Single Phase Validation of Hydra-TH for Fuel Applications
L2.THM.P9.01 (FY14.CASL.010)

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EXECUTIVE SUMMARY

This milestone is dedicated to advancing, demonstrating and assessing the Computational Fluid Dynamics (CFD) capabilities of the Hydra-TH package for fuel related single phase applications. Hydra-TH represents the CFD component adopted for the Virtual Environment for Reactor Analysis (VERA) simulation suite.

In the thermal hydraulics fuel design of Pressurized Water Reactors (PWR), knowledge of detailed local conditions is highly desirable and can be accomplished with the use of CFD. The CASL Challenge Problems (CP) are representative of this need and can greatly benefit by the advancement of the CFD accuracy, robustness and numerical efficiency. Robust application of CFD however relies on proven numerical methods and well assessed turbulence modeling representation. An extensive effort has therefore been essential, and is documented in this work, in order to develop, implement and assess the computational and modeling capabilities necessary to ensure the quality of the CFD results obtained.

The report documents the efforts in the Thermal Hydraulics Focus Area that have led to extending and assessing the capabilities of Hydra-TH in order to deliver a robust fuel simulation platform. Three key areas are discussed in this report:

- Hydra-TH Numerical Methods
- Turbulence Modeling for Fuel Related Applications
- Best Practices for Application of Hydra-TH to Fuel Analysis

The capabilities developed and assessed as part of the milestone directly support various objectives of CASL, including various CPs. These are: 1. Future extension of VERA-CS to include full core CFD as the TH component; 2. CFD based prediction of Crud induced localized corrosion (CILC); 3 CFD based turbulence force evaluation for Grid-to-Rod Fretting (GTRF) phenomena.

Specifically, the milestone work has been completed in the following areas:

1) Advancement and assessment of Hydra-TH solution algorithms.
2) Extension of turbulence modeling framework for RANS/URANS simulations.
3) Implementation and assessment of an advanced non-linear turbulence model for fuel related applications.
4) Assessment of Hydra-TH capabilities for application to GTRF predictions.
5) Testing and best practice development for fuel related applications of Hydra-TH.

The assessment of Hydra-TH for fuel related single phase applications has demonstrated the readiness of a complete CFD framework. Both RANS and LES solution methods are extremely scalable and efficient and can be applied robustly for CP related activities. The LES validation and demonstration on GTRF phenomena displayed full maturity, while the work on advanced RANS turbulence modeling will still require some improvement. Finally, while a reference best practice approach for geometry and mesh construction has been successfully implemented and assessed, more work will be required to extend the usage of Hydra-TH to a larger domain of third-party generated models.

The models and capability delivered from this milestone provide the base for supporting the application of advanced fuel modeling capabilities in VERA.
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1. MILESTONE DESCRIPTION

This milestone is dedicated to advancing, demonstrating and assessing the Computational Fluid Dynamics (CFD) capabilities of the Hydra-TH package for fuel related single phase applications. Hydra-TH represents the CFD component adopted for the Virtual Environment for Reactor Analysis (VERA) simulation suite. While the CFD approach has the demonstrated potential to overcome the limitations of current lumped-parameter methods, typically referred to as “subchannel models”, its accuracy and robustness must rely on proven numerical methods and well assessed turbulence modeling representation. The milestone report presents and critically discusses these challenges, the work that was performed to tackle them, the current status and the best practice that have been derived to support VERA usage.

1.1 CFD applications to PWR fuel design

In the thermal hydraulics design of Pressurized Water Reactors (PWR) fuel, knowledge of detailed local conditions is highly desirable and could be accomplished with the use of CFD. The CASL Challenge Problems (CP) are representative of this need and can greatly benefit by the advancement of the CFD accuracy, robustness and numerical efficiency.

Traditionally, critical heat flux (CHF) has been adopted as the key thermal performance parameter for fuel. This parameter is defined and used to ensure safe operation of the reactor core under all expected conditions. CHF is a two-phase flow phenomenon, which occurs when the fuel rod clad surface is overheated due to formation of a local vapor layer, causing dramatic reduction in heat transfer capability. While the thermal crisis is reached under two-phase flow conditions, which are much more complex to measure and model than single-phase flow, the single phase flow distribution has a dominant role in PWR conditions. It is logical and necessary therefore to start with CFD models of single phase conditions. Then, when the methodology is developed with confidence on single-phase flows, application of two-phase conditions can be achieved. This strategy makes sense not only from the complexity of the physics, but it also makes sense from a benchmark testing perspective. Figure 1 shows a representative single phase flow analysis of temperature distribution on a rod surface in proximity of a mixing vane grid, which clearly reveals the complex 3-dimensional temperature distribution and the fundamental role of CFD to support improved fuel performance.

![Figure 1: Temperature distribution on a PWR fuel rod in the vicinity of a Mixing Vane Grid [1].](image-url)
Another fundamental application area for CFD is related to the analysis of CRUD, in order to reduce uncertainty in CRUD thickness & boron uptake predictions. With a trend in the US PWR plants toward increased power upratings, longer cycles, and higher fuel burnup, understanding the local conditions in a PWR fuel assembly has become necessary to minimize the risk of future “CRUD leakers” in PWR fuel. CFD can play a fundamental role in this respect allowing designers to include in the prediction approach an accurate representation of the complex 3-dimensional flow driven effect on Crud induced localized corrosion (CILC), as demonstrated in the L2.MPO.P7.06 Milestone [3]. Figure 2 gives an illustrative example of this effect where the CRUD deposition swirl effect noticeable after the spacer is driven by the mixing vane induced flow swirl.

![Figure 2: Simulated CRUD deposition on PWR fuel rod [2].](image)

Finally, the grid-to-rod fretting (GTRF) problem in pressurized water reactors is a flow-induced vibration issue that results in wear and failure of the rod cladding. GTRF wear has been one of the leading causes for leaking nuclear fuel and has cost power utilities millions of dollars in preventive measures. CFD has shown to be a fundamental tool in order to predict accurately the turbulent excitation forces on the fuel rods, along with the coupled structural response of the rods and their supports [4]. Figure 3 shows an example of the instantaneous turbulent flow field from CFD simulation. The transient forces are computed on the fuel rods in the CFD model. The transient forces acting on the fuel rod surface are then integrated at each rod segment in two lateral components, and adopted as excitation component in the lumped VITRAN [70] model shown on the left in Fig. 3.
The discussed examples serve to clarify how improved predictions for the local fuel rod thermal-hydraulic conditions need to be obtained and understood. Testing can only provide limited information at specific locations where the instrumentation is placed and therefore CFD can be used to calculate key parameters in the whole modeling domain. Nevertheless, the complex flow field in a PWR with mixing vanes provides a very challenging problem for CFD. Therefore, an extensive effort has been necessary, and is documented in this work, in order to develop, implement and assess the computational and modeling capabilities necessary to ensure the quality of the CFD results obtained.

### 1.2 Approach and Implementation

The approach to the milestone work relies heavily on the extensive experience existing inside the CASL Thermal Hydraulics Methods (THM) Focus Area. Leveraging the existing experience has allowed focusing the implementation and assessment activities and demonstrating the effectiveness of the methods selected. The large number of fundamental mechanisms necessary to assemble the required capabilities has required a multi-stage development that has been documented in separate milestones. Below, a list of the fundamental milestones that support the current work is provided for reference, and allows appreciating the scale of the effort.

**Table 1 – THM Milestones supporting the Single Phase CFD Capabilities in Hydra-TH.**

<table>
<thead>
<tr>
<th>Code</th>
<th>Description</th>
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<td>L3:THM.CFD.P3.02</td>
<td>Deployment and testing of Hydra-TH CFD code.</td>
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<tr>
<td>L2:THM.P4.01</td>
<td>Initial assessment of Hydra-TH code on GTRF problems</td>
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<tr>
<td>L3:THM.CFD.P7.02</td>
<td>Assessment of Hydra-TH on Benchmark Problems</td>
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<tr>
<td>L3:THM.CFD.P7.09</td>
<td>Coordinate and document Hydra-TH validation, verification, and testing coverage</td>
</tr>
<tr>
<td>L3:THM.CLS.P7.04</td>
<td>ITM simulation of bubbly flow in PWR subchannel and its statistical analysis</td>
</tr>
<tr>
<td>L3:THM.CFD.P9.03</td>
<td>Hydra-TH linear algebra improvements and performance optimization</td>
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1.3 Working Group

The milestone relies on the coordinated effort from all the listed individuals, which bring together a unique set of skills and experience in collaborative research projects. A deeper look at the team members would allow appreciating a unique balance of expertise between the numerical, modeling and application expertise.

<table>
<thead>
<tr>
<th>Name</th>
<th>Subtask</th>
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<td>Best Practices</td>
<td>U-Michigan</td>
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2. HYDRA-TH NUMERICAL METHODS

Hydra-TH is the thermal hydraulics code being developed at Los Alamos National Laboratory as the CFD component for CASL VERA simulation suite [9-10].

Hydra-TH is a massively parallel code built on the Hydra Toolkit [11]. The Hydra Toolkit is written in C++ and provides a rich suite of lightweight high performance components that permit rapid application development, supports multiple discretization techniques, provides I/O interfaces to permit reading and writing multiple file formats for meshes, plot data, time-history, surface and restart output. The Toolkit also provides run-time parallel domain decomposition with data-migration for both static and dynamic load-balancing. Linear algebra is handled through an abstract virtual interface that enables the use of popular libraries such as PETSc [12] and Trilinos [13].

Hydra-TH relies on a hybrid finite-volume finite-element discretization that provides a stable and accurate discretization while preserving local conservation properties important in many thermal hydraulics applications. Hydra-TH also supports the use of hybrid meshes that permit the resolution of boundary layers on complex geometries. Hydra-TH provides interfaces for performing conjugate heat transfer and fluid-structure interaction problems using third-party radiation-conduction and structural codes.

2.1 Unstructured Grid Topology

Realistic simulation of flow fields in a PWR with mixing vanes provides a very challenging problem for CFD. Geometries are extremely complex, including very large number of small features, contacts, gaps, and have proven to be extremely challenging for most CFD tools. In order to successfully capture the geometric complexity a paramount requirement for Hydra-TH is an efficient handling of unstructured grid topologies. The central element for an effective unstructured flow solver in Hydra-TH is the use of so-called “edge-based” algorithms.

The use of edge-based algorithms for advection rely on topological grid constructs such as vertices, edges, primal and dual-grids. Figure 4 illustrates a primal grid and the associated centroidal and median dual grids. In the primal grid, each cell consists of an ordered set of vertices connected by cell edges or faces. Each vertex of the dual grid (both centroidal and median dual grids may be considered here) is associated with a cell of the primal mesh. Edges are in general lines that connect a pair of vertices. In the primal grids of interest here, the edges will be straight lines. However, the edges of the dual grids need not be straight lines as shown in Fig. 5. Edges of the dual grid intersect primal edges. In general, vertices, edges and faces of both the primal and dual grids are ordered independently.

In Hydra-TH a carefully designed and implemented edge extraction algorithm is used to construct the edge-based data structures. The concepts for the edge extraction algorithm are based on the algorithms developed in QACINA [7], but extended to treat arbitrary topology meshes comprised of multiple element types. These algorithms scale approximately as $N_{el} \log$
(N_{el}), but with a constant that is bounded and small, $2.5 \times 10^{-7} \leq C \leq 10^{-6}$. The algorithm extensions required for parallel implementation are trivial as the extraction calculation is “embarrassingly parallel”.

Figure 4: Primal, median dual, and centroidal dual grids.

