Application of Jacobian-Free Newton-Krylov Method in Implicitly Solving Two-Fluid Six-Equation Two-phase Flow Problems: Implementation, Validation and Benchmark

Ling Zou¹, Haihua Zhao, and Hongbin Zhang

Idaho National Laboratory, P.O. Box 1625, Idaho Falls, ID 83415-3870, USA

ABSTRACT

This work represents a first-of-its-kind successful application to employ advanced numerical methods in solving realistic two-phase flow problems with two-fluid six-equation two-phase flow model. These advanced numerical methods include high-resolution spatial discretization scheme with staggered grids, (high-order) fully implicit time integration schemes, and Jacobian-free Newton-Krylov (JFNK) method as the nonlinear solver. The computer code developed in this work has been extensively validated with existing experimental flow boiling data in vertical pipes and rod bundles, which cover wide ranges of experimental conditions, such as pressure, inlet mass flux, wall heat flux, exit void fraction, etc. Additional code-to-code benchmark with the RELAP5-3D code further verifies the correct code implementation. The combined methods employed in this work exhibit strong robustness in solving two-phase flow problems even when phase appearance (boiling) and realistic discrete flow regimes are considered. Transitional flow regimes used in existing system analysis codes, normally introduced to overcome numerical difficulty, were completely removed in this work. This in turn provides the possibility to utilize more sophisticated flow regime maps in the future to further improve simulation accuracy.

Keywords: Two-fluid model, fully implicit method, high-resolution spatial scheme, Jacobian-free Newton-Krylov method, validation

1. INTRODUCTION

In nuclear thermal-hydraulics, two-phase flow is an important phenomenon closely related to the normal operations and accident conditions of nuclear reactors. Accurate modeling and simulation of two-phase flow phenomena are critical to the safety analysis of nuclear reactors. During the past four decades, reactor system analysis codes, such as RELAP5 (U.S. NRC, 2001a) and TRAC (U.S. NRC, 2001b), were developed and gained worldwide success to support such safety

¹ Corresponding author, Email: ling.zou@inl.gov

analysis. These codes, most of which were originally developed in the mid- to late 1970s, are constrained with low (first) order numerical methods to solve the one-dimensional, two-phase flow equations in a reactor system. The disadvantages of using low-order numerical methods have long been recognized in the nuclear thermal-hydraulics field. It is understood that the commonly used semi-implicit time integration method introduces first-order numerical errors in time from the operator-splitting process, and it is subject to the material Courant-Friedrichs-Lewy (CFL) stability limit. Although more implicit methods, such as the Nearly-Implicit Scheme in RELAP5 (Idaho National Laboratory, 2012a), had been developed and can violate the CFL limit, these methods are still of the first order accuracy and are only suitable for slow transients. First-order upwind method is generally used in existing codes for its simplicity, stableness, and ability to preserve monotonicity. However, these schemes are highly diffusive and not always desirable in many applications.

In the past, there have been only limited attempts to investigate advanced numerical schemes to improve such a situation in the nuclear reactor thermal-hydraulics field, due to the very complex nature of two-phase flow problems encountered in nuclear reactor system analyses. The majority of these attempts also only addressed temporal or spatial schemes separately. More importantly, realistic closure correlations have rarely been considered in any of the existing work. This section provides a brief review on these attempts to introduce high-resolution spatial scheme and/or fully implicit methods in thermal-hydraulics research. High-resolution spatial discretization schemes are well accepted in the research field of computational fluid dynamics. These schemes are able to maintain higher-order accuracy in smooth regions while nonphysical spatial oscillations are removed or significantly reduced near discontinuities. Although they are widely used in computational fluid dynamics studies, they have only been applied in a few applications in reactor thermal-hydraulics. In addition, most of these work use explicit time integration schemes (Tiselj and Petelin, 1997; Munkejord, 2006; Macián-Juan, 1996; Bertolotto et al., 2011), or semi-implicit schemes already implemented in existing system analysis codes (Idaho National Laboratory, 2012a; Wang, 2012; Wang, 2013), and many of them are limited to solve the scalar transport equation only (Idaho National Laboratory, 2012a; Macián-Juan, 1996; Bertolotto et al., 2011). Fully implicit methods are not commonly seen in reactor safety analysis codes, with CATHARE (Bestion, 1990; Barre et al., 1992) as one of the rare exceptions. Attempts to apply Newton's method in solving fully implicit two-phase flow problems can be found in Frepoli's (Frepoli et al., 2003) and Abu Saleem's work (Abu Saleem and Kozlowski, 2014). It is noted that high-resolution spatial discretization scheme was also used in Abu Saleem's work (Abu Saleem

and Kozłowski, 2014), and promising results were obtained for simple cases. In recent years, the Jacobian-free Newton-Krylov method (Knoll and Keyes, 2004) has gained increasing interest in solving large nonlinear systems. In two-phase flow simulations, Mousseau did pioneering work (Mousseau, 2004, 2005, 2006) to use such a method to solve two-phase flow problems implicitly. All Mousseau's work, however, was focused on a first-order upwind spatial discretization scheme, and only highly simplified closure correlations were considered. A recent work to apply the JFNK method in solving simplified two-phase phenomenological flow problems was also done by Ashrafizadeh et al. (Ashrafizadeh et al., 2015), however with only limited success. From this review, it reveals a fact that there is a lack of a systematic study on combining these advanced numerical schemes in applications of thermal-hydraulics codes with realistic closure models.

In our previous work (Zou et al., 2015a, 2015b, 2015c, 2015d, 2015e, 2016), a systematic study was launched to investigate the aforementioned advanced numerical methods in applications of solving two-phase flow problems interested to nuclear reactor thermal-hydraulics. These advanced numerical schemes include: 1) high-resolution spatial discretization scheme with staggered grids in order to improve the spatial accuracy; 2) (high-order) fully implicit time integration schemes in order to allow for large time steps to be used, to improve the temporal accuracy, and to improve code robustness; and 3) advanced solving method, namely, the JFNK method, to efficiently solve the highly nonlinear system. Even each of these individual methods had been investigated by other authors, our successful application of combining all these methods together in solving one-dimensional single-phase and two-phase flow problems represents the original contribution. In our previous work (Zou et al., 2015a, 2015b), these methods were applied to solve two-phase flow problems using a simplified four-equation two-phase flow model without interfacial interaction being considered. It was proved that these schemes are able to provide higher order of numerical accuracy for two-phase flow problems. A series of previous studies (Zou et al., 2015c, 2015d, 2015e) have also been carried out to investigate these methods in implicitly solving phase appearance and disappearance problems commonly encountered in two-phase flow simulations. Proper numerical treatment methods have been proposed in our previous work, which successfully resolved this serious numerical challenge in two-phase flow simulations. We also made a successful attempt to introduce realistic two-phase flow closure correlations in two-phase flow simulations, however it is limited to use a four-equation drift flux model (Zou et al., 2016).

Building upon our previous successes, this paper extends these methods in solving one-dimensional two-phase flow problems interested in reactor thermal-hydraulics, using the well accepted two-fluid six-equation two-phase flow model and with realistic closure correlations. The work presented in this paper represents a successful implementation of such an extension, the first of its kind. In section 2, the commonly used two-fluid two-phase flow model along with realistic closure correlations, are reviewed. In section 3, numerical methods used in this work are discussed in details. In section 4, numerical simulations and results are presented for flow boiling in pipes and rod bundles. These results are validated using the existing experimental data, and also benchmarked with code-to-code comparison with the RELAP5-3D code. Discussions and conclusions are presented in section 5.

2. TWO-FLUID TWO-PHASE FLOW MODEL

The equations of the two-fluid single pressure two-phase flow six-equation model used in this work are almost identical to those commonly used in existing nuclear reactor system analysis codes, such as RELAP5 (U.S. NRC, 2001a), TRAC (U.S. NRC, 2001b), and CATHARE (Bestion, 1990). For simplicity, additional terms, such as the virtual mass term used in the RELAP5 code (U.S. NRC, 2001a), are not included in this current work. The six-equation system includes a set of continuity, momentum and energy equations for each phase, which are summarized as,

$$\frac{\partial(\alpha_l \rho_l)}{\partial t} + \frac{\partial(\alpha_l \rho_l u_l)}{\partial x} = -\Gamma_g \quad (1)$$

$$\frac{\partial(\alpha_g \rho_g)}{\partial t} + \frac{\partial(\alpha_g \rho_g u_g)}{\partial x} = \Gamma_g \quad (2)$$

$$\alpha_l \rho_l \frac{\partial u_l}{\partial t} + \alpha_l \rho_l u_l \frac{\partial u_l}{\partial x} + \alpha_l \frac{\partial p}{\partial x} - \alpha_l \rho_l g_x - F_{int} + F_{wall,l} + \Gamma_g (u_{int} - u_l) = 0 \quad (3)$$

$$\alpha_g \rho_g \frac{\partial u_g}{\partial t} + \alpha_g \rho_g u_g \frac{\partial u_g}{\partial x} + \alpha_g \frac{\partial p}{\partial x} - \alpha_g \rho_g g_x + F_{int} + F_{wall,g} - \Gamma_g (u_{int} - u_g) = 0 \quad (4)$$

