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# A roe-type numerical solver for the two-phase two-fluid six-equation model with realistic equation of state

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ABSTRACT

In the nuclear industry, a method based on a staggered grid is used in two-phase flow system codes such as RELAP, TRAC, and CATHARE. Solving the two-phase two-fluid model with this method is complicated. The objective of this article is to develop a new solver, which is mathematically consistent and algebraically simpler than existing codes. The extension of existing shock-capturing upwind schemes for single-phase flows is our way. A numerical solver with a Roe-type numerical flux is formulated based on a very well-structured Jacobian matrix. We formulate the Jacobian matrix with arbitrary equation of state and simplify the Jacobian matrix to a simple and structured form with the help of a few auxiliary variables, e.g. isentropic speed of sound. Because the Jacobian matrix is very structured, the characteristic polynomial of the Jacobian matrix is simple and suitable for analytical analysis. Results from the characteristic analysis of the two-phase system are consistent with well-known facts, such as the ill-posedness of the basic two-phase two-fluid model which assumes all pressure terms are equal. An explicit numerical solver, with a Roe-type numerical flux, is constructed based on the characteristic analysis. A critical feature of the method is that the formulation does not depend on the form of equation of state and the method is applicable to realistic two-phase problems. We demonstrate solver performance based on three two-phase benchmark problems: two-phase shock-tube problem, faucet flow problem, and Christensen boiling pipe problem. The solutions are in excellent agreement with analytical solutions and numerical solutions from a system code. The new solver provides essential framework for developing a more accurate and robust solver for realistic reactor safety analysis. However, improvements on the new solver is necessary for achieving a high-order accuracy and increasing the robustness.

## 1. Introduction

Two-phase flows are of great importance in reactor safety analysis. Mathematical models for two-phase flow depend on the flow configurations. For example, considering the flow of two phases, the velocity of one phase may be different from the other. For some systems, the liquid and vapor have comparable velocities; while in other systems the liquid and vapor are completely separated. Various mathematical models have been derived, some with one momentum equation for the mixture, others with a separate momentum equation for each phase. In the mixture model, one momentum equation is used for the mixture. In contrast, the two-fluid model treats the two phases separately, requiring two sets of governing equations. The more general model is the two-phase two-fluid equal pressure model proposed by averaging local field equations for each phase (Mamoru and Business, 2010). For transient two-phase flows, the two-fluid model offers more general and detailed description than the mixture model.

In the nuclear industry, a method based on a staggered grid is used in two-phase flow system codes such as RELAP (Shieh et al., 1994), TRAC (Liles and Mahaffy, 1986), and CATHARE (Barre and Bernard, 1990). In these system codes, inherent numerical dissipation and various degree of implicitness are necessary to stabilize the method. For numerical methods based on a staggered grid, scalar quantities (e.g. void fraction and pressure) are calculated at cell centers while vector quantities (e.g. velocity) are calculated at the cell boundaries. Because of this difference, the mass and energy equations are discretized differently than the momentum equations, which makes the notations for the discretized equations complicated. Solving the two-phase two-fluid model with these kind of methods is complicated. Estimation of the discretization error is important to validate a numerical solver. However, in two-phase flow simulations using the existing system codes, the discretization error is often not considered (Zou et al., 2017). The estimation of the discretization error requires continuous refinement of the mesh, which is difficult for the existing system codes. Nodalization

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is sometimes played to match the experimental data, which is highly criticized by Levy (1999). The capability of performing a rigid analysis of the discretization error through continuous mesh refinement is the basic requirement for a numerical solver. This is the main motivation for developing a new numerical solver, which is mathematically consistent and algebraically simpler than the existing system codes. The extension of existing shock-capturing upwind schemes for single-phase flows is our way.

The development of shock-capturing upwind schemes starts in early 1980s for single-phase hyperbolic systems (Euler equations of gas dynamics) by many pioneering researchers, such as Godunov (1959), Roe (1981), Van Leer (1997), Osher and Solomon (1982), and Toro (2013). The research and applications of shock-capturing upwind schemes were mainly in the aeronautical industry. Various upwind and shock-capturing schemes have been proposed for two-phase two-fluid six-equation model. Exact or approximate Riemann solver is at the heart of most upwind, shock-capturing schemes. The difficulty in constructing a Riemann solver for the two-phase system is that the eigenvalue analysis is difficult because of the coupling between the two phases and the complex equation of state (EOS). Several shock-capturing schemes have been proposed for the six-equation model. Toumi et al. (1999) proposed an approximate Riemann solver using Roe's approach assuming the liquid being non-compressible; Yeom and Chang (2006) also proposed a stable upwind scheme based on the Harten, Lax, and van Leer (HLL) Riemann solver using the stiffened EOS; Chang and Liou (2003) proposed the Advection Upwind Splitting Method (AUSM) method using stiffened EOS. Many of these schemes were based on a specific form of EOS, especially the stiffened EOS; however, the stiffened EOS is not general enough for realistic two-phase simulations.

This article provides the fundamental work on the two-phase two-fluid model for developing a Roe-type solver that is general for an arbitrary EOS. The Roe-type solver is formulated based on a very well-structured Jacobian matrix. We formulate the Jacobian matrix with an arbitrary EOS and simplify the Jacobian matrix to a structured form with the help of a few auxiliary variables, e.g. isentropic speed of sound. Because the Jacobian matrix is very structured, the characteristic polynomial of the Jacobian matrix is simple and suitable for an analytical analysis. A critical feature of the method is that the formulation does not depend on the form of EOS and the method is applicable to realistic two-phase problems. We demonstrate the solver performance with three two-phase benchmark problems: two-phase shock-tube problem, faucet flow problem, and Christensen boiling pipe problem. The convergence study of these problems shows that the Roe-type solver is mathematically consistent. Because of the analytical eigenvalues and eigenvectors, the Roe-type solver is algebraically much simpler than the existing system codes.

