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Application of implicit Roe-type scheme and Jacobian-Free Newton-Krylov method to two-phase flow problems

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ABSTRACT

A new implicit second-order accurate spatial scheme for steady-state thermal-hydraulic simulations of the two-phase two-fluid six-equation model is proposed. The new scheme is based on a Roe-type numerical flux that is formulated with the help of analytical approximate eigenvalues and eigenvectors of the two-phase system. Approximate eigenvalues and eigenvectors are obtained with a structured Jacobian matrix that is general for arbitrary Equation of State (EOS). Three issues are solved in this article: (1) A fully-implicit scheme using the backward Euler method is proposed to improve the stability and avoid the time step limit of the originally explicit scheme. The fully implicit scheme is solved with the Jacobian-Free Newton-Krylov method. (2) A second-order accurate spatial scheme is proposed by converting the first-order Roe-type numerical flux to a second-order one. The conversion is made by extending an existing procedure for single-phase flows to two-phase flows. (3) Phase appearance issue is treated with a numerical procedure, which requires little modification to the schemes. The new scheme is verified and validated with two numerical tests: the faucet flow problem and the BFBT benchmark.

1. Introduction

In a previous work (Hu and Kozlowski, 2018a), we obtained analytically the approximate eigenvalues and eigenvectors of the two-phase systems that are general for arbitrary EOS. The approximate eigenvalues and eigenvectors provide the essential framework for developing a new solver that is mathematically consistent, algebraically simpler, and numerically more accurate and robust than existing solvers for realistic thermal-hydraulic simulations. An explicit Roe-type solver was developed based on the approximate eigenvalues and eigenvectors. This solver was shown to be stable by numerical tests with both simple benchmark problems and real boiling pipe problems. However, this solver had three issues:

1. The solver is based on an explicit method. It uses very small time step because of the Courant-Friedrichs-Lewy (CFL) condition. It is not suitable for long-time simulations. The stiffness of the source terms, especially the interfacial heat transfer between the interface and gas phase, has not been considered, which puts a strict limit on the maximum time step and affects the stability of the solver. Fig. 1 shows an example (one case in the following BFBT benchmark) of the stability issue of the explicit method. For the explicit method, because of the very large interface-to-gas heat transfer coefficient, the gas temperature diverges rapidly when the time step is too large.
2. The solver is only first-order accurate in space. A very fine mesh has to be used to obtain accurate results, which is computationally expensive, because the total computational time increase quadratically with the number of meshes.
3. The solver is not capable of handling phase appearance and disappearance.

These three issues are solved in this article: (1) A fully-implicit scheme using the backward Euler method is proposed to improve the stability and avoid the time step limit of the explicit Roe-type solver, see Fig. 1. The fully implicit scheme is solved with the Jacobian-Free Newton-Krylov (JFNK) method. (2) A second-order accurate spatial scheme is proposed by converting the first-order Roe-type numerical flux to a second-order one. The conversion is made by extending an existing procedure for single-phase flows to two-phase flows. (3) Phase appearance issue is treated with a numerical procedure, which requires little modification to the scheme.

Fully implicit schemes for two-phase flows have been proposed and studied by many researchers. Recently, the JFNK method became popular as a nonlinear solver for the fully implicit

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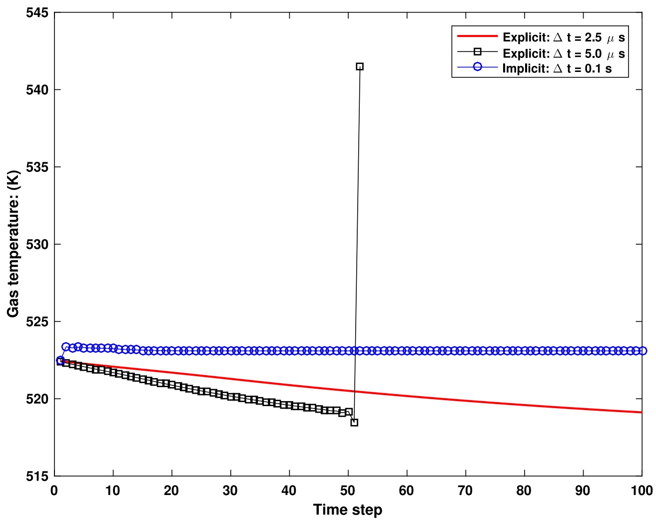

Fig. 1. Improvement of stability with an implicit scheme.

schemes. Mousseau (2004) did the pioneering work to apply the JFNK method to two-phase flows. Applications of the JFNK method to two-phase flows can also be seen in work by Ashrafizadeh et al. (2015), Abu Saleem et al. (2016), and Zou et al. (2015a, 2016b,a). Encouraging and promising results have been shown by Zou and his co-workers (Zou et al., 2015a, 2016b,a), where the fully implicit scheme was used to solve realistic two-phase flow problems, which inspired the work in this article.

