

# **EULERIAN TWO-PHASE COMPUTATIONAL FLUID DYNAMICS FOR BOILING WATER REACTOR CORE ANALYSIS**

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## **ABSTRACT**

Traditionally, the analysis of two-phase boiling flows has relied on experimentally-derived correlations. This approach provides accurate predictions of channel-averaged temperatures and void fractions and even peak assembly temperatures within an assembly. However, it lacks the resolution needed to predict the detailed intra-channel distributions of temperature, void fraction and steaming rates that are needed to address the fuel reliability concerns which result from longer refueling cycles and higher burnup fuels, particularly for the prediction of potential fuel pin cladding failures resulting from growth of tenacious crud. [1]

As part of the ongoing effort to develop a high-fidelity, full-core, pin-by-pin, fully-coupled neutronic and thermal hydraulic simulation package for reactor core analysis [2-4], capabilities for Eulerian-Eulerian two-phase simulation within the commercial Computational Fluid Dynamics code Star-CD [5,6] are being extended and validated for application to Boiling Water Reactor (BWR) cores. The extension of the existing capability includes the development of wall heat partitioning and bubble growth models, implementation of a topology map based approach that provides the necessary capability to switch between the liquid and vapor as the continuous phase on a cell-by-cell basis and the development of appropriate models for the inter-phase forces that influence the movement of bubbles and droplets.

Two applications have been identified as an initial demonstration and validation of the implemented methodology. First, the model is being applied to an Atrium-10 fuel assembly from Cycle 11 of the River Bend Nuclear Power Plant. Second, the model is being applied to an international benchmark problem for validation of BWR assembly analysis methods. [7]

*Key Words:* Computational Fluid Dynamics, Two-Phase, Boiling, Boiling Water Reactor

## **1. INTRODUCTION**

The relatively low and stable cost of commercial uranium fuel is a primary contributor to the cost competitiveness of nuclear energy with other energy sources. The long-term reliability of precision engineered and manufactured commercial fuel directly impacts an individual plant's cost of producing electricity and the cost-competitiveness of the industry as a whole. The ever-

increasing demand placed on commercial Boiling Water Reactor (BWR) fuels as a consequence of power up-rates and longer refueling cycles have led to an increase in observed fuel rod failures in many plants. While some fuel rod failures are inevitable in a reactor core containing tens of thousands of individual fuel rods and do not impact the safe operation of the reactor, each failure does impact the cost of electricity generation through increases in both plant operating cost and the cost of long term management and disposal of the failed fuel. [1]

One observed effect in today's reactor cores that may contribute to the increase in fuel failures in some BWR's is the growth of tenacious crud layers on certain individual pins. Although the growth of crud layers on fuel pins is common in BWR cores, tenacious crud is a particular challenge because it can concentrate soluble species, forming precipitates which clog porous area of the crud. This process traps steam near the clad surface a particularly insulating layer. The ability to predict specific locations on the surface of an individual fuel pin which may be susceptible to the growth of tenacious crud would be particularly valuable to core designers, but requires the ability to predict not only the axial but also the radial and azimuthal variations in neutronic and thermal hydraulic quantities within and in the vicinity of each individual pin in an entire core.

As part of an ongoing effort to develop high-fidelity full-core fully-coupled neutronic and thermohydraulic simulation capability for reactor core analysis [2-4], the commercial Computational Fluid Dynamics (CFD) code Star-CD [5] is being used as a foundation for an Eulerian two-phase boiling (E2P) model which is expected to provide the capability needed for the application of detailed CFD models to the design and analysis of Boiling Water Reactor (BWR) cores. This multi-year collaborative effort between Argonne National Laboratory and CD-adapco Group began with the implementation of an Eulerian bubbly flow model for application in the sub-cooled boiling regime. In ongoing efforts, the existing model is being expanded to allow detailed predictions throughout a typical BWR core and the tool is being applied to selected BWR assembly configurations as an initial demonstration and validation of its capabilities.