$$\frac{\partial(\alpha_l \rho_l e_l)}{\partial t} + \frac{\partial(\alpha_l \rho_l u_l e_l)}{\partial x} + p \frac{\partial \alpha_l}{\partial t} + p \frac{\partial(\alpha_l u_l)}{\partial x} - Q_{wl} - Q_{il} + \Gamma_g h_l^* + \Gamma_w h_l' = 0 \quad (5)$$

$$\frac{\partial(\alpha_g \rho_g e_g)}{\partial t} + \frac{\partial(\alpha_g \rho_g u_g e_g)}{\partial x} + p \frac{\partial \alpha_g}{\partial t} + p \frac{\partial(\alpha_g u_g)}{\partial x} - Q_{wg} - Q_{ig} - \Gamma_g h_g^* - \Gamma_w h_g' = 0 \quad (6)$$

in which, subscripts l and g denote the liquid phase and the gas phase, respectively; and subscript ‘ int ’ denotes interface. Γ_g is net vapor generation rate due to wall boiling/condensation (Γ_w), and bulk evaporation/condensation (Γ_{ig}). $F_{wall,l}$ and $F_{wall,g}$ are wall friction terms. Q_{wl} and Q_{wg} are wall-to-liquid and wall-to-gas phase heat transfer terms, respectively. Q_{il} and Q_{ig} are the interface-to-liquid and interface-to-gas phase heat transfer terms, respectively. h'_l and h'_g are phasic enthalpy carried by wall vapor generation term. h_l^* and h_g^* are phasic enthalpy carried by interfacial mass transfer term. All these parameters are explained in details in the following sections. The variables to be solved from this set of equations, in the vector form, are $\mathbf{U} = [p, \alpha_g, u_l, u_g, T_l, T_g]^T$, which are pressure, void fraction (volume fraction of the gas phase), liquid phase velocity, gas phase velocity, liquid phase temperature, and vapor phase temperature, respectively. It is noted that, $\alpha_l + \alpha_g = 1$. Additional closure correlations are summarized in the following subsections.

2.1 Flow regime map

The vertical two-phase flow regime map in the pre-CHF (critical heat flux) region concerned in this work, as shown in Figure 1, is almost identical to that used in RELAP5-3D (Idaho National Laboratory, 2012a), which includes bubbly flow, slug flow, annular mist flow, and mist flow pre-CHF in the two-phase flow region. Flow regime in each finite volume cell is determined by local geometry and thermal-hydraulics conditions, such as phasic densities, phasic velocities, pipe diameter, etc., which are documented in RELAP5-3D code manuals (Idaho National Laboratory, 2012a, 2012b). A major difference in the flow regime map used in this work, compared to RELAP5-3D (Idaho National Laboratory, 2012a) and TRAC (U.S. NRC, 2001b), is that a transition flow regime between the slug and annular mist flow regime is no longer needed. Such a transition flow regime normally serves for numerical stability purpose to avoid sudden changes in flow regime related parameters due to flow regime jump. In RELAP5-3D, the width of the transition flow regime between slug and annular mist flow is set as $\Delta\alpha = 0.05$ based on ‘engineering judgment’, see page 3-15 of RELAP5-3D code manual (Idaho National Laboratory, 2012b). In TRAC (U.S. NRC, 2001b), this transitional flow regime (interpolation region) width was set as large as 0.25 in void fraction. Such an approach was criticized for loss of accuracy; see for example on page 131 of Levy’s book (Levy, 1999). In this work, because of the strong stableness of the combined numerical methods, such a transition flow regime has been removed.

2.2 Wall heat transfer, wall boiling, and interfacial heat/mass transfer

For flow boiling conditions interested in this work, wall boiling with prescribed wall heat flux are considered. Under these conditions, wall heat flux partitioning into the liquid and the gas phase is rather simple. It is assumed that all the heat is added into the liquid phase, which will then be

used for wall boiling and to increase the liquid phase temperature. Under these assumptions, the wall heat flux terms in the liquid and gas phase energy equations become,

$$Q_{wl} = q''_w a_w \quad (7)$$

$$Q_{wg} = 0 \quad (8)$$

in which, q''_w is the prescribed wall heat flux on the wall, and a_w is the volumetric heating surface density.

For wall boiling condition, the net vapor generation rate, Γ_g term, is a result of wall boiling and bulk evaporation/condensation. Similar to RELAP5-3D (Idaho National Laboratory, 2012a), this term is modeled in two regions, the near wall region and bulk region, such that,

$$\Gamma_g = \Gamma_w + \Gamma_{ig} \quad (9)$$

in which, Γ_w and Γ_{ig} are the volumetric vapor generation rate in the near wall region and in bulk region, respectively. The near wall region volumetric vapor generation rate is determined by the method proposed by Lahey, combining with the Saha-Zuber correlation in determining the necessary conditions for net vapor generation, see section 4.7.1.1 of RELAP5-3D code manual (Idaho National Laboratory, 2012b),

$$\Gamma_w = \begin{cases} 0 & h_l < h_{cr} \\ \frac{q''_w a_w (h_l - h_{cr})}{(h_{l,sat} - h_{cr})(1 + \varepsilon_p) h_{fg}} & h_{cr} \leq h_l \leq h_{l,sat} \\ \frac{q''_w a_w}{h_{fg}} & h_l > h_{l,sat} \end{cases} \quad (10)$$

in which, ε_p is the pumping term and defined as,

$$\varepsilon_p = \frac{\rho_f [h_{l,sat} - \min(h_l, h_{f,sat})]}{\rho_g h_{fg}} \quad (11)$$

Similar to RELAP5-3D (Idaho National Laboratory, 2012a), the vapor generation rate (negative value for vapor condensation) due to interfacial heat transfer in the bulk region is modeled as,

$$\Gamma_{ig} = - \frac{H_{il}(T_{sat} - T_l) + H_{ig}(T_{sat} - T_g)}{h_g^* - h_l^*} \quad (12)$$

in which, H_{il} and H_{ig} are volumetric heat transfer coefficients of liquid-to-interface and gas-to-interface, respectively.

The interface heat transfer terms, Q_{il} and Q_{ig} , consist of two parts, interface heat transfer in the bulk and in the near wall region. For wall boiling conditions concerned in this work, the vapor-to-

interface heat transfer in the near wall region is assumed to be zero. The interface heat transfer terms and the bulk vapor condensation terms in the phasic energy equations can be manipulated to obtain,

$$Q_{il} = H_{il}(T_{sat} - T_l) - \Gamma_w(h'_g - h'_l) \quad (13)$$

and

$$Q_{ig} = H_{ig}(T_{sat} - T_g) \quad (14)$$

For more details, readers are referred to the RELAP5-3D manual (Idaho National Laboratory, 2012a), pages 3-10 to 3-14. Under wall boiling conditions, the phasic energy, h'_l and h'_g , carried by the wall vapor generation term in the phasic energy equations are defined as, $h'_l = h_l(p, T_l)$ and $h'_g = h_{g,sat}(p)$. The vapor generation rate in the bulk region is determined by the heat transfer between the two phases and the interface, which is assumed to be at the saturation condition. In subcooled flow boiling, bulk vapor phase condensation takes place, such that the phasic energies carried with the bulk vapor condensation term are defined as, $h_g^* = h_g(p, T_g)$ and $h_l^* = h_{l,sat}(p)$.

2.3 Interfacial momentum exchange

Interfacial momentum exchange consists of two terms, interfacial friction term and momentum exchange due to phase change. For interfacial drag term, we follow the same approach used in RELAP5-3D (Idaho National Laboratory, 2012a): drift flux model is used for vertical bubbly and slug flow regimes, and drag coefficient model is used in all other flow regimes. When drift flux model is used, the interfacial friction term is calculated as,

$$F_{int} = C_{int} u_R |u_R| \quad (15)$$

The interfacial drag coefficient and relative velocity are defined as,

$$C_{int} = \frac{\alpha_g \alpha_l^3 (\rho_l - \rho_g) g}{|V_{gj}| V_{gj}} \quad (16)$$

and

$$u_R = C_1 u_g - C_0 u_l \quad (17)$$

$$C_1 = \frac{1 - C_0 \alpha_g}{\alpha_l} \quad (18)$$

in which, V_{gj} is the weighted mean drift velocity, and C_0 is the distribution parameter. These two parameters are modeled using the EPRI drift flux model proposed by Chexal and Lellouche

(Chexal and Lellouche, 1986). When drag coefficient model is used, the interfacial friction is calculated as,

$$F_{int} = C_{int}(u_g - u_l)|u_g - u_l| \quad (19)$$

In this case, the interfacial drag coefficient is modeled as,

$$C_{int} = \frac{1}{8}\rho_c a_{gf} C_D \quad (20)$$

in which, ρ_c is density of the continuous phase, a_{gf} is interfacial area per unit volume, and C_D is drag coefficient. The details of modeling of these parameters can be found in Appendix 6A of RELAP5-3D code manual (Idaho National Laboratory, 2012b). There is also a major difference in the implementation of interfacial friction term in this work compared to RELAP5-3D, in which a linear interpolation was used between the drift flux model and drag coefficient model (see the discussions in the flow regime section). It is noted that such a linear interpolation is complex because of the different formulations, e.g. equations (15) and (19), used for these two flow regimes. In this work, such a transitional regime is eliminated and so is the complex linear interpolation.

