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# A multiphase-based numerical study on time-dependent melting, deforming and dripping process of Phase Change Material (PCM) induced by external heat source

(外部加熱を受ける可溶解性固体(PCM)の諸非定常過程(溶融・変形・落下)に関する数値解析)

**Yangkyun Kim**

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# Abstract

Deep understanding of fire damage triggered by combustion of electric wires is one of important issue in terms of the fire safety of automated facilities, such as factories, power plant etc. Combustion process of electric wire is, nevertheless, quite complicated since it consists of multi-phase, multi-dimensional time-dependent heat and mass transfer with chemical reactions in each phase and several fundamental processes are equally important so that it is relatively hard to simplify the system. For such reasons, very few attempts have been made at numerical study on the combustion involving multi-phase phenomenon, and no complete model which could cover combustion of electric wire with multi-phase phenomenon has been established yet. This research is particularly motivated by an interest in the establishment of numerical model for combustion of electric wire under multiphase framework.

In chapter 1, research of combustion of electric wire is briefly described first, and then possible numerical approach to simulate combustion of electric wire is introduced next, and then objective and strategy of thesis are shown last.

In chapter 2, mathematical formulation and numerical detail is described. To achieve our ultimate goal; such as propose of acceptable model of wire combustion, the most fundamental case that there is no species transport and reaction is considered first, then main part to be modeled is (1) how to consider the size change of the molten polymer, and (2) how to handle the complex melting process. In this regard, the governing equations in this chapter can only consist of the fundamental conservation equations (for mass, momentum and energy) under a multi-phase framework. We use the Enthalpy- Porosity and Volume of Fluid method (VOF) methods in order to approach the melting and dynamic motion of molten matter suspended by a metal plate. 2-D calculation domain, which consists of copper,

PCM (Phase Change Material as a model of polymer) and air, is tested under the normal gravity with exposing localized external thermal input. This simplified geometry provides a physically similar analogy of the wire combustion under normal gravity condition.

In chapter 3, validation of numerical models is described. This chapter mainly shows two types of validation; validation of modeling for liquid-gas interface and for melting front. Based on validation, it is concluded that models for liquid-gas interface and for melting front are qualitatively validated.

As results, chapter 4 shows melting and dynamic behavior of PCM (Phase Change Material) attached on metal plate by exploring various surface tension coefficients, external thermal inputs and melting temperatures. Pure effect of dynamic behavior of PCM is precisely investigated by comparing cases with/without deformation of gas-liquid interface on similar physical domain with experiment. It is found that behavior of molten polymer affects melting speed during its growth and dropping, and this dynamic effect on melting speed varies with different Stefan number and surface tension coefficient.

In chapter 5, by use of same computational configuration with same material properties used in chapter 4, thermocapillary convection effect on heat transfer, melting and dynamic behavior of PCM is examined. In order to consider thermocapillary convection, the source-based tangential force driven by surface tension, which linearly depends on the temperature, is modeled in the previous-proposed model. Numerical parameters are selected in order to investigate the thermocapillary motion in effective way, concluding that effect of thermocapillary convection on melting of Phase Change Material (PCM) is not so significant. However, it should be taken into account if the precise prediction of dripping-off timing is desired.

In chapter 6, the dynamic effect on melting speed is investigated with a moving external thermal source in order to explain the unsteady phenomena involved in experimental wire combustion. In this chapter, melting and deformation of polymeric material induced by a constant moving heat flux is investigated. The time-dependent melting and the behavior of the PCM are visualized together with the temperature distribution. The effect of the dynamic motion on the melting process with/without a deformable interface is discussed.

In appendix, gasification model based on previous-suggested model is discussed as ongoing

research.

**Keywords:** *Wire combustion, VOF (Volume Of Fluid) method, Enthalpy-Porosity method, Heat transfer, Phase change, Free surface tracking, Thermocapillary convection, Moving heat flux.*

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Title: Associate Professor, Dr. Eng.

