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# A new numerical method for solution of boiling flow using combination of SIMPLE and Jacobian-free Newton-Krylov algorithms



A. Hajizadeh <sup>a, \*</sup>, H. Kazeminejad <sup>b</sup>, S. Talebi <sup>c</sup>

a Research School of Reactor, Nuclear Science and Technology Research Institute, P. O. Box 11365-3486, Tehran, Islamic Republic of Iran

<sup>b</sup> Research School of Radiation Applications, Nuclear Science and Technology Research Institute, P. O. Box 11365-3486, Tehran, Islamic Republic of Iran

<sup>c</sup> Department of Energy Engineering and Physics, Amirkabir University of Technology (Tehran Polytechnic), 424 Hafez Avenue, P.O. Box 15875-4413, Tehran,

Islamic Republic of Iran

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# ABSTRACT

In this paper, an efficient and stable numerical approach is developed in which a different combination of Jacobian-free Newton-Krylov (JFNK) and SIMPLE methods are introduced for solution of two-phase flow in both steady state and transient conditions. It is shown that, combination of Krylov subspace methods and SIMPLE type preconditioner give a fast convergence in the solution of the Drift Flux Model (DFM). It is demonstrated that the stability problem with SIMPLE approach, for two-phase flow problems, can be avoided by combining with JFNK. RELAP5 code and experimental data are considered for verification study. For all benchmarks, the proposed methods predictions are in good agreement with experiment and RELAP5 results. The accuracy of the proposed schemes were studied and compared with the classical SIMPLE method. It was found that the present approach to two-phase flow simulation predicts accurate results over a wide pressure range; whereas the classical SIMPLE algorithm underestimated the void fraction at low pressures. Finally, a typical power transient is considered to demonstrate how the problem fastest time scale can change during the course of a transient. The present assessment of the numerical method showed that the time step control is not based on a stability time step restriction, like the material Courant limit.

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## 1. Introduction

Multi-phase flow is widely involved in the boiling channels and heat exchangers. Development of an accurate and robust tool for simulation of the two-phase flows is of great importance in the design and safety analysis of the boiling systems. Several thermalhydraulic codes such as TRAC ([TRAC, 2001](#page--1-0)) and [RELAP5 \(2001\)](#page--1-0) were developed in the mid to late 1970s for simulation of the two-phase flows. These codes employed the semi-implicit numerical approaches with temporal accuracy limited to 1st order. Moreover, the time step size was restricted to the material Coura-nt-Friedrichs-Lewy (CFL) stability limit ([Zou et al., 2015](#page--1-0)).

The two-fluid model and the Drift Flux Model (DFM) are the most precise and applicable macroscopic formulations widely used in the engineering problems ([Hibiki and Ishii, 2003\)](#page--1-0). In the twofluid model formulation, dispersed phase and continues phase

\* Corresponding author. E-mail address: [anahita\\_hajizadeh1392@yahoo.com](mailto:anahita_hajizadeh1392@yahoo.com) (A. Hajizadeh). are considered separately. Therefore, it is expressed in terms of the two sets of mass, momentum and energy conservation equations. The DFM as a mixture model comprises the diffusion model, slip flow model, and homogeneous flow model. [\(Hibiki and Ishii, 2003\)](#page--1-0). It can be applied to model a wide variety of thermal-hydraulic phenomena in pressurized water reactors (PWRs) and boiling water reactors (BWRs) since the four-equation DFM can precisely simulate a vertical boiling flow due to its ability in considering the non-equilibrium effect of the two-phase flow phenomena. Finally, to complete the field equations, the constitutive models related to the relative velocity, interfacial mass transfer, wall friction, and wall heat source should be implemented in the final computational model [\(Lee and Park, 2013](#page--1-0)).

## 11. Literature review

Because of the simplicity of semi-implicit methods, many efforts are made to develop numerical models for simulation of the twophase flow problems. For example, [Jeong et al. \(2008\)](#page--1-0) applied a semi-implicit approach for implementation of the threedimensional, transient, two-fluid, and three-field model. [Liles and](#page--1-0) [Reed \(1978\)](#page--1-0) developed a semi-implicit numerical technique to solve the equations of two-phase fluid dynamics. The Newton Block Gauss-Seidel (NBGS) method is implemented in TAPINS (Thermalhydraulic Analysis Program for INtegral reactor System) to solve the DFM governing equations [\(Lee and Park, 2013\)](#page--1-0). [Fillion et al. \(2011\)](#page--1-0) integrated the DFM and solved it by the finite volume Riemanntype solvers. [Talebi et al. \(2012\)](#page--1-0) used DFM to simulate onedimensional boiling flow in a single vertical channel. They showed that the solution obtained by DFM is simple and reliable for general transient two-phase flow modeling in a heated channel. [Khan and Yi \(1985\)](#page--1-0) used DFM to develop a BWR sub-channel code.

Development of robust and stable numerical techniques is essential in the field of nuclear thermal-hydraulic safety analysis. With modern computers, it is possible to take advantage of advanced numerical approaches to solve large nonlinear systems of partial differential equations (PDE's) using fully implicit methods with second order temporal accuracy [\(Pope and Mousseau, 2009\)](#page--1-0). Fully implicit approaches are also not restricted by any stability limit. In other words, time step could be controlled by the solution dynamical time scale. Few attempts have been made to apply Newton's method for solving the nonlinear system of equations arising from the fully implicit discretization of the field equations corresponding to two-phase flow problems [\(Bestion, 1990; Barre](#page--1-0) [et al., 1992; Frepoli et al., 2003; Abu Saleem and Kozlowski, 2014\)](#page--1-0).

