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A Multi-Year Plan for Enhancing Turbulence Modeling in Hydra-TH

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1 Executive Summary

The purpose of this milestone report is to document a multi-year plan for enhancing turbulence modeling in Hydra-TH. In Phase II of the Consortium for Advanced Simulation of Light Water Reactors (CASL) program, Hydra-TH is being developed to the meet the high-fidelity, high-Reynolds number CFD based thermal hydraulic simulation needs of the program. This work will be conducted within the thermal hydraulics methods (THM) focus area. This objective will be met by; maturation of recently added models, strategic design/development of new models and systematic and rigorous testing of existing and new models and model extensions. This report will also serve to meet the requirements of CASL level three milestone, L3:THM.CFD.P10.02, scheduled for completion March 31, 2015.

2 Introduction

Looking forward into Phase II of the CASL program, enhanced turbulence modeling capabilities have been identified as a critical component to high fidelity CFD based thermal hydraulic simulations. This includes both single- and multi-phase flows, however, only single-phase modeling will be considered in this report. Target applications include full reactor core models which will contain from tens to hundreds of millions of cells. For these models, the Reynolds Averaged Navier-Stokes (RANS) modeling methodology which is the focus of this report will be utilized.

The purpose of this planning document is to archive requirements for enhanced turbulence modeling, identify tasks and organize the work. It should also serve as a conduit for interaction and collaboration within the Hydra-TH development team. This is a multi-year plan. The major objectives are listed below.

1. Mature existing and implement new single-phase turbulence models in Hydra-TH.

2. Refactor and extend near wall model treatment.

3. Extend models to treat buoyancy driven flows, both thermal and solutal.

4. Address stretch goals.

5. Address miscellaneous items.

6. Construct a turbulence "torture test" for rigorous testing of individual models and solution verification.

Hydra-TH also contains three Large-Eddy Simulation (LES) models: implicit large-eddy simulation (ILES), Smagorinsky and wall adapted large-eddy (WALE). It also contains a hybrid RANS-LES model call detached-eddy simulation (DES) [7]. Several grid-to-rod-fretting (GTRF) studies of rod/spacer grid models using LES have been conducted with Hydra-TH [8] [9]. Several torture test problems such as the rod/spacer grid and T-Junction discussed in §10 may include using LES models along with RANS models for comparison, however, RANS model development is the main focus of this report.

The objectives listed above are discussed at length in §3-10, and a summary is given in §11.

3 Overview of Enhanced Turbulence Modeling Plan

The purpose of this document is to organize a plan for enhanced turbulence modeling capabilities in Hydra-TH for the CASL program under the THM focus area. The development plan has two major parts - design/development and rigorous testing - and spans two to three years. This document is a work in progress. It will be periodically updated as new modeling requirements emerge and as test results become available.

Currently, Hydra-TH relies on two production level RANS models; Spalart-Allmaras and RNG $k-\varepsilon$. In the first year, four proposed single-phase RANS turbulence models will be considered for development; standard $k-\varepsilon$, nonlinear $k-\varepsilon$, realizable $k-\varepsilon$ and SST $k-\omega$. The four models are in various states of development. The standard model was added after RNG to provide a baseline for all of the various versions of $k-\varepsilon$. In terms of software design, a base class for $k-\varepsilon$ models has been written with the goal that all variants will inherit from this base class. It has been exercised on only a few example problems. The nonlinear $k-\varepsilon$ has been implemented and exercised on the fuel rod sub-channel secondary flow problem § 10.17, however, additional maturing of the standard and nonlinear models will be necessary. Linearization of the equations for the fully-implicit solver is also incomplete. The SST $k-\omega$ model is documented in the theory manual but the code implementation is incomplete. Finally, the realizable $k-\varepsilon$ model development has not begun yet.

Planning for near wall treatment and buoyancy closure development will also take place in the first year. At this point in the planning process, near wall treatment encompasses both low-Reynolds number damping functions that allow for integration of the turbulence equations through the boundary layer and wall functions that replace the solution to the governing equations in the cell next to the wall with a solution derived from the law-of-the-wall.

In the second year work will begin on near wall treatment and buoyancy closure terms. Hydra-TH has one version of a wall function called the y*-insensitive model [7]. Currently the y*-insensitive wall function is used by the RNG, standard and nonlinear $k-\varepsilon$ models. The near wall treatment code will be refactored with the goal of encapsulating all modeling terms appearing in all of the governing equations to ensure consistency in the formulation and implementation and to support new near wall treatments such and low-Re damping functions.

Corrections for buoyancy driven flows both thermal and solutal are necessary for post-LOCA accident scenarios where injection of highly borated coolant is to be simulated. This area is still very much a research area. The first year objective is to review the literature and outline a development plan. Formulation and implementation will begin possibly late in FY15 and continue in FY16.

Two-phase turbulence modeling is very important to the thermal hydraulics capability. However, it will not be included in the scope of this milestone report.

Two sections and containing stretch goals and miscellaneous items are included. It is valuable to list these goals and items and archive to help assess relative importance, but the priority of these items at this time is be lower than those discussed in the previous sections.

Also in the first year a collection of turbulence benchmark problems will be constructed. This is referred to as the turbulence "torture tests". Execution of these tests by the Hydra-TH team will begin in the first year. It includes fundamental flows that have known behavior designed to rigorously test Hydra-TH for high Reynolds number flows and expose strengths and weaknesses of the individual models. The complexity of the tests increases to mimic sub-system flows encountered in reactor cores. Building from very basic to more complex will aid the development process.

The development plan is organized as follows. The proposed RANS models are presented in the next section. Because there are so many variations of $k-\varepsilon$, it is important to precisely document the motivation, references and formulation. A summary of the model formulations is presented in the appendix to help in technical discussions pertaining to formulation issues. Next, the near wall treatment refactor requirements are listed, followed by the buoyancy modeling sections. Stretch goal and miscellaneous items sections are then presented. The torture tests are presented in the next section. Each test is listed in its own sub-section. Each test has an objective, resources and task list section. As work is completed, a comment and status section will be added.

This completes the planning portion of the document. Finally, a brief summary is presented.

4 Implementation of New Turbulence Models

In this section we discuss the proposed modeling development effort which includes maturation of standard and nonlinear $k-\varepsilon$ models and two new models: Realizable $k-\varepsilon$ and SST $k-\omega$. A snapshot of RANS turbulence models is shown in Table 1. A more in depth discussion of the specific formulations can be found in the Hydra-TH theory manual [7] and a brief description of the models has can be found in the appendix of this report. It should be mentioned that the theory manual discusses two additional models, namely; $k-\varepsilon-v^2-f$ and $k-\varepsilon-\zeta-f$, however, these two models are not presently included in this development plan.

4.1 Mature Standard $k-\varepsilon$ Model

The standard $k-\varepsilon$ model has received less attention in Hydra-TH than the RNG $k-\varepsilon$ model has. It is closely related to the nonlinear $k-\varepsilon$ discussed in § 4.2. It will serve as

Model Name	Status	Documented	Regression Tested	Enhancements	Buoyancy	Near Wall Treatment
Spalart-Allmaras	production	Theory Manual	yes	curv. and rot. correction	no	yes built in
Standard $k-\varepsilon$	development	Theory Manual	no	no	Boussinesq	y*-insensitive
RNG $k-\varepsilon$	production	Theory Manual	yes	no	Boussinesq	y*-insensitive
Nonlinear $k-\varepsilon$	development	Appendix	no	no	Boussinesq	y*-insensitive
Realizable $k-\varepsilon$	formulation proposed	Appendix	NA	no	no	no
SST $k-\omega$	formulation code design	Theory Manual	NA	no	no	not necessary

Table 1: Summary list of turbulence model development activities in Hydra-TH.

a baseline with which to judge the nonlinear, realizable and SST$k-\omega$ models discussed in § 4.2, 4.3, 4.4.

Resources:

1. Jones, W.P. and Launder, B.E.,"The Prediction of Laminarization with a Two-Equation Model of Turbulence," International Journal of Mass Transfer, vol. 15, pp. 301–314, 1972.

2. Jones, W.P. and Launder, B.E.,"The Calculation of Low-Reynolds-Number Phenomena with a Two-Equation Model of Turbulence," International Journal of Mass Transfer, vol. 16, pp. 1119–1130, 1973.

3. Launder, B.E.and Spalding, D.B., "The Numerical Computation of Turbulent Flows", Computer Methods in Applied Mechanics and Engineering, vol. 3, pp. 269–289, 1974.

4. Durbin, P.A. and Pettersson Reif, B.A., "Statistical Theory and Modeling for Turbulent Flows, 2nd ed., 2011.

5. Wilcox, D.C., "Turbulence Modeling for CFD," 2nd. ed. 1998.

Tasks:

1. Construct base class for all $k-\varepsilon$ models.

2. Implementation should derive from base class.

3. Verify that the implementation is correct.

4. Verify by running select turbulence torture tests § 10.

5. Document the model in the theory and user manuals.

Comments and Status:

B. Magolan has constructed a base class for with the standard model derives from. At this point the model has been implemented and run on several example problems. It has not been rigorously verified for correctness.

4.2 Mature Nonlinear $k - \varepsilon$ Model

There are two main main differences between the nonlinear $k - \varepsilon$ and the standard $k - \varepsilon$ model. The first is that instead of a constant C_μ, it is considered a function of the mean stress which is meant to improve robustness by satisfying realizability constraints on the Reynolds stresses. The second is that the Reynolds stresses are assumed to have a quadratic and possibly cubic dependence on mean stresses. It has been argued by Baglietto and Nanokata (see resources below) that the nonlinear dependence is necessary to capture secondary flows in sub-channels.

Resources:

1. Baglietto and Nanokata, "Improved Turbulence Modeling for Performance Evaluation of Novel Fuel Designs," Nuclear Technology vol. 158, 2006.

2. Baglietto, E., "Anisotropic Turbulence Modeling of Accurate Rod Bundle Simulations," ICONE 14, 2006.

3. Magolan, B. et. al, "Non-Linear Eddy Viscosity Turbulence Modeling in Hydra-TH for Fuel Related Applications," NURETH-16, 2015.

Tasks:

1. Implementation should derive from base class.

2. Verify that the implementation of the model and linearization terms are correct.

3. Address Emilio Baglietto's concern that for symmetry boundaries, there should be a tensor reflection.

4. Verify by running the sub-channel torture test problem § 10.17.

5. Couple to low-Re damping functions

6. Document the model in the theory and user manuals.

Comments and Status:

This model has been implemented and tested extensively on the sub-channel secondary flow problem (see §10.17). Some maturation of the implementation and implicit terms remains.

