Multi-field Simulations of Liquid Film Dryout in Rod Bundle Geometry

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ABSTRACT

OpenSTREAM is a new open-source, one-dimensional, flexible computational environment designed to simulate boiling two-phase flows in single straight channels using various multi-field solvers ranging from the homogeneous equilibrium model to an advanced four-field model of annular two-phase flow. This paper applies OpenSTREAM's three-field model to simulate a series of tests conducted at the Karlstein Thermal Hydraulic (KATHY) Test Loop under Boiling Water Reactor (BWR) conditions, including core instabilities. The 10×10 rod bundle geometry is represented in the code as a three-wall channel, accounting for (1) the adiabatic fuel shroud and central water channel, (2) the fuel rod with the highest radial power peaking factor, and (3) the remaining fuel rods. Initial simulations of single- and two-phase pressure drop tests are performed to calibrate the pressure loss coefficients of the spacer grids. A feature to account for enhanced droplet deposition downstream of the spacer grids is implemented in OpenSTREAM and calibrated against critical power tests. This feature enables accurate prediction of critical power and its associated elevation, determined by iterating the power until complete liquid film dryout is achieved anywhere on the hot rod. The simulation results show consistent agreement with the experimental data for steady-state critical power across the range of tested boundary conditions. Preliminary transient simulations show that OpenSTREAM can predict dryout and rewet with time delays from inlet conditions representative of density waves.

KEYWORDS

Dryout, annular two-phase flow, rod bundle, three-field, OpenSTREAM

1. INTRODUCTION

Liquid film dryout is a relevant bounding thermal limit for Boiling Water Reactors (BWRs) core operation in which fluid in contact with the wall transitions from a two-phase mixture to vapor only, drastically decreasing the heat transfer from the surface causing the temperature to increase significantly. Thus, characterization of dryout limits is essential for determining operational margins of BWRs. Much of the analysis in literature for predicting dryout CHF in rod bundle geometries is limited to the Groeneveld look-up table [1] or phenomenological modeling in proprietary codes such as MEFISTO [2]. OpenSTREAM (Open Solvers for Two-phase flow Research, Engineering Analysis and Modeling) is a new open-source computational environment for phenomenological modeling of one-dimensional two-phase flow in straight multi-wall channels [3]. In this work, OpenSTREAM mixture and three-field solvers are validated on data from the Karlstein Thermal Hydraulic (KATHY) Test Loop using simplified equivalent geometry.

2. METHODS

2.1. OpenSTREAM

OpenSTREAM is a computational environment developed for solving steady-state and transient one-dimensional two-phase flows [3], [4]. The solver offers four frameworks for simulation: (1) mixture model, (2) two-fluid model [5], (3) three-field model [2], and (4) four-field model [6]. In this work, mixture and three-field frameworks are used. The mixture model framework uses the homogeneous equilibrium model to solve conservation equations of mass, momentum, and energy for the liquid and vapor. The void fraction and pressure drop in the channel are calculated using the assumption of homogenous flow (i.e., slip ratio equal to one) for the liquid and vapor fields without considering of liquid distribution between droplets and film. The resulting local pressure distribution is used by the three-field model, where conservation of mass, momentum, and energy equations are solved for the vapor, droplet, and liquid film fields. Additional assumptions required for the three-field framework are that the liquid film can be modeled as a continuous flow field and that the liquid mass flow is split between the droplet and film fields at the onset of annular flow using an assigned ratio, in this work an initial entrained fraction of 0.7 is used. However, the simulation results far downstream from the onset of annular flow are insensitive to the initial entrained fraction, demonstrated by identical liquid film flow rate at the end of the heated length using 0.4 or 0.7 initial entrained fraction. This is due to the coupling of entrainment and deposition models. If the initial entrained fraction is overestimated for steady-state equilibrium, it will cause increased deposition immediately after the onset of annular flow as the coupled entrainment and deposition models approach equilibrium. There is a large uncertainty in three-field parameters near the onset of annular flow due to this semi-arbitrary definition of initial entrained fraction, but since this work is concerned with regions of the heated bundle sufficiently downstream, the specific value used is irrelevant to the following analysis. Necessary closure terms for interaction between the droplets and liquid film are provided through correlations for deposition and entrainment, detailed in Section 2.2. No subcooled boiling is modeled in this work, and the evaporation of the liquid film is calculated assuming thermal equilibrium between liquid film and vapor using the latent heat of vaporization.