State of the art research demonstrates the successful implementation of the more complicated nonlinear iteration techniques, especially Jacobian-free Newton-Krylov (JFNK) as a variant of Newton's method. JFNK method is developed based on the Newton linearization approach and uses Krylov subspace to solve the correction equations at each Newton iteration. [\(Knoll and Keyes,](#page--1-0) [2004\)](#page--1-0). Although the application of JFNK in different fields is growing rapidly, few resources could be found concerning the implementation of this method for simulation of two-phase flow problems. Physics-based preconditioned JFNK method is developed by [Mousseau \(2004\)](#page--1-0) for solving the coupled two-phase flow and heat conduction equations. Their simulations demonstrate that fully implicit solution derived from JFNK method is more precise than conventional semi-implicit scheme. Discussion on JFNK method for simulation of a simplified slab reactor is made by [Pope](#page--1-0) [and Mousseau \(2009\)](#page--1-0). They concluded that there is no stability requirement for the fully implicit solution of the coupled neutronic, conduction and two-phase flow equations where the JFNK method is implemented. Three methods including explicit, Newton-Krylov (NK), and JFNK were investigated by Ashrafi[zadeh et al. \(2015\).](#page--1-0) These methods were compared for accuracy, stability and efficiency. [.Zou et al. \(2015\)](#page--1-0) developed a high-resolution spatial discretization scheme and their conclusion demonstrates the better accuracy, stability and the efficiency of the JFNK approach. Also, the application of the JFNK method as a fully implicit approach reduced the numerical errors corresponding to the temporal integration. First successful implementation of the JFNK algorithm for simulation of two-phase flow with realistic constitutive models is carried out by [Zou et al. \(2016\).](#page--1-0) They solved the two-phase four-equation DFM based on the JFNK method. In that research, a finite difference method is used to obtain the preconditioning matrix. There are two main practical difficulties with the JFNK method: 1- Newton's method convergence problem raised by inappropriate initial guess and 2- Adequate preconditioning scheme is required if Krylov method is to be successful ([Knoll and Keyes, 2004](#page--1-0)).

## 1.2. Objectives of the present study

Recently, much attention has been paid to the physics-based preconditioning. Several research studies on SIMPLE (SemiImplicit Method for Pressure Linked Equations) algorithm as a physics-based preconditioners, demonstrate its efficiency ([Elman](#page--1-0) [et al., 2008; Li and Vuiky, 2004; Segal et al., 2010](#page--1-0)). [Pernice and](#page--1-0) [Tocci \(2001\)](#page--1-0) showed that the classical pressure-correction methods such as SIMPLE can be an efficient preconditioner for the incompressible Navier-Stokes equations. The SIMPLE method is a classical algorithm in computational fluid dynamics ([Patankar,](#page--1-0) [1980\)](#page--1-0) in which pressure and velocity are coupled indirectly. Although several efforts are made to implement the Newton method and its variants for the solution of fully implicit discretized equations, no attempt is made based on the traditional powerful methods. It is noticeable that due to the iterative nature of the SIMPLE algorithm, this approach has the potential capability to linearize the nonlinear fully implicit discretized system of equations. In solving two-phase flow, this method encounters some problems such as numerical instability and lack of convergence. These problems arise from the tight coupling between the momentum and the continuity equations and also the interphase mass transfer effect [\(Miller and Miller, 2003](#page--1-0)). The tight coupling between the parameters makes the equations more dependent on the parameters evaluated in the previous iterations thus producing a destabilizing effect. To the best of our knowledge, the SIMPLE algorithm is not modified in solving the two-phase DFM. Therefore, modification of the SIMPLE method is an important contribution of the present study.

Although several studies have reported the efficiency of the JFNK approach, but little attention has been paid to its performance when used with other nonlinear solvers or their combination for better improvement.

The objectives of the present study are:

- 1. Investigation of JFNK and modified SIMPLE method as solvers for nonlinear system of equations arising from the fully implicit discretization of the DFM field equation;
- 2. Improvement of the JFNK approach by the SIMPLE method;
- 3. Modification of the SIMPLE algorithm for the two-phase flow calculations with and without using the JFNK method; and finally
- 4. Comparison of different methodologies that can be developed by the combination of the SIMPLE and the JFNK methods.

In the present study, an optimized and stable numerical solver is introduced for simulation of a boiling channel based on the combination of the SIMPLE and the JFNK methods. The present numerical technique proved viable for simulation of boiling channels thermal-hydraulics. The fully implicit discretized DFM relies on the pressure-velocity coupling based on the modified high order SIM-PLE algorithm. The SIMPLE algorithm is also used to develop a preconditioner for the JFNK method. We found that using the SIMPLE algorithm as preconditioner and the initial guess calculator can considerably improve the slow convergence of the JFNK method.

Section [2](#page--1-0) outlines a brief description of the DFM. The Fully implicit upwind scheme of the Finite Volume Method (FVM) is implemented on DFM in Section [3](#page--1-0). We successfully developed a modified fully implicit SIMPLE algorithm as explained in section [4.](#page--1-0) Section [5](#page--1-0) is devoted to the full description of the JFNK implementation in this study. Combination of the SIMPLE and the JFNK methods is illustrated in Section [6.](#page--1-0) Section [7,](#page--1-0) presents the numerical results obtained by several developed methods. Verification, accuracy, convergence and related time step control of the methods are presented in this section. Finally, Section [8](#page--1-0) summarizes our results and draws conclusions. It is shown that the developed methods based on the combination of the SIMPLE and the JFNK approaches are stable, optimized and second order accurate in time

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