INL/EXT-13-28747

Hydra-TH Simulation of Single-Phase Flow and Heat Transfer in a Rod Bundle Segment

Anh Bui
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The INL is a U.S. Department of Energy National Laboratory
operated by Battelle Energy Alliance

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Idaho National Laboratory
Idaho Falls, Idaho 83415

http://www.inl.gov

Prepared for the
U.S. Department of Energy
Office of Nuclear Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

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by Anh Bui and Hongbin Zhang

1. Objectives

The focus of this report is on the comparison of numerical prediction by Hydra-TH [1] of single-phase flow and heat transfer in a segment of Light Water Reactor (LWR) rod bundle geometries with experimental results of Krauss and Meyer [2]. This effort is to support the development of Hydra-TH code, which is a centerpiece of the CASL advanced CFD capability.

2. Problem Description

Single phase flow of air in 37-rod tube bundle is investigated. The rod bundle is similar to that used in experiments by Krauss and Mayer [2], which has a cross-section as shown in Figure 1 and a total length of 11.50 m with an unheated entrance length of 4.6 m and a heated length of 6.9. While the rod diameter is constant at 0.14 m, the pitch-to-diameter ratio P/D of the rod can be either 1.12 or 1.06. Measurements of flow temperature, velocity and turbulent characteristics are available for the cross-section located at 0.02 m from the outlet.

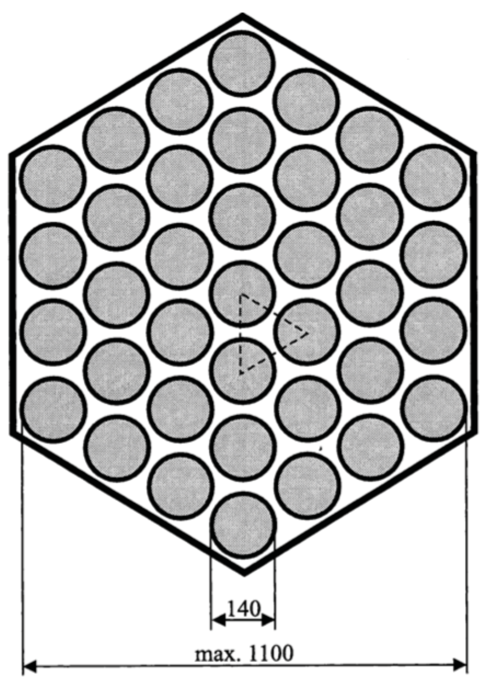


Figure 1: Cross-section of the 37-rod tube bundle used in experiments by Krauss and Mayer [2].

The experimental parameters of Krauss and Mayer's experiments are shown in Table 1.

Table 1. Experimental parameters [2].

Parameters	P/D=1.12	P/D=1.06
Bulk velocity $\overline{U}$, m/s	20.57	20.63
Bulk temperature, ^{o}C	39.7	47.0
Inlet temperature, ^{o}C	12.3	5.8
Hydraulic diameter D_h, mm	53.6	33.5
Reynolds number, Re	64590	38754
Wall heat flux, kW/m^2	1.39	0.98

3. CFD Model Information

- Solver: Hydra-TH
- Version: current
- Domain:

  By ignoring mixing between subchannels, the flow in a subchannel is assumed to be symmetrical. Consequently, only a small section of a subchannel is modeled (Figure 2). The computational domain has the cross-section as in Figure 3 and a total length of 7.88 m including a 1m unheated length and a 6.88 m heated length.

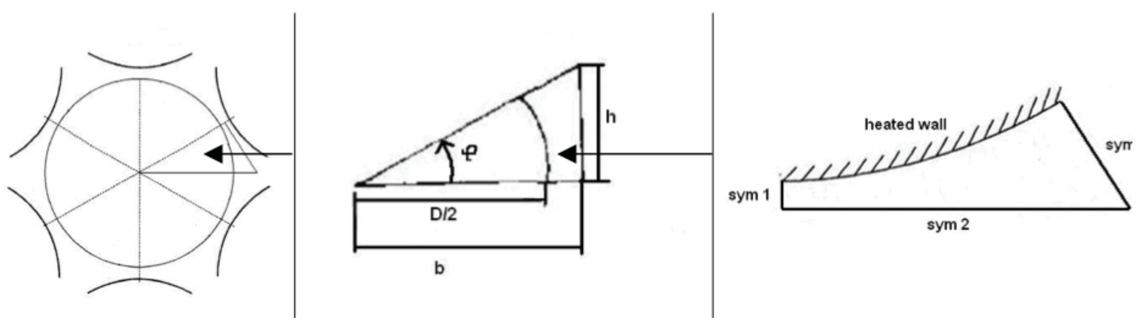


Figure 2. Computational domain being a 1/12 section of the flow channel.

- Boundary conditions:

  Symmetry boundary condition can be specified in Hydra-TH by setting the velocity component normal to a surface to zero. For the computational domain shown in Figure 2, symmetry boundary condition can easily be set for two perpendicular sides *sym1* and *sym2* (by aligning them with coordinate axes y and x and imposing zero velocities Ux and Uy, respectively, on them). However, the current version of Hydra-TH does not allow specification of symmetry boundary condition on the remaining fluid-fluid boundary using the same method. Both velocity components on this x-y plane therefore have to be set to zero. Such a “wall” type boundary condition for velocities on x-y plane will certainly affect the secondary flow driven by turbulence as shown in Figure 3.

On the heated wall, zero velocity and heat flux boundary conditions are set. Uniform velocity is specified at the inlet, and constant pressure is specified at the outlet.

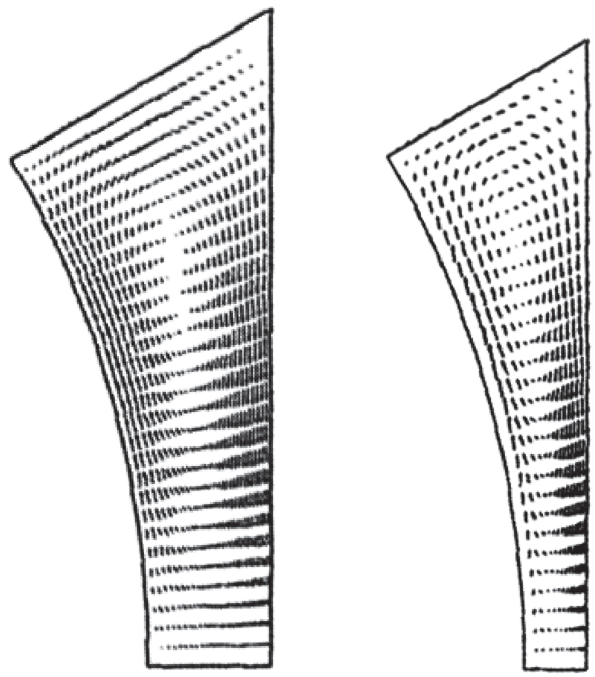


Figure 3. Turbulence-driven secondary flows predicted with SSG-RSM turbulence model [3].

- Turbulence model:

  Spalart-Allmaras turbulence model has been used. The model solves a single transport equation for turbulence that determines the turbulent viscosity [4].