2.2. Key Physics Models
2.2.1. Droplet entrainment model

OpenSTREAM allows the user to choose between several models for calculating the mass flux of droplet entrainment or to implement any user-defined model. In this work, the entrainment model of Okawa et al. [7] is modified by excluding the final branch consistent with the rod bundle modeling in Adamsson and Le Corre [2]. The resulting model for drop entrainment mass flux is given in Equations (1)-(3).

$$\pi_{ent} = \frac{f_i \rho_g J_g^2}{\sigma/\delta} \tag{1}$$

$$m_{ent} = k_{ent}\rho_l(\pi_{ent})^n \tag{2}$$

$$\begin{array}{ll} \pi_{ent} < 0.0675 & k_{ent} = 3.1 \times 10^{-2} \left[\frac{m}{s}\right] \\ & n = 2.3 \\ \pi_{ent} > 0.675 & k_{ent} = 6.8 \times 10^{-4} \left[\frac{m}{s}\right] \\ & n = 1.2 \end{array} \tag{3}$$

2.2.2. Spacer-enhanced deposition model

The deposition model from Okawa et al. [7] is used as the basis for calculating the free flow droplet deposition mass flux. A separate model was implemented in OpenSTREAM as part of this work and used to calculate a local droplet deposition enhancement factor to account for the effect of spacer grids as developed in Adamsson and Le Corre [2] and further described in Le Corre [8], reproduced in Equations (4)-(8) for convenience. The droplet deposition rate is calculated using the spacer blockage ratio Θ and two constants derived from computational fluid dynamics (CFD) calculations, B = 7.898 and D = 4.791 [2].

$$k^{MAX}_{enh\_dep} = (D\Theta + 1)(B\Theta + 1) \tag{4}$$

The deposition rate enhancement is a function of axial position to account for droplet transport in the gas core and is separated into three regions defined with respect to the axial position of the upstream spacer grid z_G [8]:

Region 1 (z_G=0 to z_2=0.05 m):
$$k_{enh\_dep} = \left(0.95 k^{MAX}_{enh\_dep} - 1\right)\frac{z - z_G}{z_2 - z_G} + 1 \tag{5}$$

Region 2 (z_2 to z_4=0.15 m):
$$k_{enh\_dep} = 0.95 k^{MAX}_{enh\_dep} \tag{6}$$

Region 3 (z_4 to z_5=0.45 m):
$$k_{enh\_dep} = \frac{1}{\left(1 - \frac{1}{0.95 k^{MAX}_{enh\_dep}}\right)\frac{z - z_4}{z_5 - z_4} + \frac{1}{0.95 k^{MAX}_{enh\_dep}}} \tag{7}$$

Finally, a tuning coefficient, k_G, is provided in the model to fit the generic spacer grid model to a specific application. This coefficient is tuned using critical bundle power data in the KATHY loop, discussed in Section 3.2.

$$m_{enh\_dep} = \left[k_G \left(k_{enh\_dep} - 1\right) + 1\right]m_{dep} \qquad (8)$$

This spacer enhanced deposition model is necessary for modeling rod bundles with local obstructions as it allows us to capture the associated increase in critical power performance along with the correct elevation of dryout below the end of the heated length.