Figure 5: Primal and median dual grids.
2.2 RANS/LES Methods

The manner in which values are approximated in the solution method has a profound effect on the stability and accuracy of the numerical scheme. Here we only provide a very concise description of Hydra-TH methods, but more details on the Hydra Toolkit and its incompressible solver are given in the Theory manual [14]. For the incompressible/low-Mach Navier-Stokes formulation all transport variables are cell-centered and treated with a locally conservative discretization that includes a high-resolution monotonicity-preserving advection algorithm. The spatial discretization is formally derived using a discontinuous-Galerkin framework that, in the limit, reduces to a locally-conservative finite-volume method. The advection algorithm is designed to permit both implicit and explicit advection with the explicit advection targeted primarily at volume-tracking with interface reconstruction. Extensive convergence studies have been performed to demonstrate the effectiveness of the methods on various types of solution grids. Figures 6 and 7 shows a sample convergence study for a mixed triangle/quadrilateral mesh.

![Figure 6: Mesh configuration for the case-a tri-quad meshes.](image)

![Figure 7: L1 errors at t = 2.5, 5.0, and 10.0 for the case-a tri-quad meshes.](image)

The Projection Method

The solution of the time-dependent incompressible Navier-Stokes equations poses several algorithmic problems due to the div-free constraint, and the concomitant spatial and temporal resolution required to perform time-accurate solutions particularly when complex geometry is
involved. Although fully-coupled solution strategies are available, the cost of such methods is generally considered prohibitive for time-dependent simulations where high-resolution grids are required. The application of projection methods provides a computationally efficient alternative to fully-coupled solution methods. The available time-integration methods include backward-Euler and the neutrally-dissipative trapezoidal method. The implicit advective treatment delivers unconditional stability for scalar transport equations and conditional stability for the momentum equation.
3. TURBULENCE MODELING FOR FUEL APPLICATIONS

3.1 RANS Models

Mainstream applications to fuel design and analysis mostly rely on Reynolds Averaged Navier Stokes (RANS) models as the most relevant approach to model the often complex geometrical configurations of fuel assemblies, at the high Reynolds number typical or reactor conditions.

Extensive use of CFD for fuel related applications in the last two decades has clearly exposed RANS turbulence modeling to still be a critical link in the development of a reliable numerical methodology. Among the many turbulence models, second order closure ones, although being attractive for their capability of simulating transport of the individual Reynolds stresses, cannot be applied with confidence due to the potential inaccuracies deriving from the inappropriate modeling of the higher order correlations. Extensive work is ongoing to try to overcome these limitations [8], but yet no clear evidence has been presented to support adequate robustness for fuel applications.

In contrast, two-equation models have undoubtedly gained prevalent popularity, thanks to their formalistic simplicity, their numerical robustness and computational economy, and especially to their wide range of testing on different applications where they have shown broad applicability. When dealing with internal flows the $k-\varepsilon$ family of closures still takes the largest roles, thanks to its proven record and the related extensive understanding of its limitations. These models still retain in fact numerous weaknesses, in particular the inability to capture anisotropy, insufficient sensitivity to secondary strains, excessive generation of turbulence at impingement zones and a violation of the realizability constraints at large strain rates.

The RANS models option that have been selected for Hydra-TH delivery are discussed below, with particular attention to the Quadratic $k-\varepsilon$ model [14-16] which has been specifically implemented as part of this milestone.

3.1.1 RNG $k-\varepsilon$ Model

Leveraging the extensive experience in the application of RANS models to complex industrial flows, the Hydra-TH package has selected the RNG (renormalization group) $k-\varepsilon$ model as a first “all-purpose” model, which was therefore implemented as the default option for two-equation RANS.

Yakhot and Orszag derived the RNG model based on Renormalization Group (RNG) methods [19]. In this approach, RNG techniques are used to develop a theory for the large scales in which the effects of the small scales are represented by modified transport coefficients. The form of the equations remains the same as that of the standard $k-\varepsilon$ model, but with modified definition and values of the coefficients. Most importantly, Yakhot and Orszag included an additional term in the epsilon equation, which is an ad hoc model not derived from RNG theory, but plays a dominant role in extending the capabilities of the RNG closure in comparison to the standard $k-\varepsilon$ approach.
\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_j} \left( \rho u_j k - \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right) = P_k - \rho \varepsilon \quad 3.1
\]

\[
\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_j} \left[ \rho u_j \varepsilon - \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] = C_{\varepsilon 1} \frac{\varepsilon}{k} P_k - C_{\varepsilon 2} \rho \frac{\varepsilon^2}{k} + \frac{C_\mu \eta^3 (1 - \eta/\eta_0) \varepsilon^2}{1 + \beta \eta^3} \quad 3.2
\]

\[\eta \equiv S \frac{k}{\varepsilon} \quad 3.3\]

The last term on the RHS in eq. 3.2 is the additional ad-hoc modification. It is this term which is largely responsible for the difference in performance of the standard and RNG models. Here the \( \eta \) term (eq. 3.3) includes “some” effect of the mean flow distortion on the turbulence dissipation, and such capability leads to improved predictions on high strain rate and high streamline curvature flows. It should be noted that from a rigorous point of view the RNG model yields much lower levels of turbulence in complex geometries, and its reduced “viscosity” leads to more realistic flow features, by grossly overestimating the level of \( \varepsilon \). In reality it is the production of \( k \) that is overestimated by the eddy viscosity assumption, and not the levels of Epsilon, and therefore the RNG model somewhat predicts the right trends for the wrong reason. The cure to the \( k-\varepsilon \) limitations should be found in a better representation of anisotropy, and essentially of the normal stresses, as discuss later.

### 3.1.2 Standard \( k-\varepsilon \) Model

The standard \( k-\varepsilon \) model has been by far the most popular two-equation model. The earliest development efforts based on this model were those of Chou 1945 [20], Davidov 1961 [21] and Harlow and Nakayama 1968 [22]. The central paper however, is that by Jones and Launder 1972 [23] that, in the turbulence modeling community is so well known that it is often referred to as the “Standard \( k-\varepsilon \)” model. Actually, Launder and Sharma, “retuned” the model’s closure coefficients and practically all researchers use the form of the model presented in their 1974 paper [24].

Recently the standard \( k-\varepsilon \) model has been largely replaced by its Realizable variant [25] and, for the case of external flow applications by the SST approach, which blends is with a near wall \( k-\omega \) closure [26]. However, due to its very extensive validation, the standard \( k-\varepsilon \) model remains the fundamental reference for evaluation of new model advancement, and therefore the model has been implemented in Hydra-TH as part of the current effort.

The standard \( k \) and \( \varepsilon \) equations are shown below:

\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_j} \left( \rho u_j k - \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right) = P_k - \rho \varepsilon \quad 3.4
\]
\[ \frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_j} \left[ \rho u_j \varepsilon - \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] = C_{e1} \frac{\varepsilon}{k} P_k - C_{e2} \rho \frac{\varepsilon^2}{k} \] \quad 3.5

The eddy viscosity in this model is defined by:

\[ \mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \] \quad 3.6

The standard values for the model parameters are:

\[ C_\mu = 0.09 \quad , \quad \sigma_k = 1.0 \quad , \quad \sigma_\varepsilon = 1.22 \quad , \quad c_{e1} = 1.44 \quad , \quad c_{e2} = 1.92 \]

When discussing the popularity of the \( \kappa-\varepsilon \) model we should not forget that well known limitations exist. In particular these models make use of the simple Boussinesq isotropic eddy-viscosity concept, which assumes that the Reynolds stresses are proportional to the mean velocity gradients. Practical engineering flows exhibit complex mean strains and are strongly affected by anisotropy, and cannot therefore be correctly predicted by this family of models. The most quoted example is the secondary flow that originates in a square duct due to the gradients of the turbulent shear stresses, and which cannot be reproduced by eddy-viscosity models. Second-moment closures offer a greater potential for predicting the anisotropic phenomena correctly, but we have previously emphasized how the inappropriate modeling of the higher-order turbulent correlations can result in serious inaccuracies and unphysical results. For this reason the next session will discuss how the most practical and reliable approach at present is to calculate the Reynolds stresses by algebraic expressions.

### 3.1.3 Reynolds Stress Anisotropy and Nonlinear Eddy Viscosity Models

The idea of creating an Explicit Algebraic Reynolds Stress Model (EARSM) was first introduced in 1975 by Pope [27], who mathematically derived a general non-linear constitutive relation using the generalized Cayley-Hamilton formulas and the invariant principles. If we define the anisotropy tensor \( \mathbf{a} \) as:

\[ a_{ij} = \frac{u_i u_j}{k} - \frac{2}{3} \delta_{ij} \] \quad 3.7

and denote the mean strain and vorticity tensors as \( \mathbf{s} \) and \( \mathbf{\omega} \), the general relationship between Reynolds stresses and strain can be expressed as:

\[ \mathbf{a} = \sum_{\lambda=4}^{10} G_{\lambda}(\eta_1,\ldots,\eta_5) T_{\lambda}(\mathbf{s},\mathbf{\omega}) \] \quad 3.8

where the \( T_{\lambda} \) are linearly-independent, symmetric, traceless tensors combination of \( \mathbf{s} \) and \( \mathbf{\omega} \), while \( \eta_\lambda \) are invariants of the form \( \{ s^a \omega^b s^c \omega^d \ldots \} \). The finite number of invariants and tensorially independent products of \( \mathbf{s} \) and \( \mathbf{\omega} \) are a consequence of the Cayley-Hamilton theorem of matrix
algebra. It has then been shown later that to obtain sensitivity to normal-stresses anisotropy and mean-streamline curvature it is sufficient to adopt a cubic stress-strain relationship, therefore we present the general cubic formulation of the stress-strain relationship that is common to all EARSM formulation:

\[
\rho U_{ij} = \frac{2}{3} \rho k \delta_{ij} - \mu_i S_{ij} 
\]

\[
+ C_1 \mu_i \frac{k}{\varepsilon} \left[ S_{ik} S_{kj} - \frac{1}{3} \delta_{ij} S_{ki} S_{kj} \right] + C_2 \mu_i \frac{k}{\varepsilon} \left[ \Omega_{ik} \Omega_{kj} - \frac{1}{3} \delta_{ij} \Omega_{ki} \Omega_{kj} \right] 
\]

\[
+ C_3 \mu_i \frac{k^2}{\varepsilon^2} \left[ \Omega_{ij} S_{ki,kl} S_{kl} + \Omega_{kl} S_{ki,jl} S_{kl} \right] + C_4 \mu_i \frac{k^2}{\varepsilon^2} \left[ \Omega_{ij} \Omega_{im} S_{mj} + \Omega_{mj} \Omega_{im} S_{ij} - \frac{2}{3} \Omega_{ij} \Omega_{im} \Omega_{ni} \delta_{ij} \right] 
\]

\[
+ C_5 \mu_i \frac{k^2}{\varepsilon^2} \left[ S_{ki} S_{kl} S_{ij} \right] + C_6 \mu_i \frac{k^2}{\varepsilon^2} \left[ \Omega_{kl} \Omega_{ki} S_{ij} \right] 
\]

where

\[
S_{ij} = \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) 
\]

3.10

and

\[
\Omega_{ij} = \left( \frac{\partial U_i}{\partial x_j} - \frac{\partial U_j}{\partial x_i} \right) 
\]

3.11

What is interesting to note is that the exact solution of the algebraic stress model in terms of \( S \) and \( \Omega \) is able to produce also the coefficients of the non-linear terms, and therefore the explicit expression should possess the main characteristics of the second-momentum closure from which it has been derived. On the opposite side, an unattractive feature of this approach is that it can render singular behaviors in complex non-equilibrium flows.

From the practical point of view, the most common approach in developing a non-linear stress-strain correlation has been to independently calibrate the coefficients of the non-linear terms. In this sense the model can be seen as a non-linear extension of a classic eddy-viscosity \( k-\varepsilon \) model. For this reason, even if having the exact same formulation of the EARSM, this class of models is generally referred to as Non-linear Eddy Viscosity Models (NLEVM).

