry representing only a fraction of the entire system remains a very difficult problem. For this class of problems solving the Reynolds averaged equations is currently the only feasible option for obtaining solutions. Unsteady RANS or large-eddy simulation may someday be feasible. Until then there is a great need to develop steady-state RANS models and push this methodology as far as it can be and understand the strengths and weaknesses and quantify uncertainties. For this reason RANS modeling capabilities are being developed in Drekar for the CASL program. Our approach is to use fully implicit and fully coupled finite element methods that are very efficient for achieving steady-state solutions and for coupled multi physics simulations (e.g., turbulent flow and conjugate heat transfer). These solutions can be obtained by integrating a transient solution to steady-state with very large time steps (pseudo-time stepping), sometimes directly to steady-state and also by parameter continuation where an initial simulation at a particular parameter value (e.g., Re) is then continued to trace out an entire solution branch (see e.g., [1]). An important feature of the Drekar infrastructure is that it supports sensitivity and uncertainty quantification (UQ) algorithms. This is in both an embedded and in a black-box mode with an existing coupling interface to DAKOTA. This technology was demonstrated in a companion VUQ milestone that carried out an initial UQ study (L3:VUQ.SAUQ.P5.02) using Drekar and two RANS models. Finally Drekar also has the potential capability to carry out parameter continuation along with bifurcation and linear stability studies as well [1].

A detailed description of Drekar is beyond the scope of this report. A theory manual was written as part of an earlier milestone and is available as a CASL archive [2]. Instead, the main ideas behind the RANS models and how they couple to the Navier-Stokes equations will be presented.

Of the many RANS models proposed two models have been chosen for an initial capability in Drekar. The first model is due to Spalart and Allmaras [3]. This model includes a single time dependent advection-diffusion-reaction PDE for the eddy viscosity. This viscosity couples to the Navier-Stokes equations using the Boussinesq approximation. Therefore, the stress tensor in the momentum equation is modified by an additional ”effective” viscosity. The second model, a variation of the classic $k-\epsilon$ two equation model, due to Lam&Bremhorst [4] is implemented. $k-\epsilon$ is also an eddy viscosity that couples to the momentum equation in the same way as Spalart-Allmaras through an effective turbulent viscosity.

Steady-state solutions to the $3 \times 3$ rod/spacer grid problem using the Spalart-Allmaras RANS turbulence model have been demonstrated and reported on earlier in the theory manual [2] and an earlier CASL milestone report (THM.CFD.P4.02) [5]. For these solutions we were able to take time steps that grew to CFL > 10,000 which allowed the code...
to quickly integrate to 2.5 seconds of physical time.

In the remaining sections, RANS models appropriate for solving incompressible isothermal high Reynolds number flows are described along with the modifications to the momentum equations necessary for coupling. Next, two CASL benchmark test cases are described. Solutions to these test cases are achieved through pseudo-transient time integration. Then results from the solution of these tests are presented. We conclude a summary of progress towards solving turbulent flows using the RANS methodology.

2 RANS MODELS for INCOMPRESSIBLE ISOTHERMAL TURBULENT FLOWS

In the Reynolds Averaged Navier-Stokes turbulence model methodology, a time filter is applied to the dependent flow variables resulting in the decomposition of the instantaneous velocity field into mean and fluctuating components,

\[ \mathbf{u} = \overline{\mathbf{u}} + \mathbf{u}' \]  

and produces new equations that are very similar to the unfiltered equations with the addition of the Reynolds stress \( \tau_t \),

\[ \tau_t = -\rho \mathbf{u}' \otimes \overline{\mathbf{u}}. \]  

This new apparent stress arises mathematically through the filter operation applied to the nonlinear advection term. It is responsible for the modification of the flow field through turbulent fluctuations. In terms of numerical simulation, it represents the “closure problem” in that additional information or equations are now required that describe \( \tau_t \) in order to close the filtered system of equations making solutions possible. Given a description of \( \tau_t \), it is added to the “real” stresses in the original momentum equation, providing the necessary coupling. A common approach is to use the Boussinesq approximation where the Reynolds stresses are related to the filtered stresses through the following;

\[ \tau_t = -\rho \mathbf{u}' \otimes \overline{\mathbf{u}} \approx \mu_t [\nabla \overline{\mathbf{u}} + \nabla \overline{\mathbf{u}}^T] - \frac{2}{3} [\mu_t \nabla \cdot \overline{\mathbf{u}} + \rho k] \mathbf{I} \]  

where \( \mu_t \) is the turbulent or eddy viscosity and

\[ k = \frac{1}{2} \mathbf{u}' \cdot \mathbf{u}' = \frac{1}{2} (u'^2 + v'^2 + w'^2) \]  

is the turbulent kinetic energy. The last term in Equation 3 is necessary for the trace of both sides of the expression to be consistent. Now the closure problem reduces to the task of calculating the eddy viscosity and turbulent kinetic energy.
3 GOVERNING FLOW EQUATIONS