## 2. EULERIAN TWO-PHASE BOILING MODEL

Analyses of multiphase flow in nuclear reactor cores and assemblies have traditionally relied upon correlation-based sub-channel analysis codes. While these codes provide reliable predictive capabilities for the channel-averaged behavior, they lack the resolution needed to simulate detailed intra-channel effects, such as localized sub-cooled boiling or highly turbulent flow around spacer grid elements, which may have significant local impacts on fuel performance. The applicability of computational fluid dynamics (CFD) to the analysis of these effects has been limited by the absence of computationally-tractable phenomenological models for two-phase boiling flows within those codes. However, recent advances in CFD modeling tools coupled with the growth of massively parallel computational platforms provides the potential for high-resolution modeling of two-phase flow phenomena in nuclear reactor assemblies.

Within the first generation of the Star-CD Eulerian-Eulerian Two-Phase Boiling Model, the entire flow field is treated as bubbly flow. While total energy balance is enforced and the axial

void profile within an assembly can be predicted with reasonable accuracy, the applicability of this approach to the pin-by-pin analysis of BWR cores is limited.

## 2.1. Transport Equations

The STAR-CD Eulerian two-phase solver tracks the mass, momentum, and energy of the liquid and vapour phases in each cell. Full details of the Eulerian two-phase flow models in STAR-CD can be found in [5] and [6]. The main equations solved are the conservation of mass, momentum and energy for each phase.

The conservation of mass equation for phase  $k$  is:

$$\frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k u_k) = \sum_{i=1}^N (\dot{m}_{ki} - \dot{m}_{ik}) \quad (1)$$

where  $\alpha_k$  is the volume fraction of phase  $k$ ,  $\rho_k$  is the phase density,  $u_k$  is the phase velocity,  $\dot{m}_{ki}$  and  $\dot{m}_{ik}$  are mass transfer rates to and from the phase, and  $N$  is the total number of phases.

The conservation of momentum equation for phase  $k$  is:

$$\frac{\partial}{\partial t}(\alpha_k \rho_k u_k) + \nabla \cdot (\alpha_k \rho_k u_k u_k) - \nabla \cdot (\alpha_k (\tau_k + \tau_k^t)) = -\alpha_k \nabla p + \alpha_k \rho_k g + M \quad (2)$$

where  $\tau_k$  and  $\tau_k^t$  are the laminar and turbulence shear stresses respectively,  $p$  is pressure,  $g$  is gravitational acceleration and  $M$  is the sum of the inter-phase forces.

The conservation of energy equation for phase  $k$  is:

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

where  $e_k$  is the phase enthalpy,  $\lambda_k$  is the thermal conductivity,  $T_k$  is the phase temperature and  $Q$  is the inter-phase heat transfer.

## 2.2. Boiling Model

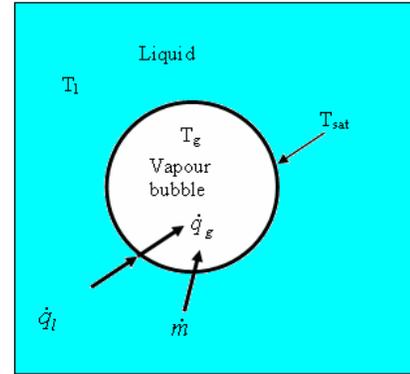
The inter-phase heat and mass transfer models were obtained by considering the heat transfers from the gas and the liquid to the gas/liquid interface, see Fig 2.1. The net heat transfer to the interface is used to compute the mass transfer rate between the two phases.

Heat transfer rate from the liquid to the interface is:

$$\dot{q}_l = h_l A_d (T_l - T_{sat}) \quad (4)$$

Heat transfer rate from the gas to the interface is:

$$\dot{q}_g = h_g A_d (T_g - T_{sat}) \quad (5)$$



**Figure 1. Heat and mass transfer between a vapour bubble and liquid.**

where  $h$  is heat transfer coefficient,  $A_d$  is interfacial area,  $T$  is temperature,  $T_{sat}$  is the saturation temperature, subscript  $l$  denotes liquid and  $g$  denotes gas phase.

The heat transferred to the interface is used in mass transfer (i.e. evaporation or condensation), the mass transfer rate can be written as:

$$\dot{m} = \frac{\dot{q}_l + \dot{q}_g}{h_{fg}} \quad (6)$$

where  $h_{fg}$  is the latent heat.

