DEVELOPMENT AND VALIDATION OF A TWO-PHASE THERMAL-HYDRAULIC CFD CODE NEK-2P

Nuclear Science and Engineering Division

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September 2020

SUMMARY

A project is underway to develop, verify and validate an advanced two-phase flow modeling capability for the highly-scalable, high-performance Computational Fluid Dynamics (CFD) code NEK5000 [1]. The goal of this work is to verify and validate the two-phase version of the NEK5000 code, named NEK-2P, to simulate the two-phase flow and heat transfer phenomena that occur in a Boiling Water Reactor (BWR) fuel bundle under various operating conditions. The NEK-2P two-phase flow models follow the approach used for the Extended Boiling Framework (EBF) [2-3] previously developed at Argonne but include more fundamental physical models of boiling phenomena and advanced numerical algorithms for improved computational accuracy, robustness, and computational speed.

The development of the NEK-2P two-phase solver and the implementation of the Extended Boiling Framework two-phase models were initially supported by Argonne National Laboratory (Argonne) through a Laboratory Directed Research and Development (LDRD) project during FY2014-2016. The development and validation of the two-phase models through analyses of selected two-phase boiling flow experiments was supported by the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program in FY2017-2020.

This report focuses on verification and validation of the water-steam boiling model NEK-2P Two-Phase, CFD code. The NEK-2P was validated with Nuclear Power Engineering Corporation (NUPEC) Pressurized Water Reactor (PWR) Sub-channel and Bundle Test (PSBT) void distribution benchmark. Three different simulations were performed and analyzed for various operating conditions such as wall-heat flux and sub-cooled inlet temperatures. Reasonably good agreement with measured data was obtained in predicting the measured void distributions.

Simulations were performed for Virginia Tech. (VT) 3x3 rod bundle geometry with and without spacers. The preliminary results were presented for Simplified Spacer Grid (SSG). In addition, the implementation of interface reconstruction model was tested with one of the Becker benchmark Critical Heat Flux (CHF) experiments.

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1 INTRODUCTION

The NEK-2P two-phase CFD code was developed at Argonne on the foundation of the high-fidelity highly-scalable CFD code Nek5000 [1] which provides general high-fidelity single-phase flow modeling capabilities. NEK-2P is designed to simulate the two-phase flow and heat transfer phenomena that occur in Light Water Reactor (LWR) fuel bundles under various operating conditions. The NEK-2P two-phase flow models utilize the Extended Boiling Framework [2] methodology previously developed at Argonne, which has been extended to include more fundamental physical models of boiling flow and heat transfer phenomena and advanced numerical algorithms for improved computational accuracy and computational speed. Previous work including the initial implementation of the Extended Boiling Framework in the CFD code STAR-CD showed promising potential for the fine-mesh, detailed simulation of fuel assembly two-phase flow phenomena [3, 4, 6], including the occurrence of Critical Heat Flux (CHF) [5].

The Extended Boiling Framework (EBF) [2-5] was developed for the fine-mesh, 3-dimensional simulation of the two-phase flow phenomena that occur in a Boiling Water Reactor (BWR) fuel assembly. These phenomena include coolant phase changes and multiple flow topologies that directly influence the reactor performance. The EBF boiling models, which describe the inter-phase mass, momentum, and energy transfer phenomena specific for various local flow topologies, allow the simulation of a wide spectrum of flow regimes expected in a BWR fuel assembly. An overview of these models is included below in Chapter 2. These models were ported to the high-performance high-fidelity CFD code NEK-2P to provide general two-phase boiling flow modeling capabilities. The NEK-2P code was validated with multiple benchmark boiling flow tests including Becker et al. [7] and Bartolemei et al. [8]. The code predicted reasonably well the onset of dryout location and wall temperature magnitudes in multiple CHF experiments [9-11]. The Conjugate Heat Transfer (CHT) model was validated through multiple benchmark simulations of Becker CHF tests including both CHF under Dryout (DO) and Departure from Nucleate Boiling (DNB) conditions [12].

The present work focuses on the verification and validation of the NEK-2P two-fluid two-phase model (2F-2P). The work reviews the EBF and Advanced Boiling Framework (ABF) models and presents results of recent NEK-2P analyses of several CHF experiments that have measured the void distribution in two-phase upward flow in a vertical channel with a heated wall. The NUPEC PSBT Void Distribution Benchmark steady-state single sub-channel benchmark selected to validate NEK-2P code. The simulated void fraction at measured plane is compared with experimental data. Good agreement with measured data was observed in predicting the vapor void fraction magnitudes, illustrating the ability of the NEK-2P code and ABF models to simulate for a wide range of thermal-hydraulic conditions. Also, simulations were performed for Virginia Tech. (VT) 3x3 rod bundle configuration. The initial results were presented for both with and without spacer configurations.