4.3 Realizable $k - \varepsilon$ Model

The realizable $k - \varepsilon$ model differs from the standard model in two main respects;

- C_μ is no longer constant, it is a function of the mean strain S_{ij} so that the Reynolds stresses remain realizable (i.e., The Schwartz inequality for the Reynolds stresses is satisfied), and

- a new dissipation rate equation is derived based on the transport equation of mean-square vorticity fluctuation.

Resources:

1. Shih et al., "A Realizable Reynolds Stress Algebraic Equation Model," NACA-TM-105993, 1993.

2. Shih et al., "A New Reynolds Stress Algebraic Equation Model," NACA-TM-106644, 1994.

3. Shih et al., "A New $k-\varepsilon$ Eddy Viscosity Model for High Reynolds Number Turbulent Flows," Computers and Fluids, 1995.

Tasks:

1. Choose the formulation.

2. Prepare a design document and vet with Hydra-TH team.

3. Implement the design.

4. Verify the model is implemented correctly.

5. Couple to low-Re damping functions and wall function.

6. Document in theory and user manuals.

4.4 SST $k-\omega$ Model

Menter's shear stress transport (SST) $k-\omega$ model [16] blends Wilcox's $k-\omega$ model [25] with the standard $k-\varepsilon$ model where the ε equation, representing the rate of turbulent kinetic energy dissipation, is rewritten as an equation for ω, which approximately represents the time scale for energy dissipation. Units for $\varepsilon \rightarrow (\ell^2/t^3)$ and for $\omega \rightarrow (1/t)$. Several motivations for choosing this model over the standard $k-\varepsilon$ or the $k-\omega$ model are;

- The $k-\omega$ model and SST version do not require the use of special near wall treatments and can be integrated to the wall directly.

- SST $k-\omega$ eliminates the sensitivity to free stream in ω that hampers the Wilcox $k-\omega$ model.

- SST $k-\omega$ incorporates transport of Reynolds stress (as the name implies) which results in better predictions in flows with strong pressure gradients.

Resources:

1. Menter, "Two-Equation Eddy-Viscosity Turbulence Models for Engineering Applications," AIAA Journal, vol. 32, 1994.

2. Menter, "Improved Two-Equation $k-\omega$ Turbulence Models for Aerodynamic Flows," NASA TM-103975, 1992.

3. Also see Hydra-TH Theory Manual [7].

Tasks:

1. Choose the formulation.

2. Prepare a design document and vet with Hydra-TH team.

3. Implement the design.

4. Verify the model is implemented correctly.

5. Document in theory and user manuals.

Comments and Status:

The formulation is documented in the Hydra-TH theory manual [7] and a skeleton of model has been coded.

5 Refactor Near Wall Model Treatment

Objectives:

1. Achieve complete coverage on all $k - \varepsilon$ models.

2. Refactor to a more flexible software design that supports multiple wall functions and low-Re damping functions.

3. Strive for "plug and play" interoperable functionality.

4. To extent possible, implement in virtual base classes.

Resources:

1. There are references available in the Hydra-TH repository, `https://hydra.lanl.gov/redmine/projects/casl-documentation/repository/references/revisions/master/show/topics/turbulence/Wall-Turbulence"`.

2. Hydra-TH has an implementation of the y*-insensitive wall function that is active when the RNG NL and STD $k - \varepsilon$ models are used.

3. There is a description of four low-Reynolds number damping functions presented in Appendix B of the Hydra-TH theory manual [7].

4. Hanjalic, K. and Launder, B., "Modelling Turbulence in Engineering, Second-Moment Routes to Closure", Cambridge University Press, 2011.

5. Wilcox, D.C., "Turbulence Modeling for CFD," 2nd. ed., pp. 187-188, 1998.

Tasks:

1. Ensure wall functions are operational for all $k - \varepsilon$ models.

2. Literature search.

3. Gather requirements.

4. Define wall function formulations.

5. Define low-Re formulations.

6. Ensure consistency between wall model surface output delegates.

7. Verify that the implementations are correct.

8. Document models in the theory and user manuals.

9. Verify by running turbulence torture tests § 10.

Comments and Status:

All variations of $k-\varepsilon$ models require some form of near wall treatment for wall bounded flows. There is a large class of problems in CASL where the quantities of interest from Hydra-TH simulations will depend on accurate surface data such as: temperature, heat flux and shear stress. Complex geometry and highly swirling flow patterns cause variations in y^+ which complicate the task of generating "optimal" meshes for the accurate wall model behavior. The y*-insensitive model is designed to handle this variable y^+ issue. This issue will have to be addressed when considering new formulations of wall models and low-Re damping functions for implementation in Hydra-TH. Additionally, it will be a challenge to ensure accurate surface output data from simulations using wall functions or low-Re damping functions.

6 Model Extensions for Buoyancy Driven Thermal and Solutal Flows

Objectives:

1. Research what is the right thing to do, open ended, research (next year).
2. Obtain references from J. Bakosi - in Hydra-TH repository, references directory topics, buoyancy driven flows.
3. Add capability in preparation for the post LOCA injection of highly borated coolant simulations (A. Stagg and S.J. Yoon).
4. Correction to the k-equation production term for buoyancy with large density variations.
5. Achieve complete coverage on all RANS turbulence models.

Resources:

1. Some references are available in the Hydra-TH repository; `https://hydra.lanl.gov/redmine/projects/casl-documentation/repository/references/revisions/master/show/topics/turbulence/Buoyancy-driven"`.
2. Davidson, L., "Second-order Corrections of the $k-\varepsilon$ Model to Account for Non-isotropic Effects Due to Buoyancy," International Journal for Heat and Mass Transfer, vol. 133, no. 12, pp. 2599–2608, 1990.
3. Hydra-TH has implemented a Boussinesq buoyancy body force in the momentum equation and a modification to the turbulent kinetic energy in the standard, RNG and Nonlinear $k-\varepsilon$ models.

Tasks:

1. Choose formulations.
2. Design code implementation.

3. Implement code design.

4. Construct and execute appropriate tests to evaluate new capabilities.

5. Document in user and theory manuals.

Comments and Status:

A baseline for modeling buoyancy driven turbulence in the context of the standard $k - \varepsilon$ model is presented in §12.2. This is based on the work of Davidson [12] and should be considered the launch point for future research and development.

7 Two-Phase Turbulence Models

Two-phase flow modeling and two-phase turbulent flow modeling are high priority capabilities for CASL THM. However, two-phase flow turbulence modeling is outside the scope of this report. As of FY2015, the plan is to follow closely the work by Layhe for turbulence closure. Only a partial citation list will be presented below.

Resources:

1. M. Lopez de Bertodano, R. T. Lahey, O. C. Jones, "Development of a k- Model for Bubbly Two-Phase Flow," J. Fluids Eng. 116(1), pp. 128-134, 1994.

2. M. Lopez de Bertodano, S.-J. Lee, R. T. Lahey, D. A. Drew, "The Prediction of Two-Phase Turbulence and Phase Distribution Phenomena Using a Reynolds Stress Model," J. Fluids Eng. 112(1), pp. 107-113, 1990.

3. G.S. Arnold, D.A. Drew, and R.T. Lahey, "Derivation of Constitutive Equations for Interfacial Forces and Reynolds Stress for a Suspension of Spheres Using Ensemble Averaging," Chem. Eng. Communications, vol. 86, pp. 43-54, 1988.

4. Antal, S., Kurul, N., Podowski, M. And Lahey, R.T., Jr., "The Development of Multidimensional Modeling Capabilities for Annular Flows, Proceedings of the International Conference on Multiphase Flow (ICMF), Lyon, France, June 8-12, 1998.

5. Lahey, R.T., Jr., A CFD Analysis of Multidimensional Two-Phase Flow and Heat Transfer Using a Four Field, Two-Fluid Model, Proceedings of the Thirteenth U.S. National Congress on Applied Mechanics, University of Florida, June 21-26, 1998.

8 Stretch Goals

Stretch goals are included in the planning because of the potential impact on turbulence modeling capability, however, the priority may be lower than development goals discussed above.

8.1 General Symmetry Boundary Conditions

Objectives:

1. Implement general (non-Cartesian axis aligned) symmetry (tensor reflection) boundary conditions.

Resources:

1. E. Baglietto is familiar with the formulation and should be consulted.

Tasks:

1. Derive symmetry conditions for arbitrarily oriented face.

2. Produce a design document.

3. Implement in Hydra-TH.

Comments and Status:
The current symmetry boundary conditions are enforced through no-penetration for velocity and no specification for scalars. This limits the use of symmetry boundary conditions to axis aligned boundaries. The user would like to be able to specify a symmetry boundary condition on an arbitrarily oriented boundary surface.

9 Miscellaneous Items

9.1 Limiting ε

Objectives:

1. Limit ε in $k-\varepsilon$ models for improving robustness.

2. Determine the best choice for limiting ε.

Resources:

1. Time scaling arguments (see M.A. Christon).

2. Implementation in Hydra-TH.

Tasks:

1. Choose the appropriate tests that express the effects limiting.

2. Determine how limiting effects robustness.

3. Evaluate time scaling arguments in test flow problems.

4. To extent possible, implement in base class.

Comments and Status:
"On the k-e models, one thing Im wondering about is a bit of probing/research on the setting the lower-bounds for epsilon. I had used a time-scale limiter similar to whats done in k-w and that the guys at Flow Sciences advocate. However, it really only works for stagnation flow. I have some scaling arguments for the lower-bound on dissipation rate and use that for setting a minimum on epsilon, but this could be an interesting and really useful small side-study to understand what is really the best choice." (M.A. Christon, 2-6-15)

9.2 Inflow Boundary Conditions

Objectives:

1. Produce a small number of generally applicable boundary conditions for specifying inflow turbulent profiles.
2. Parabolic and power law 2D and 3D channel profiles.
3. Parabolic and power law 3D pipe.
4. Specify scalars such as temperature and species.
5. Interpolate from data file.

Resources:

1. Hydra-TH does have a mechanism for specifying user defined Dirichlet BCs.

Tasks:

1. Implement user-specified, pre-programmed parabolic and power law distribution profiles for 2D and 3D geometries.
2. Add additional user defined functionality other dependent variables such scalars.
3. Implement an interface to read and interpolate boundary data.

Comments and Status:

An example of a fully developed turbulent channel flow velocity profile using a 1/7 power law is given by the function

$$U(y) = U_{in}\left(1 - 2\frac{|y - y_c|}{H}\right)^{1/7} \qquad y_{\min} \leq y_c \leq y_{\max} \quad H = y_{max} - y_{min} \tag{1}$$

where y_c is the value of the center of the channel and H is the channel width. This produces a symmetric profile about the channel center line with a 1/7 power dependence on the y coordinate. The reference velocity in this case is the value averaged across the channel which can be analytically determined by integrating the profile function. Its value is $0.875\, U_{in}$. This function serves as an example and could easily be modified to produce a parabolic profile for laminar inflow or an arbitrary power law.

