



# Modification of SIMPLE algorithm to handle supercritical natural circulation in a loop

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## ARTICLE INFO

### Article history:

Received 3 December 2016

Received in revised form 29 May 2018

Accepted 31 May 2018

### Keywords:

SIMPLE

Natural circulation

Loop

Supercritical carbon dioxide

Isothermal compressibility

## ABSTRACT

The conventional SIMPLE algorithm for the pressure–velocity coupling has been adopted by many commercial CFD codes. Since it encounters convergence problem when it is used for numerical analysis of a two-dimensional unsteady natural convection flow in a rectangular cavity with zero-isothermal compressibility, the modification of SIMPLE algorithm has been proposed for such a fluid. In this paper, differences between solutions for a one dimensional natural circulation of a super-critical carbon dioxide in a loop with a horizontal heater and a horizontal cooler configuration obtained by using the conventional SIMPLE algorithm and the modified version of the algorithm are investigated. The modification of the algorithm includes updating the density at each time step based on its value at the previous time step to satisfy the mass conservation. The differences of the velocity and temperature are relatively small comparing with the two-dimensional natural convection case. As an example of utilizing the modified SIMPLE algorithm, characteristics of the unsteady natural circulation of super-critical carbon dioxide in a rectangular loop are revealed.

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## 1. Introduction

Density wave instability in a natural circulation loop operating with supercritical fluids has been analyzed using a one dimensional simulation code [1–5]. It is worth-while to analyze this instability problem using SIMPLE algorithm [6] to reduce the computation time. A ratio of isothermal to isobaric compressibilities,  $-(\partial\rho/\partial p)_T/(\partial\rho/\partial T)_p$ , of supercritical water near the pseudo-critical point (23 MPa and 650 K) is about  $3 \times 10^{-6}$  K/Pa and that for supercritical carbon dioxide (8 MPa and 308 K) is about  $6 \times 10^{-6}$  K/Pa [7]. This ratio for water is  $1.6 \times 10^{-6}$  K/Pa at the atmospheric pressure and temperature (100 kPa and 300 K). In case of an ideal gas the ratio is expressed as  $T/p$  which is about 0.003 K/Pa at the atmospheric pressure and temperature. The ratio of isothermal to isobaric compressibilities of a supercritical fluid is small as compared to that of an ideal gas and is almost equal to that of water at atmospheric pressure and temperature. A supercritical fluid near the pseudo-critical point can be assumed as a fluid with zero-isothermal compressibility. As the pressure variation in the loop is also small, hence fluid density is treated as a

function of temperature only at a given operating pressure in the above analyses.

The SIMPLE algorithm for the pressure–velocity coupling has been adopted by many commercial and non-commercial CFD codes such as FLUENT, Star-CD, Phoenix, OpenFOAM, etc. Steady [8–11] and unsteady [8,12–14] supercritical natural circulation in a loop with a heater and a cooler were numerically analyzed by using such a code. The fluid density is also treated as a function of temperature only in these analyses. Recently, one of the authors found that if the fluid density is a function of temperature only, the conventional SIMPLE algorithm encounters a convergence problem and gives a physically unrealistic velocity profile when it is used to solve an unsteady natural convection in a two-dimensional cavity [15]. The mass of the fluid in the cavity changes with time when the fluid density is considered as a function of temperature only since the volume of the cavity is fixed. The mass conservation in the cavity is not satisfied leading to convergence problem with the conventional SIMPLE algorithm. The same convergence problem should have been observed when the conventional SIMPLE algorithm was adopted to natural circulation analysis. However, the convergence problem has not been reported in the above mentioned papers which deal with the unsteady problem.

This study deals with the modification of SIMPLE algorithm for one dimensional natural circulation in a loop. As an example of

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### Nomenclature

$a$	coefficient of discretization equation	$t$	time (s)
$A$	cross sectional area of a loop ( $\text{m}^2$ )	$T$	temperature (K)
$b$	source term of discretization equation	$u$	velocity component (m/s)
$D$	diameter of a loop (m)	$V$	volume ( $\text{m}^3$ )
$f$	friction factor ( $= \frac{-(dp/dx)D}{\rho u^2/2}$ )	$x$	coordinate (m)
$g$	gravity ( $\text{m/s}^2$ )		
$h$	specific enthalpy (J/kg)	<i>Greek</i>	
$M$	mass of fluid in a loop (kg)	$\varphi$	angle between $x$ and gravity
$N$	number of control volumes (-)	$\mu$	viscosity (Pa s)
$p$	pressure (Pa)	$\rho$	density ( $\text{kg/m}^3$ )
$\dot{q}_V$	heat input or removal per unit volume ( $\text{W/m}^2$ )	<i>subscripts</i>	
$Q$	heat input or removal (W)	$e, w$	control-volume faces
$R^C$	normalized residual of continuity equation	$in$	initial value
$R^u$	normalized residual of $u$	$nb$	neighbor-point
$Re$	Reynolds number ( $= \frac{uD}{\mu/\rho}$ )	$P$	central grid point
$S_{max}$	maximum of rate of mass imbalance in each control volume		
$S_{sum}$	rate of mass imbalance in a loop		