- Mesh information, cell type, cell count, meshing parameters:

  Coarse meshes – about 132,000 hex8 elements;
  Fine meshes – about 1,058,000 hex8 elements;

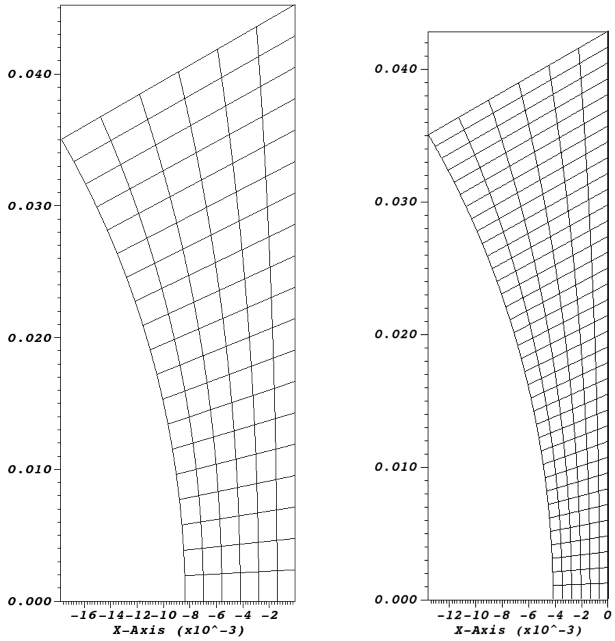


Figure 4. Cross-sections and coarse meshes of the computational domains for P/D equal 1.12 and 1.06, respectively.

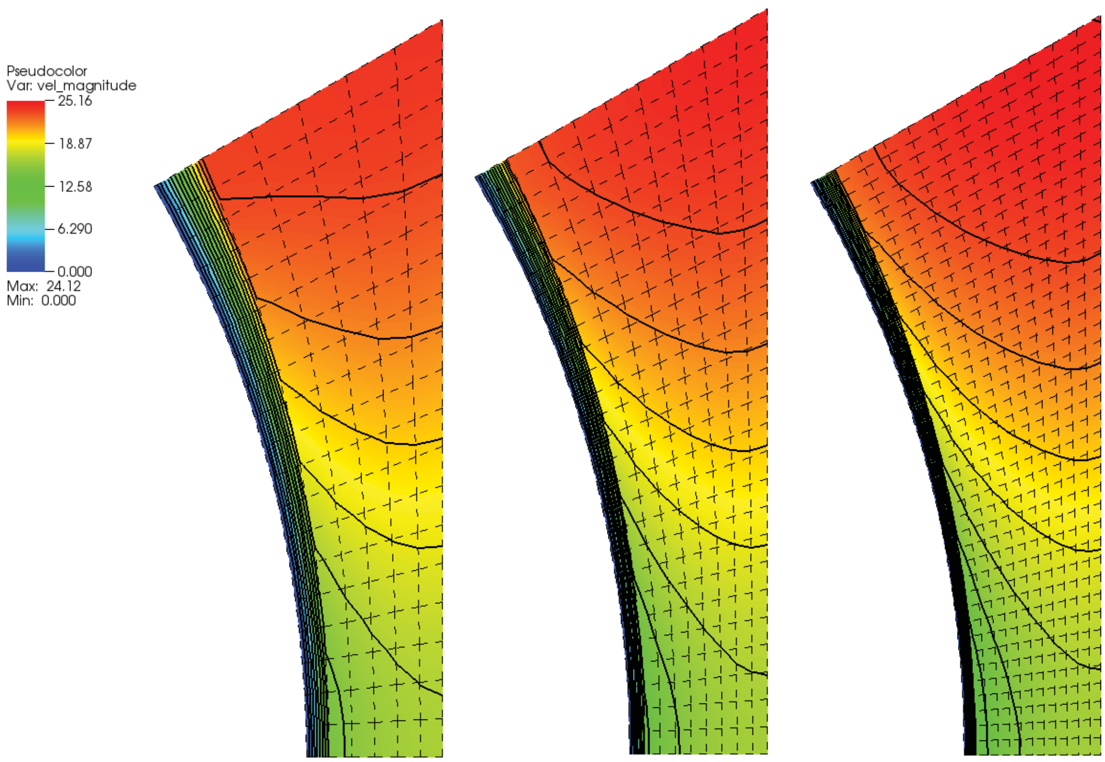


Figure 5. Effect of cross-sectional grid size reduction on prediction of velocity field at the outlet – left: 132,000 elements, middle: 280,000 elements, right: 567,000 elements.

