

Technical Guidelines for CFD Analysis in Validating Fuel Assembly CHF Test Results

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1. Introduction

The thermal-hydraulic design of nuclear fuel assemblies in pressurized water reactors (PWRs) and small modular reactors (SMRs) is fundamentally constrained by the critical heat flux (CHF), also known as departure from nucleate boiling (DNB). This phenomenon marks the point at which the efficient nucleate boiling regime transitions to an inefficient film boiling regime, leading to a sharp rise in fuel cladding temperature and potential fuel damage [1, 2].

Traditionally, CHF prediction has relied primarily on empirical correlations and one-dimensional subchannel analysis codes. However, these conventional methods are inherently limited by their strong dependence on specific experimental geometries and operating conditions, making them less reliable when applied to new fuel designs or complex flow situations. Moreover, they are unable to accurately resolve the highly complex, three-dimensional localized flow distributions, such as swirling flows, cross-flows, and spacer grid effects, that occur within tightly packed rod bundles [1-7].

While traditional subchannel analysis codes continue to depend on empirical correlations that are valid only for specific geometries and flow conditions, computational fluid dynamics (CFD) has emerged as a powerful, high-fidelity tool capable of predicting detailed local flow structures, turbulence anisotropy, and heat transfer mechanisms in complex rod bundles. CFD can effectively handle a wide range of operating conditions, including multi-dimensional flow fields and non-uniform power distributions along the fuel rods, across broad ranges of coolant temperature, pressure, and flow rates [1-12].

Based on a comprehensive literature review of CFD analysis applied to CHF in reactor fuel assemblies, this paper outlines specific technical guidelines and requirements for using CFD to validate CHF test results for new nuclear fuel assemblies. These guidelines cover key aspects such as physical modeling, geometric fidelity, verification and validation (V&V) procedures, and appropriate CHF detection criteria, with the aim of enhancing the reliability and regulatory acceptability of CFD-based CHF predictions.

2. Current status of CFD technology for simulating CHF in nuclear fuel assemblies

2.1 Physical modeling

2.1.1 Eulerian two-fluid framework

The dominant approach for simulating boiling flows in rod bundles is the Eulerian-Eulerian two-fluid model (TFM). This framework treats the liquid and vapor phases as interpenetrating continua, solving conservation equations for mass, momentum, and energy for each phase [3, 4]. Current applications assume a constant vapor density at saturation while treating liquid density as a function of temperature [5].

2.1.2 Extended wall heat flux partitioning (RPI Model)

The standard Rensselaer Polytechnic Institute (RPI) model, originally designed for subcooled boiling, partitions wall heat flux into liquid convection, quenching, and evaporation [5]. To predict CHF/DNB, state-of-the-art CFD extends this model to account for vapor contact with the heated wall.

- Vapor convection term: An additional heat flux component is introduced to model heat transfer directly to the vapor phase. This term becomes active when the local vapor volume fraction exceeds a critical threshold (e.g., 0.90–0.95), simulating the dryout condition where liquid contact with the wall deteriorates [4, 5].

- Thin film evaporation: Recent improvements include modeling the evaporation of the thin liquid film beneath vapor bubbles. Studies utilizing a thin film model demonstrated that it plays an essential role when the vapor fraction at the heated surface exceeds 0.25, significantly improving prediction accuracy for dryout trends and capturing the wall heat partition more mechanistically [6].

2.1.3 Interfacial force closure laws

Accurate phase distribution relies on empirical closure models for interfacial momentum transfer.

- Drag Force: The Ishii-Zuber model is widely adopted for calculating drag coefficients in rod bundles, correlating the drag to the local void fraction and flow regimes [7, 8].

- Non-Drag Forces: The turbulent dispersion force is identified as the most significant non-drag force for CHF predictions, as it aids in transporting vapor away from the wall to the subcooled bulk. The Lopez de Bertodano model is frequently recommended for its accuracy in predicting the onset of CHF [9].

- Lift force [10]: While critical for low-pressure bubbly flows, several studies explicitly ignore these forces in high-pressure PWR bundle simulations to improve convergence, noting they have negligible impact on CHF predictions under these specific conditions [4, 9].

2.1.4 Turbulence modeling

Capturing the complex swirling and cross-flows induced by mixing vanes requires rigorous turbulence modeling.

- Shear Stress Transport (SST) $\kappa - \omega$ model: This model is widely favored for its ability to predict flow separation and adverse pressure gradients near mixing vanes [9, 11].

