Simulation of nucleate boiling under ANSYS-FLUENT code by using RPI model coupling with artificial neural networks (Postprint)

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Abstract

The present study is to develop a new user-defined function using artificial neural networks intent Computational Fluid Dynamics (CFD) simulation for the prediction of water-vapor multiphase flows through fuel assemblies of nuclear reactor. Indeed, the provision of accurate material data especially for water and steam over a wider range of temperatures and pressures is an essential requirement for conducting CFD simulations in nuclear engineering thermal hydraulics. Contrary to the commercial CFD solver ANSYS-CFX, where the industrial standard IAPWS-IF97 (International Association for the Properties of Water and Steam-Industrial Formulation 1997) is implemented in the ANSYS-CFX internal material database, the solver ANSYS-FLUENT provides only the possibility to use equation of state (EOS), like ideal gas law, Redlich-Kwong EOS and piecewise polynomial interpolations. For that purpose, new approach is used to implement the thermophysical properties of water and steam for subcooled water in CFD solver ANSYS-FLUENT. The technique is based on artificial neural networks of multi-layer type to accurately predict 10 thermodynamic and transport properties of the density, specific heat, dynamic viscosity, thermal conductivity and speed of sound on saturated liquid and saturated vapor. Temperature is used as single input parameter, the maximum absolute error predicted by the artificial neural networks ANNs, was around 3%. Thus, the numerical investigation under CFD solver ANSYS-FLUENT becomes competitive with other CFD codes of which ANSYS-CFX in this area. In fact, the coupling of the Rensselaer Polytechnical Institute (RPI) wall boiling model and the developed Neural-UDF (User Defined Function) was found to be useful in predicting the vapor volume fraction in subcooled boiling flow.

Full Text

Preamble

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Simulation of Nucleate Boiling under ANSYS-FLUENT Code by Using RPI Model Coupling with Artificial Neural Networks

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The present study develops a new user-defined function using artificial neural networks for Computational Fluid Dynamics (CFD) simulation of water-vapor multiphase flows through fuel assemblies of nuclear reactors. Accurate material data, especially for water and steam over a wide range of temperatures and pressures, is an essential requirement for conducting CFD simulations in nuclear engineering thermal hydraulics. Contrary to the commercial CFD solver ANSYS-CFX, where the industrial standard IAPWS-IF97 (International Association for the Properties of Water and Steam-Industrial Formulation 1997) is implemented in its internal material database, the solver ANSYS-FLUENT provides only basic equations of state (EOS), such as ideal gas law, Redlich-Kwong EOS, and piecewise polynomial interpolations. To address this limitation, a new approach is implemented to incorporate the thermophysical properties of water and steam for subcooled water in the CFD solver ANSYS-FLUENT. The technique employs multi-layer artificial neural networks to accurately predict ten thermodynamic and transport properties: density, specific heat, dynamic viscosity, thermal conductivity, and speed of sound for both saturated liquid and saturated vapor. Temperature is used as the single input parameter, and the maximum absolute error predicted by the artificial neural networks (ANNs) was approximately 3%. Thus, numerical investigation using the CFD solver ANSYS-FLUENT becomes competitive with other CFD codes, including ANSYS-CFX, in this area. The coupling of the Rensselaer Polytechnical Institute (RPI) wall boiling model with the developed Neural-UDF (User Defined Function) was found to be useful in predicting the vapor volume fraction in subcooled boiling flow.

Keywords: User defined function (UDF), Computational fluid dynamics, IAPWS-IF97, ANSYS-FLUENT, Multilayer perceptron (MLP), Rensselaer Polytechnical Institute

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Introduction

The present study investigates artificial neural network support for nucleate boiling simulation, focusing on numerical simulations of preconditioned two-phase flows in a circular tube with a heated wall under pressurized conditions. Computational fluid dynamic techniques show increasing promise for simulating subcooled nucleate boiling [1]. The commercial Computational Fluid Dynamics (CFD) solver ANSYS-FLUENT is employed as the computational platform, and the Eulerian method in combination with the RPI boiling model is used, where the phases are assumed to be interpenetrating continua. This model represents the most general and complex of all multiphase flow models. The advantage of ANSYS-FLUENT lies in its variety of turbulent models adapted to special cases, while CFX has traditionally been the preferred code for turbomachinery applications.

Contributions are made toward an improved flow boiling model under Pressurized Water Reactor (PWR) conditions by conducting detailed CFD analyses based on experimental data of void distributions in heated tubes. When a heated surface exceeds the saturation temperature of the surrounding coolant, boiling on the surface becomes possible. Bubbles formed on the heated surface depart and are transported by the bulk fluid, creating a two-phase flow condition. Depending on the degree of subcooling and the length of the heated tube, the bubbles may or may not condense and collapse prior to exiting the tube. In subcooled boiling, this process results in further heating of the fluid toward the saturation temperature, while in saturated or bulk boiling, bubbles can be transported along the entire length of the heated tube without collapsing [2].