The equations governing fluid motion are the Navier-Stokes equations. These equations are listed in Table 1. They represent the conservation of mass and momentum. These equations are written in “residual” form which is typical for the discretization of these equations via the finite element method. In these equations, $\rho$ is the density (a constant),

\begin{align*}
\mathbf{u} &= \mathbf{u}_i, \quad i = 1, 2, 3 \text{ is the “Reynolds Averaged” velocity vector with index } i \text{ representing Cartesian components in the } (x, y, z) \text{ directions. } \mathbf{T} \text{ is the stress tensor for a Newtonian fluid; } \\
\mathbf{T} &= -p \mathbf{I} + \tau + \tau_t = -P \mathbf{I} + \mu_{eff}[\nabla \mathbf{u} + \nabla \mathbf{u}^T] - \frac{2}{3} \mu_{eff}(\nabla \cdot \mathbf{u}) \mathbf{I} \quad (5)
\end{align*}

where $p$ is the isotropic hydrodynamic pressure, $\mu_{eff}$ is the effective dynamic viscosity that can have contributions from turbulence models (e.g., $\mu_{eff} = \mu + \mu_t$), and $\mathbf{I}$ is the unity tensor. It is common practice to replace the pressure in the momentum equation with the sum of hydrodynamic pressure and turbulent kinetic energy;

\begin{equation}
P = p + \frac{2}{3} \rho k. \quad (6)
\end{equation}

Therefore, the equations are closed by providing an estimate of the eddy viscosity and turbulent kinetic energy.

3.1 Spalart-Allmaras Eddy Viscosity Model

The Spalart-Allmaras turbulence model equation [3] for an incompressible fluid is given in Table 2. The eddy viscosity is given by,

\begin{align*}
R_{\nu} &= \rho \frac{\partial \hat{\nu}}{\partial t} + \rho \mathbf{u} \cdot \nabla \hat{\nu} - \nabla \cdot \left( \rho \left( \nu + \hat{\nu} \right) \nabla \hat{\nu} \right) - C_{b1} \rho \hat{\nu} \hat{S} + C_{w1} f_w \rho \left( \frac{\hat{\nu}}{\sigma} \right)^2 - \frac{C_{b2} \hat{\nu}}{\sigma} (\nabla \hat{\nu} \cdot \nabla \hat{\nu}) = 0 \\
\mu_t &= \rho \hat{\nu} f_{v1}. \quad (7)
\end{align*}
Functions defining the source terms and non-conservative viscous terms in the model are listed below;

\[
f_{v1} = \frac{\chi^3}{\chi^3 + C_{v1}}, \quad f_{v2} = 1 - \frac{\chi}{1 + \chi f_{v1}}, \quad f_{w} = g \left( \frac{1 + C_{w3}}{g^6 + C_{w3}} \right)^{1/6}
\]
\[
\chi = \frac{\hat{\nu}}{\nu}
\]
\[
\begin{align*}
g &= r + C_{w2}(r^6 - r), \\
r &= \frac{\hat{\nu}}{S k^2 d^2}
\end{align*}
\]
\[
\hat{S} = (2\Omega \Omega)^{1/2} + \frac{\hat{\nu} f_{v2}}{k^2 d^2}, \quad \Omega = \frac{1}{2} (\nabla \mathbf{u} - \nabla \mathbf{u}^T)
\]

where \( \Omega \) is the rotation tensor. Model parameters are listed in Table 3.

<table>
<thead>
<tr>
<th>( k )</th>
<th>( C_{b1} )</th>
<th>( C_{b2} )</th>
<th>( \sigma )</th>
<th>( C_{w1} )</th>
<th>( C_{w2} )</th>
<th>( C_{w3} )</th>
<th>( C_{v1} )</th>
<th>( C_{v2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.41</td>
<td>0.1355</td>
<td>0.622</td>
<td>2/3</td>
<td>( \frac{C_{b1}}{C_{v2}} + \frac{1 + C_{w2}}{\sigma} )</td>
<td>0.3</td>
<td>2.0</td>
<td>7.1</td>
<td>5.0</td>
</tr>
</tbody>
</table>

Table 3: Model parameters for Spalart-Allmaras turbulence model.