The outline of the work is as follows. In Chapter 2 the two-phase CFD code NEK-2P was presented including the advanced boiling framework for two-phase flows. In Chapter 3, the NEK-2P verification and validation were presented. The preliminary results of Virginia Tech. (VT) 3x3 rod bundle boiling flows simulations were discussed in Chapter 4. The implementation of interface reconstruction model was presented in Chapter 5. Finally, future work was proposed.

2 THE NEK-2P CFD CODE TWO-PHASE MODEL

The development of the NEK-2P has followed a staged approach, beginning with the development of a homogeneous two-phase model in FY 2014, continuing with the development of a more complex two-phase drift-flux model in FY 2015, and followed with the implementation of a two-fluid two-phase (2F-2P) model for NEK-2P in FY 2016 and FY 2017. In FY18 and FY19 additional features were developed in NEK-2P such as the Departure from Nucleate Boiling (DNB) CHF model and the Conjugate Heat Transfer (CHT) model, respectively. In FY20, the NEK-2P two-phase two-fluid model validated with PSBT benchmark and preliminary simulations were initiated for Virginia Tech. (VT) 3x3 rod-bundle spacer configuration. The two-phase formulation and assumptions were described below.

2.1 HOMOGENEOUS TWO-PHASE MODEL

Because only one velocity field is available in the Low-Mach version of NEK5000, we decided to begin with the implementation of a homogeneous two-phase model. The main assumptions of the homogeneous model were: i) the local velocities of the water and vapor phases were assumed to be the same for each computational element, and ii) the local temperatures of the water and vapor phases were assumed to be the same for each computational node. The phase transition from water to vapor was due to local enthalpy changes in a reactor fuel assembly or in a heated pipe experiment are driven by the wall heat flux. The mass, momentum, and energy conservation equations can be found in Tentner et al. [9].

2.2 DRIFT-FLUX TWO-PHASE MODEL

The development of the drift-flux model was an intermediate step in the development of the two-phase NEK-2P code. The approach selected by the development team was intended to extend the capabilities of the homogeneous two-phase model described above in a manner that minimizes the changes to the one-velocity two-phase solver and to provide a test-bed for the implementation of the Extended Boiling Framework while the two-velocity two-phase solver of the NEK-2P code was being developed.

The drift-flux model accounts for the effect of different vapor and liquid velocities within the framework of the one-velocity solver. The current model allows different phase velocities, but assumes that the liquid and vapor have the same temperature in each computational cell. The calculation of the local liquid and vapor velocities requires the use of the Extended Boiling Framework as described in Tentner et al. [9].

2.3 TWO-FLUID TWO-PHASE MODEL

The NEK-2P two-fluid two-phase model development includes two sets of transport equations for mass, momentum, and energy for water and vapor phases. The full details of the transport equations and associated closures of Extended Boiling Framework (EBF) can be found in Tentner et al. [5]. The NEK-2P two-fluid two-phase model validated for both critical heat flux and subcooled boiling flow benchmark tests [6].

Nek5000 [1] is a highly-scalable open-source transient CFD code developed at Argonne National Laboratory which has been awarded the Gordon Bell prize in high-performance computing and has run on over one million processors on Argonne's massively parallel Blue Gene/Q computer Mira. The code was based on the spectral element method and it was written in FORTRAN 77 and C languages. The original Nek5000 was built for the simulation of single phase constant-density flows. A later version of the code, referred to as the Low-Mach version, was modified to allow the simulation of single-phase variable-density perfect-gas flows. The Low-Mach version of Nek5000 was selected by the project team as the platform for the implementation of two-phase boiling modeling capabilities in NEK-2P. The development of NEK-2P has followed a staged approach, beginning with the development of a homogeneous two-phase model and continuing with a more complex two-phase drift-flux model. The implementation of these two-phase models was described in Tentner et al. [9]. The development of a two-fluid two-phase solver for NEK-2P and the coupling of this solver with the EBF models have later been completed. The 2P-2F solver and the associated models which were used in the CHF experiment analyses presented in this report were reviewed below.

2.3.1 The Two-Fluid Two-Phase Conservation Equations

A new two-fluid two-phase solver has been implemented in NEK-2P, replacing the previous Nek5000 solver which could only track one fluid velocity field. The new NEK-2P Eulerian two-fluid two-phase solver calculates time evolution of the mass, velocity, and energy of the liquid and vapor phases at all mesh locations in the computational domain by solving the mass, momentum and energy conservation equations for each phase.