There has been some recent work on user defined boundary conditions. It may be possible to exploit this work for the purposes of defining turbulent inflow conditions.

9.3 Post-Processing data

Objectives:

1. Joining distributed ExodusII files into a single plot file for post-processing.
2. Provide an ExodusII based post-processing utility for extracting data from small to medium sized models for the purpose of analysis.

Resources:

1. Schoff, L.A. and Yarberry, V.R., "ExodusII: A Finite Element Data Model Sandia Report," 1994.

Tasks:

1. Write global element number and node number maps to distributed files.
2. Gather additional feature requests for post-processing.
3. Prune un-necessasary features.
4. Enrich element library by adding Pyramid5 and Wedge6 elements.
5. Add error handling.
6. Copywright the code?
7. Stretch Goal: Write a version that will process distributed files.

Comments and Status:

An incomplete example has been written and is currently being exercised. Some development effort remains. The post-processing code depends on Exodus and Netcdf. It is easily built using custom built versions or the the versions distributed with Hydra-TH. The code can be obtained from T.M. Smith.

10 Turbulence Torture Tests

The turbulence torture tests described in this section are intended to provide an archive for solution verification to diverse turbulent flows that may be encountered in nuclear reactors and validation of the turbulence modeling capabilities in Hydra-TH. As this suite of tests matures, it should facilitate rapid prototyping, solution verification and validation of future enhancements by providing information pertaining to problem setup, references, post-processing, Hydra-TH control files and mesh files.

A similar effort was undertaken by Pannala and Stagg [18] in 2012 to define THM CFD benchmark problems. The present effort incorporates several of these benchmark problems into torture test problems.

Candidate problems under consideration are listed in Table 2. Additional candidate problems will be considered based on relevancy and how well the test aligns with the requirements of THM. From the table, the objective column gives a brief description of an expected physical outcome of the solution. The mesh file column refers to whether mesh files exist. Many of these tests only require relatively simple meshes, however, several tests will require sophisticated meshes. Having multiple mesh files with varying resolution available and obtaining solutions on these meshes is necessary for establishing evidence of grid convergence, a necessary but not sufficient metric for determining the quality of the over-all solution.

Problem statements, mesh files, control files and possibly post-processing files will be archived in a separate directory within the Hydra-TH repository. Results from these tests will also be archived in a companion report. The initial version of this report will be part of a level 3 milestone (L3:THM.CFD.P11.04) scheduled for completion September, 2015.

Each test problem is presented below in its own section that describes the test, objectives, resources available, tasks, status and general comments.

Test Name	Dimensions	Objectives	Mesh Files	Status	Documented	Regression Testing
Back Step	2D	Reattachment location	Cubit available	SA, RNG	no	yes
Channel	2D	Law-of-the-wall	Cubit available	SA, RNG	Verification Manual	yes
Grid Turbulence	1D	Analytical Solution $k-\varepsilon$	three levels available	RNG, STD	Verification Manual	yes
Couette Flow	2D	Mean velocity profile	Cubit available	SA, RNG, STD	some	no
Mixing Layer	2D	spreading rate scale similarity	Cubit available	SA, RNG, STD	some	no
Jets	2D-3D	spreading rate scale similarity	none	not started	no	no
Pipe Flow	3D	Law-of-the-wall Nusselt No.	Cubit available	SA, RNG, STD	some	no
U-Channel	2D	curvature and rotation correction	Cubit available	SA, RNG, STD	some L3 milestone	no
Circular Cylinder	2D	Strouhal No.	Cubit available	SA, RNG	no	yes
Triangular Cylinder	2D	Strouhal No.	no	not started	no	no
Square Cylinder	2D	Strouhal No.	no	not started	no	no
Asymmetric Diffuser	2D	pressure induced separation	no	not started	no	no
Impinging Jet	2D	Stagnation point flow	no	not started	no	no
Jet in Crossflow	2D	complex vortical structures	no	not started	no	no
Mounted Cube	3D	Massive separation	no	not started	no	no
Square Cavity	3D	Natural Convection	no	not started	no	no
Sub-Channel Secondary Flow	3D	Secondary flow orientation	Cubit available	extensive NL, STD	presentations, NURETH-16	no
3x3 Rod/Spacer	3D	pressure drop	Cubit avail., Hexpress	extensive RNG SA, ILES	Verification Manual	no
T-Junction	3D	Velocity profiles, pressure drop	at least one available	Preliminary ILES	some	no

Table 2: Summary list of turbulence torture tests for Hydra-TH.

10.1 Backward-Facing Step

Objectives:

1. Compute re-attachment point with different models.
2. Compare solutions from different models.

Resources:

1. H. Le, P. Moin and J. Kim, "Direct numerical simulation of turbulent flow over a backward-facing step," J. Fluid Mech. 1997.
2. B. Basara. S. Jarkirlic "A new hybrid turbulence modeling strategy for industrial CFD," IJNMF, 2003.
3. Thakur et al., "Development of Pressure-Based Composite Multigrid Methods for Complex Fluid Flows," Prog. Aerospace Sci., 1996.
4. P. A. Durbin, "Separated Flow Computations with the k-e-v2 Model," AIAA J., 1995.
5. C.G. Speziale, "Analysis of an RNG Based Turbulence Model for Separated Flows," Int J. Enging. Sci., 1992.
6. Ravikanth V.R. Avancha, Richard H. Pletcher, "Large eddy simulation of the turbulent flow past a backward-facing step with heat transfer and property variations," Int. J. of Heat and Fluid Flow, 2002.
7. Cubit parametrized journal files and meshes available (contact T.M. Smith).

Tasks:

1. Generate meshes.
2. Setup control files and run.
3. Document post-processing.
4. Run different models.

Comments and Status:

An example of this flow is included in the regression test suite. Both SA and RNG $k-\varepsilon$ models are tested. These tests are the starting point for more detailed studies.

10.2 Channel Flow

Objectives:

1. Verify that the different models reproduce law-of-the-wall (y^+ vs. U^+).

Resources:

1. Moser, R.D., Kim, J. and Mansour, N.N., "Direct numerical simulation of turbulent channel flow up to $Re_\tau = 590$". Phys of Fluids. 1999.
2. See Hydra-TH V&V manual [9].

3. Cubit Aprepro parametrized journal files and meshes available (contact T.M. Smith).

Tasks:

1. Reproduce runs presented in the V&V manual for different models.

2. Run different models.

Comments and Status:

An example of this flow is included in the verification test suite. Both SA and RNG $k-\varepsilon$ models are run. From this work, it will be straight forward to run additional studies with different models.

10.3 Grid Turbulence

Objectives:

1. Exercise advection, diffusion, production, dissipation away from walls.

2. Make direct comparisons with analytical solution.

Resources:

1. See Hydra-TH V&V manual [9].

2. Three mesh files and control files for semi-implicit and fully-implicit solution strategies are available in the verification repository.

Tasks:

1. Reproduce runs presented in the V&V manual for new models.

Comments and Status:

An example of this flow is included in the regression test suite. The RNG $k - \varepsilon$ model is run. This test is also included in the verification test suite. From this work, it will be straight forward to run additional studies with different models. This test runs very quickly and quantities of interest are easy to extract from solution data.

10.4 Couette Flow

Objectives:

1. Verify that the different models reproduce mean velocity profile compared with experimental data.

2. Check for anti-symmetry in vertical profiles.

3. Test near wall treatments of the various RANS models.

4. Compare directly with experimental data.

Resources:

1. Kim, W.-W. and Menon, S., "Application of the localized dynamic subgrid-scale model to turbulent wall-bounded flows," AIAA Paper 97-0210, Jan. 6-9, 1997.

2. Aydin, E.M. and Leutheusser, H.J., "Plane-Couette flow between smooth and rough walls," Experiments in Fluids, vol. 11, pp. 302–312, 1991.

3. Cubit Aprepro parametrized journal files and meshes available (contact T.M. Smith).

Tasks:

1. Run different model.

2. Post process velocity profiles and compare with experimental data.

Comments and Status:
Preliminary tests have been run with SA, RNG, STD and NL models. Results will be included in the companion document.

10.5 Mixing Layer

The mixing layer de-emphasizes near wall modeling. It is a simple 2D benchmark problem that can be used to isolate production, dissipation, diffusion and convection mechanisms of turbulent kinetic energy and dissipation rates.
Objectives:

1. Compute the spreading rate.

2. Compare spreading rates for different models.

3. Compare profiles for scale similarity.

Resources:

1. Cubit Aprepro parametrized journal files and meshes available (contact T.M. Smith).

2. http://turbmodels.larc.nasa.gov/delvilleshear_val.html

3. Tennekes, H. and Lumley, J.L., "A First Course in Turbulence," The MIT Press, 1990.

4. F.M. White, "Viscous Flow," 2nd ed.i, McGraw Hill, 1991, pp. 476.

5. Rogers, M. M. and Moser, R. D., "Direct simulation of a self-similar turbulent mixing layer," Physics of Fluids, vol. 6, no. 2, pp.903–923, 1994.

6. Patel, R.P., "An Experimental Study of a Plane Mixing Layer," AIAA Journal, vol. 11, no. 1, pp. 67–71, 1973.

7. Mesh and control files are available (see B. Magolan and T.M. Smith).

Tasks:

1. Conduct literature search for good quality data and/or reproducible problem description.

2. Generate meshes.

3. Setup and run.

4. Compute spreading rates.

5. Run different models.

Comments and Status:

B. Magolan has conducted a study comparing the standard model to the RNG model on a validation test provided by NASA (see url above). His study includes several different splitter plate geometries as well as a no-splitter plate geometry. Results include comparison of mean velocity profiles between experiment and the two turbulence models at different down-stream locations. Near the splitter plate, discrepancies are observed, possibly due to the inflow boundary layers. Far downstream, the mean velocity profiles are slightly retarded compared to experiment. The STD and RNG predict almost identical profiles far downstream.

In a separate study, a simulation was conducted of a mixing layer without a splitter plate. Scale similarity in the mean velocity is present when the Reynolds number based on velocity difference and distance from the splitter plate $Rex = \Delta U x/\nu = 4x10^5$ (Tennekes and Lumley, pp. 129). Scale similar profiles can be extracted from the solution using the following normalizaton (White, pp. 476)

$$u^* = \frac{(\tilde{u} - U1)}{(U2 - U1)} \quad \delta = \frac{(U2 - U1)}{(\partial \tilde{u}/\partial y|_{max})}. \tag{2}$$

Results will be presented in a companion report.

