INTRODUCTION

Two-phase flow is an important phenomenon closely related to the normal and accident conditions of nuclear reactor operations. Accurate modeling and simulation of two-phase flow are critical to the safety analyses of nuclear reactors. To improve the numerical accuracy of reactor safety analysis codes, it is important to consider advanced numerical schemes and methods. Our approach includes three aspects: 1) high-resolution spatial discretization scheme to improve spatial accuracy; 2) fully implicit time integration schemes to improve temporal accuracy, e.g. to remove operator-splitting error; and 3) advanced solving method (such as the Jacobian-free Newton-Krylov (JFNK) method) to efficiently solve the highly nonlinear system. It is crucial to investigate the capabilities and robustness of these advanced methods in solving two-phase flow problems, especially when the phase appearance and disappearance phenomena are present. Such problems in two-phase flow simulations have proved to be numerically challenging, because equation system becomes singular when one phase is absent. In existing system analysis codes, such as RELAP5 [4-5] and TRAC [6], additional models are required for these parameters, and as related research work, different numerical treatments were proposed to resolve such issues. However, to our best knowledge, there are no fully consensual solutions.

Using an implicit method to solve the phase appearance/disappearance problem is even more challenging, because many known numerical treatment methods require certain level of explicit manipulations of the solutions. In a recent study done by Ashrafizadeh et al. [1], a JFNK method was used to solve one-dimensional two-phase flow problems with implicit time integration scheme. However, this work did not provide satisfactory results for the two-phase flow phase appearance/disappearance problems. Frepoli et al. [2] 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. Momentum equation of the vanishing phase is modified in order to render it non-singular. Mass and energy equations are also manipulated, when phase disappearing in expected. In our previous work [3], numerical methods were proposed and proved to be capable of solving two-phase hydrodynamic problems with phase appearance and disappearance due to advection. The treatment on the momentum equation is similar to that used in the work of Frepoli et al. [2].

In this work, it is our objective to further investigate the proposed methods in solving two-phase flow phase appearance/disappearance problem caused by phase change (boiling for example), in which the energy equations will be included and improved numerical treatments must be considered.

TWO-PHASE FLOW MODEL

The two-fluid single pressure two-phase flow equations used in this work are similar to those used in the existing system analysis codes, such as RELAP5 [4-5] and TRAC [6]. For simplicity, we do not include the wall friction terms and virtual mass terms for the flow boiling simulation. The simplified two-fluid model is summarized in equations (1)-(6):

\[
\frac{\partial (\alpha \rho)}{\partial t} + \frac{\partial (\alpha \rho u)}{\partial x} = -\Gamma_w
\]

(1)

\[
\frac{\partial (\alpha \rho u)}{\partial t} + \frac{\partial (\alpha \rho u^2)}{\partial x} = \Gamma_w
\]

(2)

\[
\alpha \rho \frac{\partial u}{\partial t} + \alpha \rho u \frac{\partial u}{\partial x} + \frac{\partial p}{\partial x} - \alpha \rho g \frac{\partial x}{\partial x} - C_i(u_i - u_j)|u_j - u_i| + \Gamma_g(u_{int} - u_j) = 0
\]

(3)

\[
\alpha \rho g \frac{\partial u}{\partial x} + \alpha \rho g u \frac{\partial u}{\partial x} + \frac{\partial p}{\partial x} - \alpha \rho g \frac{\partial x}{\partial x}
\]

(4)

\[
\frac{\partial (\alpha \rho e)}{\partial t} + \frac{\partial (\alpha \rho u e)}{\partial x} + p \frac{\partial u}{\partial t} + p \frac{\partial (\alpha u)}{\partial x} - Q_{wl} - Q_{lg} + \Gamma_w h_l = 0
\]

(5)

\[
\frac{\partial (\alpha \rho e)}{\partial t} + \frac{\partial (\alpha \rho u e)}{\partial x} + p \frac{\partial u}{\partial t} + p \frac{\partial (\alpha u)}{\partial x} - Q_{wl} - Q_{lg}
\]

(6)

\[
\frac{\partial (\alpha \rho e)}{\partial t} + \frac{\partial (\alpha \rho u e)}{\partial x} + p \frac{\partial u}{\partial t} + p \frac{\partial (\alpha u)}{\partial x} - Q_{wl} - Q_{lg}
\]

\[
- \Gamma_{ig} h_g - \Gamma_{ig} h_g = 0
\]

in which, the subscripts \( l \) and \( g \) denote the liquid phase and the gas phase, respectively. \( \Gamma_w \) is vapor generation rate due to wall boiling (\( \Gamma_{w_l} \)) and bulk condensation (\( \Gamma_{w_g} \)). \( Q_{wl} \) and \( Q_{lg} \) are the wall-to-liquid and wall-to-gas phase heat transfer terms, respectively. \( Q_{wl} \) and \( Q_{lg} \) are the interface-to-liquid and interface-to-gas phase heat transfer terms, respectively. Additional models are required for these parameters, and most of these models are readily available in existing system analysis codes, such as RELAP5 [4-5], which are not repeated in this summary. The variables to be solved from
this set of equations are, \( p, \alpha_g, u_l, u_g, T_l, \) and \( T_g, \) which are pressure, void fraction (volume fraction of the gas phase), liquid phase velocity, gas phase velocity, liquid phase temperature and gas phase temperature, respectively. It is noted that, \( \alpha_l + \alpha_g = 1. \)

**NUMERICAL SCHEMES**

The spatial discretization scheme used in this work is the same high-resolution scheme used in our previous works \([3, 7-8]\). This high-resolution spatial scheme provides a second order spatial accuracy for smooth solutions, and non-oscillating results near discontinuities. In all previous works and in this work, fully implicit time integration schemes are used (Backward Euler and BDF2), and the discretized nonlinear equation system is solved using the Jacobian-free Newton-Krylov (JFNK) method. The JFNK method proved to be a robust solver for the nonlinear two-phase flow problems in our previous works \([3, 7-9]\). In addition, comparing to the traditional Newton’s method, such as Frepoli’s work \([2]\), cumbersome derivation and implementation of complex Jacobian matrix could be avoided by using the JFNK method.

**Numerical Treatment When One Phase is Absent**

As demonstrated in our previous work \([3]\), when energy equations are not considered, the singularity issue of the equation system can be resolved by factoring out the \((\alpha p)\) term from both phasic momentum equations. However, such an approach is difficult to apply on the energy equations, such that the six-equation model raises more challenges in dealing with the phase appearance/disappearance issue. Instead, a new unified and yet simple approach is used in this work to treat the singular momentum and energy equations when one phase is absent. Using this new approach, there is no need to factor out the \((\alpha p)\) term from momentum equations.

Using the absent gas phase as an example, when the calculated void fraction is smaller than a preset small value \((10^{-9} \text{ in this work})\), the interfacial drag and the gas-to-interface heat transfer are evaluated as if the void fraction is \(10^{-9}\). As all the other terms vanish due to void fraction much smaller than \(10^{-9}\), these two treated terms bound the absent gas phase in a thermal-hydraulics state with physical meaning. For example, to simulate a boiling system, when the vapor phase does not yet physically exist (e.g. subcooled flow which precedes boiling flow), its velocity and temperature are calculated as the liquid phase velocity and the saturated temperature, respectively.

**TEST RESULTS**

The main purpose of this work is to demonstrate the capability and robustness of the proposed numerical methods in implicitly solving two-phase phase appearance problem due to boiling. It is also important to assure that such methods are capable and robust in solving single-phase problems while using the two-fluid model. In this section, two problems are presented: the first one is a single-phase flow problem with wall heating, and the second one is a subcooled flow boiling problem due to wall heating.

**Single-Phase Problem**

It is 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 codes, a residual volume fraction is used for the absent phase. Although the residual volume fraction is generally small, it introduces additional numerical errors. Ideally, for single-phase flow simulation, a zero volume fraction should be used for the absent phase. In this subsection, we will demonstrate that, for single-phase liquid flow, the proposed scheme allows zero volume fraction for the absent vapor phase and the scheme is still well behaved.

The single-phase flow test case consists of a vertical pipe with length of 1.5 m. The pipe is initially filled with single-phase liquid water and the initial void fraction \(\alpha_{g,\text{ini}} = 0.0\). Inlet conditions (bottom of the pipe) for the liquid phase are: \(G_{\text{inlet}} = 2037 \text{ kg/m}^2\text{s}, T_{\text{inlet}} = 504 \text{ K}\). Zero inlet mass flux boundary condition is used for the vapor phase. The outlet condition (top of the pipe) is set to be \(p_{\text{outlet}} = 6.81 \text{ MPa}\). A constant heat flux, which is not enough to initiate boiling, \(q''_w = 0.40 \text{ MW/m}^2\), is applied on the wall.

Numerical results were obtained in a transient simulation, with the number of finite volume cell \(N_{\text{cell}} = 40\), and time step size \(\Delta t = 10^{-2} \text{ s}\). The end of the simulation time is \(t_{\text{end}} = 5 \text{ s}\). Steady-state results were obtained at the end of the transient simulation. In the simulation results, the numerical solutions to the void fraction are in the order of \(10^{-21}\), which is effectively zero. Fig. 1 shows the distribution of phasic velocities along the pipe. It is observed that the vapor phase (absent phase) velocity is correctly bounded to the liquid phase (dominant phase) velocity. Fig. 2 shows the distribution of phasic temperatures, as well as saturation temperature, along the pipe. The liquid phase temperature increases due to wall heating, and the vapor phase temperature is correctly bounded to the saturation temperature.

**Subcooled Flow Boiling Problem**

The numerical setup of the subcooled flow boiling problem is essentially the same as the single-phase problem, except that the wall heat flux is increased to 1.13 MW/m². In this case, the applied wall heat flux is high enough to generate wall boiling. The phase appearance due to wall boiling is a numerical challenge to Newton’s method, as it generates discontinuities in the solution space. In this work, the JFNK method gave satisfactory results. As shown in Fig. 3, the void fraction becomes larger than \(0\) at \(\sim 1.0 \text{ m}\) in the axial position due to wall boiling. Fig. 4 shows the phasic velocities along the pipe length. In the single-phase region, the vapor velocity is the same as that of the liquid...
phase. In the two-phase region, the vapor phase ‘drifts’ away from the liquid phase due to buoyancy effect, and thus has a larger velocity than that of the liquid phase. The phasic temperatures are shown in Fig. 5. The liquid phase temperature increases due to wall heating, and eventually becomes close to saturation. The vapor phase temperature always remains very close to the saturation temperature, as expected.

Numerical Convergence

In this section, numerical convergences of the numerical methods and solving scheme used in this work are provided, with and without the phase appearance/disappearance numerical treatment methods proposed in this work. Using the subcooled flow boiling problem as an example, at the second time step, convergence histories are plotted in Fig. 6, with and without the numerical treatment for phase appearance and disappearance. With the numerical treatment, the JFNK method converges in 5 nonlinear iterations, with residual dropping about 9 orders of magnitudes. On the contrary, without the numerical treatment, the method did not converge and failed at the 25th nonlinear iteration due to ‘DIVERGED_LINE_SEARCH’ error. In addition, automatic time step reduction to use smaller time step size could not resolve the issue. The comparison shown in Fig. 6 clearly demonstrated the effectiveness and efficiency of the proposed numerical treatments for phase appearance and disappearance.

CONCLUSIONS

In this study, a high-resolution spatial discretization scheme and a fully implicit time integration scheme have been applied to solve one-dimensional two-phase flow problems. Numerical treatment was proposed to deal with the singularity issue when one phase is absent, and when it first appears. The treatment proved to be effective and efficient in this work. The nonlinear system is solved with the JFNK method. Two cases were tested in this work, including a single-phase problem and a subcooled flow boiling problem. Both of them demonstrated that the JFNK method is capable and robust to solve the phase appearance/disappearance problems. Comparing to the traditional numerical treatment methods, the methods proposed in this work are able to predict void fraction as zero, when the vapor phase is absent. It is expected that such methods can reduce numerical errors associated with the ‘residual’ volume fraction of the absent phase, normally used in the traditional methods.
Fig. 4. Subcooled flow boiling problem, axial phasic velocities distribution at the steady state, with $N_{cell} = 40$, $\Delta t = 10^{-2}$ s, and $t_{end} = 5$ s.

Fig. 5. Subcooled flow boiling problem, axial phasic temperatures and saturation temperature distribution at the steady state, with $N_{cell} = 40$, $\Delta t = 10^{-2}$ s, and $t_{end} = 5$ s.

Fig. 6. Convergence history of the subcooled flow boiling case, at time step = 2, with and without phase appearance/disappearance numerical treatment.

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