The conservation of mass equation for phase k is

$$\frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) = \dot{m}_{ki} - \dot{m}_{ik} \quad (1)$$

The conservation of momentum equation for phase k is

$$\begin{aligned} \frac{\partial}{\partial t}(\alpha_k \rho_k \mathbf{u}_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k \mathbf{u}_k) - \nabla \cdot (\alpha_k (\boldsymbol{\tau}_k + \boldsymbol{\tau}_k^t)) = \\ - \alpha_k \nabla P + \alpha_k \rho_k \mathbf{g} + \mathbf{M} \end{aligned} \quad (2)$$

The conservation of energy equation for phase k is

$$\frac{\partial}{\partial t}(\alpha_k \rho_k e_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k e_k) - \nabla \cdot (\alpha_k \lambda_k \nabla T_k) = Q \quad (3)$$

The momentum equations for the two phases were coupled through the pressure, which was assumed to be the same for the two phases. The mass, momentum, and energy phase conservation equations were also coupled through the corresponding inter-phase transfer terms, which were obtained using the Extended Boiling Framework (EBF) models.

The inter-phase forces considered in the model were: drag, turbulent dispersion, virtual mass, lift, and wall lubrication forces. In addition, inter-phase momentum transfer was associated with mass transfer hence $\mathbf{M}$ in Equation 2 is given by

$$\mathbf{M} = \mathbf{F}_D + \mathbf{F}_T + \mathbf{F}_M + \mathbf{F}_L + \mathbf{F}_{WL} + \dot{m}_{ki} \mathbf{u}_i - \dot{m}_{ik} \mathbf{u}_k \quad (4)$$

The treatment of the inter-phase forces covers the spectrum of flow topologies expected in a BWR fuel assembly. The drag force model, for example, covers bubbles in the sub-cooled or saturated bubbly flow topology, a mixture of Taylor bubbles and smaller bubbles in the slug-flow transition topology, and droplets in the droplet or mist topology. Details of the treatment of inter-phase forces can be found in Tentner et al. [10] and Ustinenko et al. [4]. The inter-phase heat transfer term Q in Equation 3 was obtained by considering the heat transfer from the vapor and the liquid to the gas/liquid interface assumed to be at the saturation temperature, as described in Tentner et al. [11].

The turbulence effects were currently included through an algebraic mixing-length model. An extended $k-\omega$ model that contains extra source terms that arise from the inter-phase forces present in the momentum equations is under development.

The solution of two-fluid two-phase (2F-2P) model equations implemented in NEK-2P was based on a novel low-Mach-number numerical approach, based on previous work on reactive gaseous flow [13-14]. In this approach, the pressure was assumed to be the same for both phases. The solution method was described in detail in Tentner et al. [6].

The required phenomenological closures for the continuity, momentum and the energy equations were taken from the Extended Boiling Framework (EBF) work of Tentner et al. [2]. The Advanced Boiling Framework (ABF) included in the NEK-2P code uses a four-field two-phase generalized topology representation - described below in Section 2.4 - for a more accurate prediction of interfacial area and associated mass, momentum, and energy inter-phase transfer.

2.4 THE ADVANCED BOILING FRAMEWORK

Inter-phase interactions in multiphase fluids depend on both the area and the topology of the phase interface. Sub-channel thermal-hydraulic codes rely on flow regime maps to evaluate the interface topology using cross-section-averaged flow parameters. CFD codes, which divide the flow space into much finer computational cells cannot rely on the traditional sub-channel flow regimes but must evaluate instead the local topology. The ensemble of many computational cells with relatively simple topologies can provide complex global two-phase flow topologies that include all the traditional sub-channel flow regimes. The definition of the local inter-phase surface topology and the subsequent calculation of the mass, momentum, and energy inter-phase interactions was based on the use of the Extended Boiling Framework [2, 9] which has been implemented in NEK-2P and was reviewed in this section. Flow topology changes typical for boiling flow in BWR fuel assemblies and the local topologies considered in the EBF were illustrated schematically in Figure 1.

Figure 1. Schematic view of upward boiling flow in vertical channel with heated walls

While the initial EBF models were based on a two-field representation of the local topology, the NEK-2P implementation of the EBF had been extended to include a more general four-field representation of the local topology which allows a more rigorous treatment of the inter-phase interaction terms and was referred to as the Advanced Boiling Framework (ABF). A brief discussion of the new ABF features were included below. The ABF models were integrated with the new two-fluid two-phase solver.

2.4.1 Inter-phase Surface Topology Map and Local Flow Configuration

The EBF boiling model uses a locally calculated topology variable to allow the following topologies: a) a bubbly flow topology with spherical vapor bubbles in a continuous liquid, b) a droplet or mist topology with spherical liquid droplets flowing in a continuous vapor field, and c) a transition topology which combines the features of the two previous topologies in various proportions. The local topology was determined in this model using a local topology map based on the local void fraction. The 1-dimensional topology map used for cells that were not adjacent to solid walls was illustrated in Figure 2 together with the associated local flow topologies. The topology variable which assumes values between 0-1 is based on the local vapor volume fraction and was then used in the code to determine the local topology and calculate the corresponding mass, momentum, and energy inter-phase transfer terms.

While the original Extended Boiling Framework (EBF) relies on a two-field representation of the local topology (liquid and vapor), the Advanced Boiling Framework recently implemented in NEK-2P introduces a more general four-field representation of the local inter-phase surface topology, illustrated in Figure 3.