## 2.2. Wall Heat Partitioning Model

A model describing the heat transfer between the heated wall and the coolant has also been developed. The heat flux from the wall is divided into three parts according to a wall heat partitioning model which includes convective heat for the liquid, evaporative heat for generation of steam and quench heat for heating of liquid in the nucleation sites. If the wall heat flux is specified, rather than the wall temperature, this model allows the calculation of the wall temperature that corresponds to the specified heat flux. Details of the wall heat partitioning model can be found in [5], [6] and [10].

## 2.3. Next Generation Improvements

The second generation of the boiling model that has been developed as part of this effort applies a more rigorous flow topology based approach. Within each individual computational element of a model, the flow can be represented as either bubbly flow where the liquid is the carrier phase, droplet flow where the vapor is the carrier phase, or a transition between the two. Through the application of the appropriate flow topology in each individual computational cell, the traditional flow regime map can be reproduced across the assembly as a whole without the need to superimpose flow-regime based correlations onto the CFD simulation. To support this development effort, a separate collaborative project between CD-adapco, Argonne National Laboratory and VNIIEF and Sarov Laboratories has been established to formulate and validate

the necessary models that describe the inter-phase mass, momentum, and energy exchange for all relevant boiling flow topologies. [8-10]

### 3. PRELIMINARY APPLICATIONS

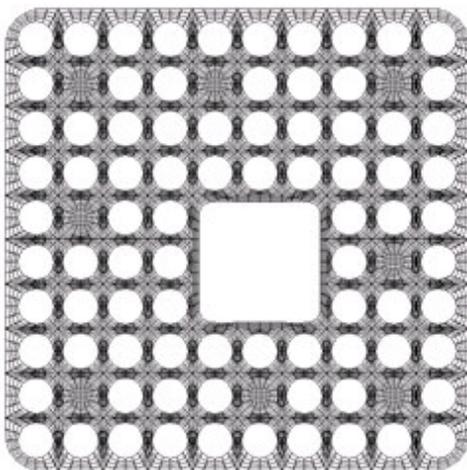
Preliminary investigations have focused on assessing the applicability of the newly developed E2P model to realistic BWR channel conditions. Two representative geometries have been selected for these investigations: 1) an AREVA Atrium-10 BWR fuel assembly, and 2) the test geometry of the OECD/NRC benchmark using the NUPEC Fine-Mesh Full-Size Boiling Water Reactor Test (BFBT) geometry.[7]

#### 3.1. Atrium-10 BWR Fuel Assembly Studies

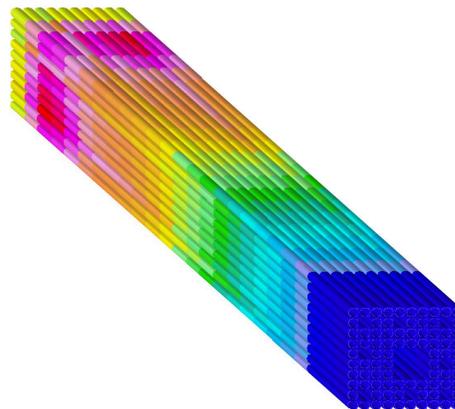
The Atrium-10 fuel assembly consists of 83 full-length and 8 partial length fuel rods configured in a 10 by 10 array. The 10 by 10 array is contained within a square assembly channel which isolates the flow through the assembly from other assemblies and the bypass flow in the gaps between individual assemblies. Within each fuel assembly, the 83 pins are held in place by a top and bottom tie plate, and seven vaned spacer grids that are typically uniformly spaced along the axis of the assembly.