In the Rensselaer Polytechnical Institute (RPI) wall boiling model or heat partitioning model, implemented in ANSYS-FLUENT version 14.5.0, the overall heat flux from the heated wall to the two-phase flow includes convective, quenching, and evaporation heat flux components. Furthermore, the heat flux partitioning model associates each heat flux contribution with a dimensionless wall area ratio to define the relative contributions [1]. A critical aspect is the knowledge and understanding of fluid behavior during heat transfer, with the thermophysical properties of water and steam representing the fundamental properties that govern this process [3].

Several approaches exist for determining thermodynamic and transport properties, including different state equations and approximation functions. In the early 1990s, the development of safety analysis codes for nuclear facilities boosted research on accuracy and expanded the range of water and steam properties. Subsequently, new IAPWS standards leveraged data and technological advances to create new formulations of thermodynamic properties [4].

Artificial neural networks are being extensively used to predict the ten thermodynamic and transport properties mentioned above. An artificial neural network (ANN) is an advanced mathematical tool that determines network output based on available experimental information and provides mathematical function ap-

proximation for both linear and nonlinear systems [3, 5].

Gibbs phase rule allows one to determine the number of degrees of freedom or variance of a system, which is useful for interpreting phase diagrams. According to this rule, $F = C - p + 2$, where F is the number of degrees of freedom, C is the number of chemical components, and p is the number of phases in the system. The number two is specified because this formulation assumes that both pressure and temperature can be varied [6]. According to this equation, in the two-phase region corresponding to the saturation curve in the $(p - T)$ diagram, the thermodynamic properties of water and steam depend on a single state variable—temperature in our case. The prediction range is valid along the entire vapor-liquid saturation line from 273.15 K to the critical temperature T_c, i.e., $273.150\,\mathrm{K} \leq T \leq 647.096\,\mathrm{K}$ [4].

The neural network training is carried out by presenting a series of input data and target output values using an experimental database covering the entire range of validity, where temperature is the single input parameter [4, 7-11].

II. Artificial Neural Networks Approach

Neural networks operate as a black box model requiring no detailed information about the system. They represent an advanced mathematical modeling procedure inspired by biological neuron systems. The ANN approach appears particularly suitable for problems where relationships between variables are nonlinear and complex. In a multi-layer structure (Fig. 1 [Figure 1: see original paper]), neurons are grouped into layers: an input neuron layer, an output neuron layer, and one or more hidden layers composed of many interconnected neurons.

Fig. 1. (Color online) Structure of the ANN.

The normalization of values is a crucial step in ANNs. Input values may differ by several orders of magnitude, which may not reflect the relative importance of the inputs in determining outlet thermophysical and transport properties. To address this, input data are normalized within the range of $[-1, 1]$ using a mapminmax algorithm, while output variables are normalized by a log function [12]. The normalization equation is given by:

$$y = \frac{(y_{\max} - y_{\min})(x - x_{\min})}{x_{\max} - x_{\min}} + y_{\min}$$

After examining numerous differently structured neural networks, the selected ANN architecture features a single hidden layer with 20 neurons and an output layer with 10 neurons. The hidden layer uses a tansig transfer function, while the output layer employs a purelin transfer function. The typical ANN structure is shown in Fig. 1, with a single input variable (T: temperature) and ten thermodynamic and transport properties as output variables: density, specific

heat, dynamic viscosity, thermal conductivity, and speed of sound for both saturated liquid and saturated vapor.

Each neuron sums the product of connection weights (w_{jk}) from neuron (j) to neuron (k) and the input (x_j), plus an additional bias weight to obtain the neuron' s sum value. The ith neuron has a summer that gathers its weighted input $w_{ij} \cdot x_j$ and bias b_i to form its net input P_i:

$$P_i = \sum w_{ij} x_j - b_i$$

where w_{ij} denotes the strength of connection from the jth input to the ith neuron, x_j is the input vector, and b_i is the ith neuron bias. An activation function $F(P_i)$, specifically the sigmoid function, calculates the neuron output given the set of inputs. To find suitable weights and biases for each neuron, a training process is essential as the first step in building an ANN. Training involves correcting the weights to produce prespecified target values (known from experiments), requiring sets of input-target pairs (X_S, Y_S). After successful training, the network should provide correct predictions for any new input X according to ANN model fundamentals, with better results obtained using more training data.

The most widely used training method for multilayered neural networks is back propagation, with the Levenberg-Marquardt (LM) algorithm applied as it is considered the most efficient in terms of speed and memory usage [13].