Figure 2. Inter-phase surface topology map used for the advanced boiling framework

The general four-field topology provides the foundation for the definition of local topologies in all the computational cells, but affects directly the topology in the interior transition cells and in the wall cells. In the interior cells with bubbly or droplet flow regimes only two fields were used (see Figure 2) and the ABF cell topology remains the same as the two-field EBF topology. In the interior transition topology cells and in the wall cells the use of the four-field ABF topology instead of the two-field EBF topology allows a more detailed treatment of the relevant two-phase flow phenomena. The use of the four-field ABF topology in the wall cells was described in the following sections.

Figure 3. General four-field inter-phase surface topology

2.4.2 Inter-phase Mass, Momentum, and Energy Transfer Models

The inter-phase surface topology map was used to evaluate the interfacial area and inter-phase interactions. Three basic local flow configurations with specific interface topology were identified

(bubbly flow, mist flow and sharp interface) and the interfacial area and inter-phase mass, momentum, and energy transfer models were defined for these configurations. In the domain identified in Figure 2 as transitional topology it was assumed that a combination of basic flow configurations was present, separated by a phase interface with geometric characteristics typical of larger Taylor bubbles. Both small bubbles with a prescribed diameter and large Taylor bubbles were considered in the transition-topology cells. The diameter of the Taylor bubbles was assumed comparable to the channel hydraulic diameter. The quantities required for closure were found by determining the appropriate combination of mass, momentum, and energy exchange terms for the local flow topology. The most general transitional topology was illustrated in Figure 3, and various other transitional topologies were obtained by retaining only a sub-set of the transition master-cell features.

As demonstrated in [15], the use of the local inter-phase surface topology map allows the modeling of complex sub-channel-scale topologies that emerge from combinations of many computational cells with one of the local topologies shown in Figure 2. E.g., the typical sub-channel annular flow regime illustrated in Figure 1 could be resolved into a distinct core flow region in which the gas phase was continuous and the local mist topology was used, separated by transition topology cells from a liquid film on the wall where the local bubbly topology and the wall-cell topology are used.

2.4.3 The Wall-cell Topology

The wall cell topology was a special case of the general cell topology discussed above. Wall cells where the local liquid volume fraction was lower than a specified value were treated in the ABF boiling model as a special liquid film and droplet topology illustrated in Figure 4. The wall cells can contain both a liquid film and liquid droplets. As the liquid volume fraction decreases the liquid film, which initially covers the entire wall surface was assumed to become unstable and to cover the wall surface only partially. This wall cell topology was representative for conditions that can lead to the occurrence of CHF under Dryout (DO) conditions.

Because the 2F-2P solver allows only one velocity and one temperature for each phase in a computational cell, the droplet and film velocities and temperatures were the same. However, the partition of the liquid between the liquid film and droplets has important implications for the heat transfer between the heated wall and the two-phase coolant. The explicit partition of liquid between the film and droplets in the wall cells allows a more detailed partition of the wall heat flux allowing an improved prediction of the CHF under DO conditions.

The CHF can occur under Departure from Nucleate Boiling (DNB) conditions at lower local void fractions due to high wall heat flux values. In this case the wall cell topology was simplified, with the liquid covering the entire wall area. The CHF can still occur due to the increasing number of departing vapor bubbles, which prevent or delay the re-wetting of the heated wall by the liquid, as illustrated in Figure 5.

Figure 4. Wall cell general four-component topology and heat flux partition

Figure 5. Wall cell topology and heat flux partition for lower void fraction conditions

2.5 CLADDING-TO-COOLANT HEAT TRANSFER MODEL

The calculation of the wall temperature and CHF prediction was based on partitioning of heat flux between six heat transfer components as illustrated in Figure 4. The new six-component heat flux partition replaces the previous five component partition presented in [6] and was designed to improve the modeling of the wall heat transfer phenomena which influence the CHF occurrence.

The wall heat flux was partitioned between the following six heat transfer components illustrated in Figure 4: a) q_{gas} , the convective heat flux from wall to the gas or vapor phase, over the wall area not covered by the liquid film; b) q_{drop} , the convective heat flux from wall to the liquid droplets, over the wall area not covered by the liquid film; c) q_{liq} , the convective heat flux from wall to the liquid phase, over the area covered by the liquid film but excluding the bubble nucleation area; d) q_{vap} , the evaporation heat flux from wall to the boiling interface, over the bubble nucleation area, during the bubble growth phase of the bubble formation and departure cycle e) q_q , the quenching heat flux from the wall to the liquid over the nucleation area, during the quenching phase of the bubble formation and departure cycle, and f) q_{dry} , the heat flux from the wall to the vapor over the nucleation area during the dry-wall phase which is assumed to follow the bubble departure and to precede the quenching phase. These heat flux components were specified per unit wall area and they decrease or become zero as the corresponding wall-contact area decreases. The wall heat flux is given by