- Solution control file: in appendix

4. Results & Discussions

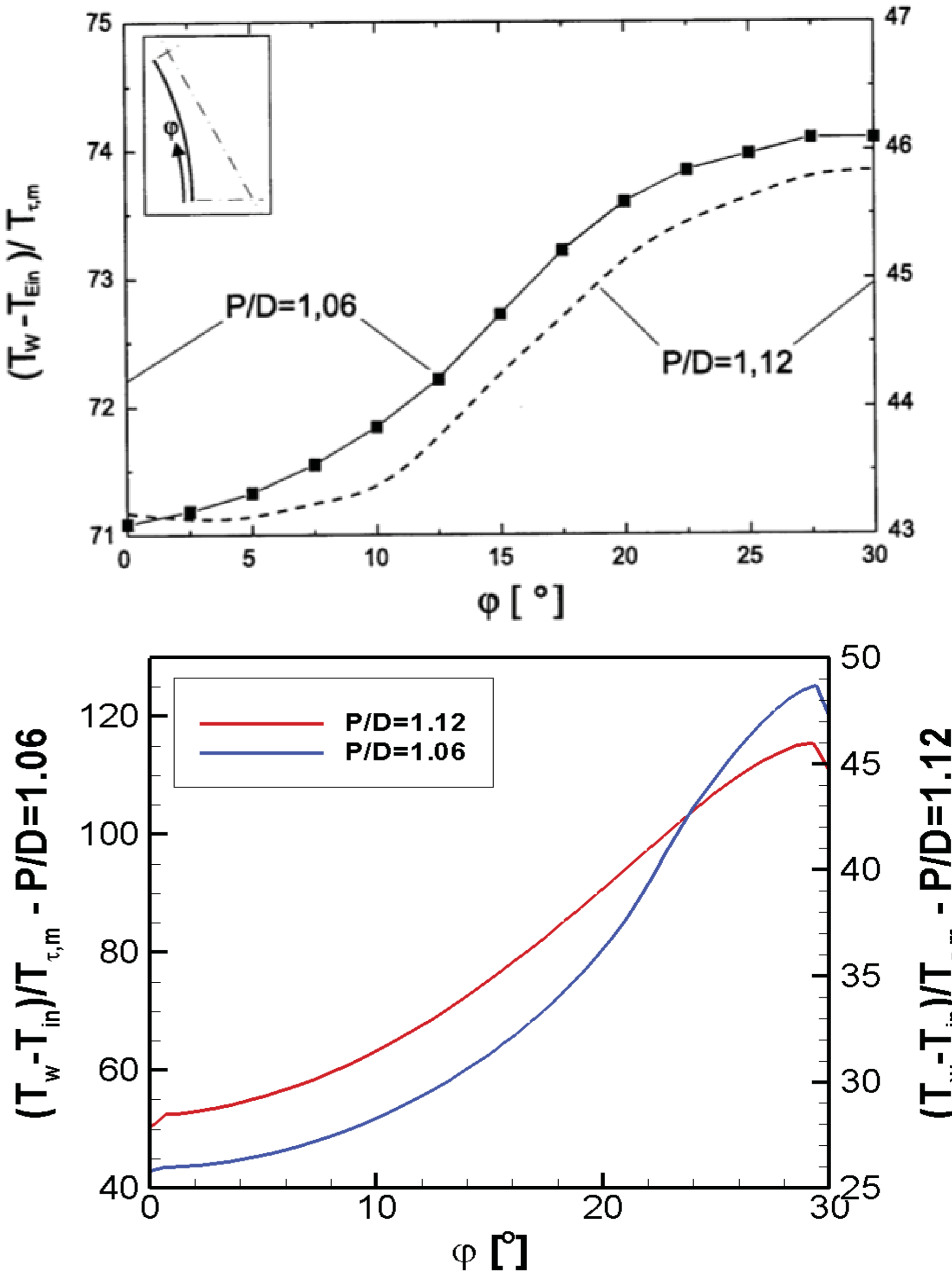


Figure 6. Dimensionless wall temperature from experiment (top) and Hydra-TH simulation (bottom).

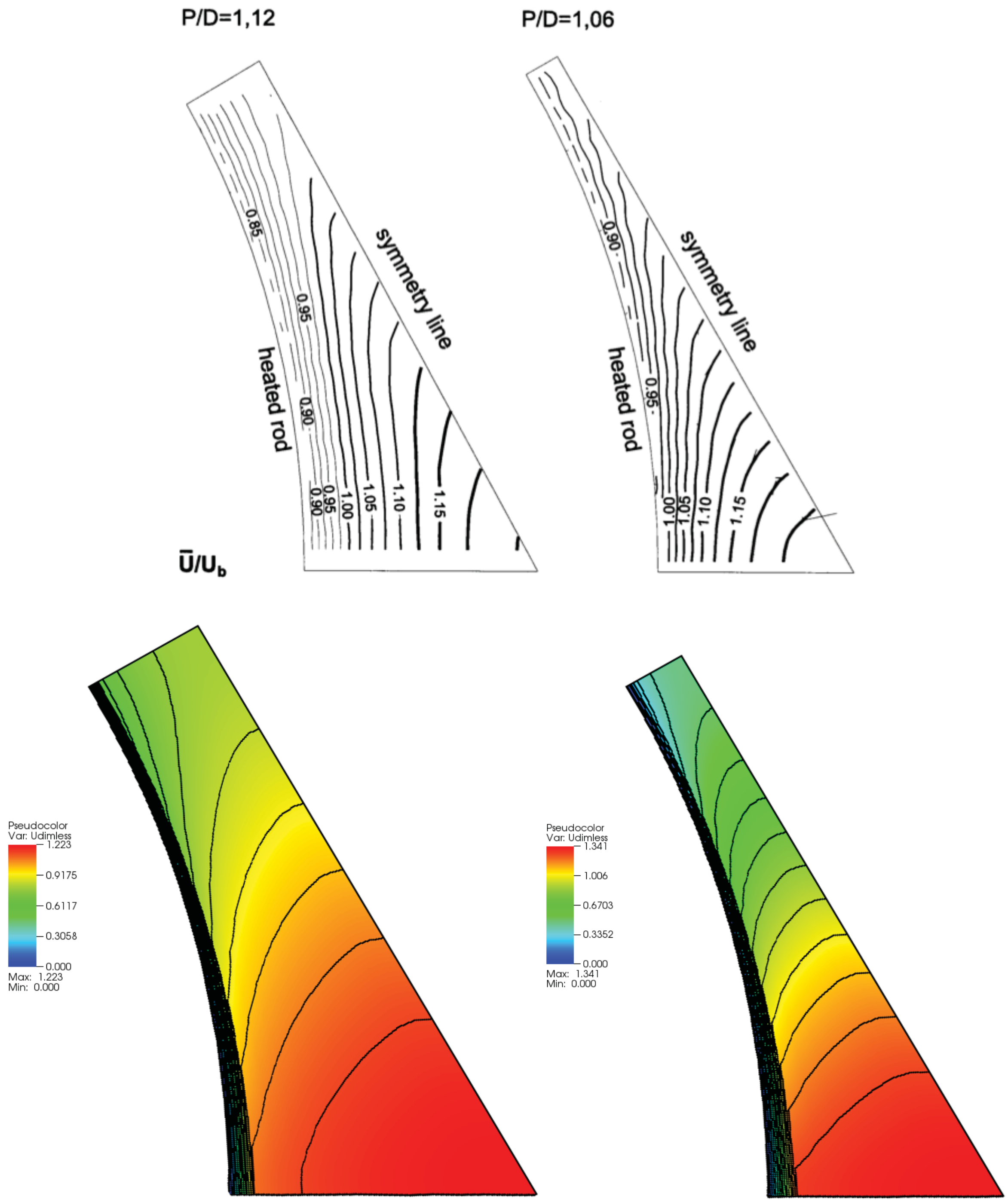


Figure 7. Distributions of velocity from experiments [2] (top) and Hydra-TH simulations (bottom).