\( k \) is von Karman’s constant, and \( d \) appearing in the source terms represents the normal distance to the wall. At a solid wall, \( \mu_t = 0 \), and therefore the boundary condition is, \( \hat{\nu}_w = 0 \). A different formula for \( \hat{S} \) has been proposed in Blazek [6] that prevents it from taking a value of zero. The modified term, \( \hat{S}_{mod} \), is:

\[
\hat{S}_{mod} = f_{v3} (2\Omega \Omega)^{1/2} + \frac{\hat{\nu} f_{v2}}{k^2 d^2},
\]
\[
f_{v2} = \left( 1 + \frac{\chi}{C_{v2}} \right)^{-3}
\]
\[
f_{v3} = \frac{(1 + \chi f_{w} v_1)(1 - f_{v2})}{\max(\chi, 0.001)}.
\]

### 3.2 \( k - \epsilon \) Turbulence Model

Many variations of the original \( k - \epsilon \) model have been proposed. We have chosen as the first candidate, the version by Lam&Bremhorst [4] due to the relative ease of implementing the low Reynolds number wall damping functions within the context of an unstructured mesh code.

For wall bounded flows, the standard \( k - \epsilon \) model must be modified in the vicinity of walls in order to capture the correct asymptotic behavior. Patel et al. [7] summarize several low Reynolds number versions of \( k - \epsilon \) turbulence models. The version from Lam&Bremhorst [4] has the advantage of not requiring \( y^+ \) locally. Instead only the normal distance from the wall is required. This simplifies the numerical implementation. However, the wall boundary condition for \( \epsilon \) is more complicated. The low Reynolds number version of \( k - \epsilon \) are written Table 4.
Table 4: $k - \epsilon$ RANS Turbulence Model Equations.

\[
R_k = \rho \frac{\partial k}{\partial t} + \rho \mathbf{u} \cdot \nabla k - \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right) - P_k + \rho \epsilon = 0
\]

\[
R_\epsilon = \rho \frac{\partial \epsilon}{\partial t} + \rho \mathbf{u} \cdot \nabla \epsilon - \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_\epsilon} \right) \nabla \epsilon \right) - \frac{\epsilon}{k} (f_1 C_1 \epsilon - f_2 C_2 \rho \epsilon) = 0
\]

The dependent variable $k$ has units of velocity squared and the dissipation rate $\epsilon$ has units of velocity squared over time. Eddy viscosity is given by;

\[
\mu_t = C_\mu f_\mu \frac{\rho k^2}{\epsilon}.
\]  

(10)

The production term is;

\[
P_k = \tau_t \otimes \nabla \mathbf{u}
\]

(11)

which for incompressible flow can be written as;

\[
P_k = \frac{\mu_t}{2} \left( \nabla \mathbf{u} + \nabla \mathbf{u}^T \right)^2.
\]

(12)

Wall damping is controlled by the following functions;

\[
f_\mu = (1 - \exp(-A_\mu Re_n))^2 \left( 1 + \frac{A_t}{Re_t} \right)
\]

(13)

\[
f_1 = 1 + (A_{C1}/f_\mu)^3
\]

(14)

\[
f_2 = 1 - \exp(-Re_t^{2})
\]

(15)

where two Reynolds numbers are defined;

\[
Re_t = \frac{\rho k^2}{\mu \epsilon} \quad Re_n = \frac{\rho k^{1/2} y_n^2}{\mu}
\]

(16)

and $y_n$ is the normal distance to the wall. A summary of the Lam&Bremhorst low Re model model parameters are presented in Table 5.

<table>
<thead>
<tr>
<th>$C_\mu$</th>
<th>$C_{\epsilon 1}$</th>
<th>$C_{\epsilon 2}$</th>
<th>$\sigma_k$</th>
<th>$\sigma_\epsilon$</th>
<th>$A_t$</th>
<th>$A_{C1}$</th>
<th>$A_\mu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.09</td>
<td>1.44</td>
<td>1.92</td>
<td>1.0</td>
<td>1.3</td>
<td>20.5</td>
<td>0.05</td>
<td>0.165</td>
</tr>
</tbody>
</table>

Table 5: Model parameters for Lam&Bremhorst $k - \epsilon$ turbulence model.

At wall boundaries $k_w = 0$. Specification of $\epsilon_w$ is more difficult. Lam&Bremhorst suggest the following,

\[
\epsilon_w = \nu \left( \frac{\partial^2 k}{\partial y_n^2} \right)w
\]

(17)

6
which is difficult to implement in an unstructured mesh code and will not be used. Patel et al. [7] suggest the natural condition;

\[
\frac{\partial \epsilon}{\partial y_{\text{wall}}} = 0
\]  

may be used. For \( \epsilon_w \), Baglietto and Ninokata [8] suggest the following boundary condition;

\[
\epsilon_w = \frac{2\nu \bar{k}}{\bar{y}^2}
\]  

where \( \bar{k} \) and \( \bar{y} \) are measures of the turbulent kinetic energy and normal-distance-to-the-wall within the cell respectively. Additional implementation details are available in the theory manual [2].

