Progress in Nuclear Energy 88 (2016) 198-210

Contents lists available at ScienceDirect

Progress in Nuclear Energy

journal homepage: www.elsevier.com/locate/pnucene

Implicitly solving phase appearance and disappearance problems using two-fluid six-equation model

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A R T I C L E I N F O

Article history: Received 12 August 2015 Received in revised form 4 November 2015 Accepted 21 December 2015 Available online 25 January 2016

Keywords: Two-phase flow Jacobian-free Newton-Krylov method Phase appearance and disappearance Implicit method

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 stag-gered 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.

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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 (U.S. Nuclear Regulatory Commission, December 2001), TRAC (U.S. Nuclear Regulatory Commission, April 2001), and TRACE (U.S. Nuclear Regulatory Commission, 2010) 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 (Zou et al., 2015a, 2015b, 2015c, 2016), several advanced numerical methods have been investigated, and they have demonstrated capabilities in improving numerical accuracy in twophase 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







(RELAP5-3D, June 2012a), 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 (Bestion, 2000). 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 (Bestion, 2000). Frepoli et al. (Frepoli et al., 2003) made an attempt to implicitly solve the onedimensional 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. (Ashrafizadeh et al., 2015), 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 (Paillere et al., 2003), 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 twofluid 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 (U.S. Nuclear Regulatory Commission, December 2001), TRAC (U.S. Nuclear Regulatory Commission, April 2001), TRACE (U.S. Nuclear Regulatory Commission, 2010) and CATHARE (Bestion, 1990). 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),

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

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

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

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

$$\frac{\partial(\alpha_{l}\rho_{l}e_{l})}{\partial t} + \frac{\partial(\alpha_{l}\rho_{l}u_{l}e_{l})}{\partial x} + p\frac{\partial\alpha_{l}}{\partial t} + p\frac{\partial(\alpha_{l}u_{l})}{\partial x} - Q_{wl} - Q_{il} - \Gamma_{l}h_{l}^{ex} = 0$$
(5)

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

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 $\Gamma_g h_{\sigma}^{ex}$ represent energy carried with the mass transfer due to phase change or injection. The variables to be solved from this set of equations are: $\boldsymbol{U} = [p, \alpha_g, u_l, u_g, T_l, T_g]^T$, 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 (Zou et al., 2014). 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,

$$Q_{wl} = q_w^{''} a_w \tag{7}$$

$$Q_{wg} = 0 \tag{8}$$

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.

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