- Realizable or Renormalization Group (RNG) $\kappa - \epsilon$ model: This model has shown superior performance in predicting peak wall temperatures in post-dryout regions and phase transitions in two-phase regimes compared to standard models [9].

- Reynolds Stress Model (RSM): Advanced simulations utilize Reynolds Stress Models (RSM) to capture the anisotropy of turbulence in tight lattice bundles, despite their higher computational demands. This capability is essential for accurate void fraction prediction in complex geometries [12].

2.2 Application to fuel assembly geometries

Current technology allows for the simulation of full-scale rod bundle segments with explicit modeling of spacer grids and mixing vanes.

2.2.1 5x5 rod bundles with mixing vanes

The 5x5 rod bundle (e.g., NUPEC-PSBT benchmark [13-15], ODN benchmark [16]) serves as the primary validation geometry.

- Swirl and decay: CFD captures the strong secondary flows (swirl) generated by mixing vane grids (MVGs). These vanes enhance mixing, but the effect decays downstream. Consequently, CHF typically occurs just upstream of a spacer grid where the mixing effect has faded and vapor accumulates [1, 2, 4]

- Correction of subchannel codes: In PSBT benchmark comparisons, CFD correctly predicted CHF on inner/peripheral rods, whereas traditional subchannel codes incorrectly predicted it on inner high-power rods. CFD attributes this to specific flow fields and lower swirling effects in peripheral regions [5].

2.2.2 Mesh strategies

State-of-the-art simulations employ hybrid meshing strategies:

- Unstructured meshes, such as polyhedral or tetrahedral elements, are deployed in the complex regions containing mixing vanes, springs, and dimples to adapt to the intricate geometry.

- Structured swept or extruded hexahedral meshes are utilized in the bare rod regions to balance computational efficiency with high accuracy.

- To ensure grid independence and effectively resolve the boundary layer, mesh counts for a full 5x5 rod bundle segment can reach upwards of 145 million cells [17].

2.2.3 SMR and low-flow conditions

Applications have extended to SMR conditions (low flow, high pressure). However, CFD models show higher deviations (relative error > 20%) at low mass fluxes (e.g., ~550 kg/m²-s). This is attributed to deficiencies in modeling the flow regime transition from bubbly to churn/slug flow [1].

2.3 Advanced phenomenological insights

CFD provides high-resolution data on local phenomena that empirical correlations cannot resolve.

- Rod bowing: CFD analysis of C-shaped bowed rods reveals that the reduced subchannel gap leads to a sharp rise in local liquid temperature and void fraction. A bowing deformation ratio of less than 0.5 causes a significant penalty in the safety margin, increasing the likelihood of early DNB [2].

- Cold wall effects: In 5x5 bundles with guide tubes (unheated "cold walls"), CFD simulations indicate that cold walls absorb heat from the coolant, reducing local void fraction. This effect was found to increase the CHF value by approximately 11.4% compared to bundles without guide tubes, as the cooled coolant mixes with fluid near heated rods [2].

- Eccentricity: In annular geometries, eccentricity promotes early CHF occurrence in narrow gap regions where liquid volume fraction reduces significantly, while delaying it in wide gap regions [9].

- Axial Power Distribution (APD): Non-uniform APD profiles, such as center-peaked or cosine shapes, show that while phase change might be delayed compared to uniform heating, the rapid accumulation of heat flux ultimately causes the wall temperature to shoot up earlier [7, 9].

2.4 Verification and validation status

2.4.1 Accuracy Metrics

- CHF Value: In complex 5x5 bundles, CFD predictions generally fall within a $\pm 25\%$ error band relative to experimental data [4]. Some tuned models achieve mean relative errors as low as 5-7% [5].

- CHF Location: CFD is highly accurate in predicting the axial and radial location of DNB, with deviations often less than 10 mm axially [5].

2.4.2. Limitations

- Empirical reliance: Despite being "mechanistic," the two-fluid model still relies on empirical closure models (e.g., for bubble departure diameter and nucleation site density) derived from low-pressure, simple-geometry experiments [2].

- Flow regime transitions: Current models struggle to predict CHF accurately under conditions involving transitions to churn or annular flow (typical of BWRs or low-flow PWR transients) [1, 9]. Under SMR operating conditions (low mass flux, high pressure), prediction errors often exceed 20% [1].

3. Technical guidelines for CFD analysis of CHF in nuclear fuel assemblies

3.1 Physical modeling guidelines

To accurately predict CHF (often referred to as DNB) in complex rod bundles, the CFD simulation must utilize a mechanistic multiphase framework rather than simple empirical correlations.