The dataset used in the ANN consists of 377 observations divided into three sections: a training set (275 data points), a test set (53 data points), and a validation set (49 data points). These subsets are obtained by selecting 72% of the dataset for training, 14% for testing, and 14% for validation.

Differences between observed and predicted values are filtered back through the system to adjust connections between layers, thereby improving performance. The root mean square error (RMSE) coefficient serves as the primary criterion for evaluating ANN performance, defined as:

$$\mathrm{RMSE} = \sqrt{\sum (y_i - y_t)^2}$$

The statistical quality of the ANN for training, test, and validation sets is evaluated using the squared correlation coefficient R, absolute error AE, and average absolute error AAE:

$$R = \frac{\sum (y_i - y_0)(y_t - y_0)}{\sqrt{\sum (y_i - y_0)^2 \sum (y_t - y_0)^2}}$$

$$AE_i = \left| \frac{|y_t| - |y_i|}{|y_t|} \right| \times 100$$

$$\mathrm{AAE} = \frac{\sum |y_i - y_t|}{n}$$

where y_i represents the ith trained, test, or validation output value, y_t is the corresponding target value, and n is the number of input vectors. The results are summarized in Table 1 .

Observed and predicted breakthrough curves (dynamic viscosity on saturated vapor as an example) shown in Fig. 2 [Figure 2: see original paper] indicate that the ANN describes the experimental data well.

Based on the modeling performance, the general model obtained from the ANN for all water and steam properties was implemented in a UDF that was compiled and hooked into the ANSYS-FLUENT solver. Figure 3 [Figure 3: see original paper] shows the incorporation of the UDF into the solver for a group of eight properties (density, dynamic viscosity, thermal conductivity, and speed of sound for saturated liquid and saturated vapor) and a group of two properties (specific heat for saturated liquid and saturated vapor). The UDF, written in C++, is a routine that can be dynamically linked with the FLUENT solver and programmed by the user.

Fig. 2. (Color online) Comparison of target and ANN predicted values for dynamic viscosity on saturated vapor at operating pressure of 4.5 MPa.

III. CFD Calculations with Developed UDF

A. Benchmark Case

The proposed benchmark exercise, experimentally studied by Bartolemei and Chanturiya [14], involves upward flow of subcooled water through a heated vertical tube of $\Phi 15.4\,\mathrm{m} \times 2\,\mathrm{m}$. The subcooled water enters from the bottom with a subcooling of 58.2 K and travels upward through the tube. A uniform heat flux of $0.57\,\mathrm{MW/m^2}$ is applied to the tube surface, and the inlet mass flux is $900\,\mathrm{kg/(m^2 s)}$. Available experimental data include temperatures along the tube wall and axis, bulk liquid temperature, and cross-sectionally averaged vapor volume fraction along the tube. The wall boiling occurs in the nucleate boiling regime [15, 16].

A parametric study is performed to investigate the effect of the developed UDF, as summarized in Table 2 .

B. Wall Boiling Model

In nucleate subcooled boiling within a heated tube, wall heat is partially used to form bubbles while the remaining portion is transferred to the liquid. Heat transfer from the wall in the vicinity of a nucleation site occurs during two distinct periods: the bubble growth time and the waiting time. According to

the RPI model, the total heat flux from a wall to liquid is partitioned into three parts [2, 17]:

$$\dot{q}_{\text{wall}} = \dot{q}_C + \dot{q}_Q + \dot{q}_E$$

where $\dot{q}_C$ is the single-phase convective heat flux, $\dot{q}_Q$ is the quenching heat flux transferred to the liquid phase during the waiting time, and $\dot{q}_E$ is the heat flux associated with phase change (evaporation).

The convective heat flux is calculated as:

$$\dot{q}_C = h_c(T_w - T_l)(1 - A_b)$$

where h_c is the liquid phase heat transfer coefficient, T_w and T_l are the wall and liquid temperatures near the wall, respectively, and A_b is the portion covered by nucleation bubbles.

The quenching heat flux is given by:

$$\dot{q}_Q = \frac{2k_l}{\sqrt{\pi\lambda_l T}}(T_w - T_l)A_b$$

where k_l and λ_l are the heat conductivity and diffusivity in the liquid phase, and T is the period of bubble detachment.

The evaporation heat flux is:

$$\dot{q}_E = V_d N_w \rho_v h_{fv} f$$

where V_d is the bubble volume based on the bubble departure diameter, N_w is the active nucleate site density, ρ_v is the vapor density, h_{fv} is the latent heat of evaporation, and f is the frequency of bubble departure.

Equations (9)-(12) require closure parameters with empirical relationships for frequency of bubble departure, bubble departure diameter, nucleate site density, etc.