For bulk vapor condensation conditions, the interfacial velocity, u_{int} , is defined as $u_{int} = u_l$ if $\Gamma_g \geq 0$, and $u_{int} = u_g$ if $\Gamma_g < 0$.

2.4 Wall friction

Closure correlations for the pressure drop due to wall friction are needed for both the single- and two-phase flows. Additional correlations are needed for the wall friction partitioning between the two phases in the two-phase flow region. The correlations used in this work are mainly based on those used in RELAP5-3D (Idaho National Laboratory, 2012a). The single-phase flow frictional factor is calculated in three flow regimes, laminar flow, turbulent flow and a transition region between these two. The two-phase flow frictional pressure drop is based on a two-phase multiplier approach:

$$\left(\frac{dp}{dx}\right)_{2\phi} = \phi_f^2 \left(\frac{dp}{dx}\right)_f = \phi_g^2 \left(\frac{dp}{dx}\right)_g \quad (21)$$

in which, ϕ_f and ϕ_g are the liquid-alone and vapor/gas-alone two-phase Darcy-Weisbach friction multipliers, respectively. Subscript ‘2 ϕ ’ denotes two-phase flow condition. The partitioning of wall friction in the two phases follows the same concept used in RELAP5-3D. More details of the implementations of frictional pressure drop can be found in Section 3.3.8 of RELAP5-3D code manual (Idaho National Laboratory, 2012b).

2.5 Water/steam properties

In the two-fluid two-phase flow model used in this work, both phases could be in stable or metastable state. Water/steam properties (such as phasic density and phasic specific internal energy) are provided as functions of pressure and phasic temperature. For example, the liquid phase density is obtained as,

$$\rho_l = \rho_l(p, T_l) \quad (22)$$

The water/steam properties used in this work are calculated by fast and accurate bilinear interpolations of the water/steam properties provided by the International Association for the Properties of Water and Steam (IAPWS). Water/steam properties are prepared in tables from the highly accurate yet expensive IAPWS function calls. When water/steam properties are needed, they are interpolated from the pre-prepared tables. The details of the implementations are documented in our previous work (Zou et al., 2014).

3. NUMERICAL AND SOLUTION METHODS

In this section, the advanced numerical methods used in this work are briefly discussed. These include: 1) a high-resolution spatial discretization scheme based on staggered grid mesh arrangement, 2) implicit time integration schemes, including BDF1 and BDF2, and 3) the JFNK method in solving the nonlinear equation system. An additional section will be devoted to describe a new numerical treatment scheme proposed in this work to overcome the numerical challenges associated with phase appearance and disappearance.

3.1 High-resolution spatial discretization with staggered grids

A high-resolution spatial discretization scheme based on staggered grids has been used in this work and in our previous work (Zou et al., 2015a, 2015b, 2015c, 2015d, 2015e; Zou et al., 2016). This section provides a brief review on this high-resolution scheme. For the staggered grid mesh arrangement, scalar variables (pressure, void fraction, phasic temperatures) are arranged at the cell centers, while vector variables (phasic velocities) are arranged at the cell edges, which are schematically shown in Figure 2. [The high-resolution spatial scheme is conceptually similar to the first-order upwind method widely used in the existing system analysis codes.](#) The key to achieve higher resolution in space is the local linear reconstruction of variables, which are then used to evaluate advection fluxes. Local linear reconstructions are done using a slope limiter, which provides higher order of spatial accuracy when solutions are smooth, and non-oscillation results when solutions contain discontinuities. [A schematic illustration of linear reconstruction of local variables is shown in Figure 3.](#) For demonstration purpose, using the gas phase mass

equation as an example, regardless whether the traditional first-order upwind method or high-resolution method is used, the advection term is semi-discretized as,

$$\left. \frac{\partial(\alpha_g \rho_g u_g)}{\partial x} \right|_i = \frac{1}{\Delta x} [(\alpha_g \rho_g u_g)_{i+1/2}^* - (\alpha_g \rho_g u_g)_{i-1/2}^*] \quad (23)$$

in which, $(\alpha_g \rho_g u_g)_{i\pm 1/2}^*$ is the numerically evaluated advection flux on cell edges. If the traditional first-order upwind method is used, it is evaluated as,

$$(\alpha_g \rho_g u_g)_{i+1/2}^* = u_{g,i+1/2} \begin{cases} \alpha_{g,i} \rho_g(p_i, T_{g,i}) & \text{if } u_{g,i+1/2} > 0 \\ \alpha_{g,i+1} \rho_g(p_{i+1}, T_{g,i+1}) & \text{otherwise} \end{cases} \quad (24)$$

On the contrary, the high-resolution discretization form of the gas phase mass flux on the cell edge is,

$$(\alpha_g \rho_g u_g)_{i+1/2}^* = u_{g,i+1/2} \begin{cases} \alpha_{g,i+1/2}^- \rho_g(p_{i+1/2}^-, T_{g,i+1/2}^-) & \text{if } u_{g,i+1/2} > 0 \\ \alpha_{g,i+1/2}^+ \rho_g(p_{i+1/2}^+, T_{g,i+1/2}^+) & \text{otherwise} \end{cases} \quad (25)$$

in which, $\alpha_{g,i+1/2}^\pm$, $p_{i+1/2}^\pm$, and $T_{g,i+1/2}^\pm$ are reconstructed void fraction, pressure, and gas phase temperature on cell edges, respectively. The linear reconstructions of local variables are performed using the slope limiter concept. As schematically shown in Figure 3, for the i^{th} finite volume cell, the reconstructed slope is,

$$\left(\frac{d\phi}{dx} \right)_i = \frac{\phi_{i+1} - \phi_i}{\Delta x} \eta(r) \quad (26)$$

in which, ϕ denotes the primitive variables, i.e., void fraction, pressure, temperature, and velocity; $\eta(r)$ is the limiter function; and $r = (\phi_i - \phi_{i-1})/(\phi_{i+1} - \phi_i)$ is the nonlinear indicator; and Δx is the mesh size. In this work, a symmetric Van Albada limiter function was used (Toro, 2009; Versteeg and Malalasekera, 2007),

$$\eta(r) = \begin{cases} \frac{r + r^2}{1 + r^2} & \text{if } r \geq 0 \\ 0 & \text{otherwise} \end{cases} \quad (27)$$

After the local slope is determined using equation (26), the reconstructed variables on cell edges can be obtained, using the left side of cell edge $i+1/2$ as an example in the following:

$$\phi_{i+1/2}^- = \phi_i + \frac{\Delta x}{2} \left(\frac{d\phi}{dx} \right)_i \quad (28)$$

The advection terms in both momentum equations are discretized slightly differently due to their primitive forms. Again, using the gas phase momentum equation as an example, the high-resolution version of the discretized advection term is formulated as,

$$\left(\alpha_g \rho_g u_g \frac{\partial u_g}{\partial x} \right)_{i+1/2} = \frac{\bar{\alpha}_{g,i+1/2} \bar{\rho}_{g,i+1/2} u_{g,i+1/2}}{\Delta x} \begin{cases} u_{g,i+1}^- - u_{g,i}^- & \text{if } u_{g,i+1/2} > 0 \\ u_{g,i+1}^+ - u_{g,i}^+ & \text{otherwise} \end{cases} \quad (29)$$

in which, $\bar{\alpha}$ and $\bar{\rho}$ are edge average values based on its two adjacent cells; $u_g^\pm$ is the linearly reconstructed variables similarly defined in equation (28). For both the first-order and the high-resolution spatial discretization schemes, the pressure gradient term is discretized using the central difference method. The $\partial(\alpha u)/\partial x$ terms in energy equations are treated similarly to the advection terms.

3.2 Time integration scheme

Two fully implicit time-integration schemes, a first order Backward Euler (BDF1) and a second order BDF2 scheme, have been implemented in this work. For the first order BDF1 scheme, using liquid phase mass equation as an example, the transient terms are simply discretized as,

$$\left. \frac{\partial(\alpha_l \rho_l)}{\partial t} \right|_i = \frac{\alpha_{l,i}^{n+1} \rho_{l,i}^{n+1} - \alpha_{l,i}^n \rho_{l,i}^n}{\Delta t} \quad (30)$$

in which, superscript ‘ n ’ and ‘ $n+1$ ’ denote the old and current time step, respectively. The $p \partial \alpha / \partial t$ term is discretized as,

$$p \left. \frac{\partial \alpha_g}{\partial t} \right|_i = p_i^{n+1/2} \frac{\alpha_{g,i}^{n+1} - \alpha_{g,i}^n}{\Delta t} \quad (31)$$

in which,

$$p_i^{n+1/2} = \frac{1}{2} (p_i^{n+1} + p_i^n) \quad (32)$$

When the BDF2 scheme is used, the transient terms are simply discretized as (still using liquid phase mass equation as an example),

$$\left. \frac{\partial(\alpha_l \rho_l)}{\partial t} \right|_i = \frac{\alpha_{l,i}^{n+1} \rho_{l,i}^{n+1} - \frac{4}{3} \alpha_{l,i}^n \rho_{l,i}^n + \frac{1}{3} \alpha_{l,i}^{n-1} \rho_{l,i}^{n-1}}{\Delta t} \quad (33)$$

in which, superscript ‘ $n-1$ ’ denote an old-old time step. The $p \partial \alpha / \partial t$ term is discretized as,

$$p \frac{\partial \alpha_g}{\partial t} \Big|_i = p_i^{n+1} \frac{\alpha_{g,i}^{n+1} - \frac{4}{3} \alpha_{g,i}^n + \frac{1}{3} \alpha_{g,i}^{n-1}}{\Delta t} \quad (34)$$