2.3. KATHY Facility and Model

Figure 1 shows the KATHY test loop consisting of a 10×10 rod bundle test section, forced flow loop, and natural circulation loop. The rod bundle test section consists of 81 full length heater rods and 10 partial length heater rods. The rods have a downskew axial heat flux profile. The test section has instrumentation to measure quantities of interest, such as bundle power, inlet mass flow rate, differential and absolute pressure, and temperature of the inner cladding wall at varying axial positions on many of the rods. A complete description of the facility and non-proprietary test data are available in [9].
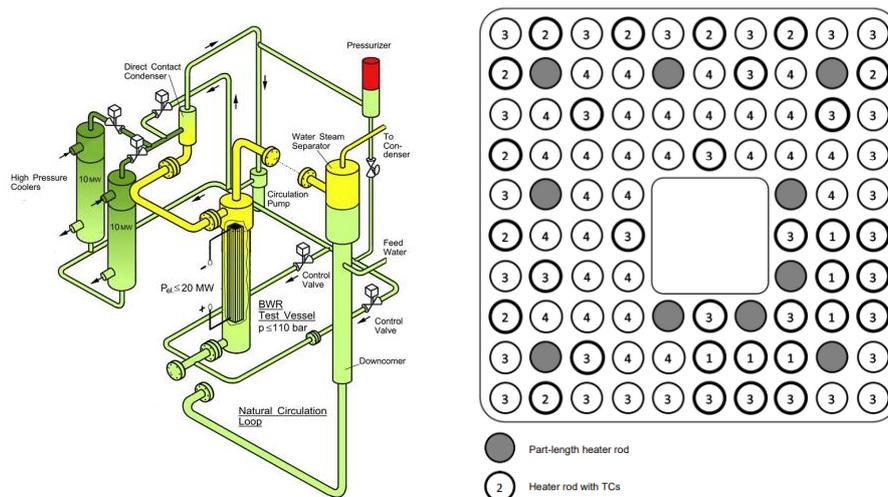

**Figure 1. KATHY Thermal Hydraulic Loop [9].**

Since OpenSTREAM is developed to model single channels, significant geometry simplifications are necessary to model a rod bundle. The KATHY loop is modeled in OpenSTREAM using three walls, preserving the heated and wetted perimeters, and the total flow area of the test loop at the bottom of the test section. The three walls modeled are (1) the adiabatic rod shroud and central water channel, (2) the rod with the highest radial power peaking factor, and (3) the remaining 90 fuel rods. Grid spacers are accounted for as local pressure losses and modeled using loss coefficients. This simplified model possesses several limitations with respect to accurately representing the experiments. First, axially variable flow area and perimeter are not currently supported in OpenSTREAM. Therefore, the partial-length heated rods are modeled as full-length heated rods. The relative error between the model and test loop for flow area, heated perimeter, and wetted perimeter above the partial length heater rods is -8%, 12%, and 10%, respectively. However, since this perimeter difference will have the greatest effect on

the "non-hot" rods, it has limited influence on the overall simulation results. Another limitation is the representation of only a single hot rod, while the experimental data showed dryout occurring on several rods depending on the conditions of the test. In this case, OpenSTREAM's treatment of the geometry as a single flow channel vs. subchannel analysis of the bundle sacrifices spatial fidelity for decreased computational expense. Additionally, since the radial power peaking factors of rods where dryout occurred most frequently across all tests are between 1.258 and 1.260, this effect of specific rod is negligible.

3. RESULTS AND DISCUSSION

3.1. Pressure Drop Tests

The first series of tests simulated in this work are the steady-state single- and two-phase pressure drop tests. The pressure loss coefficients for single- and two-phase flow for each spacer are defined using the coefficients from Duarte's analysis of KATHY data using TRACE [10]. Figure 2 shows the results of the pressure drop validation for both single-phase and two-phase flow. It is vital that the simulations can accurately capture pressure drop along the flow channel. This ensures that fluid properties are predicted with high accuracy when simulating phenomenon of greater complexity, such as flow transients or critical power. The pressure drop test simulations use only the mixture solver in OpenSTREAM and output the differential pressure and vapor quality. Figure 2 shows the OpenSTREAM calculations are within a ±10% band compared to experimentally measured values. The results provide confidence in the two-phase spacer grid loss coefficients from Duarte [10]. Therefore, the loss coefficients are used for all subsequent calculations.
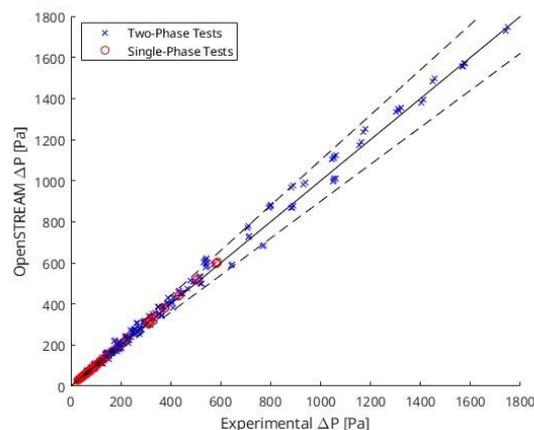