The turbulence models described above require the normal-distance-to-wall (ndtw) to evaluate the wall damping functions. This is true for Spalart-Allmaras and \( k-\epsilon \) models. The technique used in Drekar is presented by Tucker [9]. A distance scalar variable is solved for from the equation listed in Table 6. It has the boundary condition, \( \phi_w = 0 \) at walls. The normal distance is then determined from

\[
d = -\sqrt{\sum_{j=1,3} \left( \frac{\partial \phi}{\partial x_j} \right)^2} \pm \sqrt{\sum_{j=1,3} \left( \frac{\partial \phi}{\partial x_j} \right)^2 + 2\phi}
\]  

and equals the minimum absolute value of the two choices.

4 DESCRIPTION of PROBLEM GEOMETRY and FLOW CONDITIONS

This section describes the flow conditions, boundary conditions, computational domains and grids used to simulate the two CASL Benchmark Test Cases; #1 and #2 [10].

Case #1 is fully developed turbulent pipe flow. The wall surface is assumed to be smooth. The geometry is cylindrical with diameter \( D \). For this flow field periodic boundaries are assumed at the inflow and outflow planes of the geometry. With this assumption, the length of the pipe is arbitrary and is typically chosen to be 1 – 2\( D \). A Reynolds number based on \( D \) is used to parameterize the turbulence;

\[
Re_D = \frac{\rho U D}{\mu}
\]
where $U$ is the velocity magnitude at the center of the pipe. Computational grids are generated using Cubit [11]. The flow is forced by a constant volumetric pressure gradient in the $z$-component of the momentum equation.

Case #2 is circular pipe flow through a sudden expansion with and without swirl. A sketch of the geometry is shown in Figure 1. Again, the pipe surfaces are assumed to be smooth and the expansion is abrupt. A pipe with diameter $D$ and radius $R_1$ terminates into a pipe with diameter $2.5D$ and radius $R_2$. Flow is in the $z$ direction. The inlet is placed at $z = -0.05D$, the expansion plane at $z = 0$ and the outlet is at $z = 5D$. The benchmark specification has $z = 1.825D$. However, this proved to be too short causing a significant modification to the flowfield due to the outflow boundary condition. A natural boundary condition and a no-radial flow boundary condition were prescribed. Unless otherwise stated, the no-radial flow boundary condition was used in the simulations. A swirl number $S$ is defined as the ratio of angular momentum flux to linear momentum flux divided by a reference radius [12]. For this axisymmetric configuration the inflow velocity vector is described by an axial component $V_z$ and an azimuthal component $V_\theta$. $V_\theta = \omega r$ is specified as solid body rotation. Both $U_z$ and $\omega$ are constant. Given this definition for the inlet velocity, $S$ is defined as:

$$S = \frac{\omega R_1}{2U_z}.$$  \hfill (22)

The flow is specified by $Re_D$ and $S$. The walls are assumed to be no-slip. At the outflow boundary, a zero stress condition is assumed for pressure, the axial velocity component, and the transported turbulence variables. The two tangential components of velocity are set to either zero or zero stress.

Two views of the three-dimensional 62,000 element tube computational mesh are shown in Figure 2. The Cubit journal files are parameterized to allow for modification to the near wall spacing in order to adjust the mesh to achieve an appropriate value for $y^+$,

$$y^+ = u_+ y/\nu$$
where $y$ is understood to be the normal distance to the wall.

Two views of the 141,568 element sudden expansion tube computational mesh are shown in Figure 3. Similarly, the Cubit journal file allows for the control of the inlet pipe boundary layer, expansion pipe boundary layer and the shear layer grid regions.

5 BRIEF DESCRIPTION OF DREKAR

Drekar is an unstructured fully-implicit finite element Navier-Stokes solver with the capability to include coupled conjugate heat and mass transfer effects [13], [2], [5].

The temporal discretization is based on a variable-order fully-implicit multi-step backward differentiation (BDF) method that can vary from first-order (a.k.a. Backward Euler) to a fifth-order BDF method (BDF5). The spatial discretization is currently an equal-order stabilized finite element (SFE) approach that can employ linear or quadratic interpolation. Convection stabilization is achieved through the streamline-upwind-Petrov-Galerkin (SUPG) approach and discontinuity-capturing operators can also be included as part of the stabilized finite element formulation [13, 14, 15]. A parallel fully-coupled solution procedure based on an scalable algebraic multilevel preconditioned Newton-Krylov method is used to solve the discretized system of equations [14, 15]. Therefore, the RANS equations and RANS turbulence model equations are solved in a fully coupled manner.