utilizing the modified SIMPLE algorithm, characteristics of the unsteady natural circulation of super-critical carbon dioxide in a square loop are revealed.

## 2. Description of a problem

To demonstrate the modification of SIMPLE algorithm, a natural circulation square loop which is similar to Lomperski's loop [16] is considered. A schematic diagram of the loop considered is presented in Fig. 1. Both the loop height and width are  $L$ . The  $x$  is the streamwise distance and its origin is the left bottom corner of the loop. Lomperski et al. [16] used an AC direct current heater and a double tubes heat exchanger for a cooler. The heater and the cooler are located at the center of the lower and upper horizontal tubes of the loop, respectively. Therefore, it is assumed that the heater section of length  $L_H$  is heated with constant heat flux and

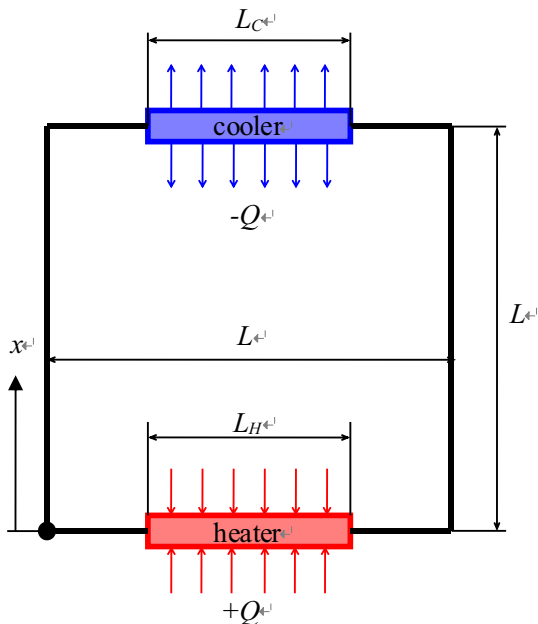


Fig. 1. A schematic diagram of a square loop.

the cooler section of length  $L_C$  is cooled with constant heat flux. The heat transfer rate in the heater and cooler sections are denoted by  $Q$  and  $-Q$ . They are located at the center of the lower and upper horizontal tubes. Initial state of the loop holds a supercritical fluid at an initial pressure  $p_{in}$  and the initial temperature  $T_{in}$ . Heating and cooling are started at  $t = 0$ .

### 2.1. Governing equations

The governing equations for one dimensional flow in a loop are well documented in the paper by Sharma et al. [14]. The continuity equation is

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0 \quad (1)$$

Integrating Eq. (1) along the loop, the following equation is obtained.

$$\frac{\partial}{\partial t} \oint \rho A dx = 0 \quad (2)$$

where  $A$  represents the cross sectional area of the loop. Eq. (2) can be rewritten as

$$\frac{\partial}{\partial t} \oint \rho A dx = \frac{\partial M}{\partial t} = 0 \quad (3)$$

where  $M$  represents the mass of the fluid in the loop. Eq. (3) expresses the mass conservation in the loop.

As mentioned before a supercritical fluid near the pseudo-critical point can be assumed as a fluid with zero-isothermal compressibility and the pressure variation in the circulation loop is not so large. This will be discussed later but it is less than 11 kPa at  $p_{in} = 8$  MPa and  $\dot{Q} = 8000$  W. The assumption that the density of the supercritical carbon dioxide is a function of temperature only, is applicable. As the volume of the loop is fixed and the fluid density is considered as a function of temperature only, the mass of the fluid in the loop changes with time after heating is started. Hence mass conservation in the loop is not satisfied. So, a special treatment for density in the continuity equation is required. This will be discussed later.

The momentum and energy equations are

$$\rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} = -\frac{\partial p}{\partial x} - \left(\frac{f}{D}\right) \frac{\rho u^2}{2} + \rho g \cos \varphi \quad (4)$$

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