##### 3.1.1. Computational Model

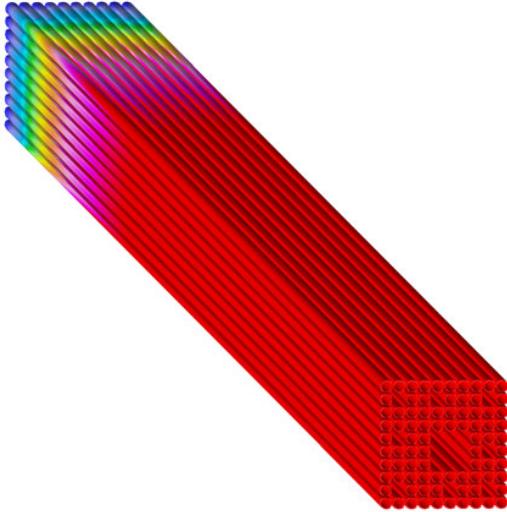
In the Atrium-10 BWR fuel assembly studies, the current computational model considers a simplified bare rod bundle geometry and does not include the effects of spacer grids and flow control vanes on the multi-phase flow field. The computational model uses approximately 1.5 million hexahedral computational cells to represent this simplified geometry. The model is divided into 240 uniform axial layers, where each layer is approximately 15mm high. Each layer contains 6016 cells in the regions where partial rods are present or 6656 cells in the regions above the partial rods. Cell dimensions were selected so that computational cells have aspect ratios less than 50 and so that the longest cell edge is parallel to the main flow direction.



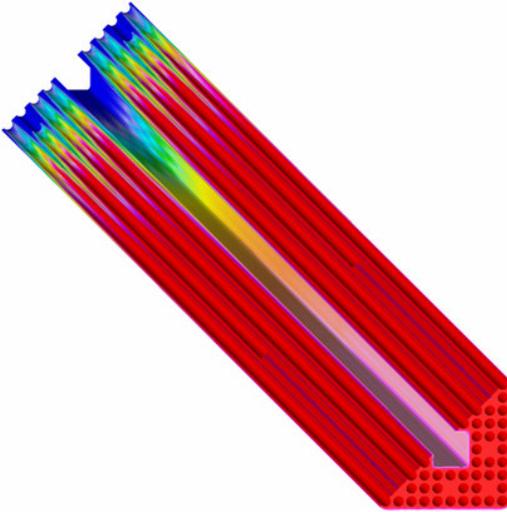
**Figure 2. Computational Mesh Geometry for Typical Boiling Water Reactor Fuel Assemblies Based on (a) the AREVA Atrium-10 Geometry.**



**Figure 3. Heat flux distribution on pin surfaces. Red indicates highest heat flux and blue indicates lowest heat flux.**



**Figure 4. Surface temperature distributions in the assembly. Red indicates temperatures greater than or equal to  $T_{sat}$ . Blue indicates temperatures less than or equal to  $T_{in}$ .**



**Figure 5. Liquid temperature distribution, shown for one diagonal half of the assembly. Red indicates temperatures greater than or equal to  $T_{sat}$ . Blue indicates temperatures less than or equal to  $T_{in}$ .**

clear that the majority of the flow field is above the saturation temperature and that the wall superheat is significant throughout the assembly. The bubbly flow model employed in the current generation model is likely applicable only in the lower regions of the assembly closer to the inlet. In other regions the bubbly flow model should be expected to predict only area- or volume-averaged quantities.

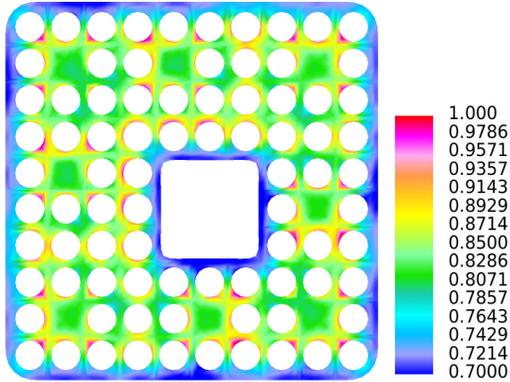
### 3.1.2. Boundary Conditions

A wall heat flux distribution is specified based on calculated axial and radial power distributions and a constant inlet velocity condition is assumed based on specified mass flux. The heat flux distribution employed in these simulations is shown in Figure 3. The can wall boundary and the surface of the water channel are assumed to have a constant temperature equivalent to the inlet coolant temperature. Although it is acknowledged that this approximation leads to an over prediction of heat rejection to the flow between the assembly cans and the flow in the water channel, the approximation simplifies comparisons between Star-CD E2P predictions and traditional 1-D approaches currently used by the vendors and utilities.