Figure 2. Single- and two-phase pressure drop calculated by OpenSTREAM against experimentally measured values from the KATHY experiments.

3.2. Critical Bundle Power Tests

For the series of steady-state critical bundle power tests, the three-field model implemented in OpenSTREAM is used to investigate the bundle power at which dryout occurs and the elevation with the highest probability of dryout occurrence. In this work, dryout is defined as any point where the magnitude of liquid film flow rate is less than 0.00001 kg/s. This criterium for dryout is the same that was used for cross validation of GRAMP, MEFISTO-T, and SCADOP [11]. To determine the critical

bundle power in OpenSTREAM, multiple calculations are run iterating on the bundle power until dryout is observed at any position along the rod. The initial guess for bundle power iteration is 75% of the experimental bundle power.

Figure 3 shows an example critical power test, with the positions of dryout marked. The axial dimension is normalized by the onset of annular flow and the end of the heated length to preserve proprietary data. A significant result seen in Figure 3 is the ability of OpenSTREAM to predict dryout at multiple locations along the hot rod due to downstream rewetting from spacer enhanced deposition. This behavior is consistent with the experimental results.
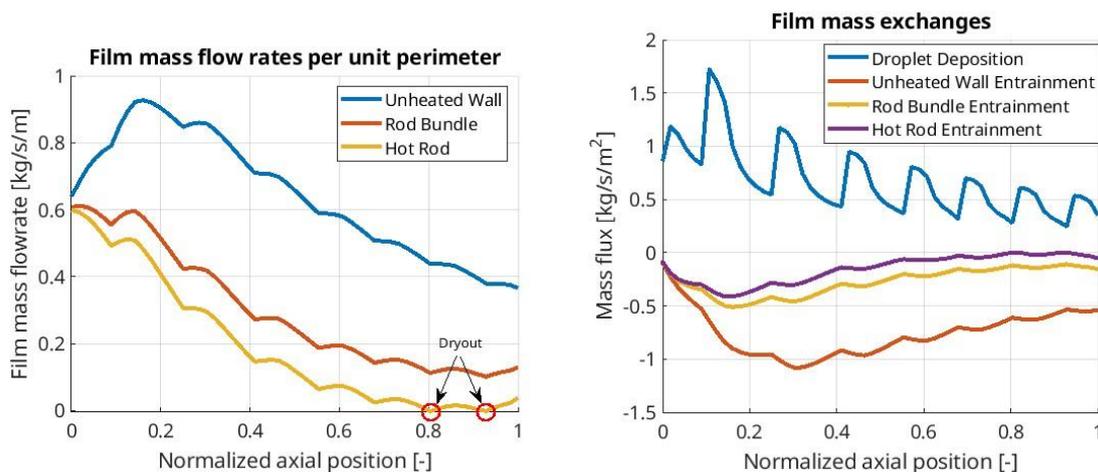

Figure 3. Sample OpenSTREAM output showing (left) liquid film mass flow rate per unit perimeter and (right) liquid film mass exchanges for each wall.