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*To my wife Kyunghee Lee*

*and to my baby Seunggwon Kim*

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# Nomenclature

|                            |                                                                 |
|----------------------------|-----------------------------------------------------------------|
| $A_{mush}$                 | Morphology constant, $\text{kg}/(\text{m}^3 \text{ s})$         |
| $c_p$                      | Specific heat at constant pressure, $\text{J}/(\text{kg K})$    |
| $c_{p, \text{ effective}}$ | Effective heat capacity, $\text{J}/(\text{kg K})$               |
| $D$                        | Diffusion coefficient, $\text{m}^2/\text{s}$                    |
| $e$                        | Internal energy, J                                              |
| $erf$                      | Error function                                                  |
| $\mathbf{F}_{\text{ST}}$   | Surface force ( <i>per unit volume</i> ), $\text{N}/\text{m}^3$ |
| $\mathbf{f}$               | Gravitational force, $\text{N}/\text{m}^3$                      |
| $\mathbf{g}$               | Gravity acceleration, $\text{m}/\text{s}^2$                     |
| $H$                        | Height, m                                                       |
| $h$                        | Enthalpy, $\text{J}/\text{kg}$                                  |
| $h_A$                      | Area-weighted enthalpy, $\text{J}/\text{kg}$                    |
| $h_{ref}$                  | Reference enthalpy, $\text{J}/\text{kg}$                        |
| $\Delta H$                 | Latent heat , $\text{J}/\text{kg}$                              |
| $k$                        | Thermal conductivity, $\text{W}/(\text{m K})$                   |
| $L$                        | Latent heat of fusion, $\text{J}/\text{kg}$                     |
| $\dot{m}'$                 | Mass source, $\text{kg}/(\text{m}^3 \text{ s})$                 |
| $\mathbf{n}_s$             | Interface normal                                                |
| $p$                        | Pressure, Pa                                                    |
| $Q$                        | Body heating, J                                                 |
| $\mathbf{q}$               | Heat flux, $\text{W}/\text{m}^2$                                |
| $R$                        | Radius of curvature of the interface, m                         |
| $S$                        | Surface, $\text{m}^2$                                           |
| $S_H$                      | Volumetric source for latent heat, $\text{W}/\text{m}^3$        |

|                     |                                                                                                                       |
|---------------------|-----------------------------------------------------------------------------------------------------------------------|
| $S_M$               | Sink term( <i>per unit volume</i> ), N/m <sup>3</sup>                                                                 |
| $Ste$               | Stefan number, $(c_p (T_E - T_{liquidus}) / L)$                                                                       |
| $T$                 | Temperature, K                                                                                                        |
| $T_E$               | Temperature at external thermal input, K                                                                              |
| $T_{liquidus}$      | Liquidus temperature, K                                                                                               |
| $T_{solidus}$       | Solidus temperature, K                                                                                                |
| $T_{ref}$           | Reference temperature, K                                                                                              |
| $t$                 | Time, s                                                                                                               |
| $U$                 | Interface moving speed, m/s                                                                                           |
| $\mathbf{v}$        | Velocity, m/s                                                                                                         |
| $\mathbf{v}_s$      | Displacement velocity, m/s                                                                                            |
| $\mathbf{v}_\Sigma$ | Interfacial velocity, m/s                                                                                             |
| $V$                 | Initial volume of air, m <sup>3</sup>                                                                                 |
| $V_{PA}$            | Pendant and detached liquid volume in initial volume of air, m <sup>3</sup>                                           |
| $V_{SP}$            | Volume of solid state PCM, m <sup>3</sup>                                                                             |
| $V_{SP}$            | Volume of solid state PCM, m <sup>3</sup>                                                                             |
| $V_{TP}$            | Volume of solid state PCM, m <sup>3</sup>                                                                             |
| $W$                 | Width, m                                                                                                              |
| $Y$                 | Mass fraction                                                                                                         |
| Greek symbols       |                                                                                                                       |
| $\alpha$            | Volume fraction                                                                                                       |
| $\alpha_p$          | Averaged pendant volume fraction                                                                                      |
| $\beta$             | Liquid fraction                                                                                                       |
| $\beta_L$           | Averaged liquid volume fraction                                                                                       |
| $\Delta\beta_L$     | Deviation of the averaged liquid volume fraction between the cases of deformable and non-deformable PCM-air interface |

|               |                                                   |
|---------------|---------------------------------------------------|
| $\sigma$      | Surface tension coefficient, N/m                  |
| $\kappa$      | Curvature of free surface, 1/m                    |
| $\rho$        | Density, kg/m <sup>3</sup>                        |
| $\mu$         | Dynamic viscosity, kg/(m s)                       |
| $\varepsilon$ | Computational constant (0.001)                    |
| $\delta_s$    | Dirac function, 1/m                               |
| $\varphi$     | Body force, N/m <sup>3</sup>                      |
| $\eta_L$      | Non-dimensional position of liquid side interface |
| $\eta_S$      | Non-dimensional position of solid side interface  |
| $\eta_{SL}$   | Non-dimensional position of interface             |
| $\Phi$        | Representative of dependent variable              |
| $\mathcal{D}$ | Viscous stress                                    |
| $I$           | Unit tensor                                       |
| $J$           | Diffusive flux, N/(m <sup>s</sup> s)              |
| $\mathcal{S}$ | Rate of strain tensor                             |
| $T$           | Surface stress tensor                             |