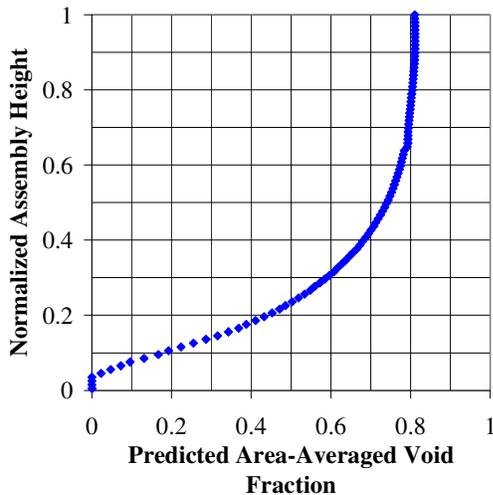
### 3.1.3. Preliminary Results

Simulations using this model were completed using 48 2.3 GHz Xeon processors on ANL's 360 processor jazz Linux cluster. The convergence criteria is defined such that all monitored residual values fall below  $10^{-3}$  and the maximum percent change in the area-averaged void fraction between the current and previous iteration falls below  $10^{-5}$ . These criteria are satisfied after approximately 3500 steady state iterations. For each iteration, each processor is active for an average of 38.22 seconds, so that 1834 total CPU seconds are used per iteration. The elapsed wall clock time per iteration is 38.44 s on average, and the total run time for the simulation is approximately 60 hours.

The surface and liquid temperature distributions within the assembly are shown in Figures 4 and 5, respectively. Based on these distributions, it is



**Figure 6. Computational Predictions of Radial Void Fraction Distribution for an Atrium-10 BWR Fuel Assembly.**



**Figure 7. Computational Predictions of Axial Void Fraction Distribution for an Atrium-10 BWR Fuel Assembly.**

A preliminary prediction of radial void distribution at the exit of the heated region is shown in Figure 6, and a preliminary axial void distribution is shown in Figure 7. Comparisons with vendor-supplied results from traditional 1-D methods are on-going, and efforts to implement second generation capabilities, including the flow-topology based extended boiling framework and improved bubble and droplet force models, are underway. It is expected that the extended capabilities of the second generation tool will significantly improve the quality of the radial void distribution predictions, yielding resolution of liquid films on the heated surfaces and accumulation of vapor at the channel center as is physically expected.

### 3.2. BFBT Fuel Assembly Studies

Although numerous configurations and conditions were considered in the NUPEC experiments, three cases have been selected as validation problems for two-phase CFD models by the benchmark program. [7] In these three cases, the assembly consists of 60 electrically heated pins organized in an 8 by 8 array. The electrically heated pins use the same cladding materials and match the outer diameter dimensions of BWR fuel pins. The test assembly includes a large circular water channel which displaces the 4 array elements at the center of the assembly. Seven ferrule spacer grids with perimeter vanes are included in the assembly test section to both restrict the motion and deformation of the pins and introduce turbulence mixing into

the flow field. The external boundary of the test geometry is representative of a standard square BWR assembly can. The external surface is assumed to be well insulated in the experiments.

Although a variety of axial and radial pin power distributions can be modeled within the test assembly by controlling the current supplied to banks of heater elements, all cases identified for the CFD benchmark exercise use a flat axial profile and the radial profile shown in Figure 8. All three cases also have a fixed inlet subcooling of 50.2 kJ/kg (approximately 10 °C) and an outlet pressure of 7.2 MPa. The flow rate through the assembly is approximately 15.3 kg/s, which results in an inlet velocity of approximately 2.33 m/s in the pin bundle. Three different exit qualities – 5, 12, and 25 percent – were achieved in the experiments considered by controlling the total current supplied to the test section.

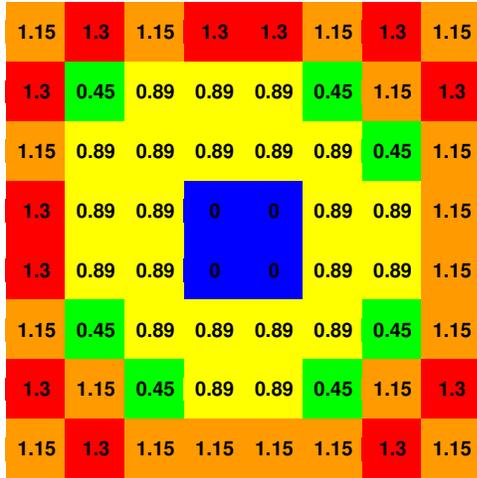


Figure 8. Radial Pin Power Distribution Used in BFBT CFD Benchmark Cases.