6 RESULTS

In the results that follow BDF1 pseudo-transient time integration is used to march the solutions to a steady-state. Pseudo-transient time integration strategies start with crude initial conditions and a relatively small initial time step. As the solution evolves, larger time steps are chosen in order to reduce the total number of time steps required to reach steady-state. In some of the expansion tube simulations, a steady-state was not achieved due to massive precession of the swirling flow. The spatial discretization is linear.
equal-order stabilized FE methods, and SUPG convection stabilization has been used in the numerical formulation to solve the turbulent flow equations described above. The results for this study were obtained by parallel runs on from 32 up to 128 cores of the SNL Redsky parallel capacity machine.

6.1 Fully Developed Turbulence in a 3D Tube

A summary of the simulations for the three-dimensional tube, and sudden expansion tube, are presented in Table 7, and Table 8, respectively. The natural boundary condition was assumed for $\varepsilon_w$ in the $k-\varepsilon$ model at solid walls.

For the 3D tube problem, The pressure gradient was chosen as $dP/dz = 50N/m^3$, the density was set equal to $1kg/m^3$, and the viscosity was specified as $1e-5kg/ms$ yielding a $Re_D = 307,800$. The meshes where designed to achieve $y^+ \approx 1$ for the finest mesh and then increased in size away from the wall. (For a summary of the 3D tube simulations refer to Table 7). Steady-state solutions are obtained by time marching from an initial state and aggressively ramping the time step size. Initial time steps correspond to CFL 1. Maximum values are presented in the Table. In all cases except mesh-I using the $k-\varepsilon$ model, a steady-state was achieved. The damping functions in the Lam&Bremhorst
Table 7: Summary of 3D tube runs.

<table>
<thead>
<tr>
<th>Mesh</th>
<th>#Elem</th>
<th>Model</th>
<th>CFL(max)</th>
<th>Time (sec.)</th>
<th>Reynolds no.</th>
<th>$y^+$</th>
</tr>
</thead>
<tbody>
<tr>
<td>G</td>
<td>52,400</td>
<td>SA</td>
<td>9,048</td>
<td>20</td>
<td>307,800</td>
<td>11.75</td>
</tr>
<tr>
<td>A</td>
<td>62,000</td>
<td>SA</td>
<td>1.88</td>
<td>20</td>
<td>307,800</td>
<td>7.71</td>
</tr>
<tr>
<td>E</td>
<td>78,000</td>
<td>SA</td>
<td>95,978</td>
<td>20</td>
<td>307,800</td>
<td>1.18</td>
</tr>
<tr>
<td>E-mod</td>
<td>78,000</td>
<td>SA</td>
<td>42,760</td>
<td>20</td>
<td>307,800</td>
<td>1.18</td>
</tr>
<tr>
<td>F-mod</td>
<td>86,000</td>
<td>SA</td>
<td>44,467</td>
<td>20</td>
<td>307,800</td>
<td>0.55</td>
</tr>
<tr>
<td>H</td>
<td>70,000</td>
<td>$k-\epsilon$</td>
<td>1,162</td>
<td>2.68</td>
<td>307,800</td>
<td>3.69</td>
</tr>
<tr>
<td>I</td>
<td>70,000</td>
<td>$k-\epsilon$</td>
<td>1.67</td>
<td>0.34</td>
<td>307,800</td>
<td>5.37</td>
</tr>
<tr>
<td>E</td>
<td>78,000</td>
<td>$k-\epsilon$</td>
<td>156,145</td>
<td>20</td>
<td>307,800</td>
<td>1.18</td>
</tr>
</tbody>
</table>

Table 8: Summary of 3D sudden expansion tube simulations.