10.6 Planar and Round Jets

The planar and round jet de-emphasizes near wall modeling. It is a simple 2D and 3D benchmark problems that can be used to isolate production, dissipation, diffusion and convection mechanisms of turbulent kinetic energy and dissipation rates. In addition, there is a well known spreading rate anomaly comparing planar versus round jet solutions that is mainly due to the dissipation rate equation ε [20]. The spreading of round jets is always smaller than the planar jet but model predictions usually contradict this observation.

Objectives:

1. Compute the spreading rate.
2. Compare the different models.

Resources:

1.

Tasks:

1. Conduct literature search and choose appropriate references with good quality data and reproducible setups.
2. Generate meshes.
3. Setup and run.
4. Compute spreading rates.
5. Run different models.

Comments and Status:

Work has not started on this test problem yet.

10.7 Fully Developed Flow in Circular Pipes

Objectives:

1. Compute y^+ vs. U^+ and y^+ vs. T^+.
2. Compute Nusselt number with different models.
3. Obtain consistency between side set outputs, boundary conditions and solution.

Resources:

1. F. M. White. Viscous Fluid Flow, 1991.
2. S.B. Pope. "Turbulent flows," 2000.
3. Kays and Crawford, "Convective Heat and Mass Transfer, 3nd ed.," 1993.
4. Smith, T.M. et al., "Thermal Hydraulic Simulations, Error Estimation and Parameter Sensitivity Studies in Drekar::CFD," CASL L3:THM.CFD.P7.05, 2013.
5. Zagarola, M. V. and A. J. Smits, "Mean-flow scaling of turbulent pipe flow." Journal of Fluid Mechanics 373: 33-79, 1998.
6. Zagarola, M. V. and A. J. Smits, "Scaling of the Mean Velocity Profile for Turbulent Pipe Flow." Physical Review Letters 78(2): 239-242, 1997.
7. Cubit meshes are available for this problem (contact T.M. Smith).

Tasks:

1. Setup control files and run.
2. Compute law-of-the-wall and Nusselt number for different RANS models.
3. Document post-processing.
4. Run additional models.

Comments and Status:

The Nusselt number is a non-dimensional number that represents the ratio of convective to conductive heat transfer. For fully developed pipe flow, it is defined as

$$Nu = \frac{hD}{\kappa} \tag{3}$$

where h is the local convection heat transfer coefficient, D is a reference length scale which in this case is the pipe diameter and κ is the thermal conductivity coefficient. The mean temperature or mixing temperature T_m is the average temperature of a cross-section of the pipe and is defined as;

$$T_m = \frac{1}{\rho V A} \int_A \rho \mathbf{u} \cdot \mathbf{n} T dA \tag{4}$$

where A is the cross-sectional area, V is the average axial component of velocity defined as;

$$V = \frac{1}{\rho A} \int_A \rho \mathbf{u} \cdot \mathbf{n} dA \tag{5}$$

and **u** is the velocity vector at a point on the surface and **n** is a unit vector normal to the surface. Newton's law of cooling can be stated as;

$$\dot{q}''_w = h(T_w - T_m) \tag{6}$$

where $\dot{q}''_w$ is the wall heat flux. The average wall heat flux is defined as;

$$\dot{q}''_w = \frac{1}{L}\oint_L \kappa \frac{\partial T}{\partial \mathbf{n}} dl. \tag{7}$$

In this case $\frac{\partial T}{\partial \mathbf{n}}$ is the temperature gradient normal to the wall and tangent to the surface for which the flux is computed and the integration is a line traversing the circumference of the tube. In a similar way, the local (axial location) reference wall temperature is computed as;

$$T_w = \frac{1}{L}\oint_L T dl. \tag{8}$$

The final definition of Nu is;

$$Nu = \frac{hD}{\kappa} = \frac{\dot{q}''_w D}{\kappa(T_w - T_m)}. \tag{9}$$

The non-dimensional wall normal distance $y+$ and velocity $U+$ are determined from the wall shear τ_w and kinematic viscosity ν;

$$y^+ = u_\tau y/\nu \quad u_\tau = \sqrt{\frac{\tau_w}{\rho}} \quad U^+ = \frac{u(y)}{u_\tau}.$$

In the viscous sub-layer of a boundary layer, viscous forces dominate and velocity fluctuations are damped due to viscosity and close wall proximity. The mean velocity scales as

$$U^+ \approx y^+$$

Away from the wall, the law of the wall describes the mean velocity by

$$U^+ = \frac{1}{0.41}\ln(y^+) + 5.2. \tag{10}$$

A difficulty arises when using a wall function, with the $y+$ of the first cell located $y+ \approx 11$, in estimating the wall shear defined by

$$\begin{aligned} (S_{ij})_w &= \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_i}{\partial x_j}\right)_w \\ t_i &= 2\mu(S_{ij})_w n_j \\ s_i &= t_i - (n_j t_j) n_i \\ \tau_w &= \sqrt{s_i s_i} \end{aligned} \tag{11}$$

where t_i is the traction vector, n_i is a unit vector normal to the surface and s_i is the shear-traction vector. The difficulty is determining the shear stress on the wall $(S_{ij})_w$, due to the coarse resolution normal to the wall imposed on the mesh by the wall model. Kays&Crawford[15] (p. 249, Equation 12-14) present a an equation for determining the shear velocity (attributed to Petukhov [19])

$$cf/2 = (2.236\ \ln(Re_D) - 4.639)^{-2} \qquad u_\tau = V\sqrt{cf/2}. \tag{12}$$

For Prandtl number near unity, Reynold's analogy states that the temperature profile will be similar to the velocity profile [15] (p. 280), thus,

$$\frac{\bar{u}}{\bar{u}_c} = \left(1 - \frac{r}{r_w}\right)^{1/7} \qquad \frac{\bar{T} - T_w}{\bar{T}_c - T_w} = \left(1 - \frac{r}{r_w}\right)^{1/7}, \tag{13}$$

where $\bar{u}_c$ and $\bar{T}_c$ are centerline values to velocity and temperature respectively. Using this assumption and the assumption that $Pr_t \approx 1.0$, Kays&Crawford [15] present correlations for Nusselt number ($Nu = Nu(Re_D, Pr)$) (Equation 14-7) for constant wall heat flux

$$Nu = 0.022\ Pr^{0.5}\ Re_D^{0.8} \qquad Re_D < 10^5 \tag{14}$$

and for constant wall temperature (Equation 14-12)

$$Nu = 0.021\ Pr^{0.5}\ Re_D^{0.8} \qquad Re_D < 10^5. \tag{15}$$

This problem will also serve as good validation test for low-Re near wall model extensions. Spalart-Allmaras model solutions capture the viscous sub-layer. Currently, the y*-insensitive wall function requires that the center of the cell adjacent to the wall be located outside the viscous-sublayer and therefore no data on the transition from log- to sub-layer is available.

10.8 U-Channel Flow

Objectives:

1. Assess the rotation/curvature correction of Dacles-Mariani et al. applied to the Spalart-Allmaras model.

Resources:

1. Spalart, P.R. and Shur, M. "On the Sensitization of Turbulence Models to Rotation and Curvature," Aerospace Science and Technology, 1997, no. 5.
2. M.L. Shur et al. "Turbulence Modeling in Rotating and Curved Channels: Assessing the Spalart-Shur Correction," AIAA J., 2000.
3. P.E. Smirnov and F. R. Menter. "Sensitization of the SST Turbulence Model to Rotation and Curvature by Applying the Spalart-Shur Correction Term," Journal of Turbomachinery, 2009.
4. Dacles-Mariani, J. et al. "Numerical/Experimental Study of a Wingtip Vortex In the Near Field," AIAA Journal vol. 33, 1995.
5. Dacles-Mariani, J. et al., "On Numerical Errors and Turbulence Modeling in Tip Vortex Flow Prediction," IJNMF, vol. 30, 1999.
6. "Enhanced Turbulence Model Capabilities in Hydra-TH," Smith, T.M. and Christon, M.A., CASL L3:THM.CFD.P9.06, 2014.
7. Cubit meshes are available for this problem (contact T.M. Smith).

Tasks:

1. Run additional models.

2. Document in V&V manual.

3. Document post-processing.

Comments and Status:

This was studied extensively and reported in [22]. To evaluate this correction, we investigated its performance in a two-dimensional U-channel flow that has a 180 degree bend. The U-channel was investigated experimentally and numerically by Monson et al. [17] and also numerically by Shur et al. [21] in the context of their version of a rotation/curvature correction. A comparison of solutions using both uncorrected and corrected versions of SA were compared.

10.9 Flow Over a Circular Cylinder

Objectives:

1. Compute Strouhal number.

2. Investigate URANS modeling strategy.

Resources:

1. M. Tutar and A. E. Holdo, "Computational modeling of flow around a circular cylinder in sub-critical flow regime with various turbulence models," IJNMF, 2001.

2. A. Travin et al., "Detached-Eddy Simulations Past a Circular Cylinder," Flow, Turbulence and Combustion, 1999.

3. P. Catalano et al., "Numerical simulation of the flow around a circular cylinder at high Reynolds numbers," Int. J. of Heat and Fluid Flow, 24, 2003.

4. Cubit meshes are available for this problem (contact T.M. Smith).

Tasks:

1. Choose the range of Reynolds numbers.

2. Generate Cubit meshes from journal files.

3. Compute Strouhal number from probe data and computed spectrum.

4. Run different models.

Comments and Status:

This problem is a regression test for SA and RNG $k-\varepsilon$ models. These tests will serve as a starting point for more detailed studies including additional models.

10.10 Flow over a Triangular Cylinder

Objectives:

1. Compute Strouhal number.
2. Investigate URANS modeling strategy.

Resources:

1. P. A. Durbin. Separated Flow Computations with the k-e-v2 Model.
2. Johansson, S., Davidson, L., and Olsson, E., "Numerical Simulation of the Vortex Shedding past Triangular Cylinders at High Reynolds Number Using a k-s Turbulence Model," International Journal of Numerical Methods in Fluids, Vol. 16, No. 6, 1993, pp. 859-878.

Tasks:

1. Generate meshes.
2. Setup control files and run.
3. Run different models.

Comments and Status:
Work has not started on this problem yet.

10.11 Flow over a Square Cylinder and Rounded Corner Cylinder

Objectives:

1. Compute Strouhal number.
2. Investigate URANS modeling strategy.

Resources:

1. D. A. Lyn, et al., "A laser-doppler velocimetry study of ensemble-averaged characteristics of the turbulent near wake of a square cylinder," J. Fluid Mech., 1995.
2. G. Bosch and W. Rodi, "Simulation of Vortex Shedding Past a Square Cylinder with Different Turbulence Models," IJNMF, 1998.
3. K. D. Squires et al., "Detached-Eddy simulation of the separated flow over a rounded-corner square," Journal of Fluids Engineering, 2005.