$$q_w = q_{gas} + q_{drop} + q_{liq} + q_{vap} + q_{qch} + q_{dry} \quad (5)$$

The heat flux components were calculated using the appropriate heat transfer coefficients and heat transfer area based on the local wall-cell topology:

$$q_{gas} = h_g \theta_{dry} (1 - \theta_{drop}) (T_w - T_g) \quad (6)$$

$$q_{drop} = h_d \theta_{dry} \theta_{drop} (T_w - T_l) \quad (7)$$

$$q_{liq} = h_l (1 - \theta_{dry}) (1 - \theta_{bn}) (T_w - T_l) \quad (8)$$

$$q_{vap} = h_l (1 - \theta_{dry}) \theta_{bn} f_{vap} (T_w - T_{sat}) \quad (9)$$

$$q_{qch} = h_q (1 - \theta_{dry}) \theta_{bn} f_{qch} (T_w - T_l) \quad (10)$$

$$q_{dry} = h_g (1 - \theta_{dry}) \theta_{bn} f_{dry} (T_w - T_l) \quad (11)$$

where θ_{dry} is the fraction of the total cell wall area covered by vapor, θ_{drop} is the fraction of the dry wall in contact with the liquid droplets, θ_{bn} is the fraction of the area covered by liquid which was covered by bubble nucleation sites, and f_{vap} , f_{qch} , f_{dry} are the fractions of the bubble formation and departure time cycle represented by the respective cycle phases shown in Eq. 12.

The formulation of the previous wall heat transfer model based on partitioning the heat flux into five components (q_{gas} , q_{liq} , q_{vap} , q_{qch} , q_{drop}) was described in [6]. This model was referred below as the CHF DO model. The sixth component of the wall heat flux q_{dry} represents the heat transferred between the heated wall and the bubble nucleation sites during the dry-out period assumed to follow the bubble departure from the wall. It has been added in order to better represent the phenomena that affect the CHF under DNB conditions. The six-component heat flux partitioning model was referred below as the CHF DO-DNB model. In the CHF DO model the bubble formation and departure cycle was divided into two phases, the bubble growth and the quenching phase, following the Kurul-Podowski model [16]. In the new CHF DO-DNB model the bubble formation and departure cycle was divided into three phases: the bubble growth phase, the dry-out phase that follows the bubble departure, and the quenching phase [17].

$$t_{BB}^{cycle} = t_{vap} + t_{dry} + t_{qch} \quad (12)$$

The length of the dry-out period t_{dry} is a function of the wall superheat and under DO conditions is equal to zero or remains small, so that the six-component heat partitioning model becomes equivalent to the five-component CHF DO model. Under DNB conditions however t_{dry} becomes significant and plays an important role in the prediction of CHF DNB as illustrated in Section 3. The length of the dry-out period t_{dry} is based on the value of the nucleation site density obtained from [2, 16]

$$n'' = (m \Delta T_{sup})^p \quad (13)$$

where $\Delta T_{sup} = T_{wall} - T_{sat}$ is the wall superheat, $m=185$ and $p=1.805$ [16]. As long as the wall area occupied by the bubbles does not exceed the total liquid film area Equation 13 is used and $t_{dry} = 0$. If the wall superheat ΔT_{sup} exceeds ΔT_{dry} when the wall area occupied by the bubbles exceeds the total liquid film area the nucleation site density cannot increase anymore and instead t_{dry} increases as a function of $(\Delta T_{sup} - \Delta T_{dry})$:

$$t_{dry} = t_{BB,o}^{cycle} C(\delta_{film}) \left(\frac{\Delta T_{sup}}{\Delta T_{dry}} - 1 \right) \quad (14)$$

where $t_{BB,o}^{cycle}$ is the length of the bubble-cycle before the occurrence of dry-out and $C(\delta_{film})$ is a coefficient that accounts for the effect of the liquid film thickness. The wall-cell topology illustrated in Figure 4 and the heat flux partitioning models described above were used the analysis of the CHF experiments described in Section 3.

3 THE NEK-2P TWO-PHASE TWO-FLUID BOILING MODEL VALIDATION WITH PSBT BENCHMARK

3.1 PSBT VOID DISTRIBUTION BENCHMARK

The void distribution and DNB measurements took place at the facility described below. The facility is able to simulate the high-pressure, high-temperature fluid conditions found in PWR's. Subcooled water enters at the bottom of the test section and flows upward. It is heated by the heat generated in the heating element and begins to boil. The detailed void fraction distribution is measured at a measuring plane, near the top of the heated region and the average cross section void fraction is also measured. The detailed void distribution in the measuring plane was not made available to the benchmark participants and only the average void distribution in the measuring plane was available for the benchmark. Although the same test loop was used for both phases of the experiment, different test sections were constructed to represent a single sub-channel and a complete rod bundle.

