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# Development of a vapor–liquid phase change model for volume-of-fluid method in FLUENT☆

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ABSTRACT

In this paper, a vapor–liquid phase change model is proposed for volume-of-fluid (VOF) method in FLUENT. This model is suitable for the case in which both unsaturated phase and saturated phase are present. In this model: (1) the unsaturated-phase thermal conductivity $\lambda_{uns}$ and specific heat $C_{p,uns}$ are actual physical parameters; (2) the saturated-phase thermal conductivity $\lambda_s$ and specific heat $C_{p,s}$ are assumed as zero and $C_{p,uns}$, respectively; (3) the interfacial mass-transfer rate $\dot{m}_s = -\dot{m}_{uns} = 2\lambda_{uns}(\nabla\alpha_{uns}\cdot\nabla T)/L$. Finally, the accuracy of the vapor–liquid phase change model is verified by one-dimensional Stefan problem and two-dimensional film boiling problem.



## 1. Introduction

Two-phase flow problems could be found in many industrial processes. But it is a great challenge to simulate these problems accurately. In the few decades, many moving interface tracking methods have been developed to simulate complex two-phase flow problems. And the most important ones include the front tracking method [1], the marker particle method [2], the level set (LS) method [3,4] and the volume-of-fluid (VOF) method [5,6]. FLUNET is the world's most widely used CFD software. The VOF method has been employed in FLUENT to simulate two-phase flow with a free surface. However, the accurate vapor–liquid phase change model is still unavailable.

In the existing models, the vapor–liquid phase change model proposed by Lee [7] has been most widely used. Its expressions are shown below:

$$\dot{m}_v = -\dot{m}_l = r\alpha_l\rho_l\frac{T-T_{sat}}{T_{sat}}, \quad T > T_{sat} \text{ (boiling process)} \tag{1}$$

$$\dot{m}_l = -\dot{m}_v = r\alpha_v\rho_v\frac{T_{sat}-T}{T_{sat}}, \quad T < T_{sat} \text{ (condensation process)} \tag{2}$$

where $r$ stands for mass-transfer intensity factor with unit $s^{-1}$. Being of an empirical coefficient, $r$ is given with different values for different problems. De Schepper et al. [8] adopted this model to simulate the flow boiling process of a hydrocarbon feedstock in the tubes of a convection section heat exchanger of a steam cracker. Here, $r$ was set as 0.1. Alizadehdakhel et al. [9] chose the same value, 0.1, to study the evaporation and condensation phenomena in a thermosyphon. However, in the references [10] and [11] $r$ was set to be 100.

Interfacial temperature is usually set as saturation temperature in the phase change process. Based on Fourier's law, the interfacial heat flux jump can be calculated by the following expression.

$$||\vec{q}_I|| = \left[\left(-\lambda_l\frac{\partial T}{\partial n}\bigg|_l\right) - \left(-\lambda_v\frac{\partial T}{\partial n}\bigg|_v\right)\right]\vec{n} \tag{3}$$

where $\vec{n}$ is the interfacial unit normal vector and points toward the vapor phase.

In References [12] and [13], the following vapor–liquid phase change model was derived according to Eq. (3).

$$\dot{m}_v = -\dot{m}_l = \frac{(\alpha_v\lambda_v + \alpha_l\lambda_l)(\nabla\alpha_l\cdot\nabla T)}{L} \tag{4}$$

because of unreasonable assumptions in the process of derivation, there is a large deviation between the computational results and the actual physical phenomena. For example, the bubble growth rate is not relevant to the vapor thermal conductivity $\lambda_v$ in the growing process of saturated bubble in superheated liquid. However, Eq. (4) contains the information of $\lambda_v$, which does not match the actual physical process.

Based on the VOF method, many authors have developed the program codes for solving the phase change problems, such as Welch and Wilson [14] and Guo et al. [15]. The key point of these methods is how to accurately calculate the interfacial heat flux on both sides, ie. $-\lambda_l\partial T/\partial n|_l$ and $-\lambda_v\partial T/\partial n|_v$ in Eq. (3). These methods can simulate the boiling and condensation problems accurately. However, the

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**Nomenclature**

| | |
|---|---|
| $C_p$ | specific heat |
| $F_V$ | interface-induced volume force |
| $g$ | gravity acceleration |
| $Gr$ | Grashof number, |
| $h$ | apparent energy with the zero defined at 298.15 K |
| $L$ | latent heat |
| $\dot{m}$ | interfacial mass-transfer rate |
| $\vec{n}$ | interfacial unit normal vector |
| $Nu$ | Nusselt number |
| $p$ | pressure |
| $Pr$ | Prandlt number |
| $\|\|\vec{q}_I\|\|$ | interfacial heat flux jump |
| $q_V$ | volume heat quantity |
| $r$ | mass-transfer intensity factor |
| $S_h$ | heat source term due to phase change |
| $t$ | time |
| $T$ | temperature |
| $v$ | velocity |
| $x, y$ | coordinates |

*Greek symbols*

| | |
|---|---|
| $\alpha$ | volume fraction |
| $\delta$ | interface position |
| $\delta x$ | cell width |
| $\kappa$ | interface curvature |
| $\lambda$ | thermal conductivity |
| $\lambda_0$ | unstable Taylor wavelength |
| $\lambda^{'}$ | characteristic length |
| $\mu$ | dynamic viscosity |
| $\rho$ | density |
| $\sigma$ | surface tension coefficient |

*Subscripts*

| | |
|---|---|
| $i$ | grid point |
| $l$ | liquid phase |
| $I$ | interfacial surface |
| $s$ | saturated phase |
| $sat$ | saturated temperature |
| $uns$ | unsaturated phase |
| $v$ | vapor phase |
| $V$ | volume |
| $w$ | wall |

solving process is complicated and needs to acquire interfacial positions and other information near interfaces. So it is very difficult to extend these methods to FLUENT.

