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Numerical implementation, verification and validation of two-phase flow four-equation drift flux model with Jacobian-free Newton–Krylov method

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A B S T R A C T

This paper presents a numerical investigation on using the Jacobian-free Newton–Krylov (JFNK) method to solve the two-phase flow four-equation drift flux model with realistic constitutive correlations ('closure models'). The drift flux model is based on Isshi and his collaborators' work. Additional constitutive correlations for vertical channel flow, such as two-phase flow pressure drop, flow regime map, wall boiling and interfacial heat transfer models, were taken from the RELAP5-3D Code Manual and included to complete the model. The staggered grid finite volume method and fully implicit backward Euler method was used for the spatial discretization and time integration schemes, respectively. The Jacobian-free Newton–Krylov method shows no difficulty in solving the two-phase flow drift flux model with a discrete flow regime map. In addition to the Jacobian-free approach, the preconditioning matrix is obtained by using the default finite differencing method provided in the PETSc package, and consequently the labor-intensive implementation of complex analytical Jacobian matrix is avoided. Extensive and successful numerical verification and validation have been performed to prove the correct implementation of the models and methods. Code-to-code comparison with RELAP5-3D has further demonstrated the successful implementation of the drift flux model.

1. Introduction

Accurate modeling and simulation of the two-phase flow phenomena are critical to the safety analysis of nuclear power reactors. Two-phase flow problems can generally be formulated using drift flux models or two-fluid models. Several existing reactor safety system analysis codes, such as RELAP5 (U.S. Nuclear Regulatory Commission, 2001) and TRACE (U.S. Nuclear Regulatory Commission, 2010), have achieved great successes by employing the two-fluid six-equation two-phase flow model that treats the two phases separately with the interfacial interactions considered by constitutive correlations ("closure models"). The drift flux models (Zuber and Findlay, 1965; Ishii, 1977; Ishii and Hibiki, 2011), on the other hand, treat the two phases as a mixture, and the models are formulated to consider the conservation laws of the mixture. The relative motion between the two phases is treated by constitutive correlations. Although the drift flux models have limitations in certain applications, they are widely used in many applications due to their simplicity and applicability to a wide range of two-phase flow problems. For example, the RETRAN-3D (Electric Power Research Institute, 1998) code uses the drift flux models and has many applications in reactor transient analyses including a small break loss-of-coolant accident. The TASS/SMR system analysis code is developed based on a three-equation drift flux model (with an additional mass equation for the non-condensable gas) for the system-integrated modular advanced reactor, SMART (Chung et al., 2012; Chung et al., 2013). Drift flux models have also been widely used in the subchannel analysis of boiling water reactor (BWR) fuel bundles Khan and Yi, 1985; Hashemi-Tilehnoee and Rahgoshay, 2013a,b, BWR core simulators (Galloway, 2010), and two-phase flow instabilities analyses (Nayak, 2007; Wang et al., 2011).

Comparing to the more complex two-fluid six-equation model, the drift flux models are relatively easier to solve and implement into a computer code. However, due to the nonlinear closure models, iterative methods are normally used in solving such equation systems to achieve convergence (Galloway, 2010; Talebi et al., 2012). The Jacobian-free Newton–Krylov (JFNK) method has gained many successes in solving nonlinear systems in different disciplines (Knoll and Keyes, 2004). Mousseau has done several pioneering works (Mousseau, 2004, 2005) to use such a method

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Nomenclatures

a_w	heating surface density, [1/m]
e	specific internal energy, [J/kg]
f	friction factor, [non-dimensional]
$\|\|E\|\|$	error norm
E_d	entrainment rate
$\boldsymbol{F}$	nonlinear function
G	mass flux, [kg/m^2-s]
h	specific enthalpy, [J/kg]
$\langle j\rangle$	two-phase volumetric flux, [m/s]
$\boldsymbol{J}$	Jacobian matrix
p	pressure, [Pa]
v	velocity, [m/s]
t	time, [s]
x	axial distance, [m]
q''	heat flux, [W/m^2]
T	temperature, [K]
$\boldsymbol{U}$	unknown vector
V_{gj}	drift velocity of gas phase, [m/s]
$\overline{V_{gj}}$	mean drift velocity of gas phase, [m/s]
$\boldsymbol{v}$	Krylov vector
x_e	equilibrium quality

Greek symbols

α	void fraction, [non-dimensional]
ε	mean absolute error
Δx	finite volume cell size, [m]
Δt	time step size, [s]
$\in$	perturbation parameter in Jacobian-free Newton–Krylov method
ρ	density, [kg/m^3]
Γ_g	volumetric vapor generation rate, [kg/m^3-s]
σ	surface tension, [N/m]