Tasks:

1. Generate meshes.
2. Setup control files and run.
3. Run different models.

Comments and Status:
Work has not started on this problem yet.

10.12 Flow in an Asymmetric Diffuser

Objectives:

1. Investigate pressure gradient induced separation.

Resources:

1. C. U. Buice and J. K. Eaton, "Experimental Investigation of Flow Through an Asymmetric Plane Diffuser," Journal of Fluids Engineering, 2000.

2. H. J. Kaltenbach et al., "Study of flow in a planar asymmetric diffuser using large-eddy simulation," J. Fluid Mech, 1999.

Tasks:

1. Generate meshes.

2. Setup control files and run.

3. Run different models.

Comments and Status:

Work has not started on this problem yet.

10.13 Impinging Jet Flow

Objectives:

1. Prediction of stagnation point flows.

Resources:

1. M. Hadziabdic and K. Hanjalic, "Vortical structures and heat transfer in a round impinging jet," J. Fluid Mech., 2008.

Tasks:

1. Generate meshes.

2. Setup control files and run.

3. Run different models.

Comments and Status:

Work has not started on this problem yet.

10.14 Jet in Crossflow

Objectives:

1. Prediction of complex vortical flows.

Resources:

1. M. R. Keimasi et al., "Numerical Simulation of Jets in a Crossflow Using Different Turbulence Models," AIAA J., 2001.

Tasks:

1. Generate meshes.
2. Setup control files and run.
3. Run different models.

Comments and Status:
Work has not started on this problem yet.

10.15 Flow over a mounted cube in a channel

Objectives:

1. Prediction of massively separated flows.
2. Investigate URANS modeling strategy.

Resources:

1. G. S. Ratnam. And S. Vengadesan, "Performance of two equation turbulence models for prediction of flow and heat transfer over a wall mounted cube," International Journal of Heat and Mass Transfer, 2008.

Tasks:

1. Generate meshes.
2. Setup control files and run.
3. Run different models.

Comments and Status:
Work has not started on this problem yet.

10.16 Square Cavity Natural Convection

Objectives:

1. Prediction of mean velocity profiles in a high Rayleigh number natural convection flow.

2. Exercises the energy equation and Boussinesq buoyancy closures.

Resources:

1. Ampofo and T.G. Karayiannis, Experimental benchmark data for turbulent natural convection in an air filled square cavity, F. Int. J. Heat Mass Transfer 46, 3551-3572, 2003.

2. Y.S. Tian and T.G. Karayiannis, Low turbulence natural convection in an air filled square cavity, Part I: Thermal and fluid flow fields, Int. J. Heat Mass Transfer 43, 849-866, 2000.

3. Y.S. Tian and T.G. Karayiannis, Low turbulence natural convection in an air filled square cavity, Part II: The turbulence quantities, Int. J. Heat Mass Transfer 43, 867-884, 2000.

4. M. Omri and N. Galanis, Numerical analysis of turbulent buoyant flows in enclosures: Influence of grid and boundary conditions, Intl. J. of Thermal Sciences 46, 727-738, 2007.

Tasks:

1. Generate Cartesian stretched meshes.

2. Setup control files and run.

3. Run different models.

Comments and Status:

There is a discussion of this test in Pannala and Stagg [18]. This test may require conjugate heat transfer to run correctly, which is being actively developed at this time.

10.17 Fuel Rod Sub-Channel Secondary Flow

Objectives:

1. Verify the nonlinear $k - \varepsilon$ model is working correctly.

2. Prediction of secondary flows in rod bundle reactor core sub-assembly flows.

3. Compare solutions from different models.

Resources:

1. Baglietto, "Anisotropic Turbulence Modeling of Accurate Rod Bundle Simulations," ICONE 14, 2006.

2. Magolan, B. et. al, "Non-Linear Eddy Viscosity Turbulence Modeling in Hydra-TH for Fuel Related Applications," NURETH-16-13336, 2015.

3. Meshes and post-processing scripts are available for this problem (contact B. Magolan or T.M. Smith).

Tasks:

1. Rerun.

2. Post-process solutions.

3. Run different models.

Comments and Status:
Emilio Baglietto and Ben Magolan have been running these simulations in conjunction with development of the nonlinear $k - \varepsilon$ turbulence model. The current status of both the model and the simulations are documented in several Power-Point slide presentations which can be obtained from Ben Magolan or T.M. Smith. A paper detailing the use of the new model will be presented at the NURETH-16 conference August 2015.

10.18 Elmahdi 3x3 V5H Rod/Spacer Grid Reactor Core Model

Objectives:

1. Comparison of turbulence models on a CASL relevant flow problem.

2. Compute heat transfer from the rods to the flow field.

3. Compare swirling flow structure between models.

4. Compare of heat transport between different models.

Resources:

1. Elmahdi, A.M. et al., "Flow induced vibration forces on a fuel rod by LES CFD Analysis," NURETH-14-365, 2011.

2. Christon, M.A. et al., "Hydra-TH L2 Milestone," LA-UR-11-07034, 2011.

3. Smith, T.M. et al., "Reactor Core Sub-Assembly Simulations Using a Stabilized Finite Element Method," NURETH-14-500, 2011.

4. Meshes are available for this problem (see. M.A. Christon or T.M. Smith).

Tasks:

1. Define metrics for comparing different models.

2. Run the simulations with the different models.

Comments and Status:
This is a very important flow problem for several reasons. First, it is the closest geometry to the reactor core. Secondly, the geometry is very complicated and the mesh includes four different cell topologies. Finally, this problem includes heat transfer from the rods to the fluid. This will test the turbulent heat flux closure.

10.19 T-Junction Pipe Flow

Objectives:

1. Comparison of turbulence models on a CASL relevant flow problem.

2. Comparison of mean velocity and temperature profiles.

Resources:

1. Some work has been done (see M.A. Christon) In addition see See the Hydra-TH V&V manual [9].

2. Report of the OECD/NEA-Vattenfall T-Junction Benchmark Exercise, NEA/CSNI/R, May 2011. This report includes OECD/NEA-Vattenfall T-Junction Benchmark Specifications (Final Version, July 2009).

3. S. Jayaraju, E. Komen, and E. Baglietto, Validation of STAR-CCM+ with the OECD/NEA T-Junction Blind Benchmark, presented at the STAR European Conference, March 22-23, 2011.

4. J-M Ndombo and R. Howard, Large Eddy Simulation and the effect of the turbulent inlet conditions in the mixing Tee, Nuclear Engineering and Design, 241, pp. 2172-2183, 2011.

Tasks:

1. Define problem, gather references.

2. Build meshes.

3. Run the simulations with the different models.

4. Document results.

Comments and Status:

Mark Christon has some resources and should be consulted before commencing with this problem. Also, Pannala and Stagg [18] have simulated this flow using Star-CCM+ [6].

11 Summary and Future Work

In this document a plan for developing enhanced turbulence modeling capabilities in Hydra-TH has been outlined. The development plan is organized into six sections and is scheduled to span two to three years. The six sections are;

1. Mature existing and implement new single-phase turbulence models in Hydra-TH.

2. Refactor and enhance near wall modeling to include both wall functions and low Re damping functions.

3. Extend models to treat buoyancy driven flows, both thermal and solutal.

4. Stretch goals.

5. Miscellaneous items.

6. Define and construct turbulence torture tests.

In the first year a collection of turbulence benchmark problems will be constructed. This is referred to as the turbulence torture tests. Also in the first year, new single-phase RANS turbulence models will be considered for development. Maturation of two existing models; standard $k-\varepsilon$ and nonlinear $k-\varepsilon$ are a high priority. Candidate new models are; realizable $k-\varepsilon$ and SST $k-\omega$. References/resources, tasks and status/comments for each of these models can be found in § 4.

In the second year work will begin in two areas; near wall treatment for different variants of the $k-\varepsilon$ models and buoyancy driven turbulence modeling. Near wall treatment work includes refactoring existing code and fundamental formulation work on low-Reynolds number damping functions and wall functions. The near wall treatment code will be refactored in order to encapsulate all modeling terms appearing in all of the governing equations to ensure consistency in the formulation, ease of implementation and to support new near wall treatments such as low-Re damping functions. Corrections/extensions for buoyancy driven flows both thermal and solutal are necessary for post LOCA accident scenarios where injection of highly borated coolant must be simulated. Two-phase turbulence modeling is very important to the thermal hydraulics capability. However, this work is beyond the scope of the work described in this report which currently deals only with single-phase flows. The final two sections contain stretch goals and miscellaneous items. This document is a work in progress. It will be periodically updated as new modeling requirements are mandated and as participation from team members grows.

12 Appendix: Hydra-TH RANS Turbulence Models

This section is intended to provide a launching point for Reynolds averaged Navier-Stokes based turbulence modeling. A richer discussion can be found in the Hydra-TH theory manual [7]. It should serve as a reference for current capabilities, future development and special topics that need to be addressed. It also helps enforce consistent nomenclature between models which is valuable during the implementation phase of development.

To develop Reynolds averaged Navier-Stokes equations, a time averaging filter is applied to the dependent variables

$$\overline{u(x_i,t)} = \frac{1}{\Delta T}\int_t^{t+\Delta T} u(x_i,\mathcal{T})d\mathcal{T}.$$

With this definition, the instantaneous "exact" value can be decomposed into a mean and fluctuating component

$$u = \overline{u} + u'.$$

For the situation where density varies, the time average is mass weighted and a Favre average is defined

$$\widetilde{u(x_i,t)} = \frac{1}{\overline{\rho}\Delta T}\int_t^{t+\Delta T} \rho(x_i,\mathcal{T})u(x_i,\mathcal{T})d\mathcal{T}.$$

Similar to the time average, the instantaneous values and their relationship to the time averaged values are

$$u = \widetilde{u} + u'' \quad \widetilde{u} = \frac{\overline{\rho u}}{\overline{\rho}}.$$

And we note that these definitions imply the following

$$\overline{u'} = 0, \quad \overline{\overline{u}} = \overline{u}, \quad \widetilde{u''} = 0, \quad \widetilde{\widetilde{u}} = \widetilde{u}.$$

Strictly speaking, the averaging operation removes temporal dependence from the dependent variables, but in practice, this dependence is retained for convenience of solution and for hybrid unsteady RANS (URANS) modeling.