3.3 Summary of discretized forms

This section gives a brief summary of the discretized forms of the two-phase flow equation system, using BDF1 time integration scheme. Replacing BDF1 scheme with BDF2 scheme would be straightforward. Discretized equations are shown as following,

$$\frac{\alpha_{l,i}^{n+1} \rho_{l,i}^{n+1} - \alpha_{l,i}^n \rho_{l,i}^n}{\Delta t} + \frac{1}{\Delta x} [(\alpha_l \rho_l u_l)_{i+1/2}^{n+1,*} - (\alpha_l \rho_l u_l)_{i-1/2}^{n+1,*}] + \Gamma_{g,i}^{n+1} = 0 \quad (35)$$

$$\frac{\alpha_{g,i}^{n+1} \rho_{g,i}^{n+1} - \alpha_{g,i}^n \rho_{g,i}^n}{\Delta t} + \frac{1}{\Delta x} [(\alpha_g \rho_g u_g)_{i+1/2}^{n+1,*} - (\alpha_g \rho_g u_g)_{i-1/2}^{n+1,*}] - \Gamma_{g,i}^{n+1} = 0 \quad (36)$$

$$\begin{aligned} & \bar{\alpha}_{l,i+1/2}^{n+1} \bar{\rho}_{l,i+1/2}^{n+1} \frac{u_{l,i+1/2}^{n+1} - u_{l,i+1/2}^n}{\Delta t} + \bar{\alpha}_{l,i+1/2}^{n+1} \bar{\rho}_{l,i+1/2}^{n+1} u_{l,i+1/2}^{n+1} \frac{[(u_l)_{i+1}^{n+1,*} - (u_l)_i^{n+1,*}]}{\Delta x} \\ & + \bar{\alpha}_{l,i+1/2}^{n+1} \frac{p_{i+1}^{n+1} - p_i^{n+1}}{\Delta x} - \frac{1}{2} (\alpha_{l,i}^{n+1} \rho_{l,i}^{n+1} g_{x,i}^{n+1} + \alpha_{l,i+1}^{n+1} \rho_{l,i+1}^{n+1} g_{x,i+1}^{n+1}) \\ & - F_{int,i+\frac{1}{2}}^{n+1} + \frac{1}{2} (F_{wall,l,i}^{n+1} + F_{wall,l,i+1}^{n+1}) + \Gamma_{g,i+1/2}^{n+1,*} (u_{int,i+1/2}^{n+1} - u_{l,i+1/2}^{n+1}) \\ & = 0 \end{aligned} \quad (37)$$

$$\begin{aligned} & \bar{\alpha}_{g,i+1/2}^{n+1} \bar{\rho}_{g,i+1/2}^{n+1} \frac{u_{g,i+1/2}^{n+1} - u_{g,i+1/2}^n}{\Delta t} + \bar{\alpha}_{g,i+1/2}^{n+1} \bar{\rho}_{g,i+1/2}^{n+1} u_{g,i+1/2}^{n+1} \frac{[(u_g)_{i+1}^{n+1,*} - (u_g)_i^{n+1,*}]}{\Delta x} \\ & + \bar{\alpha}_{g,i+1/2}^{n+1} \frac{p_{i+1}^{n+1} - p_i^{n+1}}{\Delta x} - \frac{1}{2} (\alpha_{g,i}^{n+1} \rho_{g,i}^{n+1} g_{x,i}^{n+1} + \alpha_{g,i+1}^{n+1} \rho_{g,i+1}^{n+1} g_{x,i+1}^{n+1}) \\ & + F_{int,i+\frac{1}{2}}^{n+1} + \frac{1}{2} (F_{wall,g,i}^{n+1} + F_{wall,g,i+1}^{n+1}) - \Gamma_{g,i+1/2}^{n+1,*} (u_{int,i+1/2}^{n+1} - u_{g,i+1/2}^{n+1}) \\ & = 0 \end{aligned} \quad (38)$$

$$\begin{aligned}
& \frac{\alpha_{l,i}^{n+1} \rho_{l,i}^{n+1} e_{l,i}^{n+1} - \alpha_{l,i}^n \rho_{l,i}^n e_{l,i}^n}{\Delta t} + \frac{1}{\Delta x} [(\alpha_l \rho_l u_l e_l)_{i+1/2}^{n+1,*} - (\alpha_l \rho_l u_l e_l)_{i-1/2}^{n+1,*}] \\
& + p_i^{n+1/2} \frac{\alpha_{l,i}^{n+1} - \alpha_{l,i}^n}{\Delta t} + p_i^{n+1} \frac{1}{\Delta x} [(\alpha_l u_l)_{i+1/2}^{n+1,*} - (\alpha_l u_l)_{i-1/2}^{n+1,*}] - Q_{wl,i}^{n+1} \quad (39) \\
& - Q_{il,i}^{n+1} + \Gamma_{ig,i}^{n+1} h_{l,i}^{n+1,*} + \Gamma_{w,i}^{n+1} h_{l,i}^{n+1,'} = 0
\end{aligned}$$

$$\begin{aligned}
& \frac{\alpha_{g,i}^{n+1} \rho_{g,i}^{n+1} e_{g,i}^{n+1} - \alpha_{g,i}^n \rho_{g,i}^n e_{g,i}^n}{\Delta t} + \frac{1}{\Delta x} [(\alpha_g \rho_g u_g e_g)_{i+1/2}^{n+1,*} - (\alpha_g \rho_g u_g e_g)_{i-1/2}^{n+1,*}] \\
& + p_i^{n+1/2} \frac{\alpha_{g,i}^{n+1} - \alpha_{g,i}^n}{\Delta t} + p_i^{n+1} \frac{1}{\Delta x} [(\alpha_g u_g)_{i+1/2}^{n+1,*} - (\alpha_g u_g)_{i-1/2}^{n+1,*}] - Q_{wg,i}^{n+1} \quad (40) \\
& - Q_{ig,i}^{n+1} - \Gamma_{ig,i}^{n+1} h_{g,i}^{n+1,*} - \Gamma_{w,i}^{n+1} h_{g,i}^{n+1,'} = 0
\end{aligned}$$

In these discretized equations, $\rho_{l,i} = \rho_l(p_i, T_{l,i})$ and $e_{l,i} = e_l(p_i, T_{l,i})$. In addition, $\bar{\alpha}_{l,i+1/2}^{n+1}$ and $\bar{\rho}_{l,i+1/2}^{n+1}$ are edge averaged values from its two neighbor cells. The discretized forms of all advection terms follow the similar approach defined in equations (23) and (25). $\partial(\alpha u)/\partial x$ terms in energy equations are treated similarly as if they are advection terms. For momentum exchange term due to phase change, net vapor generation rate from upstream is used (the * subscript in $\Gamma_{g,i+1/2}^{n+1,*}$ denote upstream donor cell). The discretized form of the interfacial friction term is slightly more complex, a hybrid of edge averaged and upwind donor cell values. For example, if local velocities are positive, the interfacial friction term is discretized as,

$$F_{int,i+1/2} = \frac{1}{2} (C_{int,i} + C_{int,i+1}) (C_{1,i} u_{g,i+1/2} - C_{0,i} u_{l,i+1/2}) |C_{1,i} u_{g,i+1/2} - C_{0,i} u_{l,i+1/2}| \quad (41)$$

when drift flux model is used, and,

$$F_{int,i+1/2} = \frac{1}{2} (C_{int,i} + C_{int,i+1}) (u_{g,i+1/2} - u_{l,i+1/2}) |u_{g,i+1/2} - u_{l,i+1/2}| \quad (42)$$

when drag coefficient model is used.

It is worthy of elaborating some details of the implementation of the high-resolution spatial discretization scheme in a fully implicit scheme. As shown in equations (35) - (40), it appears that the realization of the high-resolution spatial discretization scheme is based on the unknown solutions at the current $n+1$ time step. In fact, for the iterative JFNK solving method used in this work, the high-resolution realization is always based on the k^{th} iteration solutions at the current $n+1$ time step. When the iterations converge, the high-resolution realization based on the k^{th}

iteration solutions is effectively the same as that based on the $n+1$ time step solutions. More details on the iterative JFNK method are given in the next section.