Such an algebraic correlation can be mathematically derived from a second-moment closure, as shown by Pope (eq. 3.9). It has later been shown by various researchers that to obtain sensitivity to normal-stresses anisotropy it is sufficient to adopt a quadratic stress-strain relationship. It is possible to write the general quadratic formulation of the stress-strain relationship, common to all NLEVM formulation, in the following form:
\[ \rho u_i u_j = \frac{2}{3} \rho k \delta_{ij} - \mu, S_{ij} \]  

\[ + C_1 \mu_i \frac{k}{\varepsilon} \left[ S_{ik} S_{kj} - \frac{1}{3} \delta_{ij} S_{kl} S_{kl} \right] + C_2 \mu_i \frac{k}{\varepsilon} \left[ \Omega_{ik} S_{kj} + \Omega_{jk} S_{ki} \right] + C_3 \mu_i \frac{k}{\varepsilon} \left[ \Omega_{ik} \Omega_{jk} - \frac{1}{3} \delta_{ij} \Omega_{kl} \Omega_{kl} \right] \]

\[ + C_4 \mu_i \frac{k^2}{\varepsilon^2} \left[ S_{ik} \Omega_{ij} + S_{kj} \Omega_{ii} \right] S_{kl} + C_5 \mu_i \frac{k^2}{\varepsilon^2} \left[ S_{kl} S_{kl} - \Omega_{kl} \Omega_{kl} \right] S_{ij} \]

What must be noted is that the coefficients are very different, in particular in the older models. This is due to the fact that in all cases they have been recommended by (or some other feature of a simple shear, such as the normal stress level, that cannot be mimicked with a linear scheme).

A variety of values is found in literature for the coefficients in eq. 3.12. Models show a great variation in the values adopted as a consequence of solely considering the prediction of shear stress in a simple shear and, in some cases, one other complex flow. What happens is that the influence of the non-linear terms in these flows is hardly noticeable, and therefore just any sets of coefficients could in fact give the small influence necessary to obtain the required outcome.

### 3.2 Implementation of Quadratic k-ε Model

The NLEVM model variant implemented in Hydra-TH leverages a rigorous development work that has been performed to more robustly calibrate the model coefficients [16]. In particular, the adopted formulation has undergone an extensive validation work and can further leverage widespread experience in its application to fuel design [17-18-28-30]. An example of the validation and improved predictions offered by the selected model closure is shown in Fig. 4, where pressure drop predictions are calculated and compared to experiments for productions PWR spacers.

![Figure 8: Comparison of pressure loss between CFD and measurements for Standard k-ε (A) and Quadratic k-ε (B) models from Ikeda, 2009 [28].](image)
When dealing with flow inside fuel rod bundles cubic terms in the stress-strain correlation can be omitted and therefore eq. 3.12 is reduced to:

\[
\rho \ddot{u}_i u_j = \frac{2}{3} \rho k \delta_{ij} - \mu_i S_{ij} \\
+ C_i \mu_i \frac{k}{\varepsilon} \left[ S_{ik} S_{kj} - \frac{1}{3} \delta_{ij} S_{kl} S_{lk} \right] + C_2 \mu_i \frac{k}{\varepsilon} \left[ \Omega_{ik} S_{kj} + \Omega_{kj} S_{ik} \right] + C_3 \mu_i \frac{k}{\varepsilon} \left[ \Omega_{ik} \Omega_{jk} - \frac{1}{3} \delta_{ij} \Omega_{kl} \Omega_{lk} \right]
\]

Following the approach of Shih, Zhu and Lumley [30] a quadratic formulation is adopted that respects the principles of realizability, defined as the non-negativity of the turbulent normal stresses together with the Schwarz inequality between any fluctuation, which is a physical and mathematical principle that should be ensured by any turbulence model. Imposing this condition leads to a formulation of the coefficients \(C_1-C_3\) in equation 3.13 that is not constant, like in most common models, but varies with the mean flow deformation rate. The coefficients have the following formulation:

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

where \(C_\mu\) is also given as function of the shear invariant \(S\)

\[
C_\mu = \frac{2/3}{3.9 + S}
\]

\[
S = \frac{k}{\varepsilon} \sqrt{\frac{1}{2} S_{ij} S_{ij}}
\]

and \(c_{NL1}, c_{NL2}, c_{NL3}, c_{NL6}, c_{NL7}\) are the coefficients shown in Table 3.

<table>
<thead>
<tr>
<th>(c_{NL1})</th>
<th>(c_{NL2})</th>
<th>(c_{NL3})</th>
<th>(c_{NL6})</th>
<th>(c_{NL7})</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.8</td>
<td>11</td>
<td>4.5</td>
<td>1000</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Table 3 – Quadratic NLEVM Coefficients.
3.3 Wall treatment

The discussed RANS models are implemented in Hydra-TH in conjunction with a wall function approach. Wall functions bridge the viscosity-dominated thin near-wall boundary layer region with that of the fully turbulent region. Wall function methods allow simulations using a moderate number of mesh cells making large industrial problems computationally tractable. The application of CFD to PWR fuel is a perfect example, where the wall dominate complexity of the geometry makes it impossible to resolve the boundary layer region at an acceptable computational cost.

The basis for most wall-function models traces back to the modified law-of-the-wall approach used by Launder and Spalding [31]. This type of wall modeling approach is designed for use with meshes where the first near-wall cell is placed in the logarithmic layer (inertial sublayer). From an industrial point of view, for complex geometries, ensuring that all the near wall cells are outside the viscous sublayer is problematic. Also, the precise location of the logarithmic region is solution dependent and may vary during the solution process. In order to accommodate a more flexible meshing technique/mesh, we follow a \( y^* \)-insensitive wall function (also called “scalable wall function”) approach as outlined in Grotjans et al. [32].

The scalable wall function approach is based on limiting the minimum value of the scaled wall coordinate \( y^* \), such that the value of the velocity gradient at the first cell will be the same as if it was on the edge of the viscous sublayer. This constrains the lowest grid point to lie above the physical wall. Thus, this approach neglects the true fluid dynamics within the viscous sublayer, but this is also the case for the standard wall function approach where the formulation breaks down for mesh points within the viscous sublayer.

The wall element centroid \( y_p^* \) distance is scaled using:

\[
y_p^* = \frac{c_{\mu}^{1/4} \rho \sqrt{k} y_p}{\mu}
\]

where, \( k \) is the turbulent kinetic energy, \( \rho \) is the fluid density, and \( \mu \) is the molecular viscosity. The edge of the viscous sublayer is taken to be at a distance \( y_v \) from the wall (see Fig. 9) and the corresponding scaled viscous sublayer distance is given by:

\[
y_v^* = \frac{c_{\mu}^{1/4} \rho \sqrt{k} y_v}{\mu} = 11.225
\]
3.4 Subgrid-scale modeling for LES

In RANS models, as a consequence of the averaging process all scales are modeled: the flow behavior must be captured at the largest scales, the inertial subrange, as well as in the dissipation range. This is a considerable difficulty as very different physics (important at the different ranges of scales) must be captured within the same model equations. In large eddy simulation (LES) a different approach is taken. The large scales are exactly represented, while only the dissipative scales are modeled (approximated) [33]. Thus from the spectral viewpoint of the kinetic energy LES aims to resolve the energy contained in the lower wave numbers, while the energy at high wave-numbers is modeled.

The price-tag of LES is significantly higher than RANS models due to the increase in resolution requirements to represent a sufficiently large portion of the kinetic energy. However, if the second moments, e.g., the fluctuation about the mean need to be evaluated, LES is still the preferred approach. RANS models in fact compute the statistics by solving for only the mean field values and, depending on the model, the second moments. For example, the discussed $k$-$\epsilon$ model is a popular way to approximate the effects of fluctuations on the mean velocity. However, it is important to appreciate that the only goal of the $k$-$\epsilon$ model is to provide closure for mean quantities. One cannot expect a meaningful description of the fluctuations themselves, only their effect on the mean.

In LES the flow variables are filtered with a kernel function, $G$,

$$
\overline{\phi}(X,t) = \int_{-\infty}^{\infty} G(X - r, \Delta) \phi(r, t) \, dr
$$

3.19
where $\Delta$ is the filter width. Filtering results in an additive decomposition

$$\phi = \bar{\phi} + \phi'$$

3.20

The above filtering can be weighted with the fluid density, resulting in Favre filtering, in analogy with Favre averaging. Applying Favre filtering to the instantaneous conservation equations results in a set of Favre filtered equations, which formally look like the ensemble-averaged RANS equations. These equations govern the filtered flow quantities, which represent the resolved scales. The equations are unclosed: the effects of the unresolved scales must be accounted for based on some physical insight.

There are different approaches to LES filtering. Filters can be explicit or implicit. Explicit filtering explicitly performs Eq. 3.19 on the computed fluctuating flow field. Depending on the filter function, $G$, the decomposition in Eq. 3.20 yields different fields. Implicit filtering relies on the numerical grid to perform the filtering; the resulting decomposition will be different on different grids and different parts of the computational domain. The representation of the unresolved scales can also be explicit or implicit. Explicit models explicitly add model terms to the filtered continuum equations. An example is to employ the turbulent viscosity hypothesis with the turbulent viscosity computed via Smagorinsky’s model, which is analogous to Prandtl’s mixing length model in the Reynolds averaged context. Implicit models rely on the dissipative properties of the applied numerical method, resulting in implicit large eddy simulation (ILES), or, if the numerical treatment ensures monotonicity, monotonically integrated implicit LES (MILES).

Different approaches have been implemented in Hydra-TH for subgrid scale modeling as listed below. Extensive testing in Hydra-TH has shown that the monotonicity preserving advection treatment allows for an extremely efficient implementation of ILES, which has therefore been adopted for all LES cases discussed in this milestone. The current list of LES models includes:

- MILES or ILES: This family of models is obtained using a monotonicity preserving advection treatment (MILES) and is also referred to as implicit LES (ILES) [34].
- Smagorinsky model [35]
- Wall-adapted large eddy model (WALE) [36]
4. RANS MODEL APPLICATIONS

4.1 RANS Modeling Assessment

This section is dedicated to the assessment of the RANS modeling approaches implemented in Hydra-TH for application to fuel rod bundle simulations, as discussed in section 1. The validation and demonstration cases have been selected on the base of previous experience where they have shown to be particularly demanding and extremely valuable in the assessment of the simulation tools.

4.1.1 Bare Rod Bundle Validation

Among the possible effects of the anisotropy of the Reynolds stresses, one that is more evident is the formation of turbulence driven secondary flows in non-circular ducts. The existence of such secondary motion had been firstly postulated by Nikuradse in 1926 [37], who in turbulent-velocity distribution measurements in several non-circular channels found the constant-velocity lines to be distorted in a manner indicative of secondary flows. Later a phenomenological explanation was given by Nijsing and Eifler [38], but only in 1984 a detailed discussion was given by Demuren and Rodi [39]. More recently Vonka [40] has been able, with laser Doppler velocimetry, to measure the secondary flow scale for a triangularly arranged bare rod bundle. These secondary motions, also known as secondary flow of Prandtl’s second kind, are driven by the non-uniformities in the near-wall turbulence. Secondary flows have shown to have considerable effect on the turbulence levels distribution in fuel rod assemblies. In order to account for their effect a robust NLEVM has been implemented in Hydra-TH [14] as part of this effort and its assessment is shown here on dedicated tests cases.

To evaluate the influence of secondary flow and the importance of the anisotropy modeling, we can compare different turbulence models with experimental results for a simple, but significant,
case of an infinite triangular array lattice, where the domain of simulation is limited, and the effects of the secondary motion can be clearly understood. Figure 10 above shows the experimental configuration on the left (37-rod bundle) and the computation domain on the right.

The domain shown in Fig. 10 represents a series of velocity and wall shear stress measurements that where completed by Mantlik et al. [41] at NRI, Czech Republic. The experiments were performed in a wind tunnel, using a 19, 120 mm Outer Diameter (OD), rods model of a fuel assembly. The rod bundle adopted was hexagonal, with a p/d ratio of 1.17. Length of the model was 6 m and the measurements were performed inside the model at a distance of 5600 mm from the model inlet, i.e. in the region of fully developed turbulent flow, and without the back effect of outlet cross-section change. Pitot and Preston tubes of 0.8 mm OD were adopted for the shear stress and axial mean velocity measurements. The measurements were performed in a central subchannel so that it can be considered an elementary flow cell of an infinite rod bundle. The Reynolds number considered are presented in Table 4.