To start the discussion, the RANS equations for continuity, momentum and energy are shown to highlight the closure terms that must be modeled. These terms center around evaluation of eddy viscosity. The conservation of mass is written,

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial (\overline{\rho}\widetilde{v}_i)}{\partial x_i} = 0 \tag{16}$$

where the overbar $(\bar{\cdot})$ represents time average and the tilde $(\tilde{\cdot})$ represents mass weighted time average or Favre averaging. In this equation $\overline{\rho}$ is the density. The conservation of momentum is

$$\frac{\partial (\overline{\rho}\widetilde{v}_i)}{\partial t} + \frac{\partial (\overline{\rho}\widetilde{v}_i\widetilde{v}_j)}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[2\mu\widetilde{S}_{ij} - \frac{2}{3}\frac{\partial \widetilde{v}_k}{\partial x_k}\delta_{ij}\right] + \frac{\partial}{\partial x_j}(-\overline{\rho}\widetilde{v_i''v_j''}) - (\overline{\rho} - \rho_0)g_i \tag{17}$$

where $\widetilde{v}_i$ is the velocity vector, $\overline{p}$ is pressure, ρ_0 is a reference density, $\widetilde{S}_{ij}$ is the symmetric strain rate tensor

$$\widetilde{S}_{ij} = \frac{1}{2}\left(\frac{\partial \widetilde{v}_i}{\partial x_j} + \frac{\partial \widetilde{v}_j}{\partial x_i}\right) \tag{18}$$

μ is the dynamic viscosity, $-\overline{\rho}\widetilde{v_i''v_j''}$ are the Reynolds stresses that appear when the average operation is applied to the nonlinear advection term and $(v_i''(x_i, t))$ are the fluctuating velocity components in the Reynolds decomposition. A model is required to represent these stresses in order to close the momentum equations. The conservation of energy written for temperature is

$$\frac{\partial (\overline{\rho}C_p\widetilde{T})}{\partial t} + \frac{\partial (\overline{\rho}C_p\widetilde{v}_i\widetilde{T})}{\partial x_i} = -\frac{\partial \overline{q}_i}{\partial x_i} - \frac{\partial (\overline{\rho}\widetilde{h''v_i''})}{\partial x_i} + \dot{q} \tag{19}$$

where C_p is the specific heat at constant pressure and $\overline{q}_i$ is the heat flux vector assuming Fourier's law

$$\overline{q}_i = -\kappa\frac{\partial \widetilde{T}}{\partial x_i} \tag{20}$$

κ is the molecular thermal conductivity and $\dot{q}$ is a volumetric source such as radiation and $\overline{\rho}\widetilde{h''v_i''}$ is the turbulent heat flux.

The Reynolds stresses are modeled by the Boussinesq relationship

$$-\overline{\rho}\widetilde{v_i''v_j''} \approx \mu_t\left(2\widetilde{S}_{ij} - \frac{2}{3}\frac{\partial \widetilde{v}_k}{\partial x_k}\delta_{ij}\right) - \frac{2}{3}\overline{\rho}\delta_{ij}k \tag{21}$$

where μ_t is the eddy viscosity that must be determined and $k = \frac{1}{2}(\widetilde{v_k''v_k''})$ is the turbulent kinetic energy. The turbulent heat flux is modeled in a similar way dependent on the eddy viscosity and a turbulent Prandtl number (Pr_t)

$$\overline{\rho}\widetilde{h''v_i''} \approx \frac{C_p\mu_t}{Pr_t}\frac{\partial \widetilde{T}}{\partial x_i} = \kappa_t\frac{\partial \widetilde{T}}{\partial x_i}.$$

It is customary to lump the kinetic energy into the pressure

$$\hat{p} = \overline{p} + \frac{2}{3}\overline{\rho}k. \tag{22}$$

For incompressible flow, an additional Boussinesq relation is typically assumed for the body force

$$-(\overline{\rho} - \rho_0)g_i \approx -\rho_0\beta(\widetilde{T} - T_0)g_i \tag{23}$$

where $\beta = -\rho(\frac{\partial\rho}{\partial T})_p$ is a thermal expansion coefficient, g_i is the gravity vector and T_0 is a reference temperature and the divergence is zero. The RANS equations can be written in this simpler form

$$\begin{aligned}
\frac{\partial\overline{\rho}}{\partial t} + \frac{\partial(\overline{\rho}\widetilde{v}_i)}{\partial x_i} &= 0 \\
\frac{\partial(\overline{\rho}\widetilde{v}_i)}{\partial t} + \frac{\partial(\overline{\rho}\widetilde{v}_i\widetilde{v}_j)}{\partial x_j} &= -\frac{\partial\hat{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[2(\mu + \mu_t)\widetilde{S}_{ij}\right] - \beta(\widetilde{T} - T_0)g_i \\
\frac{\partial(\overline{\rho}C_p\widetilde{T})}{\partial t} + \frac{\partial(\overline{\rho}C_p\widetilde{v}_i\widetilde{T})}{\partial x_i} &= -\frac{\partial}{\partial x_i}\left[(\kappa + \kappa_t)\frac{\partial\widetilde{T}}{\partial x_i}\right] + \dot{q}
\end{aligned} \tag{24}$$

12.1 Spalart-Allmaras

The Spalart-Allmaras eddy viscosity transport model(SA) [23] is;

$$\frac{\partial\overline{\rho}\widetilde{\nu}}{\partial t} + \frac{\partial}{\partial x_j}(\overline{\rho}\widetilde{v}_j\widetilde{\nu}) = \overline{\rho}c_{b1}\widetilde{S}_a\widetilde{\nu} - \overline{\rho}c_{w1}f_w\left(\frac{\widetilde{\nu}}{d}\right)^2 + \frac{\partial}{\partial x_j}\left(\frac{\overline{\rho}}{\sigma}(\nu + \widetilde{\nu})\frac{\partial\widetilde{\nu}}{\partial x_j}\right) + \frac{\overline{\rho}c_{b2}}{\sigma}\frac{\partial\widetilde{\nu}}{\partial x_j}\frac{\partial\widetilde{\nu}}{\partial x_j}. \tag{25}$$

The eddy viscosity is given by,

$$\nu_t = \widetilde{\nu}f_{v1}. \tag{26}$$

Functions defining the damping function, source terms and non-conservative diffusion terms in the model are listed below;

$$f_w = g\left(\frac{1 + C_{w3}^6}{g^6 + C_{w3}^6}\right)^{1/6}, f_{v1} = \frac{\chi^3}{\chi^3 + C_{v1}^3}, \quad f_{v2} = 1 - \frac{\chi}{1 + \chi f_{v1}}, \tag{27}$$

$$\chi = \frac{\widetilde{\nu}}{\nu}, \quad g = r + C_{w2}(r^6 - r), \quad r = \frac{\widetilde{\nu}}{\widetilde{S}_a k^2 d^2}, \tag{28}$$

$$\widetilde{S}_a = S_r + \frac{\widetilde{\nu}f_{v2}}{k^2d^2}, \quad S_r = \sqrt{2\widetilde{R}_{ij}\widetilde{R}_{ij}}, \quad \widetilde{R}_{ij} = \frac{1}{2}\left(\frac{\partial\widetilde{v}_i}{\partial x_j} - \frac{\partial\widetilde{v}_j}{\partial x_i}\right), \tag{29}$$

where $\widetilde{R}_{ij}$ is the rotation tensor. Model parameters are listed in table 3.

k	C_{b1}	C_{b2}	σ	C_{w1}	C_{w2}	C_{w3}	C_{v1}	C_{v2}
0.41	0.1355	0.622	2/3	$\frac{C_{b1}}{k^2} + \frac{1+C_{b2}}{\sigma}$	0.3	2.0	7.1	5.0

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

A different formula for $\widetilde{S}_a$ has been proposed in Blazek [5] (also used in Hydra-TH [7]) that prevents it from taking a value of zero. The modified $\widetilde{S}_a$ is;

$$\begin{aligned} \widetilde{S}_a &= \widetilde{f}_{v3} S_r + \frac{\widetilde{\nu} f_{v2}}{k^2 d^2}, \\ \widetilde{f}_{v2} &= \left(1 + \frac{\chi}{C_{v2}}\right)^{-3} \\ \widetilde{f}_{v3} &= \frac{(1 + \chi f_{v1})(1 - \widetilde{f}_{v2})}{\chi}. \end{aligned} \tag{30}$$

k is von Karman's constant, and d appearing in the source terms represents the normal distance to the wall. At a solid wall, $\nu_t = 0$, and therefore the boundary condition is, $\widetilde{\nu}_w = 0$. At inflow boundaries $\widetilde{\nu}_{\Gamma_{Din}} \approx (3-5)\nu_\infty$ and and for outflow boundaries $\widetilde{\nu}_{\Gamma_{Nout}} = \frac{\partial \widetilde{\nu}}{\partial x_j} \hat{n}_j = 0$.

Eddy viscosity models that are used in RANS simulations such as the SA model typically contain a production source term that relates the production of eddy viscosity (in this case) to some measure of the mean shear. This is referred to as the Boussinesq approximation. The SA model makes use of the rotation tensor to estimate shear. In flows where significant vortical structure exists or geometric curvature, the eddy viscosity can be over predicted. There have been several "corrective measures" described in the literature to address this shortcoming in the model. The first correction is by Spalart and Shur [24], Shur et al. [21] (SA-S) and a second correction is due to Dacles-Mariani et al. [11] [10] (SA-DM).

The Shur et al. correction is very invasive requiring the computation of material derivatives for the symmetric stress tensor which practically amounts to solving six additional transport equations. The Dacles-Mariani et al. correction only requires a modification to the production term. The Shur et al. correction was considered to be out-side the scope of this exploratory milestone and so the Dacles-Mariani correction was pursued instead.

Examination of the production source term;

$$P(\widetilde{\nu}) = \overline{\rho} c_{b1} \widetilde{S}_a \widetilde{\nu} \tag{31}$$

shows a dependence on the magnitude of the mean rotation through $\widetilde{S}_a$ and on $\widetilde{\nu}$ itself. In flows with significant vortical structure or geometric curvature, this can lead to an over-prediction in the eddy viscosity. Dacles-Mariani et al. [11] proposed a modification to the production term that accounts for solid-body-rotation and curvature by distinguishing between mean shear and mean rotation;

$$P(\widetilde{\nu}) = \overline{\rho} c_{b1} \widetilde{\nu} \left[(S_r + 2\min(0, \quad S_s - S_r)) + \frac{\widetilde{\nu} f_{v2}}{k^2 d^2} \right]. \tag{32}$$

In this equation, S_s is the magnitude of the symmetric stress tensor;

$$S_s = \sqrt{2 \widetilde{S}_{ij} \widetilde{S}_{ij}}, \qquad \widetilde{S}_{ij} = \frac{1}{2} \left(\frac{\partial \widetilde{v}_{ij}}{\partial x_j} + \frac{\partial \widetilde{v}_{ij}}{\partial x_j} \right). \tag{33}$$

Recently, professor Hong Luo at North Carolina State University brought to our attention modifications to the Spalart-Allmaras model [1] that are receiving a lot of attention in the aerospace community. An evaluation as to whether these modifications should be incorporated into Hydra-TH will be made.