<table>
<thead>
<tr>
<th>Mesh</th>
<th>#Elem</th>
<th>Model</th>
<th>Omega</th>
<th>Swirl no.</th>
<th>CFL(max)</th>
<th>Time (sec.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>444,240</td>
<td>SA</td>
<td>20</td>
<td>0.08</td>
<td>3,688</td>
<td>2.71</td>
</tr>
<tr>
<td>B</td>
<td>141,568</td>
<td>SA</td>
<td>0</td>
<td>0</td>
<td>92,963</td>
<td>50</td>
</tr>
<tr>
<td>B</td>
<td>141,568</td>
<td>SA</td>
<td>20</td>
<td>0.08</td>
<td>108,491</td>
<td>50</td>
</tr>
<tr>
<td>B</td>
<td>141,568</td>
<td>SA</td>
<td>42.5</td>
<td>0.17</td>
<td>4,473</td>
<td>20.53</td>
</tr>
<tr>
<td>B</td>
<td>141,568</td>
<td>SA</td>
<td>100</td>
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<td>2,803</td>
<td>9.16</td>
</tr>
<tr>
<td>B-ns</td>
<td>141,568</td>
<td>SA</td>
<td>100</td>
<td>0.40</td>
<td>2,748</td>
<td>28.81</td>
</tr>
<tr>
<td>B</td>
<td>141,568</td>
<td>SA</td>
<td>162.5</td>
<td>0.65</td>
<td>958</td>
<td>7.96</td>
</tr>
<tr>
<td>C</td>
<td>175,200</td>
<td>SA</td>
<td>20</td>
<td>0.08</td>
<td>93,747</td>
<td>50</td>
</tr>
<tr>
<td>D</td>
<td>123,392</td>
<td>SA</td>
<td>20</td>
<td>0.08</td>
<td>109,012</td>
<td>50</td>
</tr>
<tr>
<td>B</td>
<td>141,568</td>
<td>$k-\epsilon$</td>
<td>0</td>
<td>0</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>D</td>
<td>123,392</td>
<td>$k-\epsilon$</td>
<td>0</td>
<td>0</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>C</td>
<td>175,200</td>
<td>$k-\epsilon$</td>
<td>0</td>
<td>0</td>
<td>—</td>
<td>—</td>
</tr>
</tbody>
</table>

Model are very sensitive to $y^+$. Departure from $y^+ \approx 1$ not only affects the solution, it also negatively impacts convergence to steady-state. For case I, $y^+ \approx 5.37$, the solver was unable to increase the time step substantially and so many time steps were necessary to achieve a steady-state. While the solution was evolving toward a steady-state, the amount of time necessary to complete the simulation was considered to be not worth the cost. A possible solution is to limit the production of turbulent kinetic energy and/or eddy viscosity in the viscous sublayer. In addition, a different low Re version of $k-\epsilon$ model that contains more robust damping functions is being considered as a replacement for the current version.

Time histories of the total kinetic energy are presented in Figures 4 and 7 for SA and $k-\epsilon$ models respectively. It has been determined that $f1$ which is responsible for increasing $\epsilon$ near the wall and thus damping the eddy viscosity becomes very stiff as the near wall normal spacing departs from $y^+ \approx 1$. The stiffness precludes taking large time steps. Simulations E-mod and F-mod use the modified source terms described above. The modified source terms improve nonlinear solver robustness.
Mean axial velocity profiles are presented in Figures 5 and 8 for SA and $k-\epsilon$ models respectively. In Figure 5 mesh convergence is alluded to by the close agreement between meshes A,E,E-mod, and F. The difference between E and E-mod are very small demonstrating the utility of using the modified source terms.

In Figure 8 mesh convergence is less convincing due to the absence of a third case. At this point we can only offer that the I-mesh is slowly approaching the a solution close to the H- and E-meshes but since it has not achieved steady-state, it was omitted from the plot.

In order to carry out validation of the RANS models the law-of-the-wall is taken from the CASL benchmark report [10] that presents and references experimental results. In the log region:

$$U^+ = \frac{1}{0.41} \ln(y^+) + 5.2$$

and in the viscous sub-layer $U^+ = y^+$. These definitions are used to validate the two RANS models in the simulation of fully developed turbulent pipe flow. Figure 6 and 9 present the comparisons between simulations and law-of-the-wall. In Figure 6, the G-mesh with $y^+ = 11.75$ stands out as too coarse compared with the other meshes. Otherwise, the agreement is good. The slight dip in the log region of the $k-\epsilon$ predictions in Figure 9 are similar in shape to those reported in Patel et al. [7] for the Lam&Bremhorst version of the model.

![Figure 4: Time history of total kinetic energy in the tube with the Spalart-Allmaras turbulence model.](image-url)
Figure 5: Mean velocity profiles for the tube with the Spalart-Allmaras turbulence model.

Figure 6: Law-of-the-Wall for the tube with the Spalart-Allmaras turbulence model.
Figure 7: Time history of the total kinetic energy in the tube with the $k - \epsilon$ turbulence model.