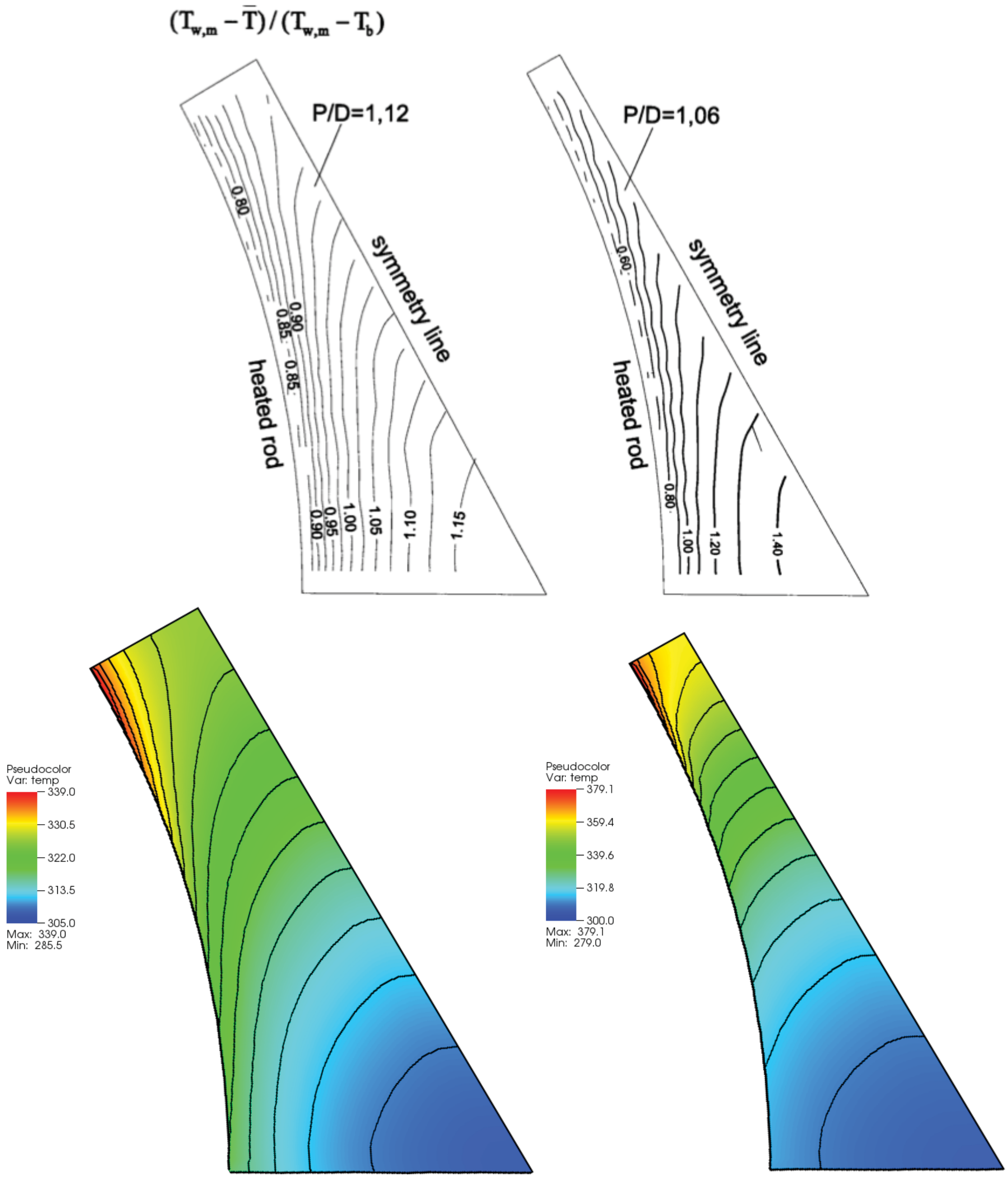


Figure 8. Distributions of dimensionless temperature from experiments [2] (top) and Hydra-TH temperature predictions (bottom).

Comparisons of the predictions of wall temperature and velocity distribution with experimental data are shown in Figures 6-8. Although similar in trends, the predicted gradients of wall temperature were found to be significantly higher than experimental data (Figure 6). The predictions of maximum velocity magnitudes were found comparable to the data, but the velocity distributions were different. These discrepancies could be caused by:

- Incorrect boundary conditions for velocity in the cross-sectional plane (as described earlier in the boundary condition setting section);
- Incorrect assumption about symmetry used in setting two other flow boundaries;
- Inadequate grid resolution near to the wall and its effect on turbulence modeling;
- Inadequacy of the chosen turbulence model. As shown in Figure 8, the choice of turbulence model could have a significant effect on the flow predictions, and all turbulence models tested in [3] could not provide predictions close to the experimental data. The modified (anisotropic) k-epsilon model proposed by Baglietto[5] was much better in predicting this flow;
- Lack of heat redistribution via thermal conduction along the wall.

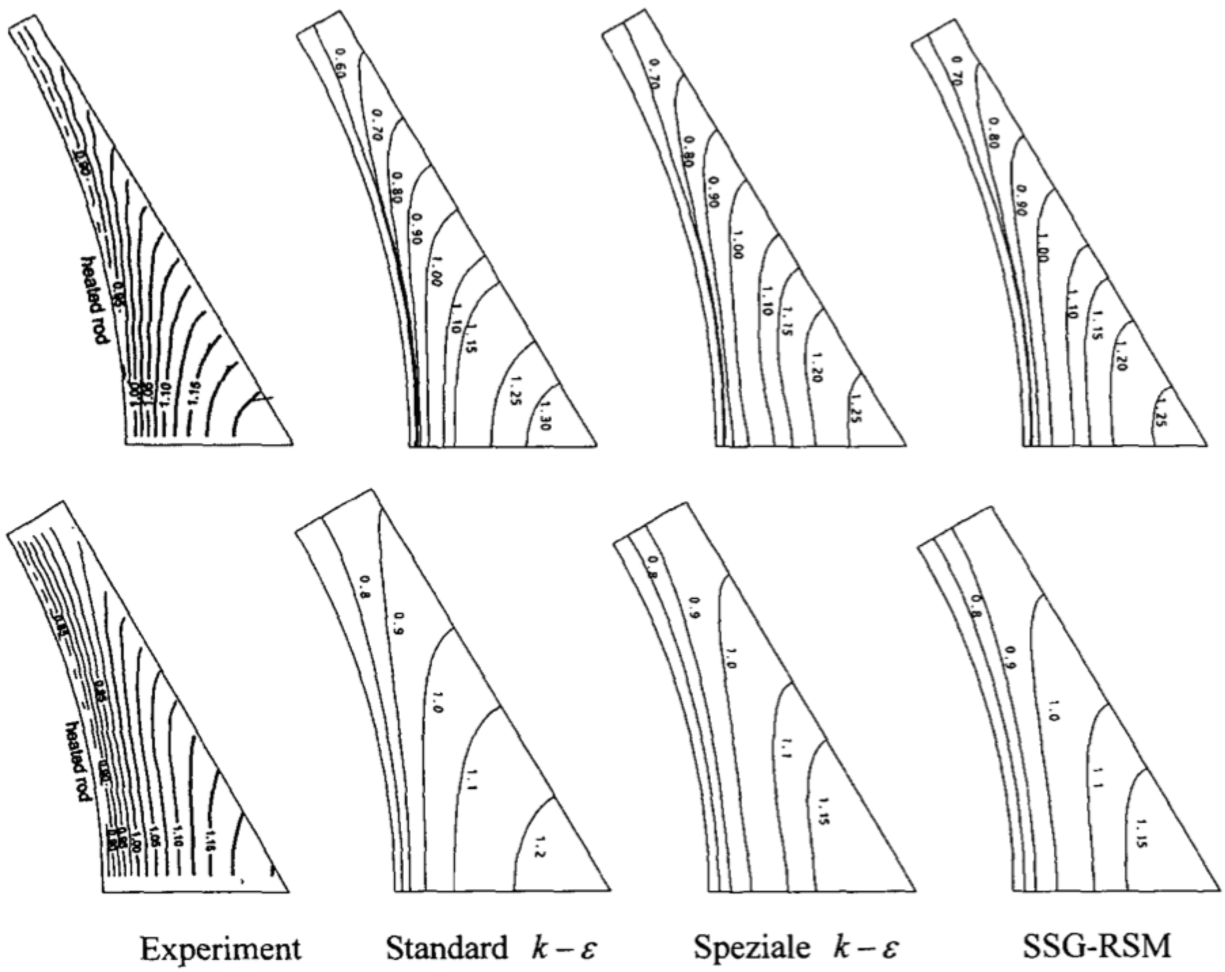


Figure 9. Comparison of CFD simulations and experimental data [3].