3.4 Jacobian-free Newton Krylov method

Equations (35) - (40) represent the discretized nonlinear equation system of a typical one-dimensional two-phase flow problem in the vector form,

$$\mathbf{F}(\mathbf{U}) = 0 \quad (43)$$

with the discretized unknown vector, $\mathbf{U} = [\dots, \alpha_{g,i}, p_i, T_{l,i}, T_{g,i}, u_{l,i+1/2}, u_{g,i+1/2}, \dots]^T$. In this work, a JFNK method is used to solve the discretized nonlinear equation system. Such a method has proved its capability in many disciplines (Knoll and Keyes, 2004) and has been used in our previous work in solving single- and two-phase flow problems (Zou et al., 2015a, 2015b, 2015c, 2015d, 2015e, 2016). The JFNK method is a variant of Newton's method, which iteratively solves the nonlinear equation system by solving a series of linearized Newton's correction equation. The iteration starts from an initial guess to the nonlinear equation system. In transient simulations, the solutions from the old time step are normally used as an initial guess. At the k^{th} step of the iterations, in order to obtain the $(k+1)^{\text{th}}$ iteration solution, one solves the linearized equation system, i.e., the Newton's correction equation,

$$\mathbb{J}^k \delta \mathbf{U}^k = -\mathbf{F}(\mathbf{U}^k) \quad (44)$$

for the Newton's correction vector $\delta \mathbf{U}^k$. In equation (44), $\mathbf{U}^k$ is the known k^{th} iteration solutions, and $\mathbb{J}^k$ is the Jacobian matrix based on the k^{th} iteration solutions. The Jacobian matrix is defined as,

$$\mathbb{J}_{mn} \equiv \frac{\partial F_m(\mathbf{U})}{\partial U_n} \quad (45)$$

in which m and n denote the index of the components of vectors $\mathbf{F}(\mathbf{U})$ and $\mathbf{U}$ respectively. After solving equation (44) for $\delta \mathbf{U}^k$, the $(k+1)^{\text{th}}$ iteration solution can then be obtained as,

$$\mathbf{U}^{k+1} = \mathbf{U}^k + \delta \mathbf{U}^k \quad (46)$$

One of the key differences between the Newton-Krylov method and traditional Newton's method is how the linear equations system, equation (44), is solved. In the Newton-Krylov framework, a key step to solve the linear equation system, for example $\mathbf{A}\mathbf{x} = \mathbf{b}$, requires the construction of the Krylov subspace,

$$\mathbf{K}_j = \text{span}(\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \mathbf{A}^2\mathbf{r}_0, \dots, \mathbf{A}^{j-1}\mathbf{r}_0) \quad (47)$$

in which, j is the size of the Krylov subspace; and $\mathbf{r}_0 \equiv \mathbf{b} - \mathbb{A}\mathbf{x}_0$ with $\mathbf{x}_0$ being the initial guess to the solution of the linear equation. One of the major costs in the Newton-Krylov framework is to construct the Krylov subspace. In most practical applications, without proper preconditioning, the efficiency of the Krylov's method could be low; e.g., a large Krylov subspace size, j , is needed. By properly choosing preconditioning schemes, the Krylov subspace size could be greatly reduced, and so is the construction cost. Either left or right preconditioning scheme can be used (Knoll and Keyes, 2004). Using the right preconditioning as an example, the original linear equations system (44) becomes,

$$(\mathbb{J}^k \mathbb{P}^{-1})(\mathbb{P} \delta \mathbf{U}^k) = -\mathbf{F}(\mathbf{U}^k) \quad (48)$$

in which, $\mathbb{P}$ is the preconditioning matrix, and $\mathbb{P}^{-1}$ is its inverse. If the preconditioning matrix $\mathbb{P}$ is properly chosen, the preconditioned matrix $\mathbb{J}^k \mathbb{P}^{-1}$ can be well conditioned, such that the Krylov subspace's size could be greatly reduced. It is noted that the preconditioned Newton-Krylov method is realized through a two-step process, in which $\mathbf{w}^k \equiv \mathbb{P} \delta \mathbf{U}^k$ is first solved from the preconditioned linear equation system, and $\delta \mathbf{U}^k$ is then solved as $\delta \mathbf{U}^k = \mathbb{P}^{-1} \mathbf{w}^k$.

As can be observed in equation (47), only the matrix-vector product operation is required in the Krylov method, while an explicit construction of the matrix is never required. Based on this fact, an additional 'Jacobian-free' step can be taken to further reduce the computational and data storage cost of the Newton-Krylov method. The Jacobian-free method to approximate the left hand side of the preconditioned linear equation system, equation (48), can be formulated as,

$$(\mathbb{J}^k \mathbb{P}^{-1}) \mathbf{w}^k \approx \frac{\mathbf{F}(\mathbf{U}^k + \epsilon \mathbb{P}^{-1} \mathbf{w}^k) - \mathbf{F}(\mathbf{U}^k)}{\epsilon} \quad (49)$$

in which, $\mathbf{w}^k \equiv \mathbb{P} \delta \mathbf{U}^k$, normally referred as the Krylov vector; and ϵ is a small perturbation parameter. One of the major advantages of using the Jacobian-free method is that the explicit formation and storage of the Jacobian matrix could be avoided. Derivation and code implementation of the analytical Jacobian matrix could be a cumbersome and error-prone task for two-phase flow system analysis codes, since many thermal-hydraulics correlations have complicated forms.

It is also worthy of noting that, the matrix-vector product operation of the preconditioning matrix, $\mathbb{P}$, is never required in the computational procedures. On the contrary, such a matrix-vector product operation of the inversed preconditioning matrix, $\mathbb{P}^{-1}$, is required. Therefore, how the $\mathbb{P}^{-1} \mathbf{w}^k$ operation is carried out is the key to different preconditioning schemes, which were thoroughly reviewed in Knoll and Keyes' work (Knoll and Keyes, 2004). One could provide an explicit analytical Jacobian matrix, or an approximated Jacobian matrix (for example, by omitting

certain terms, or by using a lower order spatial discretization scheme, etc.) as the preconditioning matrix $\mathbb{P}$. The matrix-vector product operation of $\mathbb{P}^{-1}$ can then be either obtained mathematically or formulated as a process, which is normally referred as the physics-based preconditioning scheme, see for example Mousseau's pioneering work in two-phase flow simulations (Mousseau, 2004). In our implementation of the Newton-Krylov method, the scientific computational toolkit PETSc (Balay et al., 2013) package is used. In this work, preconditioning matrix is obtained by a default finite differencing method provided in the PETSc package, such that,

$$\mathbb{P}_{mn}^k = \mathbb{J}_{mn}^k \approx \frac{F_m(\mathbf{U}^k + \epsilon \mathbf{i}_n) - F_m(\mathbf{U}^k)}{\epsilon} \quad (50)$$

in which, ϵ is a small perturbation parameter; and $\mathbf{i}_n$ is a unit vector with a non-zero n^{th} entry, $[0, \dots, 1, \dots, 0]$. Interested readers are referred to the PETSc manual (Balay et al., 2013) for more details.

3.5 Numerical treatment with phase appearance and disappearance

The phase appearance and disappearance issue presents serious numerical challenges in two-phase flow simulations using the two-fluid six-equation model. Numerical challenges arise from the singular equation system when one phase is absent, as well as from the discontinuity in the solution space when one phase appears or disappears. A numerical treatment has been implemented to treat the singular equation system when phase appearance and disappearance happen. The concept is similar to the work done in our previous studies (Zou et al., 2015c, 2015d, 2015e). Using void fraction approaching 0 as an example, gas phase momentum and energy equations, (4) and (6), become singular and thus have no unique solutions. In this work, when the solution of void fraction is smaller than α_{min} , the interfacial drag coefficient C_i is evaluated at this void fraction value, e.g., $\alpha_{min} = 10^{-5}$ replaces α in equation (16). In some cases, in equation (16), $\alpha_{min} = 10^{-3}$ gives much better code robustness. Such a change showed no obvious changes in solutions and thus was used in many cases. Similarly, the numerical treatment for the vapor phase energy equation is done on the interfacial heat transfer term, or more specifically, the H_{ig} term. When void fraction approaches to zero and is smaller than α_{min} , it is evaluated by using $\alpha_{min} = 10^{-5}$ in the closure correlations. This approach bounds the vapor phase temperature to be at saturation temperature when it is absent. Similar concept can be applied for the liquid phase when void fraction approaches to one. Note that this method only slightly changes some closure models when α approaches 0 or 1 while allowing α infinitely approaches 0 or 1. No any mass error is generated due to the numerical treatment. Therefore this is a much better method than cut-off methods (Ashrafizadeh, 2015) in which whenever the void fraction drops below a minimum

value, it will be reset at the minimum value. The cutoff method causes mass and energy errors. It should also be pointed out that RELAP5 uses a similar method like we use here to overcome the phase appearance/disappearance difficulty: for the phase that is not present, the interfacial heat transfer coefficient for that phase is computed as if the void fraction was approximately 10^{-5} instead of zero (Idaho National Laboratory, 2012a). However, due to insufficient convergence of nonlinearity inherent in the operator splitting methods, sometimes when a phase disappears, the calculated void fraction is less than zero or greater than one. When this occurs, the void fraction is then reset to zero or one, respectively. In our case, we fully resolve the nonlinearity and therefore we do not need any void fraction resetting to 0 or 1 and no mass error is generated.