Figure 8: Mean velocity profiles for the tube with Spalart-Allmaras $k - \epsilon$ turbulence models.
6.2 Turbulent Flow through an Axisymmetric Expansion Tube

The sudden expansion tube flow with swirl was simulated using the Spalart-Allmaras RANS model on four meshes. No rotation or curvature corrections were used. In each case the expansion region is 5D in length instead of 2D for reasons discussed earlier. The Reynolds number based on inner tube diameter was 10,000. The swirl number based Equation 22 ranges from 0.0 to 0.8. A summary of the different simulations is presented in Table 8. Similar to the 3D tube simulations, steady-state solutions are sought by time marching from an initial state with a modest time step and aggressively increasing the time step size. Very large values of CFL are achieved as the steady-state is approached.

During the course of investigating this problem and trying to match the experiments of Mak and Balabani [12] it became apparent that this benchmark was not characterized well enough to be a suitable benchmark for validation. The first reason is that the inflow conditions are difficult to match. The second reason is that the authors allude to a contraction in the expansion tube downstream of the measurement section that effects the flow field in the high swirl case. However, the specific change in geometry is not reported. For these reasons, we abandoned our attempt to validate our models with this as a benchmark. Instead, we ran a battery of tests with the goal of making qualitative comparisons to the experimental results. However, with slightly redesigned meshes, this benchmark could be used to perform a mesh convergence study.

In Figure 10, time histories of the total kinetic energy for different swirl numbers for the Spalart-Allmaras model are presented. As the swirl number is increased, more energy enters the system which accounts for the different energy plateaus. For S=0-0.08 the flows...
are steady. For $S=0.17-0.8$, the flows are unsteady. The average axial velocity profile for

![Expansion Tube 3D Total Kinetic Energy](image)

Figure 10: Time history of total kinetic energy in the 5D expansion tube with the Spalart-Allmaras
turbulence model.

three meshes is shown in Figure 11 at a distance of one inner-diameter down stream
from the expansion plane. The three meshes differ in the number of elements mainly in
the radial direction and so this comparison demonstrates mesh convergence in the radial
direction.

Figures 12 through 19 present images extracted from solutions on the B mesh for a
range of swirl number from 0 to 0.4. Figure 12 presents the case without swirl in the
inlet velocity. This solution has a stable radially expanding core. Primary and secondary
recirculation regions are evident from the streamlines. Figure 13 with $S=0.08$ is very
similar to the previous figure. Figure 14 presents radial plots of the axial velocity com-
ponent at four axial stations downstream from the expansion plane. The core is much
flatter than the experiment due to the obstruction in the flow upstream of the expansion
plane created by the apparatus that holds the swirl vanes in place. This makes validation
against experimental data difficult. As the swirl is increased to $S=0.17$, the simulations
are no longer steady. The core precesses around the outer wall and is flattened, no longer
circular. A time average of the unsteady solution is presented in Figure 18. From the
time average, is can be seen that the core expands radially outward more rapidly than
the smaller swirl number simulations.

Figure 16 is taken from the solution of a simulation with $S=0.4$. Again, the flow is
unsteady and the core precesses to a greater degree than the $S=0.17$ case. The time
average of this simulation is presented in Figure 19. Compared to the lower $S$ value
Figure 11: The average axial velocity profile at $z=1D$ for three different meshes; B, C, D, normalized by $U_z$ and the expansion tube radius using the Spalart-Allmaras turbulence model.

Figure 12: Image of sudden expansion tube at 50 seconds with $S=0.0$, i.e., no swirl. The flow was computed using the Spalart-Allmaras model. The image is an iso-surface of $V_z$ and the surface is colored by $V_x$ which is a cross-stream velocity component.
Figure 13: Image of sudden expansion tube at 50 seconds with $S=0.08$. The flow was computed using the Spalart-Allmaras model. The image is an iso-surface of $V_z$ and the surface is colored by $V_x$ which is a cross-stream velocity component.

Figure 14: Image of sudden expansion tube at 50 seconds with $S=0.08$. The flow was computed using the Spalart-Allmaras model. The image is $r-z$ plane colored by the value of $V_z$. The axial velocity in the radial direction at four axial locations shows the evolution of the flow field core and recirculation zones.
RANS CFD simulations: Shadid, Smith, Pawlowski, Cyr, Weber

Figure 15: Image of sudden expansion tube at 12.21 seconds with $S=0.17$. The flow was computed using the Spalart-Allmaras model. The image is an iso-surface of $V_z$ and the surface is colored by $V_x$ which is a cross-stream velocity component. The flow is unsteady and has the end of the jet precessing around the larger cylinder near the exit.

Simulations, the radial expansion is much more rapid.