3.1.1 Eulerian two-fluid model

The analysis must be based on the Eulerian-Eulerian two-fluid framework, which treats liquid and vapor phases as interpenetrating continua and solves conservation equations for mass, momentum, and energy for each phase [1-4].

3.1.2 Extended wall boiling model

A standard RPI wall boiling model is insufficient because it is limited to subcooled boiling [1, 9]. Validity requires an extended RPI model that partitions wall heat flux into four components: liquid convection, quenching, evaporation, and vapor convection [1, 6, 12]. This vapor convection term is critical as it activates when the wall is partially covered by vapor (dryout, i.e. critical void fraction > 0.90), simulating the heat transfer deterioration characteristic of DNB [1, 9].

3.1.3 Thin film evaporation

For high accuracy, particularly when the vapor fraction at the heated surface exceeds 0.25, the model should account for thin film evaporation (microlayer heat transfer) beneath vapor bubbles [6].

3.1.4 Turbulence modeling

The selection of turbulence models is crucial for capturing the swirling flow induced by mixing vanes.

- The SST $\kappa - \omega$ model is often favored for its ability to predict flow separation and adverse pressure gradients near mixing vanes [4, 18].
- The RNG $\kappa - \varepsilon$ model has shown superior performance in predicting peak wall

temperatures in post-dryout regions compared to standard models [8, 9].

- Reynolds Stress Models (RSM) are recommended to capture the anisotropy of turbulence in complex tight lattice bundles [2, 11, 12].

3.2 Interfacial force closure modeling guidelines

Proper closure models for phase interactions are mandatory for correct void fraction distributions.

3.2.1 Drag force

The simulation should employ a drag model appropriate for the expected flow regime. The Ishii-Zuber model or the Tomiyama model is technically required to properly calculate the drag coefficient across varying bubble shapes and sizes [1, 3, 4, 9].

3.2.2 Turbulent dispersion force

This is identified as the most significant non-drag force for accurate CHF prediction, as it transports vapor away from the wall. To accurately capture the migration of vapor bubbles from the heated wall into the subcooled bulk flow, a turbulent dispersion force model must be included. The Lopez de Bertodano model is strictly recommended for capturing this lateral phase distribution [4, 9].

3.2.3 Lift force

While essential for low-pressure bubbly flows, some studies indicate these may be negligible or cause convergence issues under high-pressure PWR conditions [4, 9]. Some validated models explicitly ignore them without sacrificing accuracy, while others include them with specific coefficients (e.g., lift coefficient = -0.5) [2, 4].

3.3 Geometry modeling and meshing guidelines

Validating results for fuel assemblies requires high-fidelity geometric representation to capture local flow structures.

3.3.1 Explicit geometry modeling

The simulation must explicitly model the complex features of the fuel assembly, including mixing vanes, dimples, and springs, as these drive the secondary flows that delay CHF [4, 6, 11].

3.3.2 Hybrid meshing

A hybrid strategy is often required, using unstructured (polyhedral or tetrahedral) meshes for complex spacer grid regions and structured

(swept/extruded) meshes for bare rod regions to balance accuracy and cost [4, 5, 11].

3.3.3 Grid independence:

A rigorous mesh sensitivity analysis is mandatory to ensure results (e.g., pressure drop, maximum wall temperature, lateral velocity) are independent of mesh density before moving to multiphase runs [4, 11, 12]. Validated industrial simulations for 5x5 bundles have utilized mesh counts as high as 145 million cells [17].

3.4 Verification and validation (V&V) guidelines

To confirm validity, a hierarchical V&V process is required, moving from simple to complex physics.

3.4.1 Single-phase validation

Before introducing boiling physics, the model must be validated against single-phase experiments (using LDV or PIV data) to ensure it correctly predicts pressure drop, lateral subchannel temperature distribution, lateral velocity fields, and swirl generation induced by mixing vanes [8, 11].

3.4.2 Simple two-phase validation

The model should be validated against benchmark tube or annulus experiments (e.g., Bartolomej [19], Becker [20], or DEBORA[21, 22] tests) to confirm the accuracy of void fraction and wall temperature predictions under boiling conditions [3, 8, 9, 12].

3.4.3 Bundle-scale validation

Finally, the model must be validated against rod bundle CHF data (e.g., NUPEC-PSBT [13-15] or ODEN [16] benchmarks) [5, 6]. The analysis must demonstrate the ability to predict:

- CHF value: Typically, within a $\pm 20\text{-}25\%$ error band [4, 6].
- CHF location: Accurate prediction of the axial and radial location of DNB [2, 4, 5].