In this paper, a vapor–liquid phase change model is proposed for volume-of-fluid (VOF) method in FLUENT. This model is suitable for the case, in which one of the two phases is unsaturated phase, i.e. under supercooled or overheated condition, the other is saturated phase, i.e. under saturation temperature. In the following we will introduce this model for incompressible two-phase flow and heat transfer in details.

## 2. Governing equations

VOF method was developed by Hirt and Nichols [5] in 1981. A volume fraction $\alpha$, of which the value lies between 0 and 1, is defined in this method. In each control volume, the volume fractions of all phases sum to unity.

$$\alpha_s + \alpha_{uns} = 1 \tag{5}$$

where the subscripts $s$ and $uns$ denote, respectively, the saturated and unsaturated phases.

The volume faction equations of saturated and unsaturated phases can be written as

$$\frac{\partial \alpha_s}{\partial t} + \nabla\cdot\left(\vec{v}\alpha_s\right) = \frac{\dot{m}_s}{\rho_s} \tag{6}$$

$$\frac{\partial \alpha_{uns}}{\partial t} + \nabla\cdot\left(\vec{v}\alpha_{uns}\right) = \frac{\dot{m}_{uns}}{\rho_{uns}} \tag{7}$$

where $\dot{m}_s = -\dot{m}_{uns}$.

Momentum equation:

$$\frac{\partial}{\partial t}\left(\rho\vec{v}\right) + \nabla\cdot\left(\rho\vec{v}\,\vec{v}\right) = -\nabla p + \nabla\cdot\left[\mu\left(\nabla\vec{v} + \nabla\vec{v}^{T}\right)\right] + \rho\vec{g} + F_V \tag{8}$$

where

$$\rho = \rho_s\alpha_s + \rho_{uns}\alpha_{uns} \tag{9}$$

$$\mu = \mu_s\alpha_s + \mu_{uns}\alpha_{uns}. \tag{10}$$

Surface tension is a surface force, which is converted into a volume force $F_V$ by the continuum surface force (CSF) model developed by Brackbill [16]. $F_V$ can be written as

$$F_V = \sigma\frac{\alpha_s\rho_s\kappa_s\nabla\alpha_s + \alpha_{uns}\rho_{uns}\kappa_{uns}\nabla\alpha_{uns}}{0.5(\rho_s + \rho_{uns})} \tag{11}$$

where $\sigma$ and $\kappa$ denote the surface tension coefficient and the interface curvature, respectively. The interface curvature is obtained from

$$\kappa_s = -\kappa_{uns} = -\nabla\cdot\left(\frac{\nabla\alpha_s}{|\nabla\alpha_s|}\right). \tag{12}$$

Energy equation:

$$\frac{\partial}{\partial t}(\rho h) + \nabla\cdot\left(\rho\vec{v}h\right) = \nabla\cdot(\lambda\nabla T) + S_h \tag{13}$$

where

$$h = \frac{\alpha_s\rho_s h_s + \alpha_{uns}\rho_{uns}h_{uns}}{\alpha_s\rho_s + \alpha_{uns}\rho_{uns}} \tag{14}$$

$$h_s = C_{p,s}(T-298.15), h_{uns} = C_{p,uns}(T-298.15) \tag{15}$$

$$\lambda = \lambda_s\alpha_s + \lambda_{uns}\alpha_{uns} \tag{16}$$

$$S_h = \begin{cases} -\dot{m}_s L & \text{when saturated phase is vapor phase} \\ \dot{m}_s L & \text{when saturated phase is liquid phase} \end{cases}. \tag{17}$$

## 3. Phase change model

In this section, a vapor–liquid phase change model is proposed for the volume-of-fluid (VOF) method in FLUENT. This model is suitable for the case in which both unsaturated phase and saturated phase are present. It includes the following three part contents:

Content-1: The unsaturated-phase thermal conductivity $\lambda_{uns}$ and specific heat $C_{p,uns}$ are actual physical parameters.

Content-2: The saturated-phase thermal conductivity $\lambda_s = 0$ and specific heat $C_{p,s} = C_{p,uns}$. The saturated-phase temperature equals saturated temperature everywhere and there does not exist heat conduction, so $\lambda_s$ is assumed as zero. Because of the temperature unchanged, the value of $C_{p,s}$ has no effect on the calculation results. For the convenience of calculation, $C_{p,s}$ is assumed to equal $C_{p,uns}$.