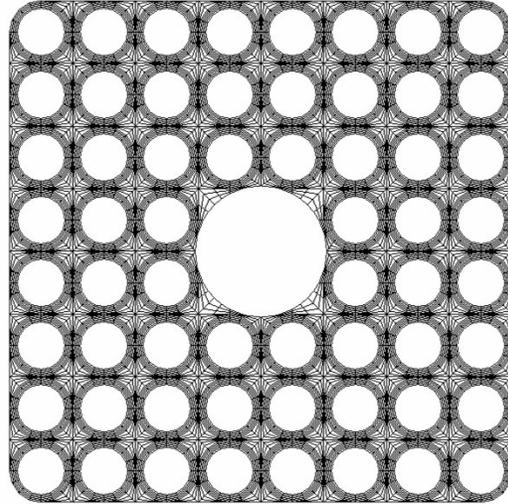


Figure 9. Radial distribution of computational cells in each axial layer.

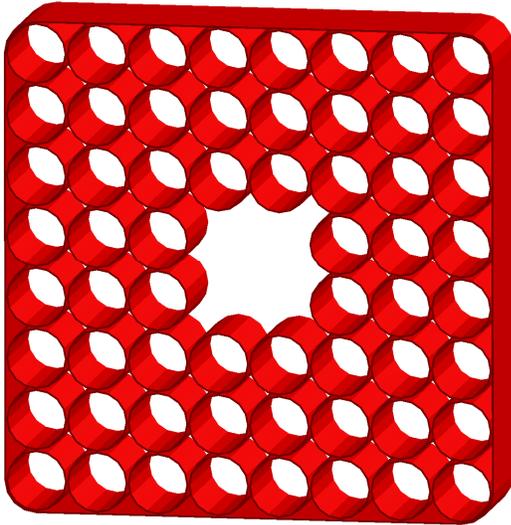


Figure 10. Detail of a simplified spacer grid.

dimensions were selected so that computational cells have aspect ratios less than 75 and the longest cell edge is parallel to the main flow direction.

The model includes a simplified representation of all 7 spacer grids, as shown in Figure 10. The simplified model includes only the ferrules themselves and the perimeter band. Spacer details such as dimples and springs are not included. The vanes along the perimeter band are also neglected. The simplified spacers are intended to capture the majority of the pressure loss associated with grids, but should not be expected to capture any significant impacts on radial void distribution. The spacer grids can be switched off or on by simply changing the material type associated with those cells.

### 3.2.1. Computational Model

The BFBT computational model is a moderately coarse model which uses approximately 3.5 million hexahedral and prismatic computational elements to describe the geometry of the test section. The model includes the heated region, a 5 cm thick extension between the top of the heated region and measurement plane, and a 15 cm extension between the measuring plane and the outlet boundary. The model is divided into 392 axial nodes, with 7680 cells in each axial layer, as shown in Figure 9. Each axial layer has a thickness of approximately 10 mm for the open bundle regions and 5 mm for the layers within the spacer grids. Cell

### 3.2.2. Boundary Conditions

In the BFBT cases, the wall heat flux distribution is specified based upon experimentally prescribed radial power distributions and a constant axial profile. A constant inlet velocity condition is assumed based on the experimentally measured mass flow rate. The benchmark specifications assume that the can wall and water channel wall are adiabatic surfaces. These conditions are used as specified to facilitate code-to-code and code-to-data comparisons planned as part of the benchmark program.

### 3.2.3. Preliminary Results

Preliminary results using the first generation models are shown below for the case with the lowest exit quality and the case with the highest exit quality.