Figure 6 shows the test section used for the central sub-channel void measurement. It consists one of the sub-channel types found in a PWR assembly. Sub-cooled water enters the pressure vessel horizontally through the coolant inlet nozzle located just below the heated section. Similar test sections were used for the central with thimble, side, and corner sub-channel types. The effective heated length is 1.555 m, and the void measurement section begins at 1.4 m from the bottom of the heated section [18].

Figure 6. Test section for central sub-channel void distribution measurement.

3.2 NEK-2P CFD MODEL

In Figure 7, CFD model of the experimental test section is shown. The CFD model includes only a 90° section of the actual geometry due to geometry symmetry.

Figure 7. CFD modeled geometry; (i) cross section view and (ii) axial view.

Figure 8. NEK-2P mesh; (i) top view and (ii) front view.

The Nek-2P mesh is shown in Figure 8. The cross section discretized with 317 elements. The total number of axial elements are 105. The dense grid was used in measured plane location. The void fraction distribution is measured at the measuring plane, near the top of the heated region. The measuring plane cells have a thickness $DZ = 5$ mm. A similar fine mesh, with $DZ = 5$ mm, is

used above and below the measuring plane, in order to avoid potential mesh-related numerical effects. The cell thickness used in the rest of the model is larger, $DZ = 20$ mm.

3.3 RESULTS OF NEK-2P SIMULATIONS OF SELECTED BOILING FLOW EXPERIMENTS

The PSBT benchmark conducted 43 central channel steady state void measurement tests, with different combinations of pressure, mass flow rate, power, and inlet temperature. Each of these parameters was varied in a range relevant for the operation of PWRs. The PSBT benchmark team selected five of these tests for the comparative computational analyses. In this work analyzed only three of these tests, identified as: 1.2211, 1.2223, and 1.2237. The physical parameters of these experiments are summarized in Table 1.

The steady state void distribution in each experiment was calculated with the NEK-2P model including the EBF models by running a transient simulation until a steady state was reached. The steady state void fraction distribution in the measuring plane was then used to calculate the average void fraction in the measuring plane. The volume averaged void fraction in the measuring plane calculated by the CFD model is shown in Table 2 together with the experimentally measured values. The distribution of the calculated local void fraction for each of the three cases analyzed is shown in Figure 9. To be noted, the bubble and droplet diameters are 0.2 and 0.1 mm, respectively.

The reasonable agreement between measured and calculated average void fractions is observed in these experiments except lower void fraction run (1.2211). The detailed void distributions exhibit features typical for two-phase flow in reactor assemblies, such as the presence of higher void fractions near the heated wall at low average void fractions (Figure 9i) and the formation of a higher void fraction region away from the wall of the channel with a low void fraction region or liquid film near the heated wall for higher average void fraction cases (Figures 9ii-iii). Figures 10-12, the vapor volume fraction, mixture velocity magnitude and liquid temperature distribution are shown over the vertical plane (YZ-plane).

Table 1. Test conditions for the central sub-channel tests analyzed

Run Number	Pressure [Kg/cm ³]	Mass Flux [10 ⁶ kg/m ² -hr]	Power [KW]	Inlet Temperature [C]
1.2211	150.1	10.91	90.0	295.4
1.2223	150.1	10.91	69.8	319.6
1.2237	150.3	10.93	60.0	329.6

Table 2. Measured and calculated average void fractions in the measuring plane

Run Number	Measured Void Fraction	STAR-CD(v3)	NEK-2P Clift=0.25
1.2211	0.038	0.039	0.106
1.2223	0.311	0.314	0.325
1.2237	0.440	0.351	0.370

Figure 9. Vapor distribution over measured plane for lift coefficient of 0.25 (Clift); (a) Run#1.2211, (b) Run#1.2223 and (c) Run#1.2237.

Figure 10. Vapor distribution over vertical plane (YZ-plane) for lift coefficient of 0.25 (C_{lift});
(a) Run#1.2211, (b) Run#1.2223 and (c) Run#1.2237.

Figure 11. Mixture velocity magnitude [m/s] over vertical plane (YZ-plane) for lift coefficient of 0.25 (Clift); (a) Run#1.2211, (b) Run#1.2223 and (c) Run#1.2237.

Figure 12. Liquid temperature [K] distribution [K] over vertical plane (YZ-plane) for lift coefficient of 0.25 (C_{lift}); (a) Run#1.2211, (b) Run#1.2223 and (c) Run#1.2237.

3.4 CONCLUSIONS

The NEK-2P validated with PSBT void distribution benchmark. Three different tests were simulated for various wall-heat flux and subcooled inlet temperatures. Reasonably good agreement was obtained between predicted and measured average vapor void fractions for the two higher void fraction cases, while for the lower void fraction run (Run#1.2211) the average void fraction in the measuring plane was somewhat over-predicted.