Attempts to apply high-resolution schemes for nuclear thermal-hydraulic simulations have been made previously by Tiselj and Petelin (1997), Wang et al. (2013), Abu Saleem et al. (2016), and Zou et al. (2015a, 2016b,a). These attempts can be classified into two groups depending on the discretization: staggered grid and collocated grid. On a staggered grid the scalar variables (void fraction, pressure, and temperature) are stored in the cell centers of the control volumes, whereas the velocity is stored at the cell faces. On a collocated grid, all variables are stored in the cell centers of the control volumes. A collocated grid is used in our scheme. The high-resolution schemes proposed by Wang, Abu Saleem, and Zou are based on the staggered grid, which can not be directly applied to our scheme. Tiselj's scheme is based on the collocated grid, but application of this scheme to two-phase flow problems using realistic EOS requires extensive work. Because our scheme has a direct link, i.e. a Roe-type numerical flux, to the existing schemes for single-phase flows, we seek a mature high-resolution scheme for single-phase flows and extend it to two-phase flows. Mature high-resolution schemes are not rare for single-phase flows. A thorough review of these schemes can be found in Van Leer (2006), Hussaini et al. (2012). Among these high-resolution schemes, the Monotone Upstream Scheme for Conservation Laws (MUSCL) of Van Leer (1997), the Total-Variation-Diminishing (TVD) scheme of Harten (1983), and the Essentially Non-Oscillatory (ENO) scheme of Harten and Osher (1987) are the most well known. In later years, the ENO schemes have been replaced by the Weighted ENO (WENO) scheme. An application of the WENO scheme to the two-phase two-fluid model can be found in a separate work by the authors (Hu and Kozlowski, 2017). Many of these schemes are a best fit of explicit schemes; however, the TVD scheme of Harten (1983) is a natural choice for developing our implicit second-order scheme, since it requires little extra numerical work once we obtain a working first-order scheme, as will be shown in Section 3.2.

Phase appearance and disappearance issue is a major challenge in two-phase flow simulations. The discontinuity in the void fraction due to the appearance and disappearance of one phase puts a strict requirement on the robustness of the numerical scheme, especially for the implicit scheme with the JFNK method. In this work, a numerical treatment which is specific for the subcooled boiling problems is proposed, inspired by Zou's (2016b) work.

This article is organized in the following way. Section 2 presents the basic two-phase two-fluid model. Section 3 presents the numerical scheme. Section 4 presents the numerical tests for demonstrating the performance of the numerical scheme. Section 5 presents the conclusion and the discussion of the current scheme.

2. Two-phase two-fluid model

For one-dimensional (1D) problems, the two-phase two-fluid six-equation model without any differential closure correlations (Ishii and Hibiki, 2010; INL, 2012a; Bajorek et al., 2008) can be written in a vector form as

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \mathbf{P}_{ix}\frac{\partial \alpha_g}{\partial x} + \mathbf{P}_{it}\frac{\partial \alpha_g}{\partial t} = \mathbf{S} \qquad (1)$$

where $\mathbf{U}$ is the vector of conservative variables, $\mathbf{F}$ is the vector of fluxes, $\mathbf{P}_{ix}$ and $\mathbf{P}_{it}$ are the vectors related to the partial derivatives of the void fraction, and $\mathbf{S}$ is the vector of source terms. They are defined as

$$\mathbf{U} \equiv \begin{pmatrix} \alpha_l\rho_l \\ \alpha_l\rho_l u_l \\ \alpha_l\rho_l E_l \\ \alpha_g\rho_g \\ \alpha_g\rho_g u_g \\ \alpha_g\rho_g E_g \end{pmatrix}, \quad \mathbf{F} \equiv \begin{pmatrix} \alpha_l\rho_l u_l \\ \alpha_l\rho_l u_l^2 + \alpha_l p \\ \alpha_l\rho_l H_l u_l \\ \alpha_g\rho_g u_g \\ \alpha_g\rho_g u_g^2 + \alpha_g p \\ \alpha_g\rho_g H_g u_g \end{pmatrix},$$
$$\mathbf{W} \equiv \begin{pmatrix} \alpha_g \\ p \\ T_l \\ T_g \\ u_l \\ u_g \end{pmatrix}, \quad \mathbf{P}_{ix} \equiv \begin{pmatrix} 0 \\ p \\ 0 \\ 0 \\ -p \\ 0 \end{pmatrix}, \quad \mathbf{P}_{it} \equiv \begin{pmatrix} 0 \\ 0 \\ -p \\ 0 \\ 0 \\ p \end{pmatrix} \qquad (2)$$

Note that one more vector $\mathbf{W}$ is introduced to denote the primitive variables. The source vector $\mathbf{S}$ depends on the physical problem and will be given later. This model assumes all pressures, including phasic pressure and interfacial averaged pressure, are equal. Let the subscript $k = l, g$ denote the liquid phase and gas phase, respectively. The variables $(\alpha_k, \rho_k, u_k, e_k)$ denote the volume fraction, the density, the velocity, and the specific internal energy of k-phase. The summation of phasic volume fraction is one, i.e. $\alpha_l + \alpha_g = 1$. p is the pressure of two phases. $E_k = e_k + u_k^2/2$ and $H_k = e_k + p/\rho_k + u_k^2/2$ are the specific total energy and specific total enthalpy, respectively.

An appropriate EOS is required to close the system. For many practical problems in the nuclear thermal-hydraulics analysis, the temperature of two phases are required to model the source terms. In such a case, a useful EOS is given by specifying the Gibbs free energy as a function of pressure and temperature T_k, i.e.

$$g_k = g_k(T_k, p), \quad \text{for } k = l, g \qquad (3)$$

After specifying the specific Gibbs free energy, the phasic density and specific internal energy are obtained from the partial derivatives of the specific Gibbs free energy. The details about specifying the EOS through the specific Gibbs free energy are referred to (Wagner and Kruse, 1998; Hu, 2018).

Closure correlations are required for simulating the behavior of a boiling system. For this type of problems, the source vector $\mathbf{S}$ is modeled as