#### 3.2.3.1. Exit Quality Equals 5 Percent

In the first case, the expected exit quality is 5 percent. The predicted axial void profile for this case is shown in Figure 11. The predicted exit void fraction for the specified condition is 47.3 percent, which is consistent with expected values based on homogeneous equilibrium assumption. The detailed predicted radial void profile at the measurement plane is shown in Figure 12. The predicted results using the first generation model indicate that the vapor is strongly concentrated near the pin walls and in the small flow spaces near the assembly edges and corners. For these flow conditions, slug flow or possibly even developing annular flow, as defined in the conventional flow regime map, should be expected to dominate at the measurement plane of the assembly, leading to a more uniform void distribution, perhaps with slight peaking near the center of the open channels. It is expected that the extended boiling framework and improved force models will result in more accurate predictions in the upper regions of the assembly. More quantitative assessments of both the first and second generation models will be completed as part of future components of the benchmark exercise.

#### 3.2.3.2. Exit Quality Equals 25 Percent

In the second case, the expected exit quality is 25 percent. The predicted axial void profile is shown in Figure 13. The predicted exit void fraction for the specified condition is 83.3 percent, which is consistent with expected values based on homogeneous equilibrium. The detailed predicted radial void profile at the measurement plane is shown in Figure 14. The predicted results using the first generation model again indicate that the vapor is strongly concentrated near the pin walls and in the small flow spaces near the assembly edges and corners. For these flow conditions, annular flow with thin wall films, as defined in the conventional flow regime map, should be expected to dominate at the measurement plane of the assembly, leading to a void distribution with little liquid in the channel beyond the film of liquid coating the heated surface. More quantitative assessments will be completed as part of future components of the benchmark exercise. It is expected that the extensions of the E2P model completed as part of this project will lead to significant improvements in accuracy of radial distributions before those comparisons are completed later this year.

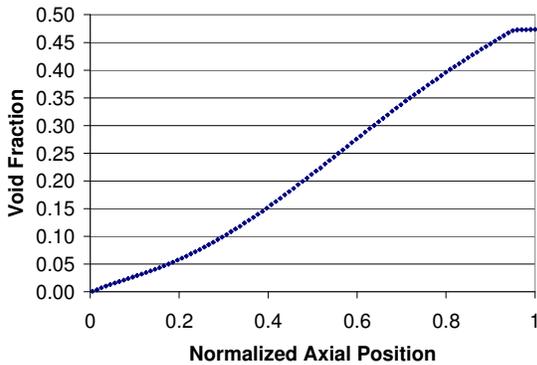


Figure 11. Predicted axial distribution of area-averaged void fraction in the BFBT test assembly for the low exit quality (5 percent exit quality) test case.

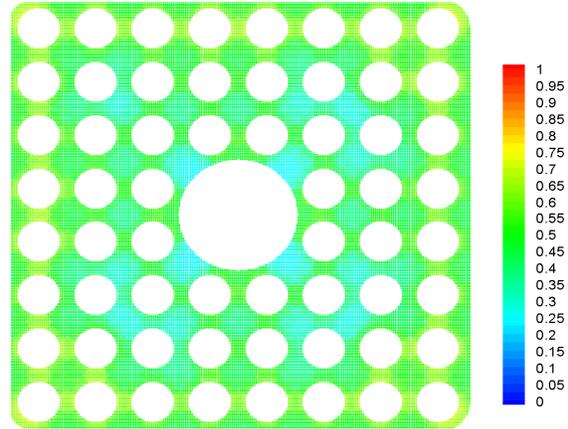


Figure 12. Radial void fraction distribution at the measurement plane in the BFBT test assembly for the low exit quality test case.

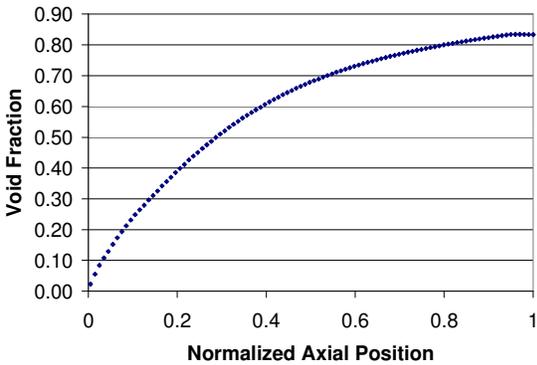


Figure 13. Predicted axial distribution of area-averaged void fraction in the BFBT test assembly for the low exit quality (25 percent exit quality) test case.