4. RESULTS AND DISCUSSIONS

In this section, Bartolomei flow boiling experimental data in vertical pipes (Bartolomei et al., 1982) and FRIGG test data in vertical bundles (Nylund et al., 1969; Skaug et al., 1968) are used to validate the computer code developed in this work. The best-estimate reactor system analysis code, RELAP5-3D (Idaho National Laboratory, 2012a), was also used to benchmark the computer code developed in this work. It is noted that both the Bartolomei and FRIGG test data are available in steady state, and therefore all code validation work was done for steady state. Nevertheless, transient simulations were run for all the cases to obtain steady-state results. Both BDF1 and BDF2 time integration schemes were used for the transient simulations, and both of them gave identical results at the steady state as expected. Boundary conditions used for all the simulations are similar, including inlet mass fluxes and temperatures for both phases, and pressure outlet boundary conditions.

4.1 Validation with Bartolomei data

In this section, the computer code is validated using Bartolomei subcooled flow boiling data (Bartolomei et al., 1982). Bartolomei data have been widely used for code validation, and have also been used in our previous work for validation purpose (Zou et al., 2016). The Bartolomei experiments were conducted using tubes with 12 mm inner diameter, 2 mm tube wall thickness, and 1.5 m heated length oriented vertically. These experiments covered a wide range of conditions: 1) pressure from 3 to 15 MPa, 2) mass flux from 405 to 2123 kg/(m²s), 3) wall heat flux from 0.42 to 2.21 MW/m², 4) inlet subcooling level from 11 to 140 K, and 5) maximum outlet void fraction up to 0.6. A summary of all the experimental conditions of the Bartolomei experimental data is presented in Table 1. It is noted that the Bartolomei experimental data (Bartolomei et al., 1982) only provide experimental measurements on void fraction distribution

along the pipe length, and were plotted against the local equilibrium quality. Measured void fraction data uncertainties were also discussed in Bartolomei's work (Bartolomei et al., 1982), in which it was stated that the maximum absolute errors of the void fraction measurements do not exceed ± 0.04 . For all the simulation cases, 20 finite volume cells are used. A typical time step of 10^{-1} s, and 100 time steps are used in transient simulations, at the end of which the steady-state solutions could be obtained. Backward Euler (BDF1) and high-resolution spatial schemes were used for all simulations reported in this section. Steady-state results are obtained in the order of 1 second of computer (wall) time, with 2.5 GHz Intel Core i7 CPU.

Errors between numerical results and experimental data on void fraction are quantitatively estimated using mean absolute error (MAE), which is defined as,

$$\varepsilon_{\alpha} = \frac{1}{N} \sum_{i=1}^N |\alpha_{num,i} - \alpha_{exp,i}| \quad (51)$$

in which, subscripts '*num*' and '*exp*' denote numerical results and experimental data, respectively; and N is the total number of data points in the two-phase region. Interpolation of numerical results is used when necessary. It is noted that the single-phase region data are excluded from the error analysis for two reasons. Firstly, only trivial errors of void fraction exist in this region. If these trivial errors were to be included, the mean absolute error would be underestimated with bias. Secondly, negative void fraction values were reported in the experimental data, which should not be used for error analysis. For all Bartolomei data, mean absolute errors for all 25 cases are summarized in Table 2. Overall, a good agreement was found between the numerical results and the experimental data. For the majority of the cases, the MAE is within or close to the maximum absolute measurement error, 0.04.

Comparisons between the numerical results and experimental data are also shown from Figure 4 to Figure 7. All data are grouped in these figures with similar parameters, the same way presented in Bartolomei's work (Bartolomei et al., 1982). It is worth mentioning Figure 4, which shows four cases with similar pressure, mass flux, wall heat flux, and inlet temperature, with apparent scattering in the experimental data. Bartolomei explained that the scattering of the experimental data could be resulted from the measurement errors of operational parameters, as well as the inaccuracy of maintaining them. On the contrary, numerical results show very little scattering due to computer code's 'deterministic' nature. It suggests the drawback of the commonly used deterministic thermal-hydraulics codes, which do not normally consider the uncertainties of the phenomenon. It can be observed that the numerical results agree very well with the experimental

data in general, with a few exceptions (for example case 18 shown in Figure 7). For this case, although the model predicts that the inception of subcooled boiling is lagged compared to the experimental data, the slope of the void fraction still agrees well with experimental data. This suggests that further investigations are needed to consider the uncertainties associated with the model in predicting the onset of net vapor generation point, e.g. the Saha-Zuber model.

4.2 Validation with FRIGG data

In the section, the computer code developed in this work is validated using the flow boiling experimental data in vertical rod bundles from the FRIGG tests (Nylund et al., 1969; Skaug et al., 1968). FRIGG is a full-scale test program for the boiling channels of the Marviken reactor, including investigations of axial and radial void distribution, single- and two-phase pressure drop, etc. The FRIGG data have also been widely used for two-phase flow closure correlations development (Chexal and Lellouche, 1986) and reactor system analysis codes validation (U.S. NRC).

FRIGG tests consist of a series of tests with different loop configurations and thermal-hydraulics conditions. In this work, ten data sets from FRIGG FT-36b series are used for code validation. For these experimental sets, the test loop consisted of 36 rods with 4.365 m uniformly heated length and 13.8 mm outer diameter. An additional unheated rod with 20 mm outer diameter was present in the center of the rod bundle. All rods are housed in a cylinder shroud, with 159.5 mm inner diameter. A schematic drawing of the test section is shown in Figure 8, reproduced from FRIGG-2 report (Nylund et al., 1969). Experimental conditions of the four sets of FRIGG FT-36b tests are summarized in Table 3. It was reported that the absolute measurement error of void fraction is 0.003, by comparing void fraction measurements with known void fraction in a mock-up facility.

Similar to the Bartolomei tests presented in the previous section, numerical results were obtained using 20 finite volume cells. Steady-state results were obtained at the end of transient simulations, using 0.1 s time step size and 200 time steps. Backward Euler (BDF1) and high-resolution spatial discretization schemes were used for all the simulations reported in this section. Each simulation takes several seconds of CPU time. It is noted that, in FT-36b tests, the radial power distribution is non-uniform, with the highest flux on the peripheral rods. In our numerical simulations, the radial power peaking factor was not considered, however an averaged wall heat flux was used instead. In addition, the effects of spacers on pressure drop are not considered in our simulations.

Numerical results obtained from in this work are plotted in Figure 9, Figure 10, and Figure 11, compared with the experimental data. Very good agreement between numerical results and experimental data is observed. Mean absolute errors for all four cases on void fraction between the numerical results and experimental data are summarized in Table 4.

4.3 Benchmark with RELAP5-3D (Idaho National Laboratory, 2012a)

The RELAP5-3D (Idaho National Laboratory, 2012a) code was developed as a best-estimate reactor system analysis code, which is successfully used to support reactor safety analyses worldwide. The two-fluid six-equation two-phase flow model and closure correlations used in this work are almost identical to those used in RELAP5-3D, except for those special numerical treatments for flow regime transitions and phase appearance/disappearance, which have been discussed in section 2 and 3.

In this section, 5 Bartolomei cases (5-9) and 4 FRIGG cases (413-147, 413-149, 413-109 and 413-117) are chosen to perform code-to-code benchmark studies. For fair comparisons, first-order spatial discretization schemes were used in this work to obtain steady-state numerical results. These numerical results along with those obtained using RELAP5-3D on void fraction are plotted in Figure 12 - Figure 15 against experimental data. From these figures, it can be observed that the numerical results obtained from this work are very close to the RELAP5-3D results.

As pointed out previously, in RELAP5-3D, for the purpose of numerical stability, a width of 0.05 in void fraction is used for the transition between the slug and annular mist flow regimes. In this work, this transition region was removed due to the good numerical stability observed for the methods used in this work. As criticized by Levy, see page 131 of Levy's book (Levy, 1999), "*to avoid sudden changes in flow regime that may be deleterious to numerical stability, transition regions covering a span $\Delta\alpha$ of at least 0.1 are included in computer system codes and that required computational flexibility overshadows any accuracy that might be derived from more exact flow regime maps.*" It is noted that $\Delta\alpha$ of 0.05 is used in RELAP5-3D. The excellent numerical stability demonstrated in this work shows that the combined methods are very promising to reduce numerical errors related to the flow regime transitions. It is potentially a practical approach to utilize more sophisticated flow regime maps to regain simulation accuracy without the need of complex numerical smoothing treatments on flow regime transitions.

Additional comparisons of numerical results between this work and the RELAP5-3D code are also provided in terms of phasic velocities and local flow regimes, for two representative cases, Bartolomei case 6 and 7. Figure 16 and Figure 18 show the local flow regimes along the pipe length predicted in this work versus using RELAP5-3D. In both cases, predicted flow regimes are identical, which have also been observed for other Bartolomei cases not shown here. Figure 17 and Figure 19 show the phasic velocities between the numerical results obtained in this work and those from RELAP5-3D predictions. Liquid phase velocities are shown in the whole pipe length, while vapor phase velocities are only plotted in the two-phase region. From both figures, it is clearly observed that the phasic velocities predicted in this work and those using RELAP5-3D agree with each other very well. There are slight deviations shown in Figure 19 near the end of the pipe between the numerical results obtained in this work and those using RELAP5-3D. From Figure 18, it can be found that these deviations take place at the transition between slug and annular mist flow regimes. Most likely, this is due to the linear interpolation used in the transitional region in the RELAP5-3D code, which is no longer needed in this work.

