



# Comparison of numerical phase-change models through Stefan vaporizing problem



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## ABSTRACT

In phase-change heat transfer, it is possible that a large amount of heat is transferred with a relatively small flow rate of working fluid because a large amount of latent heat is exchanged during the phase change process. Therefore, the phenomenon is observed in various industries. However, it is difficult to systematically investigate the phenomenon only by experiment, consequently, it is important to conduct a relevant numerical study simultaneously. In the numerical analysis, it is crucial to carefully address the thermofluidic discontinuity at the phase interface. In order to calculate the mass and energy exchange through the phase interface, various methodologies have been proposed, such as utilizing the temperature difference with the saturation temperature or the heat flux around the interface. In this study, based on the VOF method, numerical phase-change models proposed by Lee, Rattner et al., and Sun et al. were investigated and compared through the Stefan vaporization problem.

## 1. Introduction

Phase change is the phenomenon of modification of a fluid's physical phase caused by thermal conditions. Because a large amount of latent heat is transferred during the phase changing process, it is feasible that a large amount of thermal energy is transferred at a relatively small flow rate. Therefore, the phase changing phenomenon has been widely applied in various industrial applications such as power plants, refrigeration systems, desalination plants etc. However, because the shape of the phase interface continuously deforms as a result of heat transfer and the deformation is significantly chaotic in certain cases, numerical or analytical approach has been applied to limitedly simple phase-changing problems and a significant number of the previous studies of phase-change heat transfer has largely been carried out by the experimental approach notwithstanding the high costs. A variety of experimental techniques using high-speed camera, infrared image processing, and transparent electrode heater have been developed over the last decade. Because of this technical development, it has become possible to explore the phenomenon at a deeper physical consideration.

The demand for direct numerical analysis of the phase changing process, however, is still increasing because of the advantage that it allows one to observe the inside of the phenomenon without any artificial interference. However, because of the complexities of the phenomenon and resulting high computing costs, numerical studies are limited to highly straightforward phase-changing problems; moreover,

there never a consensus on the accuracy of the numerical solution. To enable the use of numerical tools for the purpose of reproducing the existing experimental results as well as solving a variety of phase changing situations appearing in real engineering problems, the characteristics of the numerical model for phase changing process must be examined in advance through a simple phase-change problem.

A number of numerical phase-change models have been presented and are steadily undergoing modifications. The existing numerical phase-change models can be classified into models using the difference between cell temperature and saturation temperature (Lee [1] and Rattner et al. [2]) and models using the heat flux data around the interface cell (sharp interface model [3] and Sun et al. [4]). All of these phase-change models predict the phase change amount using the heat transfer information, and consider the energy source as the latent heat relevant to the mass change in the interface cell when solving the energy conservation.

In the case of the Lee model [1], which has been widely used because of its simplicity, the inconsistency of the numerical coefficient that directly affects the prediction of the amount of phase change poses a challenge. It was reported that a wide range of this coefficient—from  $10^{-1}$  to  $10^8$  [5–10]—was applied on a case-by-case basis. Meanwhile, Rattner et al. [2] proposed a new model that includes the computing time interval for predicting the phase change amount. They suggested the maximum allowable time step size considering thermal diffusion stability. Sun et al. [4] developed a new numerical phase-change model

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that is a control-volume-based sharp interface model, which predicts the phase change amount using the heat flux data in the computational cell including the gas-liquid interface.

In this study, the existing Lee, Rattner, and Sun models are applied to the one-dimensional Stefan vaporization problem that does not include nonlinear convection terms and thus has a simple exact solution [3,11,12]. First, the characteristics of each model will be briefly introduced. The dependency of the numerical coefficient for the Lee model and time step dependency of the Rattner model will be addressed. The time progressions in the position of the phase interface are compared between the phase-change models. Error analysis using the exact solution will be introduced.

## 2. Numerical analysis

### 2.1. Governing equations

For the one-dimensional Stefan problem, the conservation equations of volume fraction and energy after omitting the convection terms are used as a governing equation set:

$$\frac{\partial \alpha_v}{\partial t} = \frac{\dot{m}_v}{\rho_v} \quad (1)$$

$$\frac{\partial}{\partial t}(\rho h) = \nabla \cdot (\lambda \nabla T) + S \quad (2)$$

where  $\alpha$  is volume fraction,  $t$  is time,  $\dot{m}$  is mass change rate per unit volume,  $\rho$  is density,  $h$  is enthalpy,  $\lambda$  is thermal conductivity,  $T$  is temperature,  $S$  is energy source per unit volume, and subscripts  $v$  and  $l$  represent vapor and liquid respectively.

The enthalpy of the interface cell where the vapor and liquid coexist defined by the following Eq. (3):

$$h = \frac{\alpha_v \rho_v h_v + \alpha_l \rho_l h_l}{\alpha_v \rho_v + \alpha_l \rho_l} \quad (3)$$

where  $h_l$  and  $h_v$  are defined by Eqs. (4) and (5), respectively, and  $T_{sat}$  represents the saturation temperature.

$$h_l = C_{p,l}(T - T_{sat}) \quad (4)$$

$$h_v = C_{p,v}(T - T_{sat}) \quad (5)$$

where  $C_p$  is the specific heat under constant pressure condition.