3.5 CHF detection criteria

A key technical requirement is establishing clear numerical criteria for identifying the onset of DNB within the simulation. Validated approaches include:

- Temperature excursion: Monitoring for a rapid, nonlinear jump in the maximum wall temperature as heat flux increases [1, 4, 6, 12].
- Critical void fraction: Identifying regions where the high vapor volume fraction near the wall (e.g., > 0.90) prevents liquid contact [2, 5].
- Boiling curve inflection: Plotting wall heat flux against wall superheat to identify the deviation from the nucleate boiling trend [2, 4].

Table 1. Summarized key technical guidelines for CFD analysis of CHF in nuclear fuel assemblies

Topic	Key Guidelines	Ref.
• <i>Physical Modeling</i>		
Eulerian Two-Fluid Model	Use the Eulerian-Eulerian framework to solve mass, momentum, and energy conservation equations for both liquid and vapor phases	1-4
Extended Wall Boiling Model	Use an extended RPI model with a vapor convection term to properly simulate DNB	1, 6, 9, 12
Thin Film Evaporation	Include microlayer heat transfer modeling when the surface vapor fraction exceeds 0.25	6
Turbulence Modeling	Use SST for mixing vanes, RNG for post-dryout peak temperatures, and RSM for tight lattices.	2, 4, 8, 9, 11, 12, 18
• <i>Interfacial Force Closure</i>		
Drag Force	Calculate drag using Ishii-Zuber or Tomiyama models	1, 3, 9
Turbulent Dispersion Force	Use the Lopez de Bertodano model, as this is the most critical non-drag force for vapor transport	9
Lift & Wall Lubrication Forces	May be negligible or cause convergence issues at high pressures; can often be ignored or require specific coefficients	2, 4, 9
• <i>Geometry & Meshing</i>		
Explicit Geometry Modeling	Explicitly model physical features like mixing vanes, dimples, and springs	4, 6, 11
Hybrid Meshing	Use unstructured meshes for complex grids and structured meshes for bare rod sections to optimize cost and accuracy	4, 5, 11
Grid Independence	A rigorous mesh sensitivity analysis is mandatory	4, 11, 12, 17
• <i>V&V</i>		
Single-Phase Validation	Validate pressure drop, velocity, and swirl against LDV/PIV experiments	8, 11
Simple Two-Phase Validation	Validate void fraction and wall temperature against tube/annulus benchmarks (e.g., Bartolomej, Becker, DEBORA)	3, 8, 9, 12, 19-22
Bundle-Scale Validation	Validate CHF values (within $\pm 20\text{-}25\%$ error) and locations against rod bundle benchmark data (e.g., NUPEC-PSBT, ODEN)	2, 4-6, 13-16
• <i>CHF Detection Criteria</i>		
Detection Methods	Identify DNB using clear criteria: rapid temperature excursions, critical void fractions (> 0.90), or boiling curve inflections	1, 2, 4-6, 12
• <i>Phenomenological Capabilities</i>		
Known T-H Phenomena	Ensure the model accurately captures downstream CHF, cold wall effects, and rod bowing penalties	1, 2, 4-6

3.6 Phenomenological capability guidelines

To further confirm the validity, the CFD analysis should capture the following known thermal-hydraulic phenomena;

- Downstream CHF: The model should show that CHF typically occurs just upstream of a spacer grid due to the decay of the mixing swirl generated by the previous grid [1, 2, 5]

- Cold wall effects: The analysis must account for unheated structures (guide tubes), which absorb heat and reduce local void fraction, increasing CHF margins by approximately 11.4% [2, 4].

- Rod bowing: The model must be capable of predicting the penalty on CHF caused by rod bowing, which reduces the subchannel gap and increases local void fraction [2, 6].

The technical guidelines for CFD analysis of CHF in nuclear fuel assemblies discussed above are summarized in Table 1.

4. Conclusions

This literature review demonstrates that CHF prediction technology for nuclear fuel assemblies has evolved from simple correlation-based methods to advanced multi-fluid dynamics approaches. Notably, the onset of DNB in complex 5x5 rod bundles with mixing vanes can be accurately predicted by coupling the Eulerian two-fluid model with extended wall heat flux partitioning. The application of hybrid meshes and robust turbulence models correctly predicts grid mixing and swirl decay, successfully locating CHF occurrence.

Based on these state-of-the-art findings, we derived specific technical guidelines for using CFD to validate CHF test results for new nuclear fuel assemblies. These guidelines are anticipated to provide valuable guidance for experts in the field.

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