All simulations were conducted with the CFL set to be 20. The simulations could be difficult to converge with CFL equal 40. The parallel simulation capability of Hydra-TH was found to be robust.

5. Update 1

A simulation test on the geometry with P/D=1.12 was conducted with use of the RNG k-epsilon turbulence model available in Hydra-TH. The simulation results are shown in Figures 10-12. The comparison of velocity profiles obtained with the Spalart-Allmaras and RNG k-epsilon models indicates the inadequacy of near-wall grid resolution, which has more influence on the prediction by the Spalart-Allmaras turbulence model. There is, however, little difference in the predictions of wall and flow temperatures by these two turbulence models.

Table 2. Inlet settings for k-epsilon turbulence model.

Parameters	**P/D=1.12**	**P/D=1.06**
Turbulence intensity, I	5%	5%
Turbulent kinetic energy, $k = \frac{3}{2}(\overline{U}I)^2$	1.6	1.6
Turbulent dissipation rate, $\epsilon = C_\mu^{3/4} k^{3/2} (0.07 D_h)^{-1}$	87	142

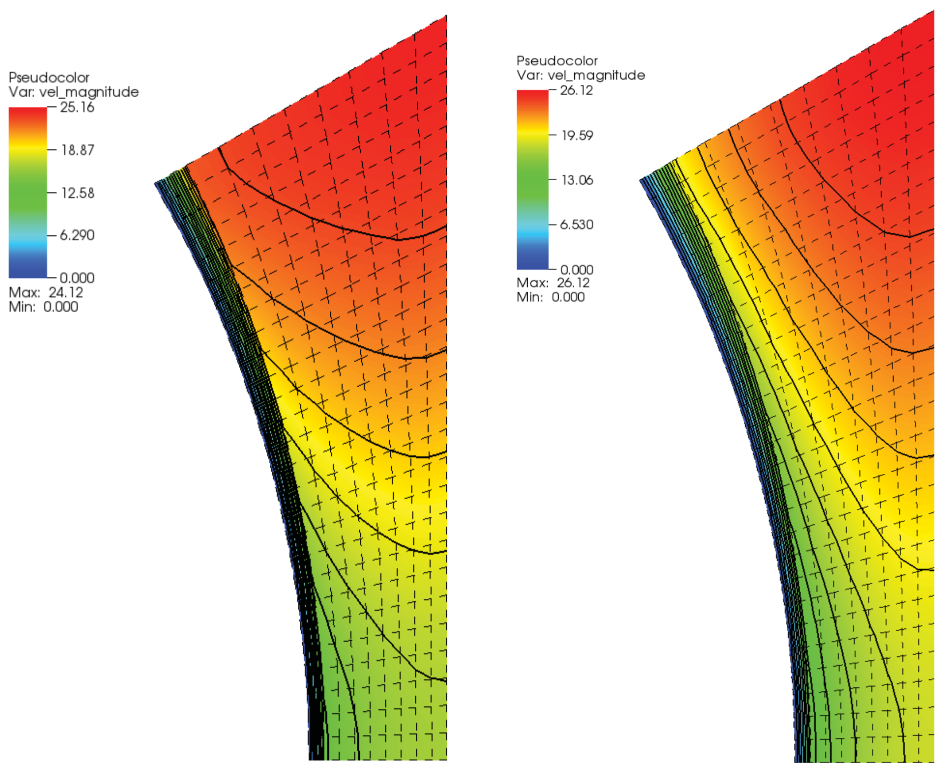


Figure 10. Comparison of velocity distribution predictions using the Spalart-Allmaras (left) and RNG k-epsilon (right) turbulence models.

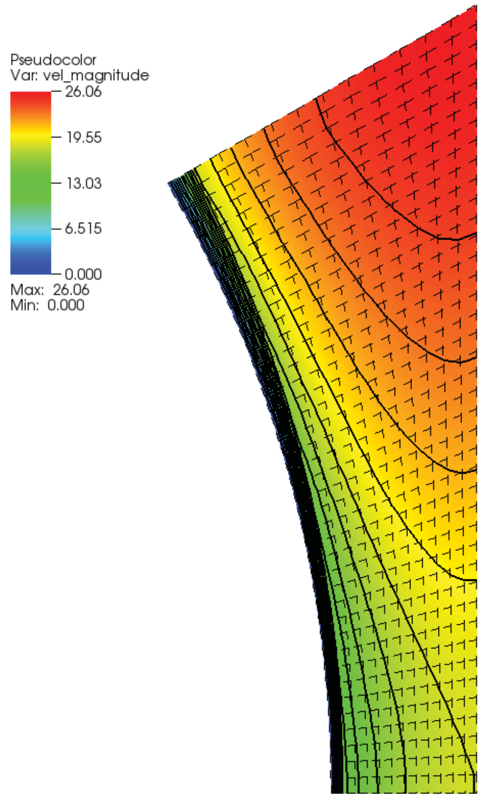
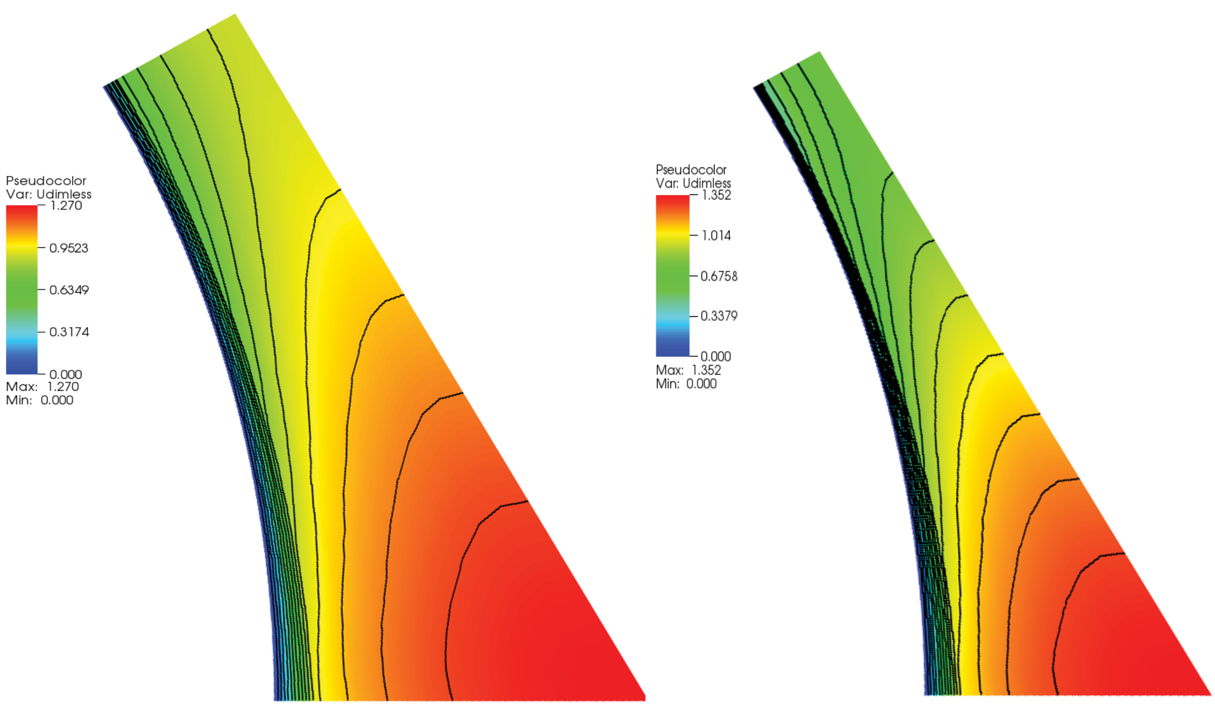


Figure 11. Prediction of velocity distribution with k-epsilon model using further refined mesh.