12.2 Standard $k-\varepsilon$ Model

See Hydra-TH theory manual [7] for a detailed discussion of the standard model. The model closure for the Reynolds stresses is reproduced from the above discussion (Equation 21)

$$-\overline{\rho}\widetilde{v_i''v_j''} \approx \mu_t \left(2\widetilde{S}_{ij} - \frac{2}{3}\frac{\partial \widetilde{v}_k}{\partial x_k}\delta_{ij} \right) - \frac{2}{3}\overline{\rho}\delta_{ij}k. \tag{34}$$

The "standard" $k-\varepsilon$ model of Jones and Launder [13] [14] for high-Reynolds number, including buoyancy effects is written

$$\begin{aligned} \frac{\partial \overline{\rho}k}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{v}_j k\right) &= \frac{\partial}{\partial x_j}\left((\overline{\mu} + \mu_t/\sigma_k)\frac{\partial k}{\partial x_j} \right) + P_k + G_B - \overline{\rho}\varepsilon \\ \frac{\partial \overline{\rho}\varepsilon}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{v}_j \varepsilon\right) &= \frac{\partial}{\partial x_j}\left((\overline{\mu} + \mu_t/\sigma_\varepsilon)\frac{\partial \varepsilon}{\partial x_j} \right) + C_{\varepsilon 1}\frac{\varepsilon}{k}P_k + C_{\varepsilon 1}\frac{\varepsilon}{k}G_B - C_{\varepsilon 2}\overline{\rho}\frac{\varepsilon^2}{k} \end{aligned} \tag{35}$$

where the production is defined as;

$$P_k = -\overline{\rho}\widetilde{v_i''v_j''}\frac{\partial \widetilde{v}_i}{\partial x_j}$$

and the eddy viscosity is define as;

$$\mu_t = \frac{C_\mu \overline{\rho} k^2}{\varepsilon}.$$

Production due to buoyancy has been modeled as (Davidson [12]),

$$G_B = -\frac{\mu_t}{\sigma_T}\beta_T g_i \frac{\partial \widetilde{T}}{\partial x_i}.$$

The model constants $C_{\varepsilon 1}$, $C_{\varepsilon 2}$, C_μ, σ_k, σ_ε and σ_T are presented in Table 4.

$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	C_μ	σ_k	σ_ε	σ_T
1.44	1.92	0.09	1.0	1.3	0.85

Table 4: Model parameters for Standard $k-\varepsilon$ turbulence model.

12.3 RNG $k-\varepsilon$ Model

The Renormalization Group Theory (RNG) model was developed by Yakhot et al. [26]. See Hydra-TH theory manual [7] for a detailed discussion of the RNG model. The model equations for k and ε are the same as the standard model equations. RNG and standard models differ by the choice of model coefficients. The model closure for the Reynolds stresses is reproduced from the above discussion (Equation 21)

$$-\overline{\rho}\widetilde{v_i''v_j''} \approx \mu_t \left(2\widetilde{S}_{ij} - \frac{2}{3}\frac{\partial \widetilde{v}_k}{\partial x_k}\delta_{ij} \right) - \frac{2}{3}\overline{\rho}\delta_{ij}k. \tag{36}$$

The model equations for high-Reynolds number are

$$\begin{aligned} \frac{\partial \overline{\rho}k}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{v}_j k\right) &= \frac{\partial}{\partial x_j}\left((\overline{\mu} + \mu_t/\sigma_k)\frac{\partial k}{\partial x_j} \right) + P_k - \overline{\rho}\varepsilon \\ \frac{\partial \overline{\rho}\varepsilon}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{v}_j \varepsilon\right) &= \frac{\partial}{\partial x_j}\left((\overline{\mu} + \mu_t/\sigma_\varepsilon)\frac{\partial \varepsilon}{\partial x_j} \right) + C_{\varepsilon 1}\frac{\varepsilon}{k}P_k - C_{\varepsilon 2}\overline{\rho}\frac{\varepsilon^2}{k} \end{aligned} \tag{37}$$

where the production is defined as;

$$P_k = -\overline{\rho}\widetilde{v_i'' v_j''}\frac{\partial \widetilde{v}_i}{\partial x_j}$$

and the eddy viscosity is define as;

$$\mu_t = \frac{C_\mu \overline{\rho} k^2}{\varepsilon}.$$

One of the main operational differences between the standard and RNG models is the definition of $C_{\varepsilon 2}$ which is no longer a constant but now depends on the mean strain rate

$$C_{\varepsilon 2} = \widetilde{C}_{\varepsilon 2} + \frac{C_\mu \eta^3 (1 - \eta/\eta_0)}{1 + \beta \eta^3}, \quad \eta = \frac{k}{\varepsilon}\sqrt{2\widetilde{S}_{ij}\widetilde{S}_{ij}}, \quad \widetilde{S}_{ij} = \frac{1}{2}\left(\frac{\partial \widetilde{v}_i}{\partial x_j} + \frac{\partial \widetilde{v}_j}{\partial x_i}\right).$$

The model constants $C_{\varepsilon 1}$, $\widetilde{C}_{\varepsilon 2}$, C_μ, σ_k, σ_ε β and η_0 are presented in Table 5.

$C_{\varepsilon 1}$	$\widetilde{C}_{\varepsilon 2}$	C_μ	σ_k	σ_ε	β	η_0
1.42	1.68	0.085	0.72	0.72	0.012	4.38

Table 5: Model parameters for RNG $k - \varepsilon$ turbulence model.

12.4 Nonlinear $k - \varepsilon$ Model Design and Implementation

This work was done in support of a level 2 milestone entitled "Single Phase Validation of Hydra-TH for Fuel Applications (FY14.CASL.010)" [3]. One objective was to design, implement and validate the nonlinear $k - \varepsilon$ model of Baglietto [2] and Baglietto and Ninkata [4] in Hydra-TH. Work remains to mature this model to point where it is production ready. A brief description of the model is included here to facilitate the task of documenting it at a later date in the Hydra-TH theory manual. The description follows closely Baglietto [2].

The "standard" $k - \varepsilon$ model of Jones and Launder [13] can be written as;

$$\begin{aligned}
\frac{\partial \overline{\rho} k}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{v}_j k\right) &= \frac{\partial}{\partial x_j}\left((\overline{\mu} + \mu_t/\sigma_k)\frac{\partial k}{\partial x_j}\right) P_k - \overline{\rho}\varepsilon \\
\frac{\partial \overline{\rho} \varepsilon}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{v}_j \varepsilon\right) &= \frac{\partial}{\partial x_j}\left((\overline{\mu} + \mu_t/\sigma_\varepsilon)\frac{\partial \varepsilon}{\partial x_j}\right) + C_{\varepsilon 1}\frac{\varepsilon}{k}P_k - C_{\varepsilon 2}\overline{\rho}\frac{\varepsilon^2}{k}
\end{aligned} \tag{38}$$

where the production is defined as;

$$P_k = -\overline{\rho}\widetilde{v_i'' v_j''}\frac{\partial \widetilde{v}_i}{\partial x_j}$$

and the eddy viscosity is define as;

$$\mu_t = \frac{C_\mu \overline{\rho} k^2}{\varepsilon}.$$

Unlike the standard model C_μ is not constant. Based upon realizability considerations, C_μ is a function of the shear and rotation invariants S and W,

$$C_\mu = \frac{C_{a0}}{(C_{a1} + C_{a2}S + C_{a3}W)}$$

where,

$$S = \frac{k}{\varepsilon}\sqrt{2\widetilde{S}_{ij}\widetilde{S}_{ij}}, \quad W = \frac{k}{\varepsilon}\sqrt{2\widetilde{\Omega}_{ij}\widetilde{\Omega}_{ij}},$$

$$\widetilde{S}_{ij} = \left(\frac{\partial \widetilde{v}_i}{\partial x_j} + \frac{\partial \widetilde{v}_j}{\partial x_i}\right), \quad \widetilde{\Omega}_{ij} = \left(\frac{\partial \widetilde{v}_i}{\partial x_j} - \frac{\partial \widetilde{v}_j}{\partial x_i}\right).$$

The Reynolds's stresses are represented by a nonlinear stress-strain relationship, necessary to capture anisotropic stress behavior which is responsible for the creation of secondary flow in fuel rod bundle flows. The quadratic stress-strain relationship is given by;

$$\begin{aligned}
\overline{\rho}\widetilde{v_i''v_j''} &= \left(\frac{2}{3}\overline{\rho}k\delta_{ij} - \mu_t\widetilde{S}_{ij}\right) \\
&+ C_1\mu_t\frac{k}{\varepsilon}\left[\widetilde{S}_{ik}\widetilde{S}_{kj} - \frac{1}{3}\delta_{ij}\widetilde{S}_{kl}\widetilde{S}_{kl}\right] \\
&+ C_2\mu_t\frac{k}{\varepsilon}\left[\widetilde{\Omega}_{ik}\widetilde{S}_{kj} + \widetilde{\Omega}_{jk}\widetilde{S}_{ki}\right] \\
&+ C_3\mu_t\frac{k}{\varepsilon}\left[\widetilde{\Omega}_{ik}\widetilde{\Omega}_{jk} - \frac{1}{3}\delta_{ij}\widetilde{\Omega}_{kl}\widetilde{\Omega}_{kl}\right]
\end{aligned}$$

where the first term on the right-hand-side is the usual linear contribution. For realizability, the three constants, (C_1, C_2, C_3) are non-constant given by;

$$C_1 = \frac{C_{NL1}}{(C_{NL6} + C_{NL7}S^3)C_\mu} \quad C_2 = \frac{C_{NL2}}{(C_{NL6} + C_{NL7}S^3)C_\mu} \quad C_3 = \frac{C_{NL3}}{(C_{NL6} + C_{NL7}S^3)C_\mu}$$

Model parameters are listed in table 6 and table 7.

σ_k	σ_ε	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	C_{a0}	C_{a1}	C_{a2}	C_{a3}
1.0	1.22	1.44	1.92	0.667	3.9	1.0	0

Table 6: Model parameters for nonlinear $k - \varepsilon$ turbulence model.

C_{NL1}	C_{NL2}	C_{NL3}	C_{NL6}	C_{NL7}
0.8	11	4.5	1000	1.000

Table 7: Model parameters for nonlinear $k - \varepsilon$ turbulence model quadratic stress terms.

The current implementation uses the y*-insensitive wall function described in the Hydra-TH theory manual. Baglietto and Ninokata [4] present damping functions to allow integration to the wall. These functions have not been implemented yet. In addition, the current implementation neglects sensitivities of the nonlinear stress terms in the implicit left-hand-side operator and so currently, the Jacobian terms for the nonlinear model are identical to the standard model. This choice was expedient and will have to be re-evaluated at a later time.

12.5 Realizable $k - \varepsilon$ Model

The Boussinesq relationship relating Reynolds stresses to the mean strain rate

$$-\overline{\rho}\widetilde{v_i''v_j''} \approx \mu_t\left(2\widetilde{S}_{ij} - \frac{2}{3}\frac{\partial \widetilde{v}_k}{\partial x_k}\delta_{ij}\right) - \frac{2}{3}\overline{\rho}\delta_{ij}k \tag{39}$$

and eddy viscosity for $k-\varepsilon$ given by

$$\mu_t = \overline{\rho} C_\mu \frac{k^2}{\varepsilon} \tag{40}$$

where $C_\mu = 0.09$ is a constant, can result in negative normal Reynolds stresses for large mean strain $\widetilde{S}$

$$\widetilde{S} = \sqrt{2\widetilde{S}_{ij}\widetilde{S}_{ij}}, \quad \widetilde{S}_{ij} = \frac{1}{2}\left(\frac{\partial \widetilde{v}_i}{\partial x_j} + \frac{\partial \widetilde{v}_j}{\partial x_i}\right), \quad \widetilde{\Omega}_{ij} = \frac{1}{2}\left(\frac{\partial \widetilde{v}_i}{\partial x_j} - \frac{\partial \widetilde{v}_j}{\partial x_i}\right)$$

and violate the Schwartz inequality for Reynolds stresses

$$\begin{aligned} \overline{(v'_\alpha v'_\alpha)} &\geq 0 \\ \overline{(v'_\alpha v'_\beta)^2} &\leq \overline{(v'_\alpha)^2 (v'_\beta)^2}. \end{aligned}$$

The model of Shih et al. [20] which will be referred to as Realizable $k-\varepsilon$ is written as

$$\begin{aligned} \frac{\partial \overline{\rho} k}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{v}_j k\right) &= \frac{\partial}{\partial x_j}\left((\overline{\mu} + \mu_t/\sigma_k)\frac{\partial k}{\partial x_j}\right) + P_k - \overline{\rho}\varepsilon \\ \frac{\partial \overline{\rho} \varepsilon}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{v}_j \varepsilon\right) &= \frac{\partial}{\partial x_j}\left((\overline{\mu} + \mu_t/\sigma_\varepsilon)\frac{\partial \varepsilon}{\partial x_j}\right) + \overline{\rho} C_1 \widetilde{S}\varepsilon - \overline{\rho} C_2 \frac{\varepsilon^2}{k + \sqrt{\nu\varepsilon}} \end{aligned} \tag{41}$$

The model constant C_1 is

$$C_1 = \max\left[0.43, \frac{\eta}{\eta + 5}\right], \quad \eta = \widetilde{S}\frac{k}{\varepsilon} \tag{42}$$

and the production is defined as;

$$P_k = -\overline{\rho}\widetilde{v''_i v''_j}\frac{\partial \widetilde{v}_i}{\partial x_j}.$$

Shih et al. [20] proposed a remedy for this deficiency by making C_μ a function of the mean strain

$$C_\mu = \frac{1}{A_0 + A_s U^* \frac{k}{\varepsilon}} \tag{43}$$

and

$$U^* = \sqrt{\widetilde{S}_{ij}\widetilde{S}_{ij} + \widetilde{\Omega}'_{ij}\widetilde{\Omega}'_{ij}} \quad \widetilde{\Omega}'_{ij} = \widetilde{\Omega}_{ij} - 2\varepsilon_{ijk}\omega_k \quad \widetilde{\Omega}_{ij} = \overline{\Omega}_{ij} - \varepsilon_{ijk}\omega_k \tag{44}$$

where $\overline{\Omega}_{ij}$ is the mean rotation rate viewed in a rotating reference frame and ω_k is the angular velocity ($rad/sec.$). For a non-rotating reference frame, $\widetilde{\Omega}'_{ij} = \widetilde{\Omega}_{ij}$, the usual definition for the rotation tensor. (This aspect of the model is a little confusing and needs to be examined more carefully.) The two model constants A_0 and A_s are given by

$$A_0 = 4.04 \qquad A_s = \sqrt{6}\cos\phi$$

where

$$\phi = \frac{1}{3}\cos^{-1}(\sqrt{6}W), \quad W = \frac{\widetilde{S}_{ij}\widetilde{S}_{jk}\widetilde{S}_{ki}}{(\widetilde{S}_{ij}\widetilde{S}_{ij})^{3/2}}. \tag{45}$$

The model constants $C_{1\varepsilon}$, C_2, σ_k and σ_ε are presented in Table 8.

$C_{1\varepsilon}$	C_2	σ_k	σ_ε
1.44	1.9	1.0	1.2

Table 8: Model parameters for Realizable $k-\varepsilon$ turbulence model.

12.6 SST $k-\omega$ Model

Menter's shear stress transport (SST) $k-\omega$ model [16] blends Wilcox's $k-\omega$ model [25] with the standard $k-\varepsilon$ model where the ε equation, representing the rate of turbulent kinetic energy dissipation, is rewritten as an equation for ω, which approximately represents the time scale for energy dissipation. Units for $\varepsilon \to (\ell^2/t^3)$ and for $\omega \to (1/t)$. Several motivations for choosing this model over the standard $k-\varepsilon$ or the $k-\omega$ model are; The $k-\omega$ model and SST version do not require the use of special near wall treatments and can be integrated to the wall directly, eliminates the sensitivity to free stream ω that hampers the Wilcox $k-\omega$ model and incorporates transport of Reynolds stress (as the name implies) which results in better predictions in flows with strong pressure gradients. See Hydra-TH theory manual [7] for a detailed discussion of the SST $k-\omega$ model. The model closure for the Reynolds stresses is reproduced from the above discussion (Equation 21)

$$-\overline{\rho}\widetilde{v_i''v_j''} \approx \mu_t \left(2\widetilde{S}_{ij} - \frac{2}{3}\frac{\partial \widetilde{v}_k}{\partial x_k}\delta_{ij} \right) - \frac{2}{3}\overline{\rho}\delta_{ij}k. \tag{46}$$

The model equations are

$$\begin{aligned}
\frac{\partial \overline{\rho} k}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{v}_j k\right) &= \frac{\partial}{\partial x_j}\left((\overline{\mu} + \mu_t/\sigma_k)\frac{\partial k}{\partial x_j} \right) + P_k - \overline{\rho}\beta^* k\omega \qquad (47)\\
\frac{\partial \overline{\rho}\omega}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{v}_j \omega\right) &= \frac{\partial}{\partial x_j}\left(\overline{\rho}(\overline{\nu} + \sigma_\omega \nu_t)\frac{\partial \omega}{\partial x_j} \right) - \frac{\gamma}{\nu_t}P_k - \overline{\rho}\beta\omega^2 + 2(1-F_1)\overline{\rho}\sigma_{\omega 2}\frac{1}{\omega}\frac{\partial k}{\partial x_j}\frac{\partial \omega}{\partial x_j}
\end{aligned}$$

where the production is defined as;

$$P_k = -\overline{\rho}\widetilde{v_i''v_j''}\frac{\partial \widetilde{v}_i}{\partial x_j}$$

and the eddy viscosity is define as

$$\nu_t = \frac{a_1 k}{\max(a_1\omega; \Omega F_2)}.$$

where $\Omega = |\nabla \times \widetilde{\mathbf{v}}|$ is taken as the absolute value of vorticity and $\mu_t = \overline{\rho}\nu_t$. The blending function is defined

$$\begin{aligned}
F_1 = \tanh(arg_1^4), \quad arg_1 &= \min\left(\max\left(\frac{\sqrt{k}}{0.09\omega y}; \frac{500\overline{\nu}}{\omega y^2} \right); \frac{4\overline{\rho}\sigma_{\omega 2}k}{CDy^2} \right)\\
CD &= \max\left(2\overline{\rho}\sigma_{\omega 2}\frac{1}{\omega}\frac{\partial \omega}{\partial x_j}\frac{\partial k}{\partial x_j}; 10^{-20} \right)\\
F_2 = \tanh(arg_2^2), \quad arg_2 &= \max\left(2\frac{\sqrt{k}}{0.09\omega y}; \frac{500\overline{\nu}}{\omega y^2} \right).
\end{aligned}$$

Constants for the inner region (set 1) and the outer region (set 2) are blended

$$g(\phi_1, \phi_2; F_1) = F_1\phi_1 + (1-F_1)\phi_2. \tag{48}$$

σ_k	σ_ω	β	γ	a_1	β^*	κ
$g(\sigma_{k1}, \sigma_{k2})$	$g(\sigma_{\omega 1}, \sigma_{\omega 2})$	$g(\beta_1, \beta_2)$	$g(\gamma_1, \gamma_2)$	0.31	0.09	0.41

Table 9: Blended model parameters for SST $k-\omega$ turbulence model.

σ_{k1}	$\sigma_{\omega 1}$	β_1	γ_1
0.85	0.5	0.075	$\beta_1/\beta^* - \sigma_{\omega 1}\kappa^2/\sqrt{\beta^*}$
σ_{k2}	$\sigma_{\omega 2}$	β_2	γ_2
1.0	0.856	0.0828	$\beta_2/\beta^* - \sigma_{\omega 2}\kappa^2/\sqrt{\beta^*}$

Table 10: Inner (set 1) and outer (set 2) parameters for SST $k-\omega$ turbulence model.

Model constants for a_1, β^*, and κ along with blended constants σ_k, σ_ω, β and γ are presented in Table 9 and the inner and outer set constants are presented in Table 10.

The free stream boundary conditions for ω, ν_t and k are

$$\omega_{\Gamma_{Din}} = (1 \to 10)\frac{V_\infty}{L}, \quad \nu_{t\Gamma_{Din}} = 10^{-(2\to 5)}\nu_\infty, \quad k_{\Gamma_{Din}} = \nu_{t\infty}\omega_{\Gamma_{Din}}.$$

The wall boundary conditions for ω and k are

$$\omega_{\Gamma_{Dwall}} = 10\frac{6\nu}{\beta_1(\Delta y_1)^2}, \quad k_{\Gamma_{Dwall}} = 0$$

where Δy_1 is the distance to the next point away from the wall. This boundary condition simulates a smooth wall where $\Delta y_1^+ < 3$ is assumed.

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