The spacer enhanced deposition model is tuned for this test bundle using all the critical bundle power tests. The tuning process takes advantage of the minimum liquid film mass flow rate per unit perimeter to being related to the power change required for dryout under otherwise identical system parameters. Figure 4 shows the sum of minimum liquid film mass flow rate per unit perimeter on the hot rod across all tests as a function of deposition tuning factor using the experimental critical bundle power. In this case, a negative liquid film flow rate simply indicates that the critical bundle power predicted by OpenSTREAM is below the experimental value. From this analysis, an optimal tuning factor of $k_G =$ 0.33 was chosen for the KATHY loop in the current work using an assumed blockage ratio of 20% for each spacer grid. However, as shown in Figure 4, a range of tuning factors ±0.05 could be used without sacrificing much accuracy of the final behavior. This is important in the fact that the deposition tuning factor is trained on a large data set in this work (71 steady-state critical power tests), and systems with less data for validation may not be able to converge on an optimal tuning factor as accurately.
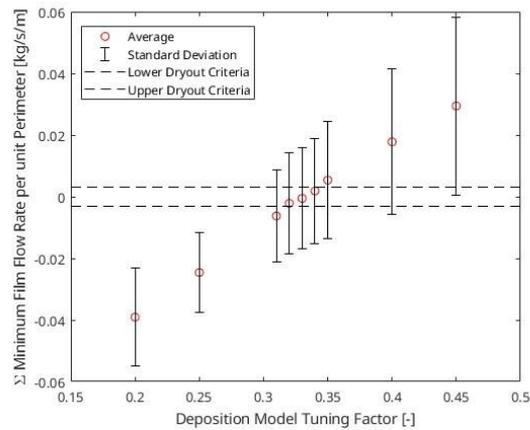
**Figure 4. Deposition tuning factor vs sum of minimum mass flow rate per unit perimeter across all tests.**

The results of critical bundle power simulations are shown in Figure 5, with and without the tuned deposition enhancement model. Using the appropriate tuning factor, OpenSTREAM can predict the critical bundle power within 5% of experimental data for the KATHY loop over a large range of system pressure, inlet mass flux and subcooling, and bundle power.
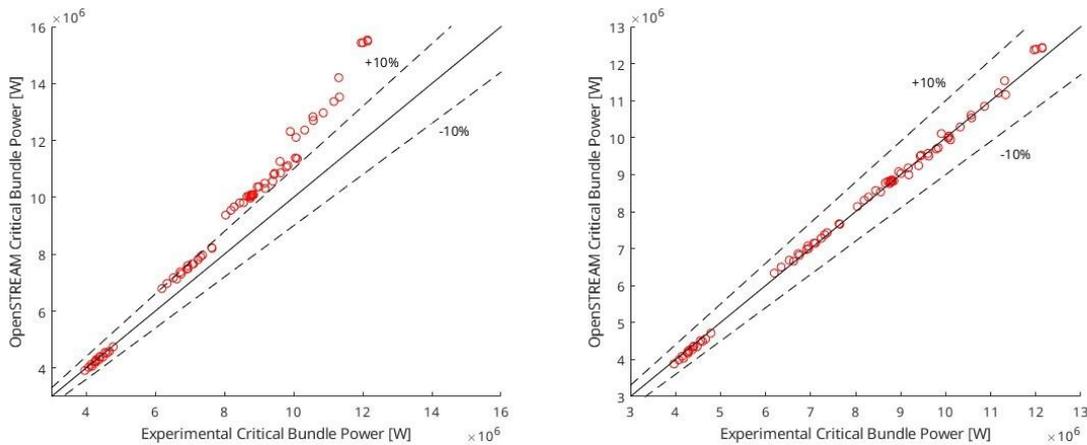
Figure 5. Experimental vs. OpenSTREAM critical bundle power with ±10% bands using (left) deposition enhancement model without tuning factor and (right) with tuning factor.