Table 4 – Experimental conditions.

<table>
<thead>
<tr>
<th></th>
<th>Density</th>
<th>Kinematic Viscosity</th>
<th>Bulk Velocity</th>
<th>Reynolds Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>1.131 kg/m³</td>
<td>1.591e-5 m²/s</td>
<td>16.73 m/s</td>
<td>64,300</td>
</tr>
<tr>
<td>Case 2</td>
<td>1.131 kg/m³</td>
<td>1.591e-5 m²/s</td>
<td>28.47 m/s</td>
<td>109,400</td>
</tr>
<tr>
<td>Case 3</td>
<td>1.131 kg/m³</td>
<td>1.591e-5 m²/s</td>
<td>47.16 m/s</td>
<td>181,200</td>
</tr>
</tbody>
</table>

**Computational Setup**

Regarding the computational model, owing to the symmetry of the problem it is sufficient to describe a smaller domain, as shown in Fig. 10, with the appropriate symmetry boundaries. The domain contains 6 unit flow cells with dimensions specified in Fig. 11.
In order to evaluate the model sensitivity to the grid resolution, three successive mesh refinements have been adopted and all computation have been performed on the successive three grids. Table 5 provides a summary of the mesh resolutions. Table 6 visually presents the adopted computations grids.

### Table 5 – Summary of adopted computational mesh resolution.

<table>
<thead>
<tr>
<th>Mesh Refinement</th>
<th># Cells</th>
<th>Characteristic Length</th>
<th>Aspect Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radial</td>
<td>Theta</td>
<td>Axial</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>20</td>
<td>60</td>
<td>72,000</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1 (10mm / Radial)</td>
</tr>
<tr>
<td>20</td>
<td>40</td>
<td>60</td>
<td>288,000</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.5 (6000mm / Axial)</td>
</tr>
<tr>
<td>30</td>
<td>60</td>
<td>60</td>
<td>648,000</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.33333333333 (z / x-y)</td>
</tr>
</tbody>
</table>

### Table 6 – Computational domain and detail of unit cell for all mesh resolutions.

<table>
<thead>
<tr>
<th>Mesh Resolution 10x20x60</th>
<th>Mesh Resolution 20x40x60</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Mesh Resolution 10x20x60" /></td>
<td><img src="image" alt="Mesh Resolution 20x40x60" /></td>
</tr>
</tbody>
</table>
Mesh Resolution 30x60x60
Calculations have been performed for the Standard k-ε model and for the Quadratic NLEVM at all 3 grid refinements and are shown next. Grid convergence is first presented followed by the analysis of the predicted secondary flows and finally the predictions of the 2 models are compared on the same grid resolution. Velocity predictions are shown for 3 location along radial coordinates and wall shear stress is shown along the angular coordinate, as schematically presented in Fig. 12.

Figure 12: Elementary flow cell dimensions.

**Grid Convergence for Standard k-ε model**
The results for the Standard k-ε model are shown in Figs. 13-15 and evidence similar trends for all three Reynolds number analyzed. The consistent behavior is to be expected and simply confirms the generality of the turbulence model at high Reynolds number. For all three cases the comparison of the grid refinement results indicate that the 2 finest grids produce practically identical results and that excellent grid convergence has been achieved. The results for the coarsest mesh (10x20x60) on the other hand do evidence appreciable numerical error. While the absolute difference between the coarse and the two fine grids is relatively small, the trends do evidence minor differences.

The comparison of CFD predictions with the experimental data evidences an overall satisfactory agreement, but with important and expected limitations. If we compare the velocity distributions in the radial direction normal to the wall, for the three locations at 0, 15 and 30 degrees we see that the experiment shows a more homogeneous distribution of the velocity, in respect to models results; the Standard k-ε model under predicts the velocity in the small gap region (0 degrees) and overpredicts it towards the channel center (30 degrees), with good agreement at the 15 degrees location. Such behavior has been consistently been observed in previous work, and it is attributed to the lack of secondary flow prediction, which would instead redistribute the turbulence levels consequently the velocity inside the flow channel.
Figure 13: Standard k-ε model results for Re=64,300.

Looking at the wall shear stress predictions, as expected the Standard k-ε model predicts a larger variation along the rod angular direction, which is again related to the missing secondary flows. Also, it is clearly noticeable how the CFD predictions produce considerably lower absolute values in comparison to the experimental data. While the same trend has been observed in previous analysis, a full justification has not been provided. It is expected that a large uncertainty could be related to the measurement techniques, which do not allow an accurate absolute calibration. Further, in absence of detailed measurement of surface roughness the wall behavior has been assumed as smooth in the near wall model treatment, but this assumption might not be fully valid. It should be observed that in the figures the difference seems to increase with the Reynolds number, due to the different plot scales used. In reality for all three cases the average difference is around 25%.

Overall, the Standard k-ε model shows very consistent predictions, with negligible grid dependency, which is a valuable characteristic of a turbulence model. The observed differences are expected and are related to the inability of Eddy viscosity models to capture the macroscopic, turbulence driven secondary flows. Peak velocity, in the channel center, and minimum velocities, in the pin-to-pin gap, are respectively overpredicted and underpredicted by around 5%.
The results for the Quadratic NLEVM are shown in Figs. 16-18. In this case the grid convergence results show more noticeable differences. The 2 fine grids show very similar results, with trends that are very similar to the previously discussed Standard k-ε model results. The coarse grid, on the other hand, produces significantly different predictions, both in trends and absolute values, for all the analyzed Reynolds number conditions. Most interestingly, the coarse grid results which should be the least converged, indicate a surprisingly close agreement with the experiment. This is true for all three Reynolds number cases, and both for the velocity and wall shear stress trends.

At first sight the coarse grid results could be discarded as simply influenced by a large spatial discretization error, but the analysis of the physical flow behavior reveals a much more interesting finding. Figure 19 show the predicted secondary flows for the coarsest mesh (10x20x60). The left side of the picture gives a view of the complete computational domain, while the right side shows the detail inside one single flow unit. The Quadratic NLEVM appears to do a good job in predicting the turbulence driven secondary flow, both in trends and scale, where the average secondary velocity is on the order of 1% of the axial bulk flow.
Looking at the secondary flow predictions for the two finer mesh sizes (Figs. 21-22) it is clear that a less consistent behavior is observed. The secondary flows do not respect the unit cell expected symmetry, and a crossflow exist between unit cells. This behavior is not consistent with experimental observation and seems to indicate some convergence issues for the NLEVM on fine grid, which will require further investigation. The same overall behavior is observed both for grid 2 and 3.

At the light of the discussion on secondary flows, the predictions of the Quadratic NLEVM are now easier to interpret. The numerical issues encountered on the finest grids hinder the prediction of consistent secondary flow in the channel, therefore leading the model to produce results very similar to a Standard $k$-$\varepsilon$ model. On the coarse grid instead the model well predicts the turbulence driven secondary flow and, as a consequence, also predicts velocity distribution very close the measured ones, and at the same time wall shear stress with much closer trend to the experimental data.

Overall, while the importance of the secondary flow predictions on the velocity redistribution is confirmed, the implemented Quadratic NLEVM evidenced some numerical issues on fine grid resolutions and will require further assessment.

Figure 15: Standard $k$-$\varepsilon$ model results for $Re=181,200$. 
Finally, the Standard k-ε model predictions and the RNG model predictions of secondary flows are shown in Figs. 22 and 23. These results are simply provided as a confirmation that the eddy viscosity model leads to the complete absence of secondary recirculation in the unit cells. The vectors are all aligned toward the channel center and the value of the secondary flow scale is less than 0.01% of the bulk flow velocity.
Figure 17: Quadratic NLEVM results for Re=109,400.

Figure 18: Quadratic NLEVM results for Re=181,200.
Figure 19: Quadratic NLEVM secondary flow predictions on Grid 1 (Re=109,400).

Figure 20: Quadratic NLEVM secondary flow predictions on Grid 2 (Re=109,400).
Figure 21: Quadratic NLEVM secondary flow predictions on Grid 3 (Re=109,400).

Figure 22: Standard k-ε model secondary flow predictions on Grid 3 (Re=109,400).
4.2 LES Application Assessment

From the engineering viewpoint the most useful information that can be obtained from simulations of turbulent flows are statistical and integrated quantities derived from the fluctuating flow field. Examples of statistics are the mean velocity, the root-mean-square (RMS) pressure, and the turbulent kinetic energy spectrum. Examples of integrated quantities are the mean drag or mean lift on an airplane wing or the power spectral density (PSD) distribution of the fluctuating forces that load the fuel rods in a pressurized water nuclear reactor.

While RANS approaches can be leveraged to compute averaged quantities in fuel assemblies, but, as discussed, one cannot expect a meaningful description of the fluctuations themselves, only their effect on the mean. If the second moments, e.g., the fluctuation about the mean, are also important, a model with a higher level of description is required. An LES approach is available in Hydra-TH to cover this fundamental application area, and has been validated against a dedicated measurement of fluctuating quantities inside a prototypical rod bundle.

4.2.1 LES validation on 5x5 TAMU data

This section presents the results of ILES calculations for a prototypical 5x5 fuel rod bundle. The geometry was provided in CAD format by Westinghouse, and corresponds to the experimental configuration used at Texas A&M, where PIV measurements were carried out. The flow domain is shown in Fig. 24. Not shown here are the exterior walls of the flow housing used in the experimental facility. Additional details on the experimental configuration and results may be found in Conner, et al. [42].

At the flow domain inlet, a prescribed velocity \( v = (0.0, 2.48, 0.0) \) m/s was used with the fluid properties for water at 24°C. This corresponds to a Reynolds number of approximately 28,000 based on the hydraulic diameter for the rod bundle. At the surfaces of the flow housing, rods,
support and spacer grids, no-slip/no-penetration velocity conditions were prescribed. Homogeneous Neumann conditions for velocity (zero normal viscous stress) along with a zero pressure condition were prescribed at the outflow plane. A fixed CFL=4 condition was used with automatic time-step control for all computations.

Figure 24: Flow domain for the 5x5 rod bundle showing rods, inlet/outlet planes, rod support, and spacer grid.

The flow domain was meshed using Numeca’s Hexpress/Hybrid mesh generator (a.k.a. Spider) following best practices that are discussed in the next chapter. A sample mesh is shown in Fig. 25. Two meshes were used, a coarse mesh with 14 million (14M) elements, and one with 96 million (96M) elements.

A series of preliminary coarse-mesh calculations were conducted to determine when a stationary turbulent state would be achieved and to test the sensitivity to mesh resolution and time-step size. Figure 26 shows the global kinetic energy, \( \int_{\Omega} \frac{1}{2} \rho (v \cdot v) d\Omega \) where \( \Omega \) is the flow domain volume, as a function of time. Based on these preliminary calculations, a time of approximately 0.2 seconds was chosen as the starting point for collecting time-averaged flow statistics with total time of 1.0 second.
Figure 25: 14M Spider mesh for the V5H 5x5 rod bundle. (a) Cut-planes of the volume mesh through the spacer grid, (b) surface mesh of the rod support (left) and the rods and spacer (right), (c) surface mesh for the spacer (left) and the outflow plane (right).
In order to compare to the experimental data provided in [8], a series of line plots were extracted from the time-averaged velocity field for the 14M and 96M meshes at locations that fall in the planes of the PIV measurements. We note here that the time-average for the computational results was performed over 0.8 seconds for the 14M calculation and approximately 0.45 seconds for the 96M mesh. In contrast, the experimental velocities were ensemble averaged with a window size of 0.8 seconds. Details on the experimental measurements are also presented in Yan, et al. [43]. All line data was measured relative to the so-called “weld-nugget” located on the spacer grid.