C. UDF-RPI Model Validation

As the problem formulation is axisymmetric, the simulated domain is only a 2D slice with width equal to the tube radius. The code manual recommends using a quadrilateral computational mesh for the Eulerian multiphase model. After several attempts to identify optimal computational meshes, a grid with 80 uniform radial elements and 1000 uniform axial elements was adopted, with finer mesh density in the contact region near the heated wall to provide better distribution of local flow parameters and achieve stable solutions.

To ensure fully-developed velocity magnitude and turbulence quantity profiles at the inlet, outlet profiles from a simulated flow field without boiling (single-phase) are used as inlet information for the boiling (multiphase) simulation.

The Eulerian-RPI method, which enables modeling of multiple separate yet interacting phases in FLUENT, is employed to predict the distribution of local flow parameters: vapor volume fraction, bubble diameter, and liquid temperature. Turbulence phenomena are described by a classical Re-Normalization Group (RNG) k-ε model combined with enhanced wall treatment for near-wall regions. A y^+ value of 5 is considered reasonable for the selected enhanced wall treatment approach. Table 3 provides a detailed list of input parameters, while Table 4 lists the boiling model correlations used in the benchmark case [18].

The saturation temperature at the selected pressure is 530.55 K. The subcooled flow boiling model assumes water properties vary with temperature, which is technically implemented through the developed UDF—the primary aim of this work.

The governing equations are nonlinear and require several iteration loops before a convergent solution is obtained. For numerical accuracy, a first-order upwind scheme is used for spatial discretization of the governing equations. As the numerical scheme is coupled with volume fractions, a low Courant number of 10 can be used to achieve faster convergence.

IV. Results and Discussion

To validate the proposed UDF in conjunction with the RPI wall boiling model, comparisons were made among the RPI model, the RPI+UDF model, and experimental data from Bartolomei and Chanturiya for a heated vertical tube at 4.5 MPa [14].

Both models were run with solution-dependent material properties defined as piecewise-linear functions of temperature using two data points at 473.15 K and 543.15 K. Figure 5 Figure 5: see original paper shows that the proposed UDF-RPI axial vapor volume fraction distribution agrees well with experimental data [14]. Similarly, the liquid temperature profile along the tube shows good agreement. Figure 5(b) demonstrates that the proposed UDF-RPI model is in good agreement with experimentally measured axial liquid temperature distributions, validating the predictions against experimental data.

Parallel to examining axial profiles of vapor volume fraction and liquid temperature, the radial distribution at various axial locations along the tube was evaluated. Figure 6 [Figure 6: see original paper] shows radial profiles of vapor volume fraction and liquid temperature at five locations for the proposed UDF in conjunction with the RPI wall boiling model [19].

In Fig. 6(a), boiling is concentrated near the heated wall for the flow regime considered. The vapor volume fraction is substantially higher adjacent to the

wall and decreases toward the center. Radial temperature profiles at five locations are shown in Fig. 6(b), revealing significant thermal non-equilibrium. Large temperature differences exist between the center and wall of the pipe at $z = 1.1\,\mathrm{m}$, where bubble production begins near the wall while the center temperature remains below saturation. Non-equilibrium conditions decrease along the pipe, with a radially uniform temperature distribution reached around $z = 1.7\,\mathrm{m}$.

Based on these comparisons, it is clear that the UDF in conjunction with the RPI wall boiling model, based on artificial neural networks, produces reasonable results. This demonstrates that the strong non-linearity of water and steam thermophysical properties often requires polynomial interpolations for defining solution-dependent material properties, which makes the difference between the two models when compared to the experimental data of Bartolomei and Chanturiya, as shown in Fig. 5.

V. Conclusion

This work focuses on the numerical study of nucleate subcooled boiling in a heated tube using the RPI wall boiling model implemented in ANSYS-FLUENT version 14.5.0, in conjunction with a developed UDF based on artificial neural networks that calculates thermodynamic and transport properties for saturated liquid and saturated vapor of water as functions of temperature. Validation was performed using experimental data under baseline case conditions. The results demonstrate that the RPI Neural-UDF method can reasonably predict vapor volume fraction distributions and liquid temperature profiles in heated vertical tubes. The computed profiles of vapor volume fraction and liquid temperature show good agreement with available experiments. It should be noted that the maximum absolute error predicted by the artificial neural networks is approximately 3%. The ANN model exhibited great potential in predicting water and steam properties with the highest R and lowest RMSE values.

The developed UDF provides a simple and fast method to calculate water and steam properties as functions of temperature, and the present model correctly represents nucleate boiling under pressurized conditions.

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Note: Figure translations are in progress. See original paper for figures.