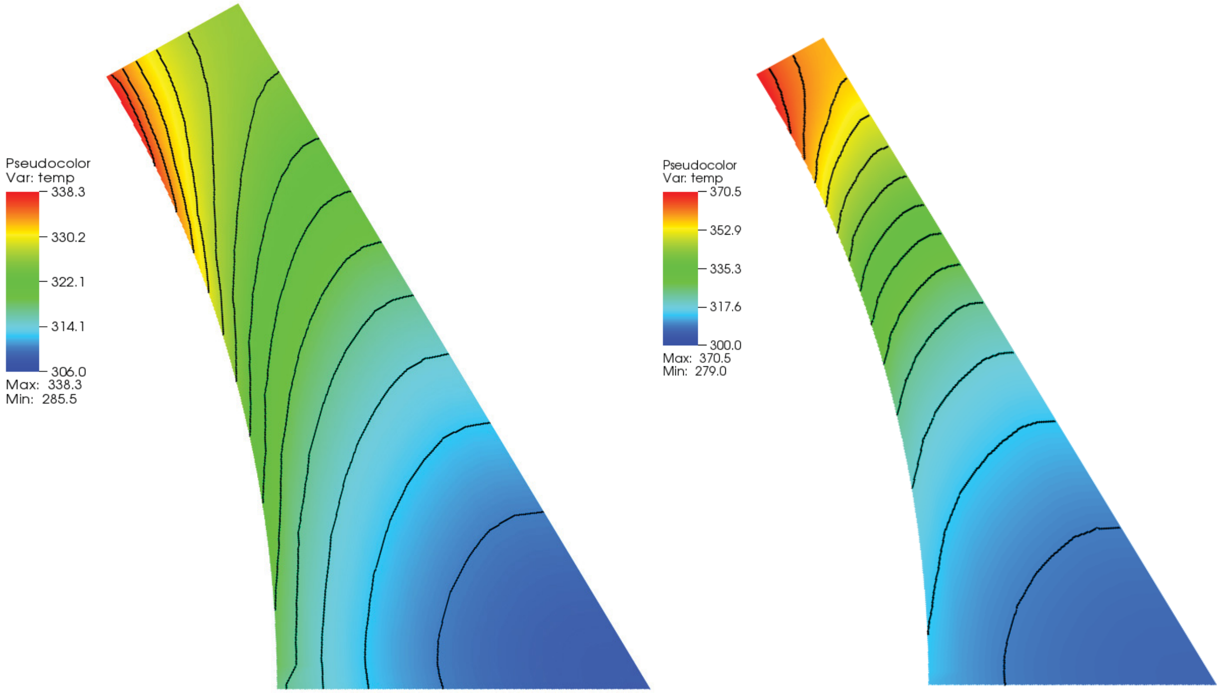


Figure 12. Predictions of dimensionless velocity (top) and temperature (bottom).

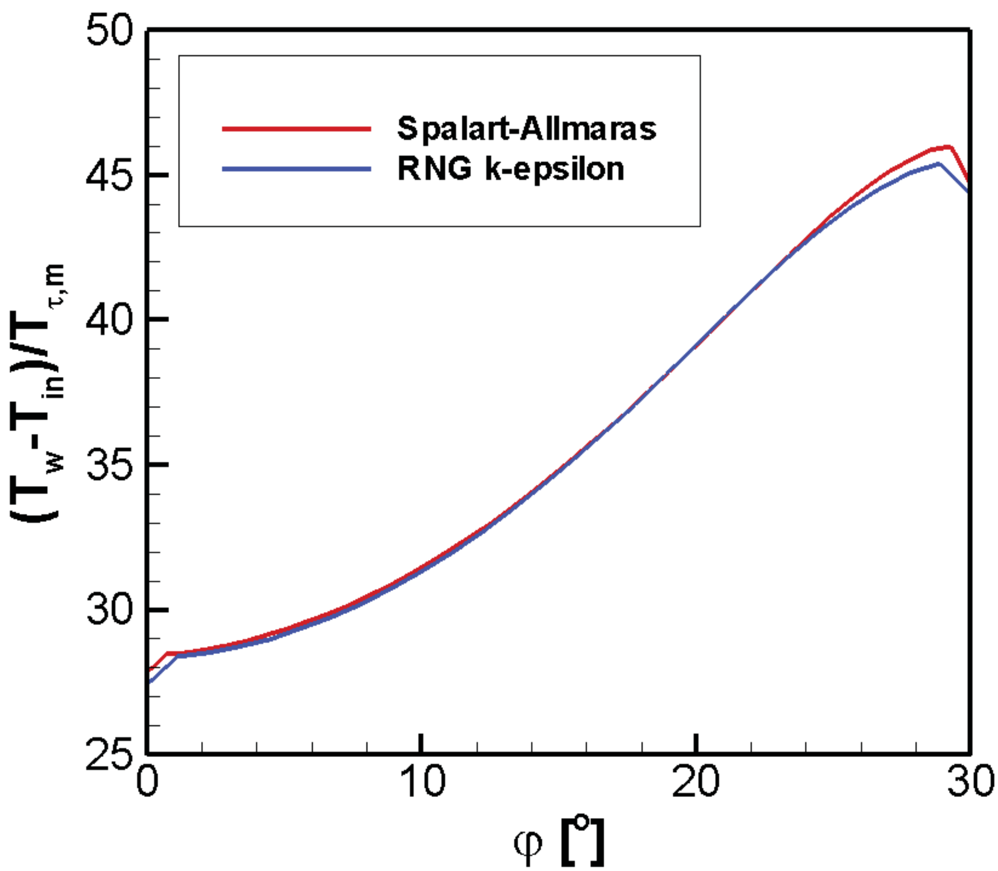


Figure 13. Comparison of wall temperature predictions.

6. Update 2

Prediction results obtained with Spalart-Allmaras and near-wall grid refinement are shown in Figures 14-16.