The “weld nugget” is located at 38.1 mm from the bottom of the spacer grid as shown in Fig. 27 (a). The line-data extracted from the computation was located at the positions indicated in Fig. 27 (b). The coordinates of the sample points A -- H are shown in Table 7, and are relative to the center of rod 13 in Figure 3 in Yan, et al. [43]. In the flow direction, the line-data is extracted for $0.05 \leq y \leq 0.09 \text{ m}$ corresponding to the region where PIV data is available downstream of the spacer grid.
Table 7 – Sample points A to H used to extract line-data for comparison with the experimental data.

<table>
<thead>
<tr>
<th>Point</th>
<th>(x,y,z) Position [10^{-3} m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>(−6.3, 50 ≤ y ≤ 90, 6.3)</td>
</tr>
<tr>
<td>B</td>
<td>(−6.3, 50 ≤ y ≤ 90, 0.0)</td>
</tr>
<tr>
<td>C</td>
<td>(−6.3, 50 ≤ y ≤ 90, −6.3)</td>
</tr>
<tr>
<td>D</td>
<td>(0.0, 50 ≤ y ≤ 90, −6.3)</td>
</tr>
<tr>
<td>E</td>
<td>(6.3, 50 ≤ y ≤ 90, −6.3)</td>
</tr>
<tr>
<td>F</td>
<td>(6.3, 50 ≤ y ≤ 90, 0.0)</td>
</tr>
<tr>
<td>G</td>
<td>(6.3, 50 ≤ y ≤ 90, 6.3)</td>
</tr>
<tr>
<td>H</td>
<td>(0.03, 50 ≤ y ≤ 90, 6.3)</td>
</tr>
</tbody>
</table>

Following Yan, et al., mean velocities are compared at points A, C, D, E, G and H for the 14M mesh as shown in Fig. 28. Here, the stream-wise velocity in the experiment corresponds to the y-velocity in the computation, while the lateral velocity corresponds to the x-velocity. In Yan, et al. [43] the systematic uncertainty in the velocities due to the PIV measurements, software data acquisition, etc., was estimated to be a maximum of 0.199 m/s. The statistical uncertainty, which is a function of the number of snapshots of the velocity, is estimated to be ±0.167 \( v_{inlet} \) in the lateral direction, and ±0.150 \( v_{inlet} \) in the axial direction, where \( v_{inlet} = 2.48 \text{ m/s} \). All experimental data has been plotted with the uncertainty bounds provided by Dominguez-Ontiveros and Hassan.

The line plots of velocity for the 14M mesh are presented in Fig. 28 for stations A to H. Inspection of Fig. 28 indicates that experimental and computed x-velocities correlate relatively well, although for points A, C, E, and G, the x-velocities are near zero. For this relatively coarse mesh, the stream-wise velocities don’t compare as well, however the general trends appear to be similar. Note that typically, the y-velocity over-predicts the stream-wise velocity, which is not surprising for this relatively coarse mesh. In comparison, the mesh used by Yan, et al. contained approximately 76 million hexahedral elements.

The line plots of velocity for the 96M mesh are presented in Fig. 28 for stations A to H. In comparison to the velocity profiles in Fig. 27 the 96M results match the experimental data more closely at all points A to H. However, the stream-wise velocity still appears to be slightly over-predicted. In contrast, the x-velocities fall within the uncertainty bounds for points A, C, E, and G, while the x-velocities at points D and H have similar profiles but are not quite within the uncertainty bounds. Overall, the 96M results compare very well to the experimental data.
Figure 28: Mean axial and lateral velocity profiles at positions A, C, D, E, G and H for the 14M Spider mesh.
Figure 29: Mean axial and lateral velocity profiles at positions A, C, D, E, G and H for the 96M Spider mesh.
Time-averaged velocities in plane-5 (see Fig 26 (b)) are shown in Fig. 30 with the computed time-averaged velocity fields. Similarly, the experimental and computed velocity fields on plane-7 are shown in Fig. 31. The velocities have been scaled relative to the 2.48 m/s inlet velocity. In this comparison, the peak velocities in the axial direction are slightly under-predicted in the Hydra-TH computations with the 7M mesh, while the lateral velocities are slightly over-predicted. This is likely due to the very coarse mesh. While the peak velocities appear to be relatively close to those found experimentally, inspection of Fig. 30 and Fig. 31 indicates that the deflection in the velocity vectors due to the mixing vanes and the flow housing is captured by the simulation. We note that the experimental data presented here was computed using a 50x40 window for time-averaging resulting in a somewhat “clumpy and rough” appearance. However, because only the true velocity vectors are used for time-averaging, the minimum/maximum velocities are based on actual velocity measurements rather than interpolation. In addition, the Hydra-TH results have been presented using the minimum/maximum velocities found in the computational results to permit direct comparison with the experimentally determined velocity bounds.

Figure 30: Experimental and computed axial (y-direction) time-averaged velocities on plane 5. Velocity magnitude has been scaled relative to 2.48 m/s inlet velocity.
Figure 31: Experimental and computed axial (y-direction) time-averaged velocities on plane 7. Velocity magnitude has been scaled relative to 2.48 m/s inlet velocity.

In order to illustrate the impact of increasing mesh resolution on the flow, Fig. 32 shows snapshots of the instantaneous helicity field for the 5x5 rod bundle. For the 14M mesh, there are relatively large coherent structures downstream of the support and spacer grid suggesting the 14M simulation is more of a VLES result. In contrast, the flow structures captured by the 96M mesh are significantly smaller and appear more randomly distributed spatially. In both cases, the influence of the mixing vanes on the spacer grid is apparent.
Figure 32: Snapshots of the instantaneous helicity field for the 14M and 96M meshes.
5. BEST PRACTICES FOR FUEL APPLICATIONS

This section is dedicated to describing the work that has been performed in order to support the delivery of an advanced boiling closure. The work has been driven by the new physical understanding derived from the innovative experimental techniques used in the THM research program. The new findings are described first, as they drive the model development and assessment. The new boiling closure formulation is then introduced providing also a graphical exemplification of the modeling ideas.

5.1 Best practices for meshing on 3x3 assembly subdomain

Hydra-TH has been used to perform computations for a 3x3 subdomain of Westinghouse V5H spacer grid. This section discusses the various meshes used in the supporting milestone work, the assessment of these meshes for use in CFD computations with various turbulence models, and the methodology used to assess the time-duration for large-eddy simulation.

5.1.1 Assessment of Cubit generated meshes

The first set of 5 computational meshes where provided by Sandia National Laboratories as journal files for the Cubit package [44]. These journal files correspond to the 672k, 1M, 3M, 6M and 12M element meshes in Table 8. Initial inspection of all 5 grids revealed a lack of mesh grading consistent with physical boundary layers on the rod and spacer surfaces as shown in Fig. 33(a). The transitions between the mesh blocks upstream and downstream of the spacer are shown in Fig. 33(b) where the abrupt change in mesh resolution from the “hex-tet” mesh around the spacer to the downstream region is apparent. For LES computations, abrupt transitions in mesh resolution from the spacer region, where small eddies are generated, to the downstream section will result in aliasing the small eddies to longer-wavelength large eddies. This is particularly unfortunate for LES computations, because this causes a numerical aliasing of energy from the small eddies generated by the spacer to larger eddies that the coarser downstream mesh can resolve. Needless to say, this is a very undesirable artifact that can’t be avoided with the Cubit meshes provided for the preliminary GTRF calculations.

<table>
<thead>
<tr>
<th>Mesh</th>
<th>No. of Elements</th>
<th>$y^+_{\text{min}}$</th>
<th>$y^+_{\text{max}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>672k</td>
<td>671,572</td>
<td>2.7388</td>
<td>86.0984</td>
</tr>
<tr>
<td>1M</td>
<td>1,049,228</td>
<td>3.4053</td>
<td>61.3910</td>
</tr>
<tr>
<td>3M</td>
<td>2,663,920</td>
<td>2.8842</td>
<td>62.1051</td>
</tr>
<tr>
<td>6M</td>
<td>5,832,718</td>
<td>0.9624</td>
<td>55.6384</td>
</tr>
<tr>
<td>12M</td>
<td>12,522,644</td>
<td>0.7452</td>
<td>45.1667</td>
</tr>
</tbody>
</table>

Table 8 – Cubit meshes used for testing, with the associated min/max $y^+$ values for the rod and spacer surfaces.
Flow Calculations

The flow conditions for the preliminary 3x3 rod bundle followed those used by Elmahdi, et al. [4]. However, the flow domain for the meshes that were provided by Sandia National Laboratories were only 17.86 diameters long compared to the approximately 32 diameter long domain used by Elmahdi, et al. For the calculations reported here, the working fluid is water at a temperature of 394.2 K, a density of 942.0 kg/m³ and a dynamic viscosity of 2.32x10⁻⁴ kg/m/s. The inlet velocity is prescribed as \( v = (0, 0, 5) \text{ m/s} \). This corresponds to a Reynolds number, based on the hydraulic diameter is \( Re_{Dh} = 4.01 \times 10^5 \). No-slip, no-penetration conditions are prescribed at the rod and spacer surfaces. At the outlet, the hydrostatic pressure is specified to be \( p_h = 0 \) in conjunction with a zero shear stress condition. For the first set of calculations, no-penetration conditions with in-plane slip in the axial flow direction were applied at the sub-channel boundaries as shown in Fig. 34.

Figure 33: Element distribution for the 3M Cubit mesh. (a) Cross-section view of the mesh in the inlet region, (b) mesh spacing on the center rod and spacer surfaces.

Figure 34: Boundary conditions on rod and spacer surfaces, and the sub-channel boundaries.
Each calculation was heavily instrumented to provide global, surface and point time-history data that included kinetic energy, RMS divergence, forces and tractions on the rod and spacer surfaces, and point-wise values of velocity and pressure. Surface forces were computed by integrating either tractions or pressures over the given surface.

Figure 35: ILES time-history data for 1M mesh showing (a) global kinetic energy, (b) zoom-in of kinetic energy, (c) pressure time-histories, and (d) lateral force time histories on the central rod.

Figure 35 shows the time-history plots of the global kinetic energy, pressure at 5 different locations and the spacer and rod forces in the cross-stream direction for the 1M mesh using the ILES model. Here, the global kinetic energy is defined as $\int \rho \frac{1}{2} (v \cdot v) d\Omega$. Although the kinetic energy and pressure appear to reach a stationary state very quickly, the startup transient is still evident in the lateral forces up to approximately 0.15 s. For this reason, mean values and turbulent statistics are collected after 0.2 seconds. A stationary state is clearly evident after approximately 0.2 seconds where there is a fluctuation around a clearly defined mean for all of the time-history data. We have tested the sensitivity of the mean quantities, specifically the rod forces, by performing averages for varying duration $0.2 \leq t \leq 0.6$ seconds and compared to the average for $0.2 \leq t \leq 1.0$. Although this is not a complete assessment of all statistical quantities, the mean forces differed by less than 0.5% for the two averages indicating that 1.0
second was a reasonable duration for these calculations. In addition to the time averages, we estimated the number of flow transits for the 1.0 second duration simulations. Given the 5 m/s inlet velocity, a 1.0 second time scale corresponds to approximately 30 flow transits through the length of the computational domain.

Three different turbulence models were tested on the 5 Cubit meshes. The turbulence models include implicit large-eddy simulation (ILES), detached-eddy simulation (DES), a blended LES/RANS method, and the Spalart-Allmaras RANS model. All calculations were performed in a time-accurate way using the neutrally dissipative second-order trapezoidal rule time-integrator for 1.0 second of physical time. A fixed CFL condition, CFL=4, was used for all calculations in conjunction with implicit second-order treatment of the advective and diffusive terms.

Figure 36 shows the in-plane velocity and pressure distribution at a location 0.1135 m downstream of the spacer grid. This location matches that used in Elmahdi, et al. The ILES results are shown in Fig. 36(a), and at this stream-wise location the pressure distribution reveals relatively strong vortical cores in the sub-channels surrounding the central rod. In addition, multiple secondary and some tertiary vortical structures are readily visible in the sub-channels. A maximum velocity magnitude of 2.982 m/s was calculated by Hydra-TH on the 3M mesh. In comparison to the results presented in Elmahdi, et al., where a mesh with 48 million elements was used, peak velocities of 3.5794 m/s were reported. Qualitatively, the secondary vortices in the rod gaps are similar, although the Hydra-TH results suggest there are stronger vortical structures in the flow than evident in the results presented by Elmahdi, et al. Here, only a qualitative comparison is made due to the truncated length and lack of boundary-layer grading for the CUBIT meshes.