The ultimate objective of this work is to develop a new solver that is mathematically consistent, algebraically simpler, and numerically more accurate and robust than existing solvers for realistic reactor safety analysis. The Roe-type solver developed in this article provides the essential framework for reaching the objective. However, improvements on the Roe-type solver is necessary for achieving a high-order accuracy and increasing the robustness, which will be discussed in a follow-up article.

This article is organized in the following way. Section 2 presents the basic two-phase two-fluid model without any differential law. Section 3 presents the thermodynamic transformations for dealing with an arbitrary EOS. Section 4 presents the characteristic analysis to the two-phase two-fluid model. Section 5 presents the construction of a Roe-type numerical solver. Section 6 presents the numerical tests for demonstrating the performance of the Roe-type solver. Section 7 presents the conclusion and the discussion of the current Roe-type solver.

## 2. Governing equation

For 1D problems, the basic two-phase two-fluid six-equation model without any differential closure law (Mamoru and Business, 2010; The RELAP5-3D Code Development Team, 2012; Bajorek et al., 2008) can be written as

$$\frac{\partial \alpha_l \rho_l}{\partial t} + \frac{\partial \alpha_l \rho_l u_l}{\partial x} = S_l^c \tag{1a}$$

$$\alpha_l \rho_l \frac{\partial u_l}{\partial t} + \alpha_l \rho_l u_l \frac{\partial u_l}{\partial x} + \alpha_l \frac{\partial p}{\partial x} = S_l^m \tag{1b}$$

$$\frac{\partial \alpha_l \rho_l e_l}{\partial t} + \frac{\partial \alpha_l \rho_l e_l u_l}{\partial x} + p\frac{\partial \alpha_l}{\partial t} + p\frac{\partial \alpha_l u_l}{\partial x} = S_l^e \tag{1c}$$

$$\frac{\partial \alpha_g \rho_g}{\partial t} + \frac{\partial \alpha_g \rho_g u_g}{\partial x} = S_g^c \tag{1d}$$

$$\alpha_g \rho_g \frac{\partial u_g}{\partial t} + \alpha_g \rho_g u_g \frac{\partial u_g}{\partial x} + \alpha_g \frac{\partial p}{\partial x} = S_g^m \tag{1e}$$

$$\frac{\partial \alpha_g \rho_g e_g}{\partial t} + \frac{\partial \alpha_g \rho_g e_g u_g}{\partial x} + p\frac{\partial \alpha_g}{\partial t} + p\frac{\partial \alpha_g u_g}{\partial x} = S_g^e \tag{1f}$$

This model assumes all pressure terms, 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 should be one, i.e. $\alpha_l + \alpha_g = 1$. $p$ is the pressure of two phases. The variables $S_k^c$, $S_k^m$, and $S_k^e$ denote the source terms for the continuity equation, the momentum equation, and the energy equation of $k$-phase. The details of $S_k^c$, $S_k^m$, and $S_k^e$ will be given for specific problems.

A conservative form of the governing equation is preferable in developing a Roe-type upwind method. Thus, we rewrite Eq. (1) as

$$\frac{\partial \alpha_l \rho_l}{\partial t} + \frac{\partial \alpha_l \rho_l u_l}{\partial x} = S_l^c \tag{2a}$$

$$\frac{\partial \alpha_l \rho_l u_l}{\partial t} + \frac{\partial (\alpha_l \rho_l u_l^2 + \alpha_l p)}{\partial x} - p\frac{\partial \alpha_l}{\partial x} = S_l^m \tag{2b}$$

$$\frac{\partial \alpha_l \rho_l \left(e_l + \frac{1}{2}u_l^2\right)}{\partial t} + \frac{\partial \left[\alpha_l \rho_l \left(e_l + \frac{1}{2}u_l^2\right) u_l + \alpha_l p u_l\right]}{\partial x} + p\frac{\partial \alpha_l}{\partial t} = S_l^e \tag{2c}$$

$$\frac{\partial \alpha_g \rho_g}{\partial t} + \frac{\partial \alpha_g \rho_g u_g}{\partial x} = S_g^c \tag{2d}$$

$$\frac{\partial \alpha_g \rho_g u_g}{\partial t} + \frac{\partial (\alpha_g \rho_g u_g^2 + \alpha_g p)}{\partial x} - p\frac{\partial \alpha_g}{\partial x} = S_g^m \tag{2e}$$

$$\frac{\partial \alpha_g \rho_g \left(e_g + \frac{1}{2}u_g^2\right)}{\partial t} + \frac{\partial \left[\alpha_g \rho_g \left(e_g + \frac{1}{2}u_g^2\right) u_g + \alpha_g p u_g\right]}{\partial x} + p\frac{\partial \alpha_g}{\partial t} = S_g^e \tag{2f}$$

Note that the source terms in Eq. (2) should change accordingly during the transformation. For the following derivations, we will also use the total energy $E_k$ and total enthalpy $H_k$

$$E_k \equiv e_k + \frac{1}{2}u_k^2 \tag{3}$$

$$H_k \equiv e_k + \frac{p}{\rho_k} + \frac{1}{2}u_k^2 \tag{4}$$

For ease of derivations and discussions, we write Eq. (2) in a vector form

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \mathbf{P}_{ix}\frac{\partial \alpha_g}{\partial x} + \mathbf{P}_{it}\frac{\partial \alpha_g}{\partial t} = \mathbf{S} \tag{5}$$

where $\mathbf{U}$ is the vector of conservative variables, $\mathbf{F}$ is the vector of flux variables, $\mathbf{P}_{ix}$ 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