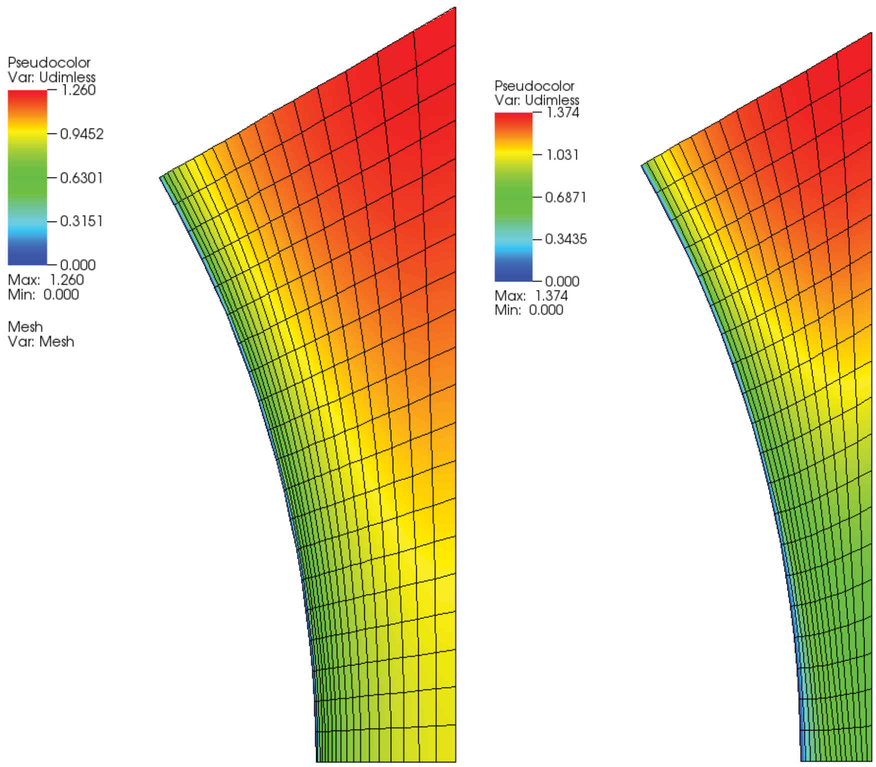


Figure 14. Velocity distributions and computational meshes.

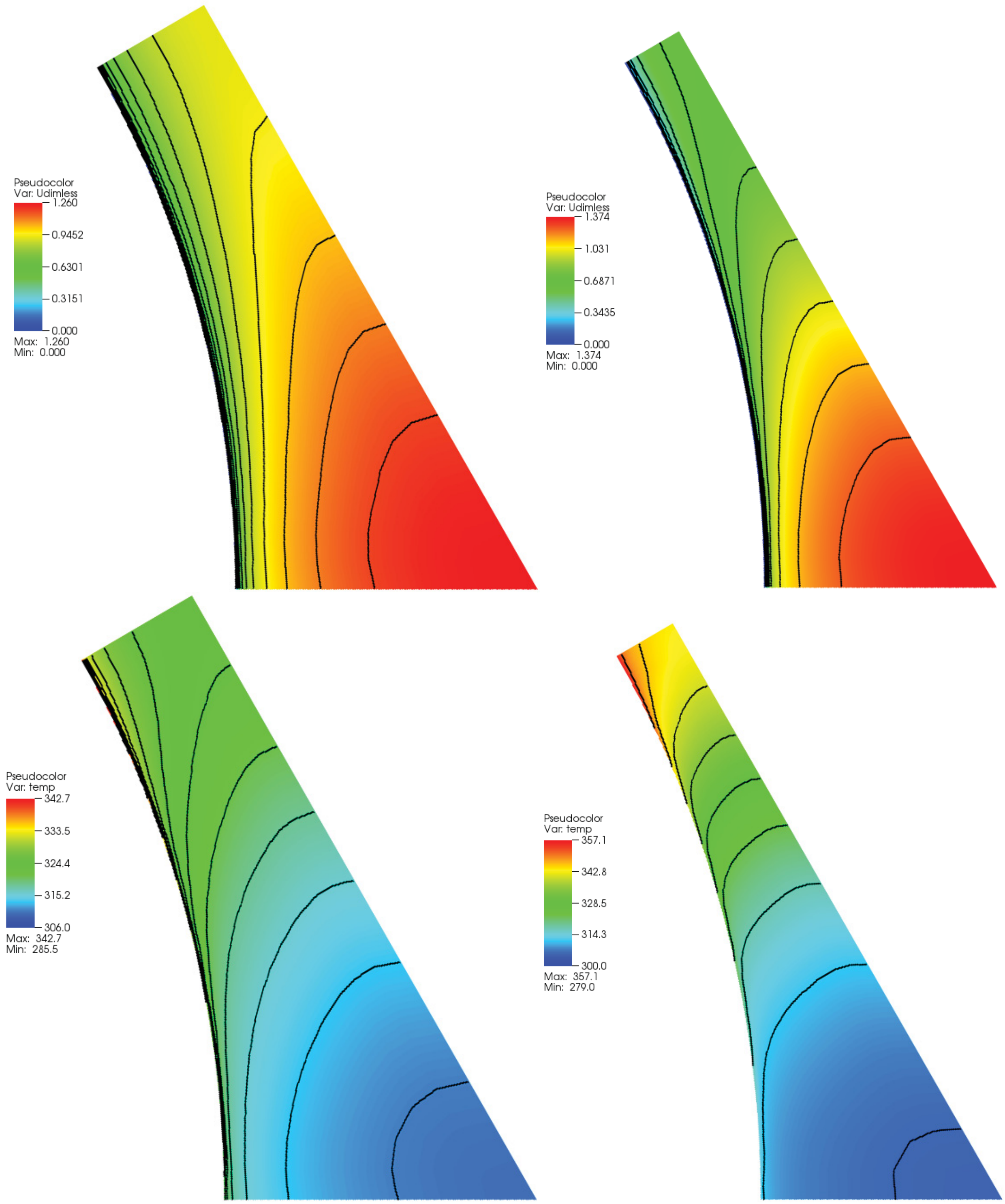


Figure 15. Predictions of dimensionless velocity (top) and temperature (bottom).

7. Recommendations for future work

For further verification and validation of Hydra-TH single-phase capabilities, it is recommended to conduct:

- Study of the effect of grid refinement near the wall;
- Testing of the Large-Eddy-Simulation (LES) capability;
- Implementation of symmetric boundary condition for boundaries not aligning with coordinate axes;
- Implementation of heat conduction model in solid walls and conjugate heat transfer coupling; The simulation results by Baglietto (Figure 16) [5] indicated the importance of heat conduction in solid rod in predicting wall temperature;
- Simulation of larger section of rod bundle domain to verify the correctness of symmetric boundary assumptions.

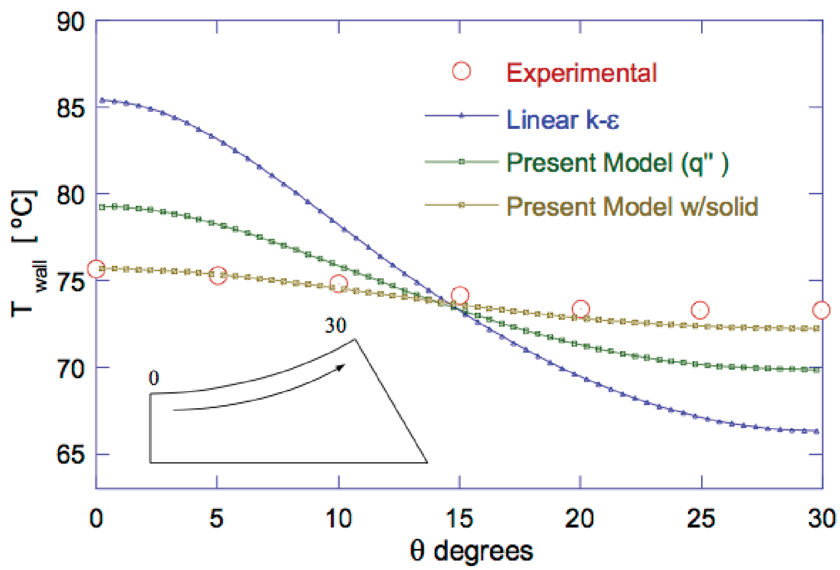


Figure 16. Predictions of wall temperature [5].