4 MODELING AND SIMULATIONS OF BOILING FLOW IN VT 3x3 ROD BUNDLE

4.1 3x3 ROD BUNDLE GEOMETRY

A facility featuring a 3x3 electrically heated rod bundle is designed and being constructed at Virginia Tech. (VT) under NEUP award. This facility is specially designed for optical measurements and is expected to provide high-quality boiling data in the future. The 3x3 rod bundle has nine (3x3) electric heaters with diameter of 15.9 mm, pitch: 21 mm [19]. The power can operate up to 14 KW for each rod, 126 kW total. The maximum designed operating pressure and temperature are upto 10 bar and 180 C, respectively. The 3x3 rod bundle geometry includes two spacer grids with mixing vanes designed by Westinghouse. For visualization and optical measurements, eight large windows were included. The 3x3 rod bundle geometry and the Simplified Spacer Geometry (SSG) are shown in Figure 13.

Figure 13. 3x3 rod bundle geometry; (a) bottom view (b) side view and (c) Simplified Spacer Grid (SSG).

The initial NEK-2P fluid simulations were performed for bare rod bundle and simplified SSG as shown in Figures 14-15. In Table 3, the operating and boundary conditions are shown for NEK-2P simulations. A full geometry (360°) was used to simulate for bare rod bundle configuration and the result are presented in Vegendla et al. [20]. In this report, the preliminary results are presented for SSG configuration. For SSG, simulations were performed for 45° slice due to limited computing time. To be noted, the presented results are yet to be converged for SSG. The transient results are shown for 0.2sec. To obtain the converged results, the simulations has to perform upto physical time of 0.6 sec. The present work focuses on BWR flow conditions for a given pressure of 70 bar.

Figure 14. A 3x3 bare rod bundle CFD model.

Figure 15. NEK-2P modeled 3x3 geometry with spacers; (a) axial view and (b) cross section view

Table 3. Geometry and operating conditions

	Units
Inlet Velocity [m/s]	1.33
Inlet Temperature [K]	549
Saturation Temperature [K]	559
Wall-heat flux [W/cm ²]	40
Heated rod diameter [mm]	15.9
Heated rod Length [m]	1.37
Pitch btw heated rods [mm]	21
Duct width or depth [m]	0.7530
Spacer location [m]	0.5 and 1

4.2 NEK-2P PRELIMINARY SIMULATION RESULTS

In Figure 16, the increased liquid phase temperatures towards an outlet were mainly due to an applied constant heat flux at fluid-solid boundary. To be noted, only fluid domain was solved by NEK-2P code.

Figure 16. Contour plots over 45° slice; (a) Liquid temperature [K] and (b) Mixture velocity [m/s]

Figure 17. Contour plots over vertical slice at center of the column; (a) Liquid temperature [K], (b) Mixture velocity [m/s] and (c) Vapor volume fraction

From Figure 17, the increased liquid phase temperatures towards an outlet were mainly due to an applied constant heat flux at fluid-solid boundary, as discussed above in Figure 16. The vapor formation increases with an increase of axial height for a given wall heat flux of 40 W/cm^2 . The disappearance of liquid was observed towards an outlet in bare rod bundle. In spacer configuration, the results are yet to be converged. The vapor formation is not observed at simulate time of 0.2 sec.

4.3 CONCLUSIONS

The initial simulations were performed for VT 3x3 rod bundle using NEK-2P CFD code. In bare rod bundle, the significant vapor formation was observed for wall heat flux of 40 W/cm^2 . Towards an outlet, the predicted higher fluid velocities were mainly due to vapor formation. The NEK-2P simulations were initiated for simplified spacer grid configuration. The SSG results were presented for physical time of 0.2 sec and the simulations are yet to be converged to form significant vapor.

5 IMPLEMENTATION OF INTERFACE RECONSTRUCTION MODEL IN NEK-2P CFD CODE

5.1 INTERFACE RECONSTRUCTION MODEL

Piecewise linear interface calculation (PLIC) schemes have been extensively employed in the volume-of-fluid (VOF) method for interface capturing in numerical simulations of multiphase flows. The PLIC scheme can keep the interface sharp while maintaining mass conservation at the expense of an extra reconstruction step [21]. In each mixed cell with the fraction value ranges from zero to unity, the interface in the PLIC method is approximated by:

$$\vec{n} \cdot \vec{X} + D = 0 \quad (15)$$

where $\vec{n}$ is the unit outward normal vector of the interface, $\vec{X}$ the position vector of the interface and D the signed distance from the origin. With the explicit description of the interfaces, the accuracy of the evaluation of the heat flux and release rate across of the interface between the liquid and vapor could be improved [22-23].

In the PLIC-VOF method, the solution of the VOF equation can be decomposed into three steps: interface orientation, reconstruction, and advection [21]. In the orientation step, the vector $\vec{n}$ is evaluated by using the volume fraction gradient $\nabla\alpha$, i.e.,

$$\vec{n} = -\frac{\nabla\alpha}{\|\nabla\alpha\|} \quad (16)$$

where the negative sign indicates that the orientation vector $\vec{n}$ point from liquid to gas. Then, the interface signed distance D is calculated by employing an analytical scheme developed in [21].