Subscripts

f	liquid phase
g	gas phase
i	finite volume cell index
inlet	inlet condition
m	mixture
sat	saturation condition
w	wall

to solve the two-fluid problems implicitly. In our previous works (Zou et al., 2015a,b), we have successfully demonstrated the applications of the JFNK method in several simplified two-fluid problems using a high-resolution spatial discretization scheme on the staggered grid. It should be pointed out that by far only simplified and continuous closure models have been used in applying the JFNK method to solve two-phase flow problems with the two fluid models (Mousseau, 2004, 2005; Zou et al., 2015a,b). Recently, the JFNK method has also been used in newly developed reactor system analysis code (Idaho National Laboratory, 2012, 2014) and its application in multi-physics simulations of nuclear reactors (Gaston et al., 2015). However, in these works, only single-phase flow model or simplified two-phase flow model was used. There are no published works showing JFNK applications with realistic closure models such as those used in the RELAP5 code with the full spectrum of flow regimes. The discontinuities in solution space, due to the discrete flow regimes, could potentially prevent the Newton's method from converging. Additionally, an effective preconditioning scheme is required to help the Krylov method converge efficiently. The same challenges are also present when applying the JFNK method to solve the drift the drift flux models. Based on these discussions, we believe that it is still lack of full understanding of the JFNK method in the applications of solving realistic two-phase flow problems. Resolving the potential issues aforementioned are critical to prove the practicability of the JFNK method applied to solving the realistic two-phase flow problems.

In this work, our objective is to investigate application of the JFNK method to solve the four-equation drift flux model with realistic and discrete closure models. Identifying and resolving numerical issues are also the purpose of this work. Section 2 provides model descriptions for the drift flux model along with the kinematic closure correlations developed by Ishii and Hibiki (2011), as well as additional constitutive correlations required to fully close the system. Section 3 presents the numerical methods to solve the drift flux model. Section 4 presents the numerical verification and validation of the code using experimental data, as well as code comparison to the RELAP5-3D (RELAP5-3D, 2012a). Section 5 presents discussions and conclusions.

2. Physical model descriptions

2.1. One-dimensional four-equation drift flux model

The one-dimensional four-equation drift flux model used in this work is directly adapted from the models developed by Isshi and his coworkers (Ishii, 1977; Ishii and Hibiki, 2011; Hibiki and Ishii, 2003, 2005). The original set of equations for the one-dimensional drift flux model includes two continuity equations (mixture and the dispersed phase), one mixture momentum equation and one mixture energy equation. In this work, the original set of equations has been simplified and is given as Eqs. (1–4):

$$\frac{\partial \rho_m}{\partial t}+\frac{\partial(\rho_m v_m)}{\partial x}=0 \tag{1}$$

$$\frac{\partial(\alpha\rho_g)}{\partial t}+\frac{\partial(\alpha\rho_g v_m)}{\partial x}+\frac{\partial}{\partial x}\left(\frac{\alpha\rho_g\rho_f}{\rho_m}\overline{V_{gj}}\right)=\Gamma_g \tag{2}$$

$$\begin{aligned}\frac{\partial v_m}{\partial t}+v_m\frac{\partial v_m}{\partial x}=&-\frac{1}{\rho_m}\frac{\partial p}{\partial x}-g_x-\frac{f_m}{2D}v_m|v_m|\\&-\frac{1}{\rho_m}\frac{\partial}{\partial x}\left[\frac{\alpha\rho_g\rho_f}{(1-\alpha)\rho_m}\overline{V_{gj}}^2\right]\end{aligned} \tag{3}$$

$$\begin{aligned}&\frac{\partial(\rho_m e_m)}{\partial t}+\frac{\partial(\rho_m h_m v_m)}{\partial x}+\frac{\partial}{\partial x}\left[\frac{\alpha\rho_g\rho_f}{\rho_m}\Delta h_{gf}\overline{V_{gj}}\right]\\&=q''_w a_w+\left[v_m+\frac{\alpha(\rho_f-\rho_g)}{\rho_m}\overline{V_{gj}}\right]\frac{\partial p}{\partial x}\end{aligned} \tag{4}$$

in which the subscripts m, g and f denote the mixture, gas phase, and liquid phase, respectively. $\overline{V_{gj}}$ is the mean drift velocity of the gas phase. Comparing to the original equations in Hibiki and Ishii's 2003 journal article (Hibiki and Ishii, 2003) and Ishii's 2011 book (Ishii and Hibiki, 2011), there are several noticeable changes that need explanations: (1) the mixture momentum equation has been rewritten in the primitive form, which was done in a similar way to obtain the primitive momentum equation for the single-phase Euler equations; (2) in the mixture energy equation,