The detached-eddy results shown in Fig. 36(b) are similar to the ILES results, in that the pressure distribution reveals relatively strong vortical structures in the sub-channels surrounding the central rod. In addition, multiple secondary and some tertiary vortical structures are readily visible in the sub-channels. A maximum velocity magnitude of 2.933 m/s was calculated by Hydra-TH on the 3M mesh. These values are just slightly lower than the in-plane velocities predicted using the ILES model. As with the ILES calculations, the secondary vortices in the rod gaps are qualitatively similar to the structure reported by Elmahdi, et al.

In Fig. 36(c) the velocity and pressure distribution is shown for the Spalart-Allmaras (RANS) model. Relative to the ILES and DES results, the vortical structures are in general smoother, the eddy sizes larger, and the low-pressures associated with the vortical structures are reduced as expected. The peak velocity magnitudes are about 28% lower than those calculated with the ILES model. In addition, the secondary eddies in the sub-channels between rods are weak and barely detectable.

The planar velocity distributions in Fig. 36 suggest the presence of strong helical structures that propagate downstream from the mixing vanes on the spacer. This is shown explicitly in the instantaneous helicity isosurfaces in Fig. 37 for the ILES, DES and Spalart-Allmaras models. Here, the correlation between the stream-wise velocity component and the vorticity, i.e., the helicity, is shown in pairs of counter-rotating eddies whose directions are aligned in the primary flow direction. The ILES and DES results are similar in that there are small vortical structures
generated on the surface of the spacer, with large coherent and persistent helical structures in the wake of the mixing vanes. The overall structure of the wake is very similar for the ILES and DES results. The helicity fields for the ILES and DES results indicate qualitatively that the vortices generated by the mixing vanes are correlated with the flow velocity, and the strength of the helical structures is such that the longitudinal vortices propagate a considerable distance downstream. Note that we consider these calculations to be under-resolved and the coherent structures to be an artifact of the low mesh resolution. The Spalart-Allmaras results shown in Fig. 37(c) indicate that the flow structures are smeared out, but still reveal significant helical structures in the flow field downstream of the spacer mixing vanes.

Figure 36: Snapshots of instantaneous velocity and pressure on cut-plane for the 3M mesh at t = 1.0 second for (a) the ILES, (b) detached-eddy simulation, and (c) Spalart-Allmaras models.
Figure 37: Instantaneous isosurface snapshots of helicity ($v \cdot \omega$) for the 3M element mesh at $t = 1.0$ second for the (a) ILES, (b) DES, and (c) Spalart-Allmaras models. Isosurface values +/- 5000 m/s$^2$. 
This discussed investigation on the 3x3 spacer subdomain calculations provides useful information and best practices for application of Hydra-TH to fuel simulations. In general, the overall quality of the Cubit meshes is relatively poor and not recommended for LES calculations with unresolved boundary layers and rapid jumps in mesh resolution. In effect, the ILES and DES calculations reported here are essentially very large-eddy simulation, or put more simply "dirty LES".

In passing, we note that, due to the coarse meshes and inconsistent distribution of mesh points, the behavior of the trends in the overall pressure drop and RMS forces were not monotonic with respect to mesh resolution, this made it impossible to perform any serious solution verification. Regardless, we were able to extract the convergence rate based on the time-averaged global kinetic energy, which for the ILES computations was

$$ KE = 0.7779 - 0.01142 \left( \frac{h_2}{h_1} \right)^{2.5155} $$

where $h_2/h_1$ is the ratio of the average mesh resolution for two different grids. Similar second-order spatial convergence was extracted for the DES and Spalart-Allmaras calculations.

A qualitative comparison between the velocity distributions computed by Elmahdi, et al. [4] and this work show reasonable agreement in terms of the vortical structure and in-plane velocity magnitude. The presence of relatively strong vortical motion at the outflow boundary suggests that this boundary is too close to the spacer in the Cubit meshes – a consequence of using a 50% shorter domain length. Despite using a time-accurate RANS approach with Spalart-Allmaras, the time-history force data indicate that this approach is not a viable for GTRF calculations where the mean and RMS forces are of interest. In addition, it may be worthwhile to investigate additional turbulent statistics rather than only considering mean and RMS values of forces.

### 5.1.2 Assessment of Spider generated meshes

In this section, we discuss the application of Numeca’s Hexpress/Hybrid mesh generator, aka Spider, to the 3x3 and 5x5 rod bundles with the V5H spacer grid. Special attention is devoted to mesh characteristics desirable for LES, which are more stringent than requirements for RANS and include:

- Sufficient overall mesh resolution for capturing the important energy-containing features of the flow. A highly resolved LES calculation requires that about 80% of the energy spectrum be mesh resolved.
- Smooth transitions in regions downstream of the spacer to avoid non-physical aliasing of kinetic energy from smaller to larger scales.
- High quality boundary layers that adequately but economically resolve the complex turbulent flow in the vicinity of walls. In future calculations with heat transfer, this may be particularly important due to (1) the highly inhomogeneous and anisotropic nature of the flow at walls and (2) the potentially first-order influence of the quality of the simulation at walls to compute (and possibly the design of RANS models for) accurate heat transfer.
Spider's shrink-wrap meshing technology is quite different from that of Cubit and allows for automatic generation of body fitted meshes on arbitrarily complex geometries. Spider meshes are unstructured, hex-dominant, and conformal, containing hexahedra, tetrahedra, wedges, and pyramids. As a consequence, extremely complex geometries can be discretized. Furthermore, Spider is capable of generating high-quality boundary layer meshes; its configuration is based on a simple text file, though a graphical interface is also available; and it is easy to use in batch mode, yielding fast throughput of a series meshes for convergence studies and uncertainty quantification.

We have generated a series of Spider meshes for the V5H GTRF geometry for both 3x3 and 5x5 rod bundles with the V5H spacer grid. The approximate cell count for the 3x3 meshes are 2 million (M), 7M, 14M, 30M, 47M, 80M, and 185M, and for the 5x5 meshes are 14M and 96M. The 7M and 47M meshes for the 3x3 rod bundle are shown in Fig. 38. Visual inspection of these meshes reveal relatively uniform cell sizes inside the flow domain with targeted refinement in corners and edges in the vicinity of the spacer and symmetry planes (not shown). Compared to the Cubit meshes, discussed above, there are no visible transitions in cell sizes downstream of the spacer and there are smooth transitions from refined corners towards inside the domain. These features are promising from the viewpoint of obtaining quality LES results.

Figure 38: 7M and 47M Spider surface meshes for the V5H GTRF 3x3 rod bundle.
Some representative snapshots of the coarser 14M mesh for the 5x5 bundle have been shown in Fig. 25 where the grid was adopted for ILES validation. The images reveal that the 14M mesh may be somewhat coarse for a fully resolved LES simulation. Neither series of meshes contain targeted boundary layer refinement close to no-slip walls. This approach is adopted in conjunction with a wall-modeled LES method.

In summary we are very pleased with Spider as a tool for mesh generation: it is relatively easy to use, fast, and automatically generates high-quality meshes for extremely complex geometries, required for the GTRF problem. As an example, the 96M 5x5 mesh was generated in only 80 minutes on an 8-core workstation with 48GB RAM. Spider is a shared-memory parallel code and its approximate memory requirement is 0.5GB RAM per million cells generated; it can save in the latest EXODUSII file format with an HDF5 [45] container which is required for mesh sizes beyond ~60M cells.

A Priori Quantitative Mesh Assessment

Based on the preliminary scoping studies and mesh assessment using the Sandia-supplied Cubit meshes, a more quantitative method of mesh assessment for turbulent flow calculations was developed. In this section, the method for quantitative assessment of unstructured meshes for turbulent flows where no-slip boundary conditions are imposed is described. This is followed by an evaluation of the so-called “Spider” meshes.

In the application of computational fluid dynamics to engineering problems, it is common practice to use the wall-normal distance, $y^+$, to assess the mesh quality at no-slip walls. The distance from the wall measured in viscous lengths, or wall-units, is defined by

$$y^+ = \frac{y}{\sqrt{v/\tau_w/\rho}}$$

where $y$, $v$, $\tau_w$, and $\rho$ denote the (dimensional) normal distance from the wall, kinematic viscosity, wall-shear stress, and fluid density, respectively. As $y^+$ is similar to a local Reynolds-number, its magnitude can be expected to determine the importance of turbulent processes relative to viscous effects. The value of $y^+$ can be computed in each computational cell along no-slip walls for a given Reynolds number and mesh, yielding a different value in each cell. For unstructured meshes, the $y^+$ field is non-uniform along a surface. Typically, $y^+ \approx 1$ for wall-resolved LES, and $y^+ \gtrsim 30$ is typical for RANS models with wall-functions.

The approach proposed to assess a mesh before a full-blown LES computation leverages specific capabilities in Hydra-TH. In a numerical solution of the Navier-Stokes equations the $y^+$ field obtained after the first time step can be used to assess the mesh if (and only if) the initial and boundary conditions are consistent with the dynamical level of approximation of the computed flow. In incompressible, single-phase flows, this consistency amounts to constructing a divergence-free velocity field and a consistent pressure, both satisfying the prescribed initial and boundary conditions. The incompressible Navier-Stokes flow solver in Hydra-TH is based on a second-order implicit projection algorithm that uses a pressure-Poisson equation to continuously project the velocity field to a divergence-free velocity space at each time step. Given a set of
user-prescribed initial and boundary conditions the initial startup procedure at \( t = 0 \), Hydra-TH computes the solution of a Poisson equation for a Lagrange multiplier. Then a subsequent projection of the prescribed velocity field to a divergence-free subspace ensures that (1) the initial velocity field is divergence-free, (2) the velocity is consistent with the pressure, and (3) both fields satisfy the prescribed initial and boundary conditions for an incompressible flow. This procedure guarantees that basic solvability conditions are satisfied at \( t = 0 \), and that a mathematically and numerically well-posed Navier-Stokes problem is integrated for \( t > 0 \).

The \( y^+ \) fields, discussed below, have been obtained after the div-free startup procedure described above, and after a single time step, and serve as the basis of the mesh quality assessment described here. We emphasize that the \( y^+ \) field computed after the first time step is approximate: it depends on the mesh, the Reynolds number, and the turbulence model employed to compute \( \tau_w \), and is only constant when the flow is statistically stationary. Ideally, a more accurate \( y^+ \) could be obtained after the flow has reached a statistically stationary state. However, for large meshes obtaining a statistically stationary state may require many thousands of time steps and thus it is not economical as a quick \textit{a priori} mesh assessment. Instead, we rely on the approximate but physically and mathematically consistent \( y^+ \) field after the div-free start-up and first time step.