Similar simulation using $k-\epsilon$ with $S=0$ and $S=0.8$ are currently underway and the results will be updated as these are completed. It should be noted that the Drekar implementation of $k-\epsilon$ is less mature than Spalart-Allmaras model and because of the defined role of Drekar in the current CASL THM effort there has been just a limited amount of effort put into refining the convergence of this model. At this point something is preventing the code from increasing the time steps as large as the SA RANS model and so the code is time marching at a relatively small constant value compared to the SA RANS model. Stiffness may be due to; inflow conditions, wall boundary conditions for $\epsilon$ or the source terms. We believe a modest effort is required to rectify this inadequacy in the $k-\epsilon$ model implementation.

7 CONCLUSIONS

This milestone is a continuation of the THM Level 3 Milestone THM.CFD.P5.01 completed June 30, 2012 in which a demonstration of a new RANS turbulent flow simulation capability was presented. In the current report, two CASL THM CFD benchmark problems where chosen to validate the new RANS capability. The first benchmark was fully developed turbulent pipe flow with a relatively high Reynolds number. The second benchmark was an axisymmetric sudden expansion pipe without and with swirl. Pseudo-transient time integration was used to march solutions to steady-state.
Figure 16: Image of sudden expansion tube at 3.1 seconds with $S=0.4$. The flow was computed using the Spalart-Allmaras model. The image is an iso-surface of $V_z$ and the surface is colored by $V_x$ which is a cross-stream velocity component.

Figure 17: Image of sudden expansion tube at 26.3 seconds with $S=0.4$. The flow was computed using the Spalart-Allmaras model. The image is an iso-surface of $V_z$ and the surface is colored by $V_y$ which is a cross-stream velocity component. Zero stress conditions were imposed on pressure and all velocity components. The four time history plots at the bottom of figure are; maximum $\nu$ in the domain, $\nu$, pressure and $V_x$ at a single grid vertex.
Figure 18: Image of sudden expansion tube with $S=0.17$. The flow was computed using the Spalart-Allmaras model. The image is an iso-surface of $V_z$ and the surface is colored by $V_x$ which is a cross-stream velocity component. The flow is unsteady and has the end of the jet precessing around the larger cylinder near the exit. This image is a time-average and indicates the time-averaged spread of the swirling jet.

Figure 19: Image of sudden expansion tube with $S=0.4$. The flow was computed using the Spalart-Allmaras model. The image is an iso-surface of $V_z$ and the surface is colored by $V_x$ which is a cross-stream velocity component. This image is a time-average and indicates the time-averaged spread of the swirling jet.
In the pipe flow problem, for both Spalart-Allmaras and the Lam&Bremhorst version of $k - \epsilon$, the law-of-the-wall was validated using a variety of meshes that mainly differed by the near wall spacing. In the context of the implicit solution methods the Spalart-Allmaras model can be time marched at very large time steps with $CFL > 10,000$ in a number of cases for reasonable meshes and $y^+$. This was also shown to be the case with the the $k - \epsilon$ model for this problem however the degradation of the time step sizes for poor quality meshes was much more severe.

The second benchmark dealing with sudden expansion without and with swirl was based on an experiment. Through the course of trying to reproduce the experimental results, it was determined that this benchmark is ill-defined and is not a good candidate for validation at this time. Instead, a battery of simulations using Spalart-Allmaras were run and qualitative comparisons with the experiment were made. The code was able to take very large time steps to achieve steady-state solutions for no swirl and low swirl cases. For high swirl numbers, the flow field is three-dimensional and unsteady. The unsteady aspect of this problem at high swirl numbers, the difficulty of reproducing the inflow velocity profile and the sensitivity of the outlet boundary conditions make the use of this problem difficult without further refinement. In a qualitative sense the geometry of the expanding jet, the existence of the primary and secondary recirculation, and the influence of swirl on this complex flow has been captured by the simulations. In general the simulations qualitatively correspond to the available experimental results as well as computational data furnished as part of the THM problem #2 benchmark.

For this problem simulations with $k - \epsilon$ model are still on-going. Due to stiffness in the model, the code can not increase the time step size to an acceptable value as in the 3D tube problem. This renders the time for the simulation times larger than we believe it should be. A modest effort will be required to resolve this issue.

In general this study has demonstrated the validation of the Drekar RANS models on a well characterized CFD turbulence problem, benchmark #1 (3D fully-developed turbulent pipe flow). It has also been demonstrated that the fully-implicit solution approach has some promise for this class of problems. It has also pointed out issues with the challenging TH-M problem #2. The results of this work could be used to further refine this problem or to point to a definition of a steady/transient problem that has some promise for evaluating the characteristics of RANS type models and also CFD solution methods.
REFERENCES