It should be noted that the first two steps, interface orientation and reconstruction, have been implemented in the framework of NEK-2P. The basic idea is creating dummy control volumes around the Gauss-Legendre points in each element (see Figure 18). The interface has then been reconstructed in these dummy cells (solid blue lines in Figure 18(b)).

(a) Elements in Nek-2P [1]

(b) Created dummy cells

Figure 18. Illustration of the elements and created dummy cells around the Gauss-Legendre points (lx1,ly1,lz1).

The dummy control volumes are created only once before the simulation starts for the consideration of computational efficiency. Each element will have $(lx1-2)*(ly1-2)*(lz1-2)$ dummy

cells, which will be treated as an unstructured mesh, i.e., the point coordinates, point-face and face-cell topology information will be calculated and stored.

The reconstructed interfaces could be imported in *.obj format for post-processing in the current implementation. The reconstructed interfaces from different threads in a parallel simulation will be collected and stored into a single file (see Figure 19).

Figure 19. Illustration of the reconstructed interface collection in a parallel simulation.

5.2 RESULTS

The previously published NEK-2P results for one of the Becker benchmark validation case was tested to reconstruct the interface in the post-processing step. The analysis of experiment C (highlighted in Table 4) was used to test the interface reconstruction model. The Becker boiling flow experiments are Critical Heat Flux (CHF) experiments performed in a vertical heated tube as shown in Figure 20. The inner and outer diameter and length of the vertical pipe are 14 mm, 10 mm and 7m, respectively.

Figure 20. Schematic diagram of the Becker experiment [7].

Table 4. Parameters of the CHF Dryout (DO) experiments analyzed with NEK-2P.

Exp	G [kg/s-m ²]	q_w [W/m ²]	$T_{in}-T_{sat}$ [K]	q_w/G [J/kg]	Pressure [bar]
A	497.0	35.0e4	-10.3	704	70
B	1009.6	40.1e4	-10.3	397	70
C	1008.9	49.9E4	-10.3	495	70
D	1495.0	79.7E4	-10.3	533	70
E	1994.9	79.6E4	-10.3	399	70
F	2482.9	80.0e4	-10.3	322	70

Figure 21 shows the clip view of the reconstructed interfaces (solid white lines) at different cross-section locations in a CHF simulation. The detailed analysis of the results and model improvements will be carryout in future work.

Figure 21. Illustration of the reconstructed interfaces for experiment C from Table 4.

5.3 CONCLUSIONS

The developed NEK-2P interface reconstruction model was tested for one of the Becker CHF benchmark tests. Reasonable results were obtained from interface reconstruction model. The future work includes the implementation of the interface advection, interphase smoothness enhancement and computational efficiency improvement, and the addition of models that describe the mass, momentum, and enthalpy transfer phenomena associated with the interface.

6 FUTURE WORK

NEK-2P development and validation will continue with a focus on CHF models enhancement and simulation of both Dryout (DO) and Departure from Nucleate Boiling (DNB) experiments. The development and validation of the interface reconstruction models will also continue. The boiling flow simulations will be continued for VT 3x3 rod bundle simplified spacer geometry. The development and validation of the NEK-2P conjugate heat transfer capability with a focus on rod-bundle simulations is also planned. The focus of the future effort mainly will be on modeling of two-phase boiling flow in fuel pin bundles with realistic spacer geometry: (a) evaluate the effect of spacers on vapor distribution and flow topologies, (b) evaluate the effect of spacers on CHF and (c) evaluate the effect of CHT in the presence of spacers.

NOTATION

A	wall area [m^2]
C_p	specific heat [J/kg.K]
d	diameter [m]
g	gravity [m/s^2]
h	enthalpy [J/kg]
h_{fg}	latent heat of vapor [J/kg]
m	mass [kg]
q	heat flux [W/m^2]
t	time [sec]
T	temperature [K]
V	volume [m^3]
α	volume fraction
ρ	density [kg/m^3]
σ	surface tension [N/m]
θ	phase topology [-]
λ	thermal conductivity [W/m.K]

Subscripts

b	bubble
c	continuous fluid (or) convection
d	disperse fluid
g	vapor
L	liquid
q	quench
w	wall
drop	droplet
dry	dryout
sat	saturation
sup	super heat
vap	vaporization

ACKNOWLEDGMENTS

This work was funded by the U.S Department of Energy, Office of Nuclear Energy, Nuclear Energy Advanced Modeling and Simulation (NEAMS) program, under Argonne contract DE-AC02-06CH11357.

We gratefully acknowledge the computing resources provided on Blues and Bebop, a high-performance computing cluster operated by the Laboratory Computing Resource Center at Argonne National Laboratory.

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