Figure 39 shows the spatial \( y^+ \) distribution on the spacer for the same geometry and Reynolds number for two different meshes. The first mesh was generated using Numeca’s Hexpress/Hybrid, aka Spider, and the second with Cubit for the 3x3 rod-bundle with the V5H spacer grid. While the smallest and largest \( y^+ \) values on these two meshes are comparable, the fields are very different. The \( y^+ \) on the Spider mesh appears to be much smoother and low \( y^+ \) values indicate highly refined edges and corners. Compared to the Spider mesh, the Cubit mesh exhibits a much more checkerboard-like pattern, indicating a larger spatial variation of \( y^+ \) on the surface – nearly a factor of 10 in many locations. A uniform \( y^+ \) distribution is desired for a predictable simulation quality. For example, sudden changes in \( y^+ \), i.e., sudden changes in the cell sizes along walls, will perturb an otherwise smooth boundary layer resulting in artificial adverse pressure gradients and non-physical boundary-layer separation. This is particularly important in wall-resolving LES as the simulation must faithfully represent the highly inhomogeneous and anisotropic nature of the turbulence in the vicinity of walls. In RANS simulations, a smoothly varying \( y^+ \) is very desirable given the highly nonlinear nature of the models in the near-wall region that respond poorly to rapid changes in mesh resolution.
Quantitative *a priori* metrics that can be used to assess the non-uniform $y^+$ fields on a complex surface, such as the spacer grid and mixing vanes in the GTRF problem, may be defined based on the statistical distributions of the $y^+$ field. Such a distribution may be generated by counting up the $y^+$ values of the cells adjacent to a surface and grouping them to equal-sized bins between their extremes. Instead of counting each occurrence as a unit value, a weighted histogram is obtained if the values of the corresponding cell area are counted. Such an area-weighted histogram is displayed in Fig. 40 which corresponds to the $y^+$ distributions in Fig. 39.

Figure 40: Cell-area weighted histograms of $y^+$ for the 7M Spider and 8.3M meshes for the V5H GTRF 3x3 rod bundle. The histograms correspond to the $y^+$ distributions in Fig 39.
The mean of the histograms in Fig. 40 may be used as one quantitative metric to assess the average $y^+$ on a complex surface with no-slip boundary conditions. The mean can be computed by numerically estimating the integral

$$
(y^+) = \int y^+ f(y^+) dy^+ \approx \sum y^+ f(y^+) \Delta y^+
$$

where $f(y^+)$ denotes the function values of the area-weighted histogram as shown in Fig. 40, and the integral of the histogram is unity, i.e., $\int f(y^+) dy^+ = 1$. In addition to the mean, the standard deviation suggests how much variation in $y^+$ may be expected on the surface.

The spatial uniformity of the $y^+$ field is also of interest. To define a useful metric that characterizes the uniformity, the spatial variation of $y^+$ is used. The variation of $y^+$ is computed by visiting each surface cell and finding the maximum difference between the $y^+$ of the given cell and that of its neighbors. This yields a new scalar field, which we call $dy^+$, whose area-weighted histogram is computed using the same method as that of $y^+$ discussed previously. We note in passing that the weighted sum of the non-zero differences could also be used to indicate the variation in the $y^+$ field.

The spatial distribution of the $dy^+$ field for the 7M Spider and 8.3M Cubit meshes are shown in Figure 41. This confirms the earlier observation that the Spider mesh is smoother, while the $y^+$ varies more significantly in the Cubit mesh. This is quantified in the histograms shown in Fig. 42. Compared to the $y^+$ histograms, the $dy^+$ histograms are only defined for $dy^+ > 0$. The perfect mesh would be characterized by the theoretically ideal $dy^+$ histogram which is a Dirac-delta function at $dy^+ = 0$. In Fig. 41, larger function values in the histogram indicate a larger
surface area covered by a given $y^+$ variation. While the $dy^+$ histogram for the Spider mesh has a large peak close to 0, the peak for the Cubit mesh is displaced to the right, indicating that there is significant variation in $y^+$ for most of the spacer surface area. The difference in uniformity of $y^+$ can be explained by the different mesh generation strategy. The Spider meshes are generated using a layer of similar-sized cells of varying type inserted along the boundary without truncating the cells or the geometry. Using Cubit, the mesh was first generated using tetrahedra that were then dissected to yield an all-hex mesh, resulting in non-uniform cell sizes along walls. Fig. 42(b) shows the $dy^+$ histogram for a 47M-cell Spider mesh. Here, the variation in $y^+$ is significantly reduced relative to the coarser 7M mesh.

![Image](image.png)

**Figure 42:** Cell-area weighted histograms of the $y^+$ variation for the 3x3 rod bundle. (a) $dy^+$ histograms for the 7M Spider and 8.3M Cubit meshes, (b) $dy^+$ histogram for the 47M Spider mesh.

To quantify the uniformity of $y^+$ with a single scalar value, one can estimate the total variation of $y^+$ by computing the total surface area under the $dy^+$ histograms as

$$TV(y^+) = \int g(dy^+) \, d(dy^+) \approx \sum g(dy^+) \Delta(dy^+)$$

where $g(dy^+)$ denotes the function values of the area-weighted $dy^+$ histogram, such as in Fig. 42. The total variation (TV), mean $y^+$, along with additional metrics, computed for all the meshes considered in [3,4], are shown in Table 9. The Spider meshes used for the metrics in Table 9 are hex-dominated hybrid meshes, containing hexahedra, pyramids, tetrahedra, and wedges. In contrast, the Cubit meshes contain pure hexahedra generated by splitting tetrahedral elements. The $y^+$ fields are computed along the spacer surfaces, the most complex part of the geometry where no-slip/no-penetration boundary conditions are imposed. The Reynolds number for the 3x3 rod bundle is $Re_{Dh} = 4.01 \times 10^5$, corresponding to the work in Elmahdi, et al. [4]. The Reynolds number for the 5x5 rod bundle is $Re_{Dh} = 28.0 \times 10^3$, corresponding to the work reported by Yan, et al. [43]. The extremes of the $y^+$ fields, $y^+_\text{min}$ and $y^+_\text{max}$, denote the extents of the $y^+$ histograms, while $\langle y^+ \rangle$ and the (total variation) $TV(y^+)$ represent the mean of the $y^+$ histograms and the integral of the $dy^+$ histograms respectively. The total variation, $TV(y^+)$, is normalized by the total surface of the spacer, $A$. 
Table 9 – Mesh statistics for the 3x3 and 5x5 rod bundles with the V5H spacer grid.

<table>
<thead>
<tr>
<th>Rod Bundle</th>
<th>Mesh</th>
<th>Generator</th>
<th>No. of Elements</th>
<th>$y^+_{\text{min}}$</th>
<th>$y^+_{\text{max}}$</th>
<th>$\langle y^+ \rangle$</th>
<th>$TV(y^+) \quad A$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3x3</td>
<td>3.9M</td>
<td>Cubit</td>
<td>3,879,436</td>
<td>1.87</td>
<td>61.38</td>
<td>34.52</td>
<td>0.40</td>
</tr>
<tr>
<td></td>
<td>8.3M</td>
<td>Cubit</td>
<td>8,301,944</td>
<td>1.99</td>
<td>53.80</td>
<td>31.23</td>
<td>0.35</td>
</tr>
<tr>
<td></td>
<td>18.6M</td>
<td>Cubit</td>
<td>18,665,148</td>
<td>0.85</td>
<td>45.41</td>
<td>27.20</td>
<td>0.30</td>
</tr>
<tr>
<td>3x3</td>
<td>2M</td>
<td>Spider</td>
<td>2,639,781</td>
<td>1.55</td>
<td>73.41</td>
<td>41.58</td>
<td>0.38</td>
</tr>
<tr>
<td></td>
<td>7M</td>
<td>Spider</td>
<td>7,835,811</td>
<td>0.82</td>
<td>53.57</td>
<td>36.85</td>
<td>0.27</td>
</tr>
<tr>
<td></td>
<td>30M</td>
<td>Spider</td>
<td>29,980,627</td>
<td>0.72</td>
<td>43.18</td>
<td>28.26</td>
<td>0.21</td>
</tr>
<tr>
<td></td>
<td>47M</td>
<td>Spider</td>
<td>46,794,662</td>
<td>0.70</td>
<td>40.92</td>
<td>25.85</td>
<td>0.20</td>
</tr>
<tr>
<td></td>
<td>80M</td>
<td>Spider</td>
<td>83,212,438</td>
<td>0.34</td>
<td>34.25</td>
<td>22.25</td>
<td>0.15</td>
</tr>
<tr>
<td></td>
<td>185M</td>
<td>Spider</td>
<td>185,445,954</td>
<td>0.35</td>
<td>29.87</td>
<td>18.10</td>
<td>0.16</td>
</tr>
<tr>
<td>5x5</td>
<td>14M</td>
<td>Spider</td>
<td>14,238,181</td>
<td>0.29</td>
<td>22.04</td>
<td>15.24</td>
<td>0.11</td>
</tr>
<tr>
<td></td>
<td>96M</td>
<td>Spider</td>
<td>96,366,083</td>
<td>0.21</td>
<td>16.42</td>
<td>12.41</td>
<td>0.09</td>
</tr>
</tbody>
</table>

The following observations can be made based on the data in Table 9:

- The mean $y^+$ monotonically decreases with increasing cell count, signaling an overall uniform increase of refinement with larger meshes, a prerequisite for meaningful mesh convergence studies and uncertainty quantification.
- The total variation of $y^+$ also monotonically decreases with increasing cell-count, i.e., relatively larger surface area is covered by more uniform-size elements at the no-slip walls. This is an assurance of increasing mesh quality at walls, which minimizes non-physical perturbations in the wall-treatment, important for both LES and RANS simulations with wall-functions.
- Based on the $dy^+$ histograms and the total variation of $y^+$ the quality of Spider meshes are clearly superior to those produced using Cubit.

Figure 43 shows a graphical representation of the $\langle y^+ \rangle$ column in Table 9. Here, $\langle y^+ \rangle$ is plotted for both series of Spider meshes for the 3x3 and 5x5 geometries, as well as, for the 3x3 Cubit meshes. While the Reynolds number is the same for the respective Cubit and Spider series of meshes for the 3x3 geometry, the $\langle y^+ \rangle$ for the 5x5 meshes are computed for a lower Reynolds number. This is the main reason for a significantly lower $\langle y^+ \rangle$ for the 5x5 meshes for similar total cell counts when compared to the 3x3 meshes. Both the Spider and Cubit meshes exhibit a monotonic decrease in the mean $y^+$ with increasing cell count. The trends are all logarithmic. This is expected as none of these meshes have graded boundary-layer meshes at walls. The logarithmic fit in Fig. 43 extrapolates the trend for the 3x3 Spider meshes and predicts that to achieve $\langle y^+ \rangle \approx 1$ with this meshing strategy would require approximately 5 billion cells. Since the trend is the same for the Cubit meshes, the asymptotic mesh estimate is expected to be the same. The next step in mesh generation is to add power-law-graded boundary layer refinement, a relatively straightforward exercise with the Spider mesh generator. With graded boundary layer meshes, it is estimated that meshes with less than 50 million elements will be required to achieve $\langle y^+ \rangle \approx 1$ for the 3x3 rod bundles.
5.2 Alternative approaches

In order to further extend the flexible application of Hydra-TH, a separate task was dedicated to developing non-proprietary CFD models of a single pin and a 5x5 subassembly with spacers and mixing vanes, adopting a fully hexahedral commercially available block structured mesher. The constructed mesh could be used for future code-to-code comparisons and further for testing various multiphysics coupled simulations (CFD/chemistry, CFD/neutronics, etc.). The 5x5 subassembly geometry corresponds to a selected region of the Seabrook fuel assemblies analyzed in the L2.MPO.P7.06 milestone [46] and could therefore be adopted for a follow up milestone for the validation of HYDRA-TH/MAMBA.

5.2.1 Single Pin Block Structured Mesh

The first test problem consists of a typical PWR pin cell. The dimensions of the pin are summarized in Table 10, while the geometry is presented in Fig. 44. Three grid spacers are modeled in the upper regions of the pin.

Table 10 – Dimensions of fuel pins and guide tubes.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pin radius</td>
<td>0.4025 cm</td>
</tr>
<tr>
<td>Clad radius</td>
<td>0.4759 cm</td>
</tr>
<tr>
<td>Active fuel height</td>
<td>365.76 cm</td>
</tr>
<tr>
<td>Inlet velocity</td>
<td>5.278 m/s</td>
</tr>
</tbody>
</table>
The CFD mesh has been developed taking advantage of the problem symmetry. Therefore, at first only 1/4 part of the geometry was meshed. This mesh was then replicated azimuthally in order to cover the entire model domain. The volume occupied by the grid spacers was not meshed (i.e. it was left as void), since our interest is focused on the fluid-dynamics effect of the grid spacers and mixing vanes only.