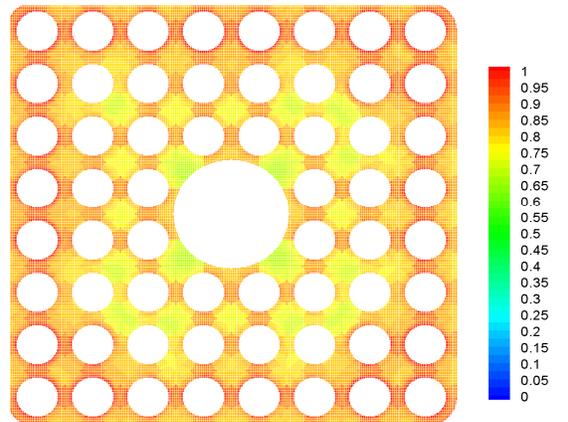


Figure 14. Radial void fraction distribution at the measurement plane in the BFBT test assembly for the high exit quality test case.

#### 4. CONCLUSIONS

In response to the fuel reliability challenges being faced in today's high performance Boiling Water Reactor cores, a fully-integrated three-dimensional simulation capability is being developed to assess pin-by-pin variations in neutronic and thermal hydraulic characteristics within a full BWR core. As part of this effort, an Eulerian-Eulerian two-phase boiling model has been implemented within the commercial CFD code Star-CD. A preliminary demonstration of the applicability of this capability to realistic BWR geometries and conditions has been completed. Additional demonstration cases and a preliminary validation of the model are underway.

## 5. ACKNOWLEDGMENTS

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## 6. REFERENCES

1. Taylor Moore, “The Challenge of Nuclear Fuel Reliability,” *EPRI Journal*, pp 18-25, Fall (2005).
2. T. Sofu, et al., “Treatment of Multi-Physics Phenomena Influencing Reactor Core Design,” *Proceedings of ICAPP '04*, Pittsburgh, PA USA, June 13-17, 2004, Paper 4218 (2004).
3. D. P. Weber et al., “The Numerical Nuclear Reactor – A High Fidelity, Integrated Neutronic, Thermal-Hydraulic and Thermo-Mechanical Code,” *Proceedings of Intl. Mtg. on Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications*, Palais des Papes, Avignon, France, September 12-15 (2005).
4. T. Sofu, et al., “Coupled BWR Calculations With The Numerical Nuclear Reactor (NNR) Software System,” *Proceedings of Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007)*, Monterey, California, April 15-19 (2007).
5. *STAR-CD Version 3.20 Methodology Manual*, Chapter 13, CD-adapco, UK (2004).
6. S. Lo, “Modelling multiphase flow with an Eulerian approach”, *von Karman Institute Lecture Series - Industrial Two-Phase Flow CFD*, May 23-27, von Karman Institute, Belgium (2005).
7. B. Neykov, et. Al., *OECD-NEA/US-NRC/NUPEC BWR Full-size Fine-mesh Bundle Test (BFBT) Benchmark, Volume I: Specifications*, NEA No. 6212, NEA/NSC/DOC(2005)5, ISBN 92-64-01088-2 (2006)
8. V. Ustinenko, et al., “Validation Of CFD-BWR, A New Two-Phase Computational Fluid Dynamics Model For Boiling Water Reactor Analysis,” *Proceedings of CFD4NRS: OECD/NEA International & International Atomic Energy Agency (IAEA) Workshop on Benchmarking of CFD Codes for Application to Nuclear Reactor Safety*, Garching, Munich, Germany, 5 - 7 September (2006).
9. A. Tentner, et al. “Advances In Computational Fluid Dynamics Modeling Of Two Phase Flow In A Boiling Water Reactor Fuel Assembly,” *Proceedings of ICONE14, the 14<sup>th</sup> International Conference on Nuclear Engineering*, Miami, FL, USA, July 17-20, 2006, ICONE14-89158 (2006).
10. A. Tentner, et al. “Computational Fluid Dynamics Modeling Of Two Phase Flow In A Boiling Water Reactor Fuel Assembly,” *Proceedings of Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications*, Palais des Papes, Avignon, France, September 12-15, 2005, on CD-ROM Palais des Papes, Avignon, France, September 12-15 (2005).