8. References

[1] M. Christon, J. Bakosi and R. Lowrie, "Hydra-TH User's Manual, Version: LA-CC-11120," Tech. report LA-UR-12-23181, LANL, 2011.

[2] T. Krauss and L. Meyer, "Experimental investigation of turbulent transport of momentum and energy in a heated rod bundle," *Nucl Eng Design,* vol. 180, pp. 185-206, 1998.

[3] W.-K. In, C.-H. Shin, D.-S. Oh and T.-H. Chun, "Numerical analysis of the turbulent flow and heat transfer in a heated rod bundle," *J Korean Nucl Soc,* vol. 36, no. 2, pp. 153-164, 2004.

[4] C. Rumsey, "Turbulence Modeling Resource," NASA Langley Research Center, [Online]. Available: http://turbmodels.larc.nasa.gov/spalart.html.

[5] E. Baglietto, "Anisotropic turbulence modeling for accurate rod bundle simulations," in *Proc of Int Conf on Nuclear Eng (ICONE)-14*, Miami, Florida, 2006.

Appendices

Brief Description of Hydra-TH

Hydra-TH [1] is a hybrid finite-element/finite-volume Computational Fluid Dynamics (CFD) code built with use of the Hydra toolkit. The code has been designed to simulate a broad class of incompressible, viscous fluid dynamics problems involving convective heat transfer. The new multiphase flow modeling capability is currently being added to the code. Hydra-TH has been chosen to be integrated with CASL Virtual Environment for Reactor Analysis (VERA) for predictive advanced simulation of Light Water Reactors (LWRs).

Hydra-TH solves the system of incompressible/low-March number Navier-Stokes equations. All equations are cell-centered and treated with a conservative discretization that includes a high-resolution monocity-preserving advection algorithm. The spatial discretization is derived using a discontinuous-Galerkin framework that, in the first-order limit, reduces to a locally-conservative finite-volume method. The time-integration methods include backward-Euler and the neutrally-dissipative trapezoidal method. The current implementation of numerical method is found to be stable for CFL in the range from 20 to 40.

The solution algorithm of Hydra-TH is based on a second-order projection method. The projection method allows a fully coupled solution of momentum and mass conservation equations. Hydra-TH has a number of options for linear algebraic solvers that include, for instance, the conjugate-gradient (CG), bi-conjugate gradient squared (BCGS), generalized minimum residual (GMRES), etc. Both linear algebraic libraries Petsc and Trilinos can be used for preconditioning and algebraic equation solution.

The Hydra-TH flow solver can make use of hybrid meshes comprising hex, tet, pyramid and wedge elements to permit meshing extremely complex geometries.

The current CFD features that Hydra-TH provides include the following [1]

- Solution of energy equation which may be in temperature or enthalpy form;
- Multiple turbulence models including large-eddy simulation (LES), detached-eddy simulation (DES) Spalart-Allmaras, and RNG k-epsilon with wall function treatment;
- Model of flow in porous media;
- Time-dependent boundary and source terms;

- Generalized body forces;
- Automatic time-step control;
- Different boundary conditions including Dirichlet boundary conditions for scalar and velocity, symmetry velocity conditions, pressure boundary condition, and heat flux wall boundary condition;
- Fluid-structure interaction using an arbitrary Lagrangian-Eulerian (ALE) formulation with mesh deformation;
- Coupling interface for use with 3rd-party codes for conjugate heat transfer and fluid-solid interaction.

Hydra-TH accepts meshes in Exodus-II format and produces outputs which can be visualized using different visualization software based on VTK, such as LLNL Visit, Paraview, etc.

Hydra-TH Inputs for P/D=1.12

```
title
Flow in a tube-bundle section
cc_navierstokes
 energy   temperature
 nsteps   2000
 deltat   0.0001
 term     2.0

 time_integration
  type    fixed_cfl
  CFLinit 1.0
  CFLmax  20.0
  dtmax   0.25
  dtscale 1.025
  thetaa  1.0
  thetak  1.0
  thetaf  1.0
 end

 # Output options
 pltype exodusii
 filetype serial
 plti   50
 ttyi   10
 dump  500

 # Turbulence model
 tmodel spalart_allmaras

 # Material model definition
 material
  id  1
```

```
  rho 1.127
  mu  19.238e-6
  Cp  1005.0
  Cv  718.0
  k11 0.0271
  gamma 1.4
end

materialset
  id 1
  material 1
  block 1
end

plotvar
  elem vel
  elem volume
  elem density
  elem div
  elem temp
  node vel
  node pressure
  node temp
  node turbnu
end

histvar
  elem 10 temp
end

# Simple IC's
initial
  velx 0.0
  vely 0.0
  velz 20.57
  temperature 285.45
  turbnu 1.0e-6
end

# Fixed pressure outlet
pressure
  sideset 20 -1 1.0e5
end

# Turbulent viscosity
turbnu
  sideset 30 -1 0.0
  sideset 31 -1 0.0
end

# Normal distance
distance
```

```
  sideset 30 -1 0.0
  sideset 31 -1 0.0
end

# Velocity BC's
velocity
 # Inlet
 velx sideset 10 -1 0.0
 vely sideset 10 -1 0.0
 velz sideset 10 -1 20.57
 # Wall
 velx sideset 30 -1 0.0
 vely sideset 30 -1 0.0
 velz sideset 30 -1 0.0
 velx sideset 31 -1 0.0
 vely sideset 31 -1 0.0
 velz sideset 31 -1 0.0
 # Symmetry
 velx sideset 40 -1 0.0
 vely sideset 50 -1 0.0
 velx sideset 60 -1 0.0
 vely sideset 60 -1 0.0
end

temperature
  sideset 10 -1 285.45
end

heatflux
        sideset 30 -1 1390.0
        sideset 31 -1 0.0
        sideset 40 -1 0.0
        sideset 50 -1 0.0
        sideset 60 -1 0.0
end

ppesolver
  type  AMG
  smoother ILU
  cycle W
  itmax 250
  itchk 1
  coarse_size 100
  diagnostics off
  convergence off
  eps 1.0e-8
end

momentumsolver
  type  ILUFGMRES
  itmax 50
  itchk 2
```

```
    restart 20
    diagnostics off
    convergence off
    eps   1.0e-8
  end

  transportsolver
    type  ILUFGMRES
    itmax 50
    itchk 2
    restart 20
    diagnostics off
    convergence off
    eps   1.0e-8
  end

end

exit
```