Implicitly Solving Phase Appearance and Disappearance Problems Using Two-Fluid Six-Equation Model

Ling Zou¹, Haihua Zhao, and Hongbin Zhang

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

ABSTRACT

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. In this work, a high-resolution spatial discretization scheme on staggered grids and fully implicit methods were applied for the simulation of two-phase flow problems using the two-fluid six-equation model. A Jacobian-free Newton-Krylov (JFNK) method was used to solve the discretized nonlinear problem. An improved numerical treatment was proposed and proved to be effective to handle the numerical challenges. **The treatment scheme is conceptually simple, easy to implement, and does not require explicit truncations on solutions, which is essential to conserve mass and energy.** Various types of phase appearance and disappearance problems relevant to thermal-hydraulics analysis have been investigated, including a sedimentation problem, an oscillating manometer problem, a **non-condensable** gas injection problem, a single-phase flow with heat addition problem and a subcooled flow boiling problem. Successful simulations of these problems demonstrate the capability and robustness of the proposed numerical methods and numerical treatments. Volume fraction of the absent phase can be calculated effectively as zero.

Keywords: Two-phase flow, Jacobian-free Newton-Krylov method, phase appearance and disappearance, implicit method

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

1. INTRODUCTION

In the nuclear engineering field, 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 are critical to the safety analyses of nuclear reactors. During the last four decades, several nuclear reactor system analysis codes have been developed to solve the one-dimensional two-phase flow equations to represent the complex reactor systems. These codes, such as RELAP5 [1], TRAC [2], and TRACE [3] have gained great successes in supporting reactor safety analyses, as well as design and licensing of new reactors. Low order spatial discretization scheme (such as first-order upwind method) and operator-splitting type of time integration schemes (such as semi-implicit method) are commonly used in these codes. It is well understood that these low-order numerical schemes generally introduce excessive numerical errors. Consequently, advanced numerical methods are essential to improve the numerical accuracy of reactor safety analysis codes. In our previous work [4-7], several advanced numerical methods have been investigated, and they have demonstrated capabilities in improving numerical accuracy in two-phase flow simulations. These advanced numerical schemes and methods include: 1) a high-resolution spatial discretization scheme using staggered grid mesh arrangement to improve spatial accuracy; 2) fully implicit time integration schemes to improve temporal accuracy, to allow for larger time step to be used, as well as to enhance code robustness; and 3) a Jacobian-free Newton-Krylov (JFNK) method to efficiently solve the highly nonlinear system. It is critical to investigate these methods in the simulations of phase appearance and disappearance two-phase flow problems using the six-equation two-fluid model, commonly used in existing reactor system analysis codes.

The phase appearance and disappearance problems present serious numerical challenges in the two-phase flow simulations. Existing reactor safety analysis codes use different kinds of numerical treatments for such problems. In the RELAP5-3D code [8], different strategies are used

for different scenarios, one-phase to one-phase, two-phase to one-phase, etc. The strategy used in CATHARE to deal with numerical difficulties associated with the phase appearance/disappearance phenomenon is described by Bestion [9]. When the void fraction tends to the prescribed minimum value of $\alpha_{min}=10^{-5}$ or the maximum values of $\alpha_{max}=1-10^{-6}$, interfacial mass and energy transfers are conditioned so that the predicted void fraction does not exceed these limiting values [9]. Frepoli et al. [10] made an attempt to implicitly solve the one-dimensional three-field two-fluid two-phase flow equations using Newton's method. Special treatment was proposed for the phase appearance/disappearance problem. In his work, the momentum equation of the vanishing phase is modified to avoid singularity, and mass and energy equations are manipulated when one of the two phases is expected to vanish. In a recent study done by Ashrafizadeh et al. [11], a JFNK method was used to solve one-dimensional two-phase flow problems with an implicit time integration scheme. An extended AUSM+ scheme and a phase appearance/disappearance treatment strategy, originally proposed in [12], were adapted in Ashrafizadeh's work. However, the same treatment, which has been proved to be effective for explicit time integration scheme, did not give satisfactory results when implicit schemes were used.

Based on reviews of existing literatures, implicitly solving phase appearance and disappearance problems still remains a great numerical challenge in two-phase flow simulations. Although our previous work has successfully demonstrated capabilities of advanced numerical methods in improving numerical accuracy of two-phase flow simulations, it is crucial to investigate these methods when applied to solve the phase appearance and disappearance problems. The main objective of this study is to investigate proper numerical treatments, when applying the aforementioned methods to implicitly solve phase appearance and disappearance phenomena problems. These methods will be tested with a wide range of applications relevant to thermal-hydraulics analysis, including a sedimentation problem, an oscillating manometer problem, a gas

injection problem, a single-phase flow with heat addition problem and a subcooled flow boiling problem. In the following sections, the single-pressure six-equation two-fluid two-phase flow model, which is commonly used in existing reactor safety analysis codes, will be presented. A high-resolution spatial discretization scheme on staggered grid, implicit time integration schemes, and the JFNK method will be briefly discussed for the purpose of completeness. Numerical results of the aforementioned test cases will be presented and discussed.

2. ONE-DIMENSIONAL TWO-FLUID TWO-PHASE FLOW MODEL

The six-equation two-fluid single-pressure two-phase flow equations used in this work are similar to those used in existing nuclear reactor system analysis codes, such as RELAP5 [1], TRAC [2], TRACE [3] and CATHARE [13]. [For simplicity, wall friction terms and virtual mass terms are not included in this work.](#) The six-equation system includes a set of continuity, momentum and energy equations for each phase, and is summarized in Eqs. (1)-(6),

$$\frac{\partial(\alpha_l \rho_l)}{\partial t} + \frac{\partial(\alpha_l \rho_l u_l)}{\partial x} - \Gamma_l = 0 \quad (1)$$

$$\frac{\partial(\alpha_g \rho_g)}{\partial t} + \frac{\partial(\alpha_g \rho_g u_g)}{\partial x} - \Gamma_g = 0 \quad (2)$$

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

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

$$\frac{\partial(\alpha_l \rho_l e_l)}{\partial t} + \frac{\partial(\alpha_l \rho_l u_l e_l)}{\partial x} + p \frac{\partial \alpha_l}{\partial t} + p \frac{\partial(\alpha_l u_l)}{\partial x} - Q_{wl} - Q_{il} - \Gamma_l h_l^{ex} = 0 \quad (5)$$

$$\frac{\partial(\alpha_g \rho_g e_g)}{\partial t} + \frac{\partial(\alpha_g \rho_g u_g e_g)}{\partial x} + p \frac{\partial \alpha_g}{\partial t} + p \frac{\partial(\alpha_g u_g)}{\partial x} - Q_{wg} - Q_{ig} - \Gamma_g h_g^{ex} = 0 \quad (6)$$

in which, the subscripts l and g denote the liquid phase and the gas phase, respectively. Γ_g is the net gas/vapor generation rate due to phase change or external injection. Γ_l is the net liquid generation rate due to phase change. Q_{wl} and Q_{wg} are the 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. F_{int} is the interfacial drag term. $\Gamma_l h_l^{ex}$ and $\Gamma_g h_g^{ex}$ represent energy carried with the mass transfer due to phase change or injection. The variables to be solved from this set of equations 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, $\alpha_l + \alpha_g = 1$. Water/steam properties are provided as functions of pressure and phasic temperature, using a package based on IAPWS1995 standard [14]. Properties of nitrogen, which is used in the nitrogen injection test case, are provided using ideal gas law. In order to close the equation system, constitutive models are required to model the source terms in each of these equations. The following subsections present detailed descriptions of the constitutive models including the modeling of subcooled boiling.

2.1 Wall heat transfer

For the subcooled flow boiling conditions, wall heat flux partitioning into the liquid and the gas phase is rather simple. Under such conditions, it is normally 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 isothermal test cases, wall heat fluxes are set to be zeros for both phases, such that,

$Q_{wl} = Q_{wg} = 0$. Different heat flux partitioning would be necessary for other conditions, such as two-phase flow with large void fraction and single-phase steam flow, which are not investigated in this work.

2.2 Non-condensable gas injection

When non-condensable gas is injected from an external source, and liquid injection is not considered,

$$\begin{aligned}\Gamma_g &= \Gamma_{injection} \\ h_g^{ex} &= h_{g,injection} \\ \Gamma_l &= 0\end{aligned}\tag{9}$$

where $\Gamma_{injection}$ is volumetric gas injection rate, and $h_{g,injection}$ is the enthalpy of the injected gas phase from external source. Heat transfer rate between the two phases is estimated using a simplified correlation, which assumes a constant interfacial heat transfer coefficient between them,

$$Q_{il} = -Q_{ig} = H_{lg}(T_g - T_l)\tag{10}$$

where H_{lg} is the interfacial heat transfer coefficient between the liquid and gas phase.

2.3 Wall boiling and interfacial heat/mass transfer

When wall boiling is considered, the total net vapor generation rate, Γ_g term, is a result of wall boiling and bulk condensation. Similar to RELAP5-3D [8], this term is modeled in two regions, the near wall region and bulk region,

$$\Gamma_g = \Gamma_w + \Gamma_{ig}\tag{11}$$

and

$$\Gamma_l = -\Gamma_g\tag{12}$$

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 void generation (section 4.7.1.1 of [15]).

Similar to RELAP5-3D [8], the vapor generation rate (negative value for vapor condensation) due to interfacial heat transfer is modeled as,

$$\Gamma_{ig} = -\frac{H_{il}(T_{sat}-T_l) + H_{ig}(T_{sat}-T_g)}{h_g^* - h_l^*} \quad (13)$$

in which, H_{il} and H_{ig} are volumetric heat transfer coefficients of liquid-to-interface and gas-to-interface, respectively. The separate effects from the wall boiling and bulk condensation also have to be considered in the energy source terms due to phase change,

$$\Gamma_l h_l^{ex} = -\Gamma_{ig} h_l^* - \Gamma_w h_l' \quad (14)$$

$$\Gamma_g h_g^{ex} = \Gamma_{ig} h_g^* - \Gamma_w h_g' \quad (15)$$

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 $h_l^* = h_{l,sat}(p)$.

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. Under wall boiling conditions, 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,

$$-Q_{il} + \Gamma_w h'_l = -H_{il}(T_{sat} - T_l) + \Gamma_w h_{g,sat} \quad (16)$$

and

$$-Q_{ig} - \Gamma_w h'_g = -H_{ig}(T_{sat} - T_g) - \Gamma_w h_{g,sat} \quad (17)$$

For more details, readers are referred to Ref. [8], pages 3-10 to 3-14.

2.4 Interfacial momentum exchange

Interfacial momentum exchange consists of two terms, interfacial drag term and momentum exchange due to phase change or injection. For interfacial drag term, a simplified approach similar to the drag coefficient method used in RELAP5-3D [8] and the model used in Städtke's work [16] is used. The model has also been tested in our previous work and showed good results [6]. The interfacial drag term is modeled as,

$$F_{int} = C_i(u_g - u_l)|u_g - u_l| \quad (18)$$

and the drag coefficient is modeled as,

$$C_i = \frac{1}{8} C_d a^{int} \rho_m \quad (19)$$

in which, the interfacial area density is estimated as,

$$a^{int} = \frac{3\alpha(1 - \alpha)}{r_p} \quad (20)$$

and the mixture density is defined as,

$$\rho_m = \alpha \rho_g + (1 - \alpha) \rho_l \quad (21)$$

and, C_d is the drag coefficient, r_p is the particle (vapor bubble in flow boiling) size. In this work, a constant value of 0.44 is used for C_d , the same as in [16]. The bubble size, r_p , is calculated based upon the concept of critical Weber number (section 4.1.1.1.1 of Ref. [15]). 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 $\Gamma_g < 0$.

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) two fully implicit time integration schemes - the first order backward Euler (BDF1) and the second-order BDF2 methods, 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 upwind spatial discretization scheme based on staggered grids has been used in this work and in our previous work [4-7]. This section provides a brief review on this high-resolution scheme. This high-resolution spatial discretization scheme is conceptually similar to the first-order upwind method widely used in existing system analysis codes. A key difference is that linear reconstructions of variables, using the concept of slope limiter, are used to achieve higher-order of accuracy, as schematically shown in Figure 1. This can be illustrated using the gas phase continuity equation as an example. At first, the advection term of the gas phase continuity equation is semi-discretized as,

$$\left. \frac{\partial(\alpha_g \rho_g u_g)}{\partial x} \right|_i = \frac{1}{\Delta x} [(\alpha_g \rho_g u_g)_{i+1/2}^* - (\alpha_g \rho_g u_g)_{i-1/2}^*] \quad (22)$$

If the traditional first order upwind method is used, the numerical gas phase mass flux on the cell edge, $i+1/2$, is evaluated as,

$$(\alpha_g \rho_g u_g)_{i+1/2}^* = u_{g,i+1/2} \begin{cases} \alpha_i \rho_g(p_i, T_{g,i}) & \text{if } u_{g,i+1/2} > 0 \\ \alpha_{i+1} \rho_g(p_{i+1}, T_{g,i+1}) & \text{otherwise} \end{cases} \quad (23)$$

When the high-resolution scheme is used, the numerical gas phase mass flux on the cell edge, $i+1/2$, is evaluated as,

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

in which, $\alpha_{g,i+1/2}^\pm$, $p_{i+1/2}^\pm$, and $T_{g,i+1/2}^\pm$ are the reconstructed void fraction, pressure, and gas phase temperature on cell edges, respectively, as shown in Figure 1. The slope limiter concept is standard to any modern finite volume method. Such a spatial discretization scheme is able to provide a second-order of spatial accuracy if the solutions are spatially smooth, and it provides spatially non-oscillation numerical results if there is a spatial discontinuity in solutions.

Figure 1. Schematic illustration of the first-order and high-resolution spatial discretization schemes for the staggered grid mesh. Positive velocities are assumed in this plot. ϕ represents scalar properties (such as pressure and void fraction), and u is velocity.

3.2 Time integration schemes

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

$$\left. \frac{\partial(\alpha_l \rho_l)}{\partial t} \right|_i = \frac{\alpha_{l,i}^{n+1} \rho_{l,i}^{n+1} - \alpha_{l,i}^n \rho_{l,i}^n}{\Delta t} \quad (25)$$

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

$$p \left. \frac{\partial \alpha_g}{\partial t} \right|_i = p_i^{n+1/2} \frac{\alpha_{g,i}^{n+1} - \alpha_{g,i}^n}{\Delta t} \quad (26)$$

in which,

$$p_i^{n+1/2} = \frac{1}{2} (p_i^{n+1} + p_i^n) \quad (27)$$

For BDF2, these terms are discretized as,

$$\left. \frac{\partial(\alpha_l \rho_l)}{\partial t} \right|_i = \frac{\alpha_{l,i}^{n+1} \rho_{l,i}^{n+1} - \frac{4}{3} \alpha_{l,i}^n \rho_{l,i}^n + \frac{1}{3} \alpha_{l,i}^{n-1} \rho_{l,i}^{n-1}}{\Delta t} \quad (28)$$

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

$$p \left. \frac{\partial \alpha_g}{\partial t} \right|_i = p_i^{n+1} \frac{\alpha_{g,i}^{n+1} - \frac{4}{3} \alpha_{g,i}^n + \frac{1}{3} \alpha_{g,i}^{n-1}}{\Delta t} \quad (29)$$

3.3 Summary of discretized equations in residual forms

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

$$res_{mass,l,i} = \frac{\alpha_{l,i}^{n+1} \rho_{l,i}^{n+1} - \alpha_{l,i}^n \rho_{l,i}^n}{\Delta t} + \frac{1}{\Delta x} [(\alpha_l \rho_l u_l)_{i+1/2}^{n+1,*} - (\alpha_l \rho_l u_l)_{i-1/2}^{n+1,*}] + \Gamma_{l,i}^{n+1} \quad (30)$$

$$res_{mass,g,i} = \frac{\alpha_{g,i}^{n+1} \rho_{g,i}^{n+1} - \alpha_{g,i}^n \rho_{g,i}^n}{\Delta t} + \frac{1}{\Delta x} [(\alpha_g \rho_g u_g)_{i+1/2}^{n+1,*} - (\alpha_g \rho_g u_g)_{i-1/2}^{n+1,*}] - \Gamma_{g,i}^{n+1} \quad (31)$$

$$\begin{aligned} res_{momentum,l,i+1/2} &= \bar{\alpha}_{l,i+1/2}^{n+1} \bar{\rho}_{l,i+1/2}^{n+1} \frac{u_{l,i+1/2}^{n+1} - u_{l,i+1/2}^n}{\Delta t} \\ &+ \bar{\alpha}_{l,i+1/2}^{n+1} \bar{\rho}_{l,i+1/2}^{n+1} u_{l,i+1/2}^{n+1} \frac{[(u_l)_{i+1}^{n+1,*} - (u_l)_i^{n+1,*}]}{\Delta x} + \bar{\alpha}_{l,i+1/2}^{n+1} \frac{p_{i+1}^{n+1} - p_i^{n+1}}{\Delta x} \\ &- \frac{1}{2} (\alpha_{l,i}^{n+1} \rho_{l,i}^{n+1} g_{x,i}^{n+1} + \alpha_{l,i+1}^{n+1} \rho_{l,i+1}^{n+1} g_{x,i+1}^{n+1}) - F_{int,i+\frac{1}{2}}^{n+1} \\ &- \Gamma_{l,i+1/2}^{n+1,*} (u_{int,i+1/2}^{n+1} - u_{l,i+1/2}^{n+1}) \end{aligned} \quad (32)$$

$$\begin{aligned} res_{momentum,g,i+1/2} &= \bar{\alpha}_{g,i+1/2}^{n+1} \bar{\rho}_{g,i+1/2}^{n+1} \frac{u_{g,i+1/2}^{n+1} - u_{g,i+1/2}^n}{\Delta t} \\ &+ \bar{\alpha}_{g,i+1/2}^{n+1} \bar{\rho}_{g,i+1/2}^{n+1} u_{g,i+1/2}^{n+1} \frac{[(u_g)_{i+1}^{n+1,*} - (u_g)_i^{n+1,*}]}{\Delta x} \\ &+ \bar{\alpha}_{g,i+1/2}^{n+1} \frac{p_{i+1}^{n+1} - p_i^{n+1}}{\Delta x} - \frac{1}{2} (\alpha_{g,i}^{n+1} \rho_{g,i}^{n+1} g_{x,i}^{n+1} + \alpha_{g,i+1}^{n+1} \rho_{g,i+1}^{n+1} g_{x,i+1}^{n+1}) \\ &+ F_{int,i+\frac{1}{2}}^{n+1} - \Gamma_{g,i+1/2}^{n+1,*} (u_{int,i+1/2}^{n+1} - u_{g,i+1/2}^{n+1}) \end{aligned} \quad (33)$$

$$\begin{aligned} res_{energy,l,i} &= \frac{\alpha_{l,i}^{n+1} \rho_{l,i}^{n+1} e_{l,i}^{n+1} - \alpha_{l,i}^n \rho_{l,i}^n e_{l,i}^n}{\Delta t} + \frac{1}{\Delta x} [(\alpha_l \rho_l u_l e_l)_{i+1/2}^{n+1,*} - (\alpha_l \rho_l u_l e_l)_{i-1/2}^{n+1,*}] \\ &+ p_i^{n+1/2} \frac{\alpha_{l,i}^{n+1} - \alpha_{l,i}^n}{\Delta t} + p_i^{n+1} \frac{1}{\Delta x} [(\alpha_l u_l)_{i+1/2}^{n+1,*} - (\alpha_l u_l)_{i-1/2}^{n+1,*}] - Q_{wl,i}^{n+1} \\ &- Q_{il,i}^{n+1} - \Gamma_{l,i}^{n+1} h_{l,i}^{ex,n+1} \end{aligned} \quad (34)$$

$$\begin{aligned}
res_{energy,g,i} = & \frac{\alpha_{g,i}^{n+1} \rho_{g,i}^{n+1} e_{g,i}^{n+1} - \alpha_{g,i}^n \rho_{g,i}^n e_{g,i}^n}{\Delta t} \\
& + \frac{1}{\Delta x} [(\alpha_g \rho_g u_g e_g)_{i+1/2}^{n+1,*} - (\alpha_g \rho_g u_g e_g)_{i-1/2}^{n+1,*}] + p_i^{n+1/2} \frac{\alpha_{g,i}^{n+1} - \alpha_{g,i}^n}{\Delta t} \\
& + p_i^{n+1} \frac{1}{\Delta x} [(\alpha_g u_g)_{i+1/2}^{n+1,*} - (\alpha_g u_g)_{i-1/2}^{n+1,*}] - Q_{wg,i}^{n+1} - Q_{ig,i}^{n+1} - \Gamma_{g,i}^{n+1} h_{g,i}^{ex,n+1}
\end{aligned} \tag{35}$$

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 adjacent cells. The * superscript denotes upwind treatment described in section 3.1. These quantities are similarly defined for the gas phase. The discretized forms of all advection terms follow the similar approach defined in equations (22) and (24). $\partial(\alpha u)/\partial x$ terms in energy equations are treated similarly as if they are advection terms. It is also noted that, for improved efficiency, a scaling factor of 10^{-6} is used for energy equations for both phases, i.e., equations (34) and (35).

3.4 Jacobian-free Newton Krylov method

In this work, the JFNK method is used to solve the discretized nonlinear equation system, (30) - (35). Such a method has proved its capability in many disciplines [17] and has been used in our previous work in solving single- and two-phase flow problems [4-7]. As was discussed previously, one of the major advantages of using the JFNK method is that explicit formation of the Jacobian matrix could be avoided. Derivation and code implementation of 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. In our implementation of the Newton-Krylov method, the scientific computational toolkit PETSc [18] package is used, with more details could be found in our previous work [4-7]. It is important to point out that, a JFNK method generally needs a good preconditioning scheme to be effective and efficient. There are different ways to precondition the JFNK method, which were reviewed in Ref. [17]. In our work,

the preconditioning matrix is obtained by a default finite differencing method provided in the PETSc package.

3.5 Numerical treatment with phase disappearance

When one of the two phases is absent, the equation system becomes singular. This is evident from the discretized phasic momentum and energy equations. As an example, if the gas phase is absent ($\alpha_g=0$), physically all the source terms become zeros, and thus equations (33) and (35) admit infinitely many solutions to gas phase velocity and temperature, i.e.,

$$res_{momentum,g,i+1/2} = 0 \quad (36)$$

for any given $u_{g,i+1/2}^{n+1}$. Many different methods have been proposed to overcome such a numerical challenge, as reviewed in the Introduction section. In this work, a new numerical treatment has to be used to treat the singular equation system when phase appearance and disappearance happen. The numerical treatment proposed in this work is rather simple and unified for both the momentum and energy equations. Using void fraction equal to 0 as an example, the numerical treatment is described in the following.

When the solution of void fraction is smaller than α_{min} (10^{-9} for example), the interfacial drag coefficient C_i is evaluated with this void fraction value, e.g., α_{min} replaces α in equation (20), such that the numerically treated interfacial drag coefficient $\tilde{C}_i \neq 0$ as α approaches 0. Therefore, the originally underdetermined gas phase discretized momentum equation is no longer underdetermined as α approaches 0,

$$res_{momentum,g,i+1/2} = O(0) + \tilde{C}_i(u_{g,i+1/2} - u_{l,i+1/2})|u_{g,i+1/2} - u_{l,i+1/2}| \quad (37)$$

This numerical treatment prevents the vapor phase momentum equation from becoming singular and drives the absent vapor phase velocity to be the same as the liquid phase velocity, as the void fraction approaches zero. Similarly, the numerical treatment for the vapor phase energy equation is done on the interfacial heat transfer term, or more specifically, H_{ig} term. The approach is

conceptually similar however not exactly the same as that used in the momentum equation. The evaluations on H_{ig} and H_{il} follow the suggestions made in the RELAP5-3D manual [8]. As void fraction approaches zero, H_{il} becomes a trivial number close to zero while H_{ig} is calculated as a nontrivial number. The numerical treatment can be illustrated by considering the gas phase energy equation when void fraction approaches zero and no wall boiling is considered,

$$res_{energy,g,i} = O(0) - Q_{ig,i} - \Gamma_{g,i} h_{g,i} \quad (38)$$

Substituting equations (13) and (17) into equation (38), it is easy to find that this reduced residual is proportional to $(T_{sat} - T_g)$ under the conditions that $H_{il} \approx 0$ and $H_{ig} \neq 0$. This approach drives the vapor phase temperature to be at saturated temperature when it is absent, and $\Gamma_{ig} = 0$. Similar concept can be applied for the liquid phase when void fraction approaches one.

As the numerically treated equations (30) - (35) provide continuous residual functions, no explicit numerical treatment is needed for single- to two-phase transition. The same set of discretized equations is solved for single-phase, two-phase, and single- to two-phase flow transition. The method proposed here is conceptually simpler and easier to implement than many existing treatment methods. It does not require a residual volume fraction for the absent phase, and thus it is mathematically simpler than the CATHARE treatment [9]. It provides continuous residual functions and does not require dynamic changes in residual forms as used in Frepoli's work [10]. Additionally, it does not involve any explicit truncation on solutions as used in Ashrafizadeh's work [11], which is essential to conserve mass and energy.

4. NUMERICAL TESTS

In this section, four test cases are included to demonstrate the capability and robustness of the proposed numerical methods in solving the six-equation two-phase flow problems, when various types of phase appearance and disappearance phenomena are considered. [For all the test cases,](#)

BDF2 time integration scheme and the high-resolution spatial discretization scheme are used. An additional section is provided to summarize mass and energy errors for all the test cases.

4.1 Sedimentation problem

The sedimentation problem is a test problem originally proposed by Youngs [19] for testing the phase separation due to gravity effect. The test consists of a vertical pipe initially filled with a two-phase mixture having a uniform void fraction $\alpha = 0.5$. Due to the gravity effect, the two phases will eventually separate into two single-phase zones with the heavier liquid phase settling down at the bottom, and the lighter phase at the top of the pipe. **No mass transfer is considered for this test problem.** A schematic drawing of the sedimentation problem is shown in Figure 2. There are two numerical challenges in the simulation of the sedimentation test, 1) a dynamically developed phase disappearance phenomenon due to phase separation; and 2) a sharp interface existing between the separated two phases. Table 1 summarizes configurations and parameters used for the sedimentation test problem. Numerical results were obtained by using 50 cells, **BDF2 scheme** and a time step size of 1×10^{-2} s ($CFL \approx 0.375$ based on largest velocity observed at ~ 1.5 m/s). The residual history of the simulation is shown in Figure 3. The total residual norm is defined as,

$$\|res\| = \sqrt{\sum_{i=1}^{N_{unknown}} (res_i)^2} \quad (39)$$

where, $N_{unknown}$ is the total number of unknowns in the system. For the residual norm of the liquid mass equation, it is defined as,

$$\|res\| = \sqrt{\sum_{i=1}^{N_{cell}} (res_{mass,l,i})^2} \quad (40)$$

where N_{cell} is the total number of finite volume cells, and $res_{mass,i}$ is defined in equation (30). The residual norms for other equations are defined similarly. It is also noted that, residual norms are evaluated at the beginning of a time step for the residual norms plot.

In Figure 3, it can be found that the simulation reaches steady state at about 21 seconds. However it was observed that void fraction and pressure profiles do not change significantly after 10 seconds. Figure 4 and Figure 5 show the transient void fraction and pressure distribution along the pipe. Two discontinuous void fronts could be found to move upward and downward, and eventually merged in the center of the pipe at about 10 seconds. Numerical results obtained in this work are found to be very close to those from Städtke [16]. Numerical results of void fraction at the bottom part of the pipe are in the order of 10^{-10} , which is effectively zero.

Figure 2, Schematic drawing of the sedimentation test problem.

Table 1. Parameters, initial and boundary conditions for the sedimentation problem

Parameter	Value	Unit
Pipe length (L)	2.0	[m]
Gravity (g_x)	-9.81	[m/s ²]
$u_{l,init}$	0.0	[m/s]
$u_{g,init}$	0.0	[m/s]
$T_{l,init}$	300	[K]
$T_{g,init}$	300	[K]
$\alpha_{g,init}$	0.5	
p_{init}	10^5	[Pa]
<i>Inlet</i>	Non-penetrating wall	
<i>Outlet</i>	Non-penetrating wall	
N_{cell}	50	
Δt	10^{-2}	[s]
$N_{timestep}$	4000

Figure 3, Residual history of the sedimentation test case, with $N_{cell} = 50$, $\Delta t = 1 \times 10^{-2}$ s.

Figure 4, Void fraction distribution at different time for the sedimentation test problem, with $N_{cell} = 50$, $\Delta t = 1 \times 10^{-2}$ s.

Figure 5, Pressure distribution at different time for the sedimentation test problem, with $N_{cell} = 50$, $\Delta t = 1 \times 10^{-2}$ s.

4.2 Oscillating manometer problem

The oscillating manometer test problem was originally proposed as a numerical benchmark test for two-phase flows [19]. The problem consists of a “U” tube manometer, which is partially filled with liquid and vapor (see Figure 6 (left) for the schematic drawing). This problem provides a test for the modeling of inertia and body force effects. Different than the sedimentation test, two phases are already initially separated in the oscillating manometer problem. In the numerical test, a straight pipe with different local gravity constants is used to simulate the manometer problem. **No mass transfer is considered for this test problem.** A schematic drawing and nodalization of the manometer problem is shown in Figure 6 (right). Parameters, boundary and initial conditions for the numerical tests are summarized in Table 2. In this study, numerical results of the manometer test problem were obtained using 20 cells, BDF2 and a time step of 10^{-2} s ($CFL \approx 0.02$ corresponding to largest velocity observed at ~ 2 m/s), a total number of time steps of 1500. **The numerical setup is similar to that used in the RELAP5-3D assessment manual [20].** For this test case, $\alpha_{min} = 10^{-9}$ gave less satisfactory convergence behavior. Instead, the value of α_{min} was set to 10^{-6} . **This test case does not admit a steady-state solution, and therefore residual history was not provided.** Numerical results of the liquid phase velocity at the bottom of the “U” tube and liquid level in the left leg of the manometer are plotted in Figure 7 and Figure 8, respectively. The liquid level was determined by calculating the total amount of liquid in the left leg of the U-tube. **In both figures, numerical results agree well with the analytical solutions, with excellent agreement in tracking the oscillation magnitudes in both liquid phase velocity and level. The simulation showed much better numerical accuracy compared to other work, such as the results presented in the RELAP5-3D assessment manual (figure 3.6-7 in [20], without mixture level tracking) and Ashrafizadeh’s work [11].**

Figure 6, Schematic drawing (left) and nodalization (right) of the oscillating manometer problem.

Table 2. Parameters, initial and boundary conditions for the oscillating manometer problem

Parameter	Value	Unit
Pipe length (L)	20	[m]
Gravity (g_x)	$\begin{cases} 9.81 & 0 \leq x < 10 \\ 0 & x = 10 \\ -9.81 & 10 < x \leq 20 \end{cases}$	[m/s ²]
$u_{l,init}$	-1.0	[m/s]
$u_{g,init}$	-1.0	[m/s]
$T_{l,init}$	300	[K]
$T_{g,init}$	300	[K]
$\alpha_{g,init}$	$\begin{cases} 0.0 & \text{if } 5 \leq x \leq 15 \\ 1.0 & \text{otherwise} \end{cases}$	
p_{init}	$10^5 + \rho_{init}g/h$	[Pa]
$\alpha_{g,left,bc}$	1.0	
$\alpha_{g,right,bc}$	1.0	
$p_{left,bc}$	10^5	[Pa]
$p_{right,bc}$	10^5	[Pa]
N_{cell}	20	
Δt	10^{-2}	[s]
$N_{timestep}$	1500

Figure 7, Liquid velocity at the bottom of the manometer, with $N_{cell} = 20$, $\Delta t = 10^{-2} s$, and $N_{timestep} = 1500$.

Figure 8, Height of the liquid level on the left leg of the manometer, with $N_{cell} = 20$, $\Delta t = 10^{-2} s$, and $N_{timestep} = 1500$.

4.3 Nitrogen injection problem

In this test case, gas phase appearance is induced by external injection of nitrogen gas from the side wall of the pipe. The test case consists of a vertical pipe of length 2.0 m, with pipe inner diameter (I.D.) of 0.0512 m. Liquid water enters into the pipe from the bottom with a mass flux boundary condition, $G_{l,inlet} = 400 \text{ kg/m}^2\text{-s}$, and temperature $T_{l,inlet} = 300 \text{ K}$. Outlet pressure, $p_{outlet} = 10^5 \text{ Pa}$ is set at the top of the pipe. Nitrogen injection is introduced from the side-wall of the pipe at $z = 0.5 \text{ m}$ (from the bottom), with injection rate corresponding to $\sim 0.06 \text{ m/s}$ of gas superficial velocity. The setup is similar to the experimental work done by Prasser et al. [21]. For simplicity, a constant value, $10^4 \text{ W/m}^3\text{-K}$, is used for the volumetric phase-to-phase heat transfer coefficient, H_{lg} . In the transient simulation, 40 finite volume cells were used, with a time step size $\Delta t = 0.02 \text{ s}$ (CFL ≈ 0.4 corresponding to 1 m/s velocity), and a total number of time steps $N_t = 500$. At the end of the transient simulation, steady state solutions were obtained. The residual history of the simulation is shown in Figure 9. Numerical results at the steady state are shown in Figure 10 and Figure 11. Figure 10 shows the calculated void fraction distribution. Before the injection, void fraction values are kept at zero; and after the injection, the void fraction jumps from zero to ~ 0.06 . The void fraction keeps increasing with elevation as a result of system depressurization (gravity effect). Figure 11 shows the distribution of phasic velocities. Before the injection, the velocities of both phases are the same. After the injection, the gas phase accelerates and then ‘drifts’ away from the liquid phase, and both phasic velocities slightly increase along the pipe length as a result of system depressurization.

Table 3. Parameters, initial and boundary conditions for the nitrogen injection test case

Parameter	Value	Unit
Pipe length (L)	2.0	[m]
Pipe I.D.	0.0512	[m]
$u_{l,init}$	0.4	[m/s]
$u_{g,init}$	0.4	[m/s]
$\alpha_{g,init}$	0.0	
$T_{l,ini}$	300	[K]
$T_{g,ini}$	300	[K]
p_{init}	10^5	[Pa]
$\alpha_{g,inlet}$	0.0	
$G_{l,inlet}$	400.0	[kg/m ² -s]
$G_{g,inlet}$	0.0	[kg/m ² -s]
$T_{l,inlet}$	300	[K]
$T_{g,inlet}$	300	[K]
p_{outlet}	10^5	[Pa]
$\Gamma_{injection}$	1.5*	[kg/m ³ -s]

* Nitrogen injection ($\Gamma_{injection} = 1.5 \text{ kg/m}^3\text{-s}$) is applied at the 10th finite volume only

Figure 9, Residual history of the nitrogen injection test case.

Figure 10, Numerical results of the void fraction of the nitrogen injection test problem.

Figure 11, Numerical results of the phasic velocities of the nitrogen injection test problem.

4.4 Single-phase flow and subcooled flow boiling problems

In this section, a single-phase flow with wall heat addition and a subcooled flow boiling problems are investigated. Although numerical simulations of single-phase flow problems are well-studied topics, it still remains a numerical challenge using the two-fluid two-phase model to simulate single-phase flow with zero (or one) void fraction. In many existing research work and analysis codes, a residual volume fraction is normally used for the absent phase. The residual volume fraction is generally small, however it could introduce additional numerical errors. Ideally, for single-phase flow simulation, a zero volume fraction should be used for the absent phase. The single-phase flow test case consists of a vertical pipe of length 1.5 m, with pipe inner diameter (I.D.) of 0.012 m. The pipe is initially filled with single-phase liquid water and thus the initial void fraction $\alpha_{g,ini} = 0.0$. A summary of the geometry parameters, initial and boundary conditions are listed in Table 4. In the transient simulation, 40 finite volume cells were used, with a time step size $\Delta t = 0.01$ s (CFL ≈ 0.35 corresponding to 1.3m/s velocity at exit), and a total number of time steps $N_t = 500$. At the end of the transient simulation, steady state solutions are obtained. The residual history of the simulation is shown in Figure 12. The numerical results are plotted in Figure 13 and Figure 14. In this case, heat is applied on the wall, but it is not high enough to initiate wall boiling. As a result, the void fraction remains at zero. In the simulation results, the numerical solutions to the void fraction are calculated in the order of 10^{-21} , which is effectively zero. Figure 13 shows the phasic velocities of the numerical results, from which it can be seen that the vapor phase velocity is correctly bound to the liquid phase velocity. Figure 14 shows the phasic temperatures and the saturation temperature. It shows that the absent vapor phase temperature is correctly bound to the local saturation temperature. An increased liquid phase temperature along the axial direction reflects the effect of wall heating.

The subcooled flow boiling test case is similar to the single-phase test case, except that the prescribed wall heat flux is increased to 0.44 MW/m^2 . This test case is the same as one of the Bartolomei subcooled flow boiling experimental test case (row 1 of figure 2(a) in Ref. [22]). All

other parameters are the same and are listed in Table 4. Similar to the single-phase simulation, in the transient simulation, 40 finite volume cells were used, with a time step size $\Delta t = 0.01$ s (CFL ≈ 0.6 corresponding to 2.2m/s velocity at exit), and a total number of time steps $N_t = 500$. At the end of the transient simulation, steady state solutions were obtained. The residual history of the simulation is shown in Figure 15. The numerical challenges of this test case are two-fold: 1) the singularity in the single-phase region, which has been resolved in the single-phase flow test case, and 2) the discontinuities in the solution space when jumping from single to two-phase region. If improperly treated, such discontinuities normally prevent Newton's method from being converged, as shown with the numerical difficulties encountered by Ashrafizadeh et al. (section 4.3 in Ref. [11]) in which void fraction was set to be equal to 0.001 when it is less than 0.001. In this test case, the proposed scheme shows strong robustness and stabilities in handling both challenges. It correctly handles the zero void fraction in the single-phase region, as well as when vapor starts to appear due to boiling. The numerical results are shown in Figure 16, Figure 17, and Figure 18. As shown in Figure 16, the void fraction becomes larger than 0 at ~ 0.8 m in the axial position due to wall boiling. Figure 17 shows the phasic velocities along the pipe length. In the single-phase region, the vapor velocity is the same as the liquid phase; and in the two-phase region, the vapor phase 'drifts' away from the liquid phase due to buoyancy effect, and thus has larger velocity than the liquid phase. The phasic temperatures are shown in Figure 18. The liquid phase temperature increases due to wall heat, and eventually becomes close to saturation. The vapor phase temperature is always close to the saturation temperature, as expected.

Table 4. Parameters, initial and boundary conditions for the single-phase and subcooled flow
boiling test case

Parameter	Value	Unit
Pipe length (L)	1.5	[m]
Pipe I.D.	0.012	[m]
Wall heat flux (q''_w)	0.22/0.44*	[MW/m ²]
$u_{l,init}$	1.0	[m/s]
$u_{g,init}$	1.0	[m/s]
$\alpha_{g,init}$	0.0	
$T_{l,ini}$	521	[K]
$T_{g,ini}$	558	[K]
p_{init}	6.81	[MPa]
$\alpha_{g,inlet}$	0.0	
$G_{l,inlet}$	998.0	[kg/m ² -s]
$G_{g,inlet}$	0.0	[kg/m ² -s]
$T_{l,inlet}$	521	[K]
$T_{g,inlet}$	558	[K]
p_{outlet}	6.81	[MPa]

* 0.22 MW/m² for single-phase, and 0.44 MW/m² for subcooled flow boiling

Figure 12, Residual history of the single-phase flow test problem.

Figure 13, Numerical results of the phasic velocities of the single-phase flow test problem.

Figure 14, Numerical results of the temperature of the single-phase flow test problem.

Figure 15, Residual history of the subcooled flow boiling test problem.

Figure 16, Numerical results of the void fraction of the subcooled flow boiling test problem.

Figure 17, Numerical results of the phasic velocities of the subcooled flow boiling test problem.

Figure 18, Numerical results of the temperatures of the subcooled flow boiling test problem.

4.5 Mass and energy balances

The fully implicit methods used in this work are able to fully resolve the nonlinearity in the equation system, and thus the traditional ‘mass error’ due to operator splitting process in traditional codes is eliminated. In addition, the numerical methods used in this work to treat phase appearance and disappearance do not involve any explicit truncations on solutions, and thus the mass error from solution truncations is also avoided. However, it is essential to numerically verify the balance of mass and energy in these test cases. This section provides a summary of the mass and energy balances in all the cases studied in this work. Due to the different nature of all the test cases, transient vs. steady state, open system vs. closed system, etc., mass and energy balances are done differently for these cases.

For the manometer problem, mass and energy balances are done for the liquid phase only, as the mass is not conserved for the gas phase for this open system. The mass and energy balance errors are defined as,

$$\varepsilon_{mass,l} = \frac{\sum_{i=1}^{N_{cell}} \alpha_l \rho_l - \sum_{i=1}^{N_{cell}} \alpha_{l,0} \rho_{l,0}}{\sum_{i=1}^{N_{cell}} \alpha_{l,0} \rho_{l,0}} \quad (41)$$

$$\varepsilon_{energy,l} = \frac{\sum_{i=1}^{N_{cell}} \alpha_l \rho_l e_l - \sum_{i=1}^{N_{cell}} \alpha_{l,0} \rho_{l,0} e_{l,0}}{\sum_{i=1}^{N_{cell}} \alpha_{l,0} \rho_{l,0} e_{l,0}} \quad (42)$$

where, subscript ‘0’ denotes the initial condition. Because the interfacial heat transfer and work related terms in the energy equation are difficult to evaluate in such a transient simulation, they were not considered in the energy balance analysis. Therefore, the energy error defined in equation (42) is not precise. However, these terms are insignificant compared to the internal energy term, although they introduce additional numerical errors. Nevertheless, equation (42) is still used for energy balance calculations.

For the sedimentation problem, as a closed system without phase change, mass balance is evaluated for both phases, and the energy balance is done for two-phase mixture only because of interfacial heat transfer. The mass balance error for both the liquid and gas phases is defined similarly to equation (38), and the two-phase mixture energy error is defined as,

$$\varepsilon_{energy,2\phi} = \frac{\sum_{i=1}^{N_{cell}} (\alpha_l \rho_l e_l + \alpha_g \rho_g e_g) - \sum_{i=1}^{N_{cell}} (\alpha_{l,0} \rho_{l,0} e_{l,0} + \alpha_{g,0} \rho_{g,0} e_{g,0})}{\sum_{i=1}^{N_{cell}} (\alpha_{l,0} \rho_{l,0} e_{l,0} + \alpha_{g,0} \rho_{g,0} e_{g,0})} \quad (43)$$

where, subscript ‘2 ϕ ’ denotes two-phase mixture. Again, work related term is ignored in equation (43).

For the nitrogen injection test case, as an open system, mass balances are done for both phases at the steady state,

$$\varepsilon_{mass,l} = \frac{(\alpha\rho u)_{outlet,l} - (\alpha\rho u)_{inlet,l}}{(\alpha\rho u)_{inlet,l}} \quad (44)$$

and

$$\varepsilon_{mass,g} = \frac{(\alpha\rho u)_{outlet,g} - G_{injection,g}}{G_{injection,g}} \quad (45)$$

The energy error is evaluated on the two-phase mixture with work related term considered,

$$\varepsilon_{energy,2\phi} = \frac{\left\{ [(\alpha\rho ue)_{outlet,l} + (\alpha\rho ue)_{outlet,g}] + \sum_{i=1}^{N_{cell}} p_i \left(\frac{\partial \alpha_l u_l}{\partial x} + \frac{\partial \alpha_g u_g}{\partial x} \right) dx - [(\alpha\rho ue)_{inlet,l} + (Ge)_{injection,g}] \right\}}{[(\alpha\rho ue)_{inlet,l} + (\alpha\rho ue)_{inlet,g}]} \quad (46)$$

For the single-phase with heat addition test case, mass and energy balances are done for the liquid phase only as the vapor phase is absent. The mass error of the liquid phase is defined the same as that defined in equation (44). The liquid phase energy balance error, with the work related term considered, is defined as,

$$\varepsilon_{energy,l} = \frac{(\alpha\rho ue)_{outlet,l} + \sum_{i=1}^{N_{cell}} p_i \left(\frac{\partial \alpha_l u_l}{\partial x} \right) dx - (\alpha\rho ue)_{inlet,l} - q_{wall} a_w L}{q_{wall} a_w L} \quad (47)$$

For the flow boiling test case, mass and energy balances are done for two-phase mixture because of phase change. The errors are defined as,

$$\varepsilon_{mass,2\phi} = \frac{(\alpha\rho u)_{outlet,l} + (\alpha\rho u)_{outlet,g} - (\alpha\rho u)_{inlet,l}}{(\alpha\rho u)_{inlet,l}} \quad (48)$$

and

$$\varepsilon_{energy,2\phi} = \frac{\left\{ [(\alpha\rho ue)_{outlet,l} + (\alpha\rho ue)_{outlet,g}] - [(\alpha\rho ue)_{inlet,l} + (\alpha\rho ue)_{inlet,g}] + \sum_{i=1}^{N_{cell}} p_i \left(\frac{\partial \alpha_l u_l}{\partial x} + \frac{\partial \alpha_g u_g}{\partial x} \right) dx - q_{wall} a_w L \right\}}{q_{wall} a_w L} \quad (49)$$

Based on these definitions, mass and energy balance errors are summarized in Table 5 for all the test cases presented in this work. Overall, satisfactory mass and energy balances were found for

all the test cases. Slightly larger errors were found for energy balance for the sedimentation and manometer test problems due to insignificant however numerically nontrivial terms omitted. For all the other mass/energy balances, excellent results were obtained. In addition, Figure 19 shows the relative mass balance error for the liquid and gas phases of the sedimentation test problem, plotted with time. It indicates that there is no accumulated mass error along with simulation time, which is very important in reactor safety analysis. Similar trends were observed for the other cases.

Table 5. Relative mass and energy balance errors for all the test cases

Test cases	Mass Balance Error			Energy Balance Error		
	Liquid	Gas	Two-phase	Liquid	Gas	Two-phase
Sedimentation	$O(10^{-13})$	$O(10^{-12})$	-	-	-	$O(10^{-8})^*$
Manometer	$O(10^{-11})$	-	-	$O(10^{-6})^*$	-	-
Nitrogen injection	$O(10^{-14})$	$O(10^{-15})$	-	-	-	$O(10^{-13})$
Single-phase	$O(10^{-13})$	-	-	$O(10^{-12})$	-	-
Flow boiling	-	-	$O(10^{-14})$	-	-	$O(10^{-14})$

* Errors are relatively larger due to terms omitted when evaluating energy balance.

Figure 19, Relative mass balance error for the sedimentation test problem.

5. Conclusions and Future Work

In this study, high-resolution spatial discretization and fully implicit time integration schemes have been applied to solve one-dimensional two-phase flow problems with various types of phase appearance phenomena considered. The JFNK method was used to solve the discretized nonlinear equations. A [conceptually simple and easy to implement](#) numerical treatment was proposed in this work for phase appearance/disappearance. [The treatment method does not involve explicit truncations on solutions](#), thus it does not introduce mass and energy errors. Five test problems were presented in this study to test the proposed numerical methods, including a sedimentation problem, an oscillating manometer problem, a nitrogen gas injection problem, a single-phase flow with heat addition problem, and a subcooled flow boiling problem. These numerical methods demonstrated robust and stable behaviors in solving singular problems when one phase is absent or when it first appears. [Mass and energy balance errors were estimated for all the test cases, and satisfactory results were obtained](#). The discontinuity in solution space due to phase appearance, normally a numerical challenge for Newton-type of solving schemes, has also been successfully treated with the proposed numerical methods.

[This work will be extended in the future to include more challenging problems, such as steam injection into subcooled water, two-phase flow during the reflood phase of a postulated loss-of-coolant-accident, complete dryout conditions, etc. These challenging problems would require more realistic and sophisticated two-phase closure correlations to be implemented, which will be investigated in the future.](#)

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