#### Subscript

|                |                  |
|----------------|------------------|
| $e$            | East             |
| $F$            | Fuel             |
| $g$            | Gas              |
| $k$            | Phase            |
| $L\text{-PCM}$ | Liquid state PCM |
| $l$            | Liquid           |
| $MG$           | Mixture gas      |
| $m$            | Melting          |
| $mush$         | Mushy zone       |

|          |                 |
|----------|-----------------|
| $n$      | North           |
| $ref$    | Reference       |
| $S$      | Surface         |
| $s$      | South           |
| $S-PCM$  | Solid state PCM |
| $SP$     | Solid state PCM |
| $TP$     | Total PCM       |
| $V$      | Volume          |
| $w$      | West            |
| $\Sigma$ | Interface       |

# Chapter 1

## INTRODUCTION

### 1.1 Background and motivation

#### 1.1.1 Thermal decomposition of polymeric material

Many objects are composed of synthetic polymer, such as furniture, home appliance, pipe line and thermal insulator in building, factory, vehicle, etc. Today, synthetic polymer materials are rapidly replacing more traditional materials such as steel and nonferrous metals, natural rubber and so on. The objects composed by synthetic polymer potentially have fire hazard when exposed to fire [1]. Figure 1.1 shows different modes in which fuel vapor is generated from a solid. Such routes are determined by mechanisms of thermal decomposition based on molecular structure of polymers. Looking at process in Fig. 1.1, one can see that thermal decomposition route ‘b’, ‘c’, and ‘d’ undergo melting process while route ‘a’ and ‘e’ do not have melting process. When we put certain heating above a particular temperature, some polymers that have cross-linked structure, such as polyacrylonitrile and poly(oxy-m-xylene), undergo route ‘a’, then polymer is decomposed, evolving volatile species. Most are directly changed to gases from solid state polymer without passing through a liquid stage, leaving behind carbonaceous residue. On the contrast, polymers which decomposed by random scission (e.g., polyethylene and polystyrene) undergo route ‘b’, ‘c’, and ‘d’, thus, considerable molten polymers that undergo route ‘b’, ‘c’, and ‘d’ can results in potential cause of fire growth. Generally these kinds of polymers are called “thermoplastic materials” [2].

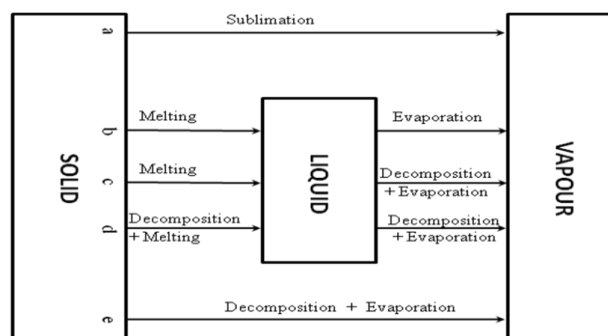


Figure 1.1 Modes of plastic thermal decomposition [2]

### **1.1.2 Fire hazard of polymeric material involving melting, deforming and dropping**

Thermoplastic materials that undergo melting process can cause considerably complicated fire scenario. This is because burning molten polymer can affect the flame spreading rate by changing its shape, and sometime induce a pool fire over the burnable objects. The pool fire may accelerate the flame spread of thermoplastic and thus generate more molten polymer to increase its intensity. This phenomenon can inevitably render much more heat and heavier toxic smoke, and will be a potential hazard to occupants and fire fighters. Consequently, it is important to investigate mechanisms that dominate the melting of thermoplastic material involving dynamic behavior during the fire. Several researches have been done for melting and dynamic behavior of thermoplastics. Sherratt [3] examined various types of potential secondary fire induced by pool fire. He found that chain breaking mechanism is the main factor to control the rate of decrease of the average chain length, which dominates the flow rate. Ohlemiller et al. [4] studied the role of polymer melt viscosity and flammability behavior when vertically oriented thermoplastic is irradiated by radiant heat flux. They reported that the burning behavior of a thermoplastