INTRODUCTION

In the nuclear engineering, 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. Several nuclear reactor system analysis codes have been developed to solve the simplified one-dimensional two-phase flow equations to represent the complex reactor systems. These codes, such as RELAP5 [1-2] and TRAC [3], have gained great successes in supporting reactor safety analyses, as well as design and licensing of new reactors.

First-order numerical schemes in both space and time were widely used in these codes. However, these schemes are highly diffusive and not always desirable in many applications such as boron solute transport. As we aim 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. These include: 1) high-resolution spatial discretization scheme in order to improve the spatial accuracy; 2) fully implicit time integration schemes in order to allow large time step and to improve the temporal accuracy; 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, and especially when phase appearance/disappearance presents. Frepoli et al. [4] made an attempt to solve the one-dimensional three-field two-fluid two-phase flow equations using a Newton’s method. Several problems were tested, however, only limited success was achieved. As the authors stated, there were many unresolved issues. However, this work provided many significant insights on practical issues when using Newton’s method to solve two-phase flow problems, such as the singularity issue at single-phase region, convergence criteria, time step control, and numerical Jacobian evaluation. Moussau has done pioneering works [5-7] to use the Newton-Krylov method to solve the two-phase flow problem with fully implicit method. His work provided important insights on time step control, preconditioning scheme for JFNK method in solving two-phase flow problems. Many challenging issues of the two-phase problems, such as the singularity issue, were not addressed in his works. In a recent study done by Ashrafizadeh et al. [8], a Jacobian-free Newton Krylov (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.

In this work, it is our objective to investigate the Newton-Krylov method in the applications of solving two-phase flow problems, when high-resolution spatial discretization scheme and fully implicit methods are used. We are specifically interested in the robustness of the Newton-Krylov method in dealing with singular two-phase flow problems due to phase disappearance/appearance, which has been a challenging two-phase flow simulations.

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 [1-2] and TRAC [3]. For simplicity, we focus on the two-phase hydrodynamics problems. In addition, without considering the mass transfer between the two phases and wall friction, the six-equation system is reduced to a four-equation system,

\[
\frac{\partial (1 - \alpha \rho_l)}{\partial t} + \frac{\partial (1 - \alpha \rho_l) u_l}{\partial x} = 0
\]

\[
\frac{\partial (\alpha \rho_l u_l)}{\partial t} + \frac{\partial (\alpha \rho_l u_l)}{\partial x} = 0
\]

\[
\frac{\partial u_l}{\partial t} + u_l \frac{\partial u_l}{\partial x} + \frac{1}{\rho_l} \frac{\partial p}{\partial x} - g_x - \frac{C_l}{1 - \alpha \rho_l} (u_g - u_l) |u_g - u_l| = 0
\]

\[
\frac{\partial u_g}{\partial t} + u_g \frac{\partial u_g}{\partial x} + \frac{1}{\rho_g} \frac{\partial p}{\partial x} - g_x - \frac{C_g}{\alpha \rho_g} (u_g - u_l) |u_g - u_l| = 0
\]

in which, the subscripts l and g denote the liquid phase and the gas phase, respectively. The variables to be solved from this set of equations are, \( p, \alpha, u_l, \) and \( u_g, \) which are pressure, void fraction (volume fraction of the gas phase), liquid phase velocity, and gas phase velocity, respectively. The system is closed with linearized equations of state for both phases,

\[
\rho_l(p) = 1000 + 10^{-7} (p - 10^5);
\]

\[
\rho_g(p) = 0.5 + 10^{-6} (p - 10^5)
\]

in which, \( p \) is density in \([kg/m^3]\), and \( p \) is pressure in [Pa]. An interfacial drag model similar to the model used in Städtke’s work [9] is used in this work.
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\[ C_i = \frac{1}{8} C_d a^{\text{int}} \rho_m \]  
(6)

where, the interfacial area density is estimated as,

\[ a^{\text{int}} = \frac{3\alpha(1 - \alpha)}{r_p} \]  
(7)

and the mixture density is defined as,

\[ \rho_m = \alpha \rho_g + (1 - \alpha) \rho_l \]  
(8)

Constant values, 0.44 for \( C_d \), and 0.5×10^{-3} \( m \) for \( r_p \) were used in this work, the same as in [9].

**NUMERICAL SCHEMES**

In this section, the numerical schemes for spatial discretization and time integration, as well as the Newton-Krylov method, are briefly discussed.

**High-resolution Staggered Grid Method**

In this work, the traditional staggered grid mesh arrangement is used, in which scalar variables (\( \rho, \alpha, \rho_i, \) and \( \rho_g \)) are arranged in the cell centers, while vector variables (\( u_i \) and \( u_g \)) are arranged on the cell edges. Spatially high-resolution results could be obtained by combining the donor cell upwind method with local linear reconstruction of variables. Using mass equation as an example, the mass flux is evaluated on the cell edge as,

\[ (\alpha \rho_g u_g)_i^{+1/2} = u_g^i \left\{ \begin{array}{ll} a_{i+1/2}^{+1/2} & \text{if} \ u_g^{i+1/2} > 0 \\ a_{i+1/2}^{-1} & \text{otherwise} \end{array} \right. \]  
(9)

in which, \( a_{i+1/2}^{+1} \) and \( a_{i+1/2}^{-1} \) are the reconstructed variables on the cell edge, \( i + 1/2 \), which are schematically shown in Fig. 1 (b). Similar approach is used for the momentum advection term with a slight difference (due to its primitive form),

\[ u_g \frac{\partial u_g}{\partial x} \bigg|_{i+1/2} = \frac{1}{\Delta x} \left( u_g^{i+1} - u_g^i \right) \left\{ \begin{array}{ll} u_g^{i+1} & \text{if} \ u_g^{i+1/2} > 0 \\ u_g^i & \text{otherwise} \end{array} \right. \]  
(10)

For more details of the spatial discretization schemes, readers are referred to the work done by Stelling and Duinmeijer [10].

**Newton-Krylov Method**

As fully implicit methods, such as the first-order and second-order backward differentiation formula (BDF1 and BDF2), are used for the time integration scheme, it is necessary to use iterative solving scheme, such as the Newton-Krylov method.

For a discretized nonlinear system, such as the discretized two-phase equations we are interested in, one solves,

\[ F(U) = 0 \]  
(11)

for the unknown vector, \( U = [\rho, \alpha, u_i, u_g]^T \). The solution to the nonlinear system is obtained by iteratively solving a series of Newton’s linear correction equations,

\[ J^k \delta U^k = -F(U^k) \]  
(12)

where, \( J^k \) is the Jacobian matrix; \( U^k \) is the \( k \)th nonlinear step solution; and \( \delta U^k \) is the correction vector. In the JFNK frame, the linear system, equation (12), could be effectively solved with a Krylov’s method. In the Krylov’s method, only a matrix-vector product would be required and thus it does not require the explicit form of the Jacobian matrix. It is worth noting that it is an important feature in applications using Newton’s method, since the derivation and code implementations of analytical Jacobian matrix could be a cumbersome and error-prone task for two-phase flow system analysis codes. After the correction vector, \( \delta U^k \), is solved from the linear system, the \((k + 1)\)th nonlinear step solution could be updated as,

\[ U^{k+1} = U^k + \delta U^k \]  
(13)

Fig. 1. A schematic drawing of the first-order and high-resolution spatial discretization for scalar variables. \( i - 1, i, \) and \( i + 1 \) are cell centers. \( i - 1/2 \) and \( i + 1/2 \) are cell edges. \( U \) is the scalar quantity, such as pressure and void fraction.

In our implementation of the Newton-Krylov method, the scientific computational toolkit PETSc [11] is used to solve the discretized nonlinear fluid equations.

**TEST RESULTS**

Two hydrodynamics test problems are presented in this section, including a two-phase linear advection problem and a sedimentation problem, both of which involve phase disappearance/appearance due to advection. The phase disappearance/appearance phenomenon is a challenging problem in the simulation of two-phase flows. In many applications special numerical treatments (such as limiting the minimum volume fraction of the disappearing phase) are required to treat such a singular flow condition. In this section, we will show that the Newton-Krylov method is very robust in dealing with such flow conditions, and no
special numerical treatment is required for conditions that one of the two-phase vanishes.

**Linear Advection Problem**

In the two-phase linear advection test, a 1 m long pipe is initially filled with two-phase mixtures with $\alpha = 1$, 0, and 1 in three consecutive sections, moving at the same speed at 1 m/s. The pipe is frictionless, and a same pressure is given for the inlet and the outlet. Analytically, the three columns of fluid would simply advect with their initial velocity and sharp void fraction discontinuities will maintain. First-order numerical methods (either spatial or temporal) are generally too dissipative to capture this sharp interface. With the help of high-resolution spatial scheme and high-order time integration scheme, the numerical diffusion could be significantly reduced, with the results shown in Fig. 2.

![Fig. 2. Numerical results of void fraction distribution for the linear advection test problem, with $N_{cell} = 100/400$, $\Delta t = 10^{-3}$, and $N_{timestep} = 100$](image)

The first-order results using 400 cells are only comparable to the high-order results using 100 cells. It is clear that the high-resolution spatial and high-order temporal schemes can significantly reduce numerical errors.

In addition, the JFNK method showed extremely robust and stable behaviors in solving such a singular problems without any special numerical treatments in the single-phase regions, which has never been demonstrated before.

**Sedimentation Problem**

The sedimentation problem is a test problem originally proposed by Youngs [12] for testing the phase separation due to gravity. 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 would 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. This test, the singularity is dynamically developed from the phase separation process, which is different than that of the previous advection problems.

In this test, numerical results were obtained by using 50 cells and a time step of $5 \times 10^{-3}$ s. Fig. 3 shows the transient void fraction distribution along the pipe. Two discontinuous void fronts could be found to move upward and downward, and eventually merged at the 10 second. The transient pressure profiles are shown in Fig. 4. There is no analytical solution for the transient pressure distribution and such transient profiles have been rarely reported in existing literatures. We have found our results are very similar to what Städtke have predicted [9], which is somewhat expected since similar interfacial drag terms were used.

Again, the Newton-Krylov method is able to handle the situation when singularity is dynamically developed, i.e., the void fraction values could reach 0 and 1 due to phase separation without special numerical treatments.

![Fig. 3. Void fraction distribution at different time for the sedimentation test problem, with $N_{cell} = 50$, $\Delta t = 5 \times 10^{-3}$ s](image)

![Fig. 4. Pressure distribution at different time for the sedimentation test problem, with $N_{cell} = 50$, $\Delta t = 5 \times 10^{-3}$ s](image)

**CONCLUSIONS**

In this study, high-resolution spatial discretization and high-order time integration schemes have been applied to solve one-dimensional two-phase flow problems. The nonlinear system is solved with a Newton-Krylov method. Such a method shows great robustness in dealing with
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singular two-phase problems when one of the two phases disappears/appears due to advection. Future studies will be focused on the phase disappearance/appearance phenomenon due to source terms, such as boiling and condensation. Realistic water/steam properties and closure models will also be added in the future such as the robustness of the algorithms presented in this work can be compared with other system analysis codes.

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