Clearly, the spacer enhanced deposition model is critically important for accurate prediction of dryout in rod bundles. The low uncertainty of OpenSTREAM calculated critical bundle power compared to experimental data shows that the method of calculating droplet deposition in this system works well across all tested boundary conditions. This warrants deeper analysis on the sensitivity of OpenSTREAM critical bundle power as a function of system inlet parameters, shown in Figure 6. The prediction of critical bundle power seems insensitive to inlet subcooling and system pressure but positively correlated with the inlet mass flow rate. The tuning factor optimization process is biased by the number of tests with low and medium flow rates relative to the number of tests with high flow rates. Additionally, the deposition enhancement model used in this work inherently does not account for the effect of the droplet velocity within the vapor core on their deposition and rather relies on an approach based on position (Equations 5-8). Intuitively, a higher vapor core velocity resulting from higher inlet mass flux would

lead to enhanced deposition further downstream due to the time delay between increased turbulence at the obstruction and resulting deposition. Thus, a model for droplet deposition based on time may be more universally applicable. Regardless, this effect is largely negligible for the present data set.
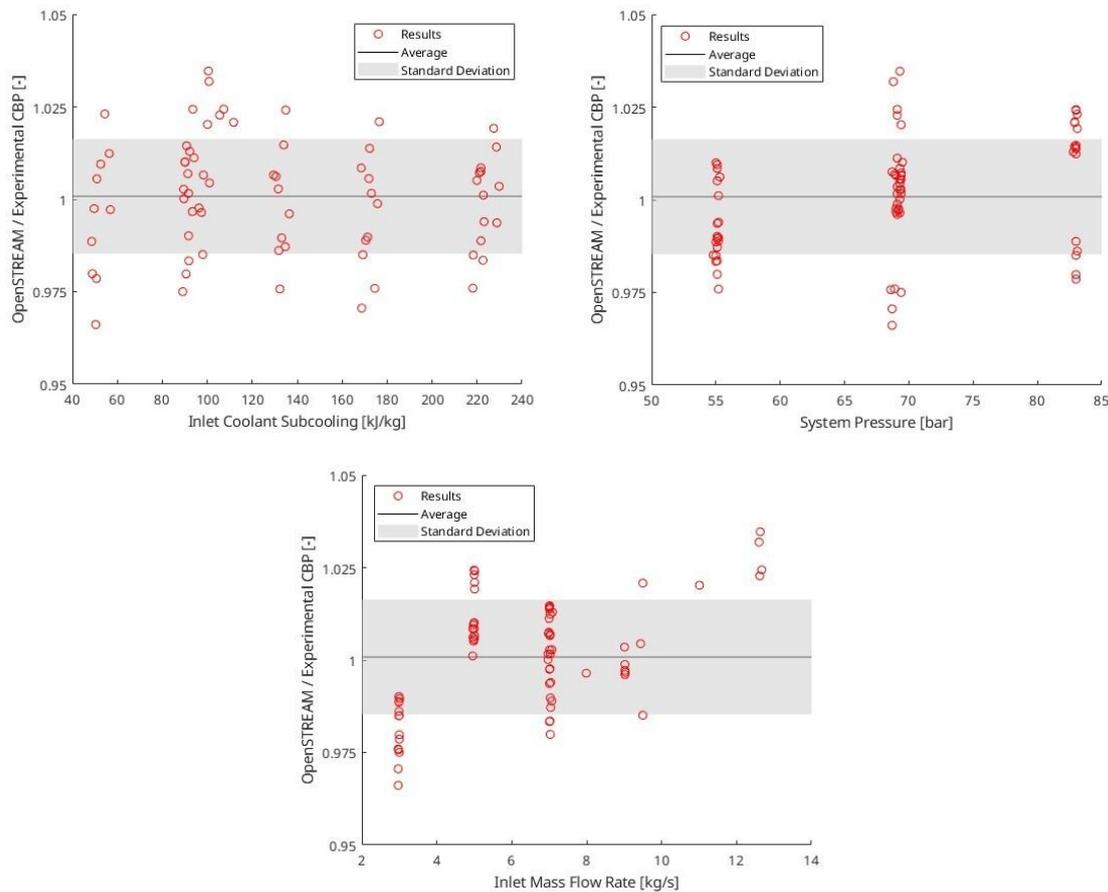
Figure 6. OpenSTREAM to experimental critical bundle power (CBP) ratio as a function of KATHY system parameters.
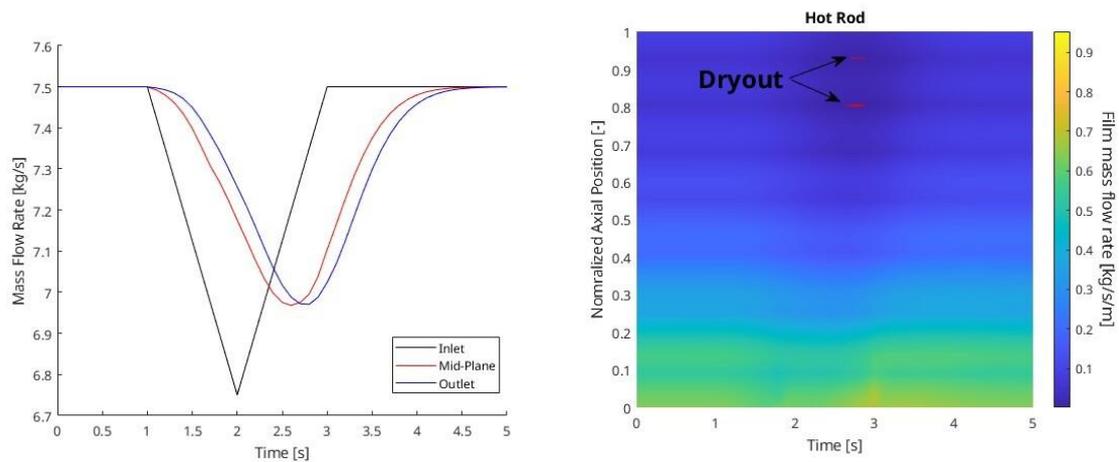
Another limitation of the results in Figure 5 is that the simulations are insensitive to dryout position. However, Figure 7a shows strong predictive capability of dryout elevation on the rod except for the tests where dryout occurred at TC 5Z. Here, the (-1) bin represents a test in which OpenSTREAM shows the lowest dryout occurring at TC (N)Z while experimental data showed dryout at TC (N-1)Z.   Figure 7b shows that when iterating the power until dryout occurs at the correct position, the resulting critical bundle power is nearly indistinguishable from Figure 5, except for the tests where dryout occurs at TC 5Z which have approximately 10% difference between experimental and OpenSTREAM critical bundle power. Even when enforcing dryout at the experimental position, OpenSTREAM shows comparable accuracy to the results from Duarte using TRACE V5.840 without considering axial position of dryout [10].
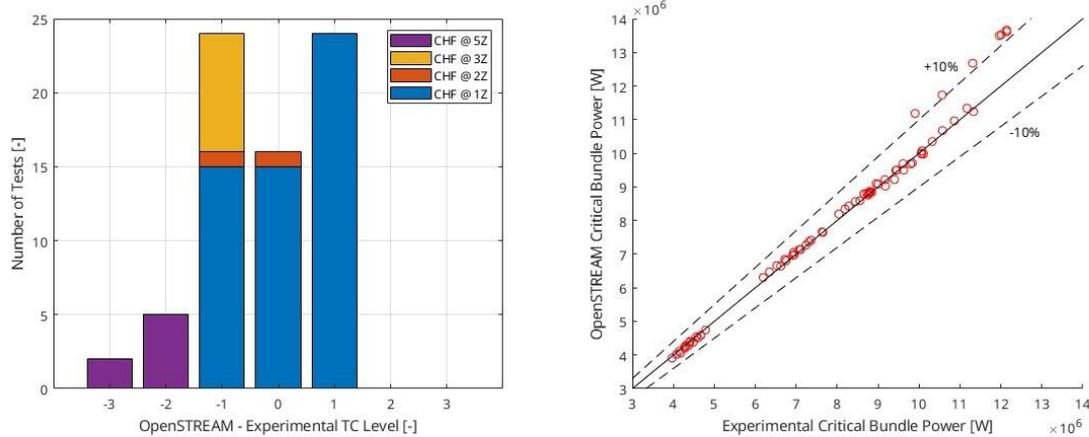
Figure 7. (left) Dryout position error histogram and (right) critical bundle power forcing lowest dryout position to match experimental data.

3.3. Transient Tests

Work on simulating the instability transients performed in the KATHY loop is ongoing. Preliminary analysis on solver kinetics, ability to predict transient dryout, and prediction of rewetting has been performed. A mock transient is run using constant power and variable mass flow rate as shown in Figure 8a. While there is no physical data to compare the results to, the output should provide intuitive results with physical meaning. The delay in mass flow downstream from the inlet is caused by a density wave due to increased void production upstream, inducing a delay in the local pressure drop [12] causing phenomena downstream to be out of phase with the inlet oscillations [10]. This is shown by the two dryout regions occurring around 2.5 seconds into the transient, even though the inlet mass flow is increasing at this time. Once this increase in mass flow reaches the dry region, the liquid film mass flow surpasses the dryout criterion and the rod is considered rewetted. The three-field parameters return to steady-state values identical to the beginning of the transient once the density wave has propagated through the entire channel, demonstrating the stability of the solver. The preliminary transient demonstrates the general capability of OpenSTREAM in simulating transient dryout and rewet cycles. Future work in transient modeling will include validation of the time delay caused by the density wave against experimental measurements, and simulation of KATHY instability tests with and without power feedback.

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Figure 8. Mock transient results showing (left) mass flow rate at various axial positions and (right) dryout and subsequent rewet at two locations on the hot rod.

3.4. Limitations

While the steady-state critical bundle power and preliminary transient simulation results are encouraging, there are some limitations in using a 1D approach for inherently 3D configurations such as rod bundles. The geometric smearing to accommodate a 1D approach can allow for increased field interactions that would be impossible due to proximity in the bundle. For example, the deposition mass flux is calculated based on the total droplet concentration in the bundle and appropriated to each wall based on its perimeter. The droplet concentration in a rod bundle will not be uniform, and will have a non-uniform radial, axial, and azimuthal distribution within the bundle based on the position of unheated channels, partial length rods, and peaking factors of specific rods, affecting the local deposition on any given rod. Another limitation of the 1D approach for steady-state critical bundle power is that only the rod with the highest power peaking factor will exhibit dryout, when even in the experimental data dryout was seen for multiple rods in the bundle, likely because of radial geometric smearing. As OpenSTREAM is designed for test section geometries with limited 3D effects, its application to complex 3D systems is limited, but can provide knowledge about some physics of the system without requiring computationally expensive simulations to resolve the 3D phenomena.

4. CONCLUSIONS

The OpenSTREAM computational environment can model the KATHY loop rod bundle geometry using a simplified three-wall approach. Validation of the flow predictions was performed by comparing differential pressure across the channel for steady-state single and two-phase flows. The application of a spacer grid deposition enhancement model provided excellent agreement for critical bundle power to achieve dryout. Further investigation demonstrated similar agreement of critical bundle power even when enforcing dryout at the correct position. The tests with dryout at TC 5Z showed a 13% deviation from experimental bundle power. Analysis of the deposition enhancement tuning factor revealed that it was insensitive to all system parameters except for mass flow rate, which biased the tuning factor due to the limited spread of data. This result may be due to the inherent simplicity of the deposition enhancement model. There is a need for improved models to be developed based on droplet velocity (i.e., time) instead of relative position. Using this validated steady-state model, a transient simulation

was performed which showed mass flow time delays in the channel caused by the density wave, and dryout and rewet at two locations on the hot rod. These results are encouraging for future application of the OpenSTREAM to model transient instability, such as dryout and rewet cycles like those captured in experiments performed using the KATHY loop.

NOMENCLATURE

f_i	Interfacial friction factor [-]
J	Superficial velocity [m/s]
m	Mass flux [kg/s/m^2]
n	Empirical constant
z	Axial coordinate [m]

Greek

δ	Liquid film thickness [m]
π	Non-dimensional entrainment number [-]
ρ	Density
σ	Surface tension [N/m]

Subscripts

dep	Deposition
enh	Enhancement
ent	Entrainment
g	Gas
l	Liquid

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