The values of density and thermal conductivity applied in the energy conservation Eq. (2) are the weighted averages determined using the volume fraction of each phase.

$$\rho = \alpha_v \rho_v + \alpha_l \rho_l \quad (6)$$

$$\lambda = \alpha_v \lambda_v + \alpha_l \lambda_l \quad (7)$$

The  $\dot{m}$  (mass change rate per unit volume) and  $S$  (energy source per unit volume) in the governing Eqs. (1) and (2) are differently obtained for each phase-change model.

### 2.2. Phase-change models

#### 2.2.1. Lee model

In the Lee model, the mass change rate per unit volume is obtained using the difference between the cell temperature and saturation temperature and the volume fraction following Eq. (8):

$$\begin{cases} \dot{m}_v = -\dot{m}_l = r \alpha_l \rho_l \frac{T - T_{sat}}{T_{sat}} & \text{(for vaporization)} \\ \dot{m}_l = -\dot{m}_v = r \alpha_v \rho_v \frac{T - T_{sat}}{T_{sat}} & \text{(for condensation)} \end{cases} \quad (8)$$

where  $r$  is a numerical coefficient with  $s^{-1}$  dimensions. As mentioned previously, significantly different values of  $r$  were used on a case-by-case basis. A few researchers defined  $r$  as the mass transfer time relaxation [13] or empirical coefficient [8].

In actuality, the temperature at the phase interface is to be maintained as the saturation temperature. However, as the numerical simulation progresses, the cell temperature in the interface cell tends to deviate significantly from the saturation temperature as a result of the heat transfer between the saturated and unsaturated phases. To compensate for this and maintain the cell temperature of the interface cell to be equal to the saturation temperature, the energy source term is added to the right-hand side of energy conservation Eq. (2). Its magnitude is determined by the following Eq. (9):

$$S = \begin{cases} -|\dot{m}| h_{lv} & \text{(for vaporization)} \\ |\dot{m}| h_{lv} & \text{(for condensation)} \end{cases} \quad (9)$$

where  $h_{lv}$  is the latent heat for the phase change.

#### 2.2.2. Rattner model

To overcome the solution's dependency on the numerical coefficient in the Lee model, the following phase-change model was proposed by Rattner et al. [2].

$$S = \begin{cases} -\min(S_1, S_2, S_3) & \text{(for vaporization)} \\ \min(S_1, S_2, S_3) & \text{(for condensation)} \end{cases} \quad (10)$$

where,  $S_1$ ,  $S_2$ , and  $S_3$  are defined as follows.

$$S_1 = \left| \frac{(\rho C_p)_{eff} (T - T_{sat})}{\Delta t} \right| \quad (11)$$

$$S_2 = \begin{cases} \frac{\alpha_l \rho_l h_{lv}}{\Delta t} & \text{(for vaporization)} \\ \frac{\alpha_v \rho_v h_{lv}}{\Delta t} & \text{(for condensation)} \end{cases} \quad (12)$$

$$S_3 = \frac{h_{lv}}{\Delta t} \left( \frac{1}{\rho_v} - \frac{1}{\rho_l} \right)^{-1} \quad (13)$$

The parameter  $S_1$  is the magnitude of the heat source calculated from the phase change amount for a single computing time interval ( $\Delta t$ ); the phase change amount is obtained from the deviation between the cell temperature and saturation temperature. The parameter  $S_2$  represents the limit of the energy source because it is not practicable for the phase change amount exceed the amount of the saturated phase remaining in the cell. The parameter  $S_3$  is a device for numerical stability that limits the growth rate of the interface and is known as the Courant-Friedrichs-Lewy (CFL) condition.

The mass change rate per unit volume to be applied to the volume fraction conservation Eq. (1) is calculated by the following Eq. (14).

$$\dot{m}_v = -\dot{m}_l = -\frac{S}{h_{lv}} \quad (14)$$

This model successfully removed the ambiguous numerical coefficient in the Lee model; however, there is a likelihood of time step dependency because of the inclusion of the computing time interval for obtaining the phase change amount, as illustrated in Eqs. (11)–(13). Rattner et al. [2] suggested the following maximum allowable time step size considering the thermal diffusion stability:

$$\Delta t \leq \frac{1}{6} \left[ \Delta x^2 / \left( \frac{\lambda}{\rho C_p} \right)_{eff} \right] \quad (15)$$

where  $\Delta x$  is the grid size.

In this study, when applying the various time step sizes, the accuracy of this model is addressed through one-dimensional Stefan problem.

#### 2.2.3. Sun model

To overcome the dependency of the numerical coefficient for the Lee model and time step size for the Rattner model, Sun et al. [4] suggested the numerical phase-change model that uses the total heat

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