The mesh was built using a multi-block structured approach, available in the ANSYS ICEM CFD mesh generator. Following this approach, the entire geometry has to be divided in hexahedral mesh blocks, and the interfaces of contiguous blocks need to be conformal. The meshing domain, selected for the construction of the block structure, starts from the middle plane of a grid spacer and extends up to the middle plane of the coolant channel region existing between two consecutive spacers, as indicated in Fig. 45. The block structure created for this domain allows meshing the region that includes the mixing vanes. Then, the mesh created for this domain is extended over the entire pin domain by mirroring and copying operations, as illustrated in Fig. 46. The inlet and outlet parts of the fuel pin are created by extrusion. The approach sketched in Fig. 46 significantly reduces the meshing time and ensures identical meshing for each grid spacer.
The block structure and the corresponding hexahedral mesh generated are shown in Fig. 47 and Fig. 48 respectively. This mesh contains about 110 blocks and can be easily extended to a full $2\pi$ (360 deg.) model thanks to the conformal matching of all vertical interfaces. The block structure and corresponding mesh are fully consistent with the channel geometry and the mesh block side/edge/vertex is associated with the corresponding geometry surface/curve/point. A significant number of additional geometrical features were included in the channel geometry (see Fig. 49) in order to have extensive control over the definition of the block structure.
The mesh quality was evaluated using the ANSYS ICEM CFD mesh diagnostic tool. The “Quality” and “Determinant” criteria were used. The “Determinant” is defined as the ratio between the smallest and the largest determinant of the Jacobian matrix, where each determinant is computed at each node of the mesh element. The “quality” is defined as a weighted average of the “Determinant” (between -1 and 1), the maximum deviation from orthogonality “Max Orthogls” (normalized between -1 and 1; if deviation from orthogonality is greater than 90 degrees, then the normalized value will be smaller than 0) and “Max Warpgls” (normalized between 0 and 1; warpage of 0 degrees is 1, warpage of 180 degrees is 0). For both criteria, a value of 1 indicates a perfectly regular mesh element, a value of 0 indicates an element degenerated in one or more edges, and negative values indicate inverted elements. The mesh quality results are shown in Fig. 50.
Figure 56 Fine hexahedral (Section)
Figure 57 Coarse hexahedral (Section)
Figure 58 Fine polyhedral mesh (Section)
Figure 59 Coarse polyhedral mesh (Section)
Figure 60 Fine trimmed mesh (Section)
The block meshing approach shown for the single pin application can also be extended to a full non-proprietary 5x5 assembly domain, which is shown in Fig. 61, and contains approximately 124M elements in 543 blocks. Unfortunately, difficulties were experienced in the conversion of large 5x5 hexahedral mesh to the EXODUSII format supported by HYDRA-TH. Currently, several commercial and open-source meshing tools have been tested for the conversion, without success, indicating an important aspect that should be addressed to allow more flexible use of Hydra-TH regardless of the available meshing approach.

![Figure 61 Non-proprietary fully hexahedral block structured 5x5 Mixing Vane Model.](image)

In order to estimate the performance of the developed hexahedral mesh, seven simulations were performed using 3 different CFD codes (STAR-CCM+, ANSYS CFX, and Hydra-TH). Coolant properties and boundary conditions were kept equal for all simulations.

Two mesh resolutions (a coarse and a fine one) have been selected for the present study, resulting in two hexahedral meshes of 3.3M and 11.2M cells respectively (see meshes side-view in Fig. 51 and Fig.52, and meshes cross-section views in Fig. 56 and Fig. 57). The two meshes have been used to run simulations with STAR-CCM+, ANSYS CFX and HYDRA-TH in order to have a code-to-code comparisons and to assess the computational performance of each code.

Three additional simulations have been carried out with STAR-CCM+, using a fine polyhedral mesh (7.2M see Fig. 53 and Fig. 58 for side- and cross-sections views respectively), a coarse polyhedral mesh (1.9M see Figure 54 and Figure 59) and a fine trimmed mesh (5.6M see Fig. 55 and Fig. 60) respectively. This study allows estimating the sensitivity to mesh structured between different codes which adopt relatively dissimilar discretization approaches.
A qualitative comparison could be performed comparing Velocity Magnitude (Fig. 62, Fig. 64) and Turbulent Kinetic energy (Fig. 63, Fig. 65) profiles plotted right downstream of the first spacer at Z=2.535m. Preliminary quantitative comparison could be done using velocity profiles plotted at four locations (z=2.530, 2.535, 2.540, 2.545m see Fig. 67 – Fig 74) downstream the first spacer.
Fine polyhedral mesh

Coarse polyhedral mesh

Fine hexahedral

Fine trimmed mesh

Figure 65 TKE magnitude, obtained on different meshes using STAR-CCM+ (first spacer proximity at Z=2.535m).

Figure 66 Velocity plot locations.
Figure 67 Velocity magnitude at Z=2.530 (STAR-CCM+, ANSYS® CFX, Hydra-TH).

Figure 68 Velocity magnitude at Z=2.535 (STAR-CCM+, ANSYS CFX, Hydra-TH).
Figure 69 Velocity magnitude at Z=2.540 (STAR-CCM+, ANSYS CFX, Hydra-TH).

Figure 70 Velocity magnitude at Z=2.545 (STAR-CCM+, ANSYS CFX, Hydra-TH).
Figure 71 Velocity magnitude at Z=2.530 Star-CCM+ on different meshes.

Figure 72 Velocity magnitude at Z=2.535 Star-CCM+ on different meshes.
In conclusion, a valuable tests was performed on the use of block structured hexahedral meshes for simulation of PWR fuel rod bundles. Hexahedral meshes have been successfully developed for non-proprietary single-pin and 5x5 assembly problems, including spacers and mixing vanes.
The meshes can be used to test codes and models performance within the CASL project. The block structured grids makes the mesh particularly useful during testing, allowing also large applicability for code-to-code comparison and multiphysics application.

While the block structured approach is excessively cumbersome for production application of CFD, and therefore this study was important in demonstrating that the fully hexa approach does not offer particular advantages and more general unstructured meshers can be used with confidence. The hexahedral for the single-pin problem has been successfully used with HYDRA-TH, STAR-CCM+, and ANSYS-CFX. The results obtained with the different codes were consistent.

5.3 Solver settings for massively parallel applications

The following is a list of best-practice guidelines accumulated running relatively large problems on large numbers of compute cores, using the single-phase incompressible Navier-Stokes solver:

**Load balancing:** The third-party ParMetis [47] and Zoltan [48] libraries are used for load-balancing computational meshes for parallel execution. Our experience shows that for compute core counts larger than 2,000 ParMetis is less reliable than Zoltan. Zoltan’s algorithms, e.g., RCB (recursive coordinate bisection), or RIB (recursive inertial bisection), are recommended for large core counts. An example syntax for setting the load balance algorithm in the control file is:

```plaintext
load_balance
method rcb # Select recursive coordinate bisection of Zoltan end
```

**Solution of the pressure-Poisson equation:** One of the most compute-intensive parts of the incompressible solver is the solution of the pressure, for which algebraic multi-grid (AMG) is recommended. Available algorithms for computing a preconditioner include ML (multi-level), and Hypre. Experience shows that ML frequently outperforms Hypre for small to relatively modest-size meshes, e.g., up to a few thousand cells, while for larger meshes, e.g., in the order of millions and above, Hypre’s performance is superior. ML has been known to run out of memory on compute core counts larger than approximately 2,000. Therefore, ML is recommended for smaller cases, while Hypre for larger problems and larger core counts. Additionally, we have found that (for the pressure-Poisson operator) Hypre performs best with the **strong threshold** parameter set to at least 0.8 (and higher, but not exceeding 1.0). One way to reduce the memory requirement of AMG with ML is to increase the **coarse size** of the mesh the algorithm attempts to coarsen the mesh to at every AMG cycle. As a result less AMG levels and less memory are required (for the price of more computation per cycle). Example `ppesolver -- end block using Hypre for large problems:`
ppesolver
  type AMG        # Select algebraic multi-grid
  amgpc hypre    # Select Hypre as preconditioner
  itmax 40       # Stop after this many AMG cycles
  itchk 1        # Number of iterations before checking convergence

  strong threshold 0.85 # Strength threshold, largely influences convergence
  levels 12       # Maximum number of AMG levels/cycle
  diagnostics off # Don’t echo detailed solver diagnostics to screen
  convergence off # Don’t echo detailed convergence diagnostics
  eps 1.0e-5      # Convergence criteria for the linear solver
end

Solution of the momentum and other transport equations: Depending on the time stepping scheme, i.e., a semi-implicit algorithm for time-accurate transient solutions or a fully implicit algorithm for quickly reaching a steady-state solution, different strategies work better for the numerical solution of the momentum, energy, and various other transport equations. As an example, for a time-accurate large-eddy simulation, as the time-steps must be relatively small, e.g., CFL=4-10, the dynamics change less during a time step, so a simpler preconditioner, set by the solver type, GMRES or FGMRES, su ces for the transport equations. On the other hand, for the larger time steps occurring during convergence to steady-state, using an implicit scheme, e.g., CFL=50-100, a more elaborate preconditioner, such as incomplete LU, set by, e.g., ILUFGMRES, will perform better. Example

momentumsolver type FGMRES        # Select flexible generalized minimum residuals
  itmax 100       # Maximum number of linear solver iterations
  itchk 1         # Check convergence after every iteration
  restart 20      # Use this many GMRES restart vectors
  diagnostics on  # Echo detailed solver diagnostics to screen
  convergence on  # Echo detailed convergence statistics to screen
  eps 1.0e-5      # Convergence criteria for the linear solver
end
6. SUMMARY

The work presented in this milestone report has been focused on advancing, demonstrating and assessing the CFD capabilities of the Hydra-TH package for fuel related single phase applications. The report supports the work in the Thermal Hydraulics Focus Area that have led to extending and assessing the capabilities of Hydra-TH in order to deliver a robust fuel simulation platform.

The milestone first has documented the effort in the advancement and assessment of Hydra-TH solution algorithms. The methods have shown good maturity on very large complex industrial applications. Hydra-TH has in particular demonstrated a clear aptitude towards transient turbulence resolving applications, as those related to the GTRF issue. LES was validated firstly against dedicated PIV measurements and further applied to a complex 5x5 prototypical spacer with excellent performance. Best practices have been collected for massively parallel application of the LES methodology.

In order to deliver low computational cost averaged quantities, an advanced RANS model capable of resolving the Reynolds stress anisotropy in fuel assemblies has been implemented in Hydra-TH. The model has been tested on the very challenging case of turbulence driven secondary flow, showing an excellent potential and some open challenges related to its application on fine grids. The standard k-ε model was also implemented in Hydra-TH in addition to the existent RNG variant: both models have shown very robust performance on fuel simulations.

Finally extensive assessment of the CFD process, including different meshing approaches, have been performed in order to accumulate consistent best practice guidelines. A series of isothermal turbulent flow calculations of the grid-to-rod-fretting (GTRF) problem have been carried out on a 3x3 rod bundle with the V5H spacer grid which allowed deriving optimal processes:

- Mesh generation: Numeca's Hexpress/Hybrid mesh generator, a.k.a., “Spider”, has been used successfully to generate high quality meshes of production spacers.
- A quantitative a priori mesh assessment has been introduced for complex unstructured meshes with no-slip walls and used to assess a series of meshes generated for the GTRF problem by two mesh generators. Numeca's Hexpress/Hybrid provided the highest quality grids jointly to the most flexible process.
- Quantitative comparison of RMS forces on a rod show an order-of-magnitude difference between Cubit and Spider meshes, stressing the importance of high quality grids for turbulence resolving LES simulations. Predicted RMS forces, integrated for the whole rod, are an order of magnitude larger using the higher-quality Spider meshes compared to Cubit meshes.
- Tests with different commercially available meshing software have shown a lack of good quality commercial converter for EXODUSII files for large models, which could currently limits the flexibility of the approach.
7. REFERENCES


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