As a short summary, from the comparisons with the RELAP5-3D results, numerical results obtained in this work showed excellent agreement with RELAP5-3D. The good agreements between this work and the RELAP5-3D results further validate the correct implementation of the physical models and numerical methods used in this work.

5. Conclusions

In this work, we demonstrated a successful application to employ advanced numerical methods in solving two-fluid two-phase six-equation model with the full coverage of all the pre-CHF flow regimes for vertical upward channels. High-order staggered grid finite volume method and fully implicit methods (BDF1 and BDF2) were used for the spatial discretization and time integration schemes, respectively. The JFNK method was used as the nonlinear solver. To our best knowledge, this work represents the first-of-its-kind successful application of the JFNK method to solve the two-fluid two-phase flow models with high order numerical methods and with realistic closure models. Extensive code validation was performed, by comparing the numerical results to flow boiling experimental data in vertical pipes and rod bundles. For all cases, the numerical results agree well with experimental data. Code-to-code comparison with RELAP5-3D was also performed to verify the code implementation. Numerical results were compared to those obtained using RELAP5-3D, and good agreement between them was obtained.

The combined methods are robust and efficient even without implementing the analytical Jacobian matrix, which is typically required for traditional Newton's methods. The Jacobian-free feature yields significant savings in developing a fully implicit system analysis code. Due to the numerical difficulty in traditional codes, transitional flow regimes are added in existing system analysis codes to avoid sudden jump in flow regime dependent parameters. This causes loss of accuracy that has been widely criticized. A strongly robust performance was achieved in this work, and thus such transitional flow regimes were completely removed. Potentially, more sophisticated flow regime maps could be utilized, and therefore simulation uncertainty could be further reduced.

Extensive code validation work has been done in this work focused on flow boiling under steady-state conditions. Although we have previously demonstrated the advantages of using second-order fully implicit time integration schemes, additional work is needed to validate the code for transient two-phase flow simulations. The work will also be extended to include additional flow regimes, such as those in horizontal pipes.

6. Acknowledgement

This work is supported by the U.S. Department of Energy, under Department of Energy Idaho Operations Office Contract DE-AC07-05ID14517. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

Table 1, Experimental conditions of the Bartolomei flow boiling tests in vertical pipes
(Bartolomei et al., 1982)

Case Index	P (MPa)	Mass flux (kg/m ² -s)	Wall heat flux (MW/m ²)	T _{inlet} (K)	$\Delta T_{sub,inlet}$ (K) [†]	Notes
1	6.89	985	1.13	464	94.04	Figure 1, row 1, (Bartolomei et al., 1982)
2	6.78	1071	1.13	465	91.96	Figure 1, row 2, (Bartolomei et al., 1982)
3	6.84	961	1.13	465	92.55	Figure 1, row 3, (Bartolomei et al., 1982)
4	6.84	995	1.15	466	91.55	Figure 1, row 4, (Bartolomei et al., 1982)
5	6.81	998	0.44	521	36.25	Figure 2 (a), row 1, (Bartolomei et al., 1982)
6	6.89	965	0.78	493	65.04	Figure 2 (a), row 2, (Bartolomei et al., 1982)
7	6.84	961	1.13	466	91.55	Figure 2 (a), row 3, (Bartolomei et al., 1982)
8	6.74	988	1.7	416	140.58	Figure 2 (a), row 4, (Bartolomei et al., 1982)
9	7.01	996	1.98	434	125.24	Figure 2 (a), row 5, (Bartolomei et al., 1982)
10	14.79	1878	0.42	603	11.26	Figure 2 (b), row 1, (Bartolomei et al., 1982)
11	14.74	1847	0.77	598	16.00	Figure 2 (b), row 2, (Bartolomei et al., 1982)
12	14.75	2123	1.13	583	31.06	Figure 2 (b), row 3, (Bartolomei et al., 1982)
13	14.7	2014	1.72	545	68.79	Figure 2 (b), row 4, (Bartolomei et al., 1982)
14	14.99	2012	2.21	563	52.37	Figure 2 (b), row 5, (Bartolomei et al., 1982)
15	6.89	405	0.79	421	137.01	Figure 3 (a), row 1, (Bartolomei et al., 1982)
16	6.89	1467	0.77	519	39.06	Figure 3 (a), row 3, (Bartolomei et al., 1982)
17	6.79	2024	0.78	520	37.10	Figure 3 (a), row 4, (Bartolomei et al., 1982)
18	11.02	503	0.99	494	97.43	Figure 3 (b), row 1, (Bartolomei et al., 1982)
19	10.81	966	1.13	502	88.01	Figure 3 (b), row 2, (Bartolomei et al., 1982)
20	10.81	1554	1.16	563	27.05	Figure 3 (b), row 3, (Bartolomei et al., 1982)
21	10.84	1959	1.13	563	27.26	Figure 3 (b), row 4, (Bartolomei et al., 1982)
22	3.01	990	0.98	445	62.49	Figure 4 (a), row 1, (Bartolomei et al., 1982)
23	4.41	994	0.9	463	66.55	Figure 4 (a), row 2, (Bartolomei et al., 1982)
24	14.68	1000	1.13	533	80.65	Figure 4 (a), row 5, (Bartolomei et al., 1982)
25	6.81	2037	1.13	504	53.30	Figure 4 (b), row 1, (Bartolomei et al., 1982)

† The inlet subcooling levels are calculated from the inlet pressure, which is not available in the references and were obtained from numerical results. These values are presented for purpose of references only, and they should not be used as ‘known’ experimental conditions.

Table 2, Mean absolute error (MAE) of void fraction, ε_a , between numerical results and Bartolomei experimental data (Bartolomei et al., 1982)

Case	ε_a	Case	ε_a	Case	ε_a	Case	ε_a	Case	ε_a
1	0.026	6	0.061	11	0.015	16	0.037	21	0.025
2	0.080	7	0.051	12	0.018	17	0.030	22	0.025
3	0.055	8	0.041	13	0.019	18	0.076	23	0.042
4	0.048	9	0.029	14	0.028	19	0.047	24	0.071
5	0.009	10	0.034	15	0.122	20	0.057	25	0.039

Table 3, Experimental conditions of the FRIGG FT-36b flow boiling tests in a vertical rod bundle (Nylund et al., 1969; Skaug et al., 1968)

Case Index	P (MPa)	Mass flux (kg/m ² -s)	Averaged wall heat flux (MW/m ²)	$\Delta T_{sub,inlet}$ (K)
413-127	3.00	524	0.217	3
413-145	3.00	1110	0.439	3
413-147	3.00	755	0.664	3.1
413-149	3.03	514	0.439	25.2
413-109	5.00	992	0.664	3.3
413-117	4.98	520	0.439	30.4
413-118	5.00	736	0.664	2.9
413-125	7.00	950	0.664	15.3
413-140	8.68	1606	0.738	2.3
413-141	8.68	981	0.439	2.3

Table 4, Mean absolute error (MAE) of void fraction, ε_a , between numerical results and FRIGG FT-36b experimental data (Nylund et al., 1969; Skaug et al., 1968)

Case	ε_a	Case	ε_a
413-127	0.057	413-117	0.015
413-145	0.053	413-118	0.029
413-147	0.023	413-125	0.033
413-149	0.009	413-140	0.026
413-109	0.022	413-141	0.016

Figure 1, Flow regimes in vertical channels used in this work.

Figure 2, Schematic drawing of the staggered grid mesh arrangement.

Figure 3, Schematic illustration of the linear reconstruction of variables using the slope limiter method. ϕ is the piecewise constant variables before linear reconstruction. $\phi^{+/-}$ is the reconstructed variables on cell edges after the linear reconstruction.

Figure 4, Comparisons between numerical results (NUM) and experimental measurements (EXP). Group 1, with similar pressure $\sim 6.8\text{MPa}$, similar mass flux $\sim 1000\text{ kg/m}^2\text{s}$, similar wall heat flux, 1.13 MW/m^2 , and similar inlet temperature, $\sim 465\text{K}$. See Figure 1 of Bartolomei paper (Bartolomei et al., 1982).

Figure 5, Comparisons between numerical results (NUM) and experimental measurements (EXP). Group 2, with similar pressure $\sim 6.8\text{MPa}$, similar mass flux $\sim 1000\text{ kg/m}^2\text{s}$, wall heat flux increasing while inlet temperature decreasing. See Figure 2 (a) of Bartolomei paper (Bartolomei et al., 1982).

Figure 6, Comparisons between numerical results (NUM) and experimental measurements (EXP). Group 3, with similar pressure $\sim 15\text{MPa}$, similar mass flux $\sim 2000\text{ kg/m}^2\text{s}$, wall heat flux increasing while inlet temperature decreasing. See Figure 2 (b) of Bartolomei paper (Bartolomei et al., 1982).

Figure 7, Comparisons between numerical results (NUM) and experimental measurements (EXP). Group 5, with similar pressure ~ 11 MPa, similar wall heat flux ~ 1.1 MW/m², both mass flux and inlet temperature increasing. See Figure 3 (b) of Bartolomei paper (Bartolomei et al., 1982).

Figure 8, Cross section of the FRIGG FT-36b tests, reproduced from FRIGG-3 Report (Nylund et al., 1969).

Figure 9, Comparisons between numerical results (NUM) and FRIGG FT-36b experimental measurements (EXP). Pressures are at ~30 bars.

Figure 10, Comparisons between numerical results (NUM) and FRIGG FT-36b experimental measurements (EXP). Pressures are at ~50 bars.

Figure 11, Comparisons between numerical results (NUM) and FRIGG FT-36b experimental measurements (EXP). Pressure is at ~70 bars for case 413-125, ~90 bars for cases 413-140 and 413-141.

Figure 12, Comparisons among numerical results obtained in this work (NUM), numerical results obtained using RELAP5-3D (RELAP5), and experimental measurements (EXP), for Bartolomei cases 5, 7, and 9.

Figure 13, Comparisons among numerical results obtained in this work (NUM), numerical results obtained using RELAP5-3D (RELAP5), and experimental measurements (EXP), for Bartolomei cases 6 and 8.

Figure 14, Comparisons among numerical results obtained in this work (NUM), numerical results obtained using RELAP5-3D (RELAP5), and experimental measurements (EXP), for FRIGG test cases 413-147 and 413-149.

Figure 15, Comparisons among numerical results obtained in this work (NUM), numerical results obtained using RELAP5-3D (RELAP5), and experimental measurements (EXP), for FRIGG test cases 413-147 and 413-149.

Figure 16, Comparisons between numerical results obtained in this work (NUM) and numerical results obtained using RELAP5-3D (RELAP5) on local flow regimes for Bartolomei case 6.

Figure 17, Comparisons between numerical results obtained in this work (NUM) and numerical results obtained using RELAP5-3D (RELAP5) on phasic velocities for Bartolomei case 6.

Figure 18, Comparisons between numerical results obtained in this work (NUM) and numerical results obtained using RELAP5-3D (RELAP5) on local flow regimes for Bartolomei case 7.

Figure 19, Comparisons between numerical results obtained in this work (NUM) and numerical results obtained using RELAP5-3D (RELAP5) on phasic velocities for Bartolomei case 7.

Abu Saleem, R.A., and Kozlowski, T., “Development of Accurate and Stable Two-Phase Two-Fluid Model Solver”, *Proceedings of ICAPP 2014*, Charlotte, USA, April 6-9, (2014).

Ashrafizadeh, A., Devaud, C.B., and Aydemir, N.U., “A Jacobian-free Newton–Krylov Method for Thermalhydraulics Simulations”, *Int. J. Numer. Meth. Fluids*, DOI: 10.1002/fld.3999, (2015).

Balay S., et al., “PETSc Users Manual, Reversion 3.4”, ANL-95/11 (2013).

Barre, F., Parent, M., and Brun, B., “Advanced Numerical Methods for Thermalhydraulics”, Proceedings of the CSNI Specialist Meeting on Transient Two-phase Flow, Aix-en-Provence, France, April 6-8, (1992).

Bartolomei, G.G., et al., “An Experimental Investigation of True Volumetric Vapor Content with Sub-cooled Boiling in Tubes,” *Thermal Engineering* **29** (3), 132–135, (1982).

Bertolotto, D., Manera, A., Macián-Juan, R. and Chawla, R., “Improvement of the one-dimensional dissolved-solute convection equation using the QUICKEST-ULTIMATE algorithm”, *Nuclear Engineering and Design*, **241**, 245-256 (2011).

Bestion, D., “The physical closure laws in the CATHARE code”, *Nucl. Eng. and Des.*, **Vol. 124**, 229 (1990).

Chexal, B., and Lellouche, G., A Full-Range Drift-Flux Correlation for Vertical Flows (Revision 1), EPRI NP-3989-SR, Electric Power Research Institute, September (1986).

Frepoli, C., Mahaffy, J.H., and Ohkawa, K., “Notes on the implementation of a fully-implicit numerical scheme for a two-phase three-field flow model”, *Nuclear Engineering and Design*, **225**, 191-217 (2003).

Idaho National Laboratory, “RELAP5-3D Code Manual Volume I: Code Structure, System Models and Solution Methods”, INEEL-EXT-98-00834, Revision 4.0, June (2012a).

Idaho National Laboratory, “RELAP5-3D Code Manual Volume IV: Models and Correlations,” INEEL-EXT-98-00834, Revision 4.0, June (2012b).

Knoll, D.A., and Keyes, D.E., “Jacobian-free Newton-Krylov Methods: a Survey of Approaches and Applications”, *J. Comp. Phys.*, **193**, 357-397 (2004).

Levy, S., Two-Phase Flow in Complex Systems, ISBN 0-471-32967-3, John Wiley & Sons, (1999).

Macián-Juan, R., “A study of high order solute tracking in system codes”, Ph.D. Dissertation, Pennsylvania State University (1996).

Mousseau, V.A., “Implicitly Balanced Solution of the Two-phase Flow Equations Coupled to Nonlinear Heat Conduction”, *J. Comp. Phys.*, **200**, 104-132 (2004).

Mousseau, V.A., “Accurate Solution of the Nonlinear Partial Differential Equations from Thermal Hydraulics”, *Nuclear Technology*, **158**, 26-35 (2005).

Mousseau, V.A., “A Fully Implicit, Second Order in Time, Simulation of a Nuclear Reactor Core”, Proceedings of ICONE-14, International Conference on Nuclear Engineering, Miami, Florida, USA, July 17-20, (2006).

Munkejord, S.T., “Analysis of the two-fluid model and the drift-flux model for numerical calculation of two-phase flow”, PhD Dissertation, Norwegian University of Science and Technology, (2006).

Nylund O., et al., “Hydrodynamic and Heat Transfer Measurements on a Full-Scale Simulated 36-Rod Marviken Fuel Element with Non-uniform Radial Heat Flux Distribution,” FRIGG Loop Project, FRIGG-3, (1969).

Skaug, J.A., Eklund, R., and Nylund, O., “FT-36b: Results of Void Measurements,” FRIGG Loop Project, FRIGG-PM--15, (1968).

Tiselj, I. and Petelin, S., “Modeling of Two-Phase Flow with Second- Order Accurate Scheme”, *J. Comp. Phys.*, **Vol. 136**, 503-521 (1997).

Toro, E.F., Riemann Solvers and Numerical Methods for Fluid Dynamics: A Practical Introduction, Springer Science & Business Media, (2009).

U.S. Nuclear Regulatory Commission, “RELAP5/MOD3.3 Code Manual Volume I”, NUREG/CR- 5535 ed., December, (2001a).

U.S. Nuclear Regulatory Commission, “TRAC-M/FORTRAN 90 (Version 3.0) Theory Manual”, NUREG/CR-6724 ed., April, (2001b).

U.S. Nuclear Regulatory Commission, “TRACE V5.0 Assessment Manual, Appendix B: Separate Effects Tests.”

Versteeg, H.K. and Malalasekera, W., An Introduction to Computational Fluid Dynamics, the Finite Volume Method, Second Edition, Pearson Education Limited, (2007).

Wang, D., “Reduce numerical diffusion in TRACE using the high-resolution numerical method ENO”, *Transactions of the American Nuclear Society*, **107**, (2012).

Wang, D., et al., “Implementation and assessment of high-resolution numerical methods in TRACE”, *Nuclear Engineering and Design*, **263**, 327-341 (2013).

Zou, L., et al., “C++ Implementation of IAPWS Water/Steam Properties”, INL/EXT-14-31502, (2014).

Zou, L., Zhao, H., and Zhang, H., “Applications of high-resolution spatial discretization scheme and Jacobian-free Newton-Krylov method in two-phase flow problems,” *Annals of Nuclear Energy*, **Vol. 83**, pp. 101-107, (2015a).

Zou, L., Zhao, H., and Zhang, H., “On the Analytical Solutions and Numerical Verifications of the Two-Phase Water Faucet Problem”, Proceedings of the 16th International Topical Meeting on Nuclear Reactor Thermalhydraulics (NURETH-16), August 30 – September 4, Chicago, Illinois, USA, (2015b).

Zou, L., Zhao, H., and Zhang, H., “Newton-Krylov Methods in Applications of Two-Phase Flow Problems with Phase Appearance/Disappearance,” *Transactions of the American Nuclear Society*, **Vol. 112**, pp. 974-977, (2015c).

Zou, L., Zhao, H., and Zhang, H., “Solving Phase Appearance/Disappearance Two-Phase Flow Problems with High Resolution Staggered Grid and Fully Implicit Schemes by Jacobian-Free Newton-Krylov Method”, *Computers and Fluids*, Under Review, (2015d).

Zou, L., Zhao, H., and Zhang, H., “Implicitly Solving Phase Appearance and Disappearance Problems Using Two-Fluid Six-Equation Model”, *Progress in Nuclear Energy*, Accepted Article, <http://dx.doi.org/10.1016/j.pnucene.2015.12.006>, (2015e).

Zou, L., Zhao, H., and Zhang, H., “Numerical Implementation, Verification and Validation of Two-Phase Flow Four-Equation Drift Flux Model with Jacobian-free Newton Krylov Method”, *Annals of Nuclear Energy*, **Vol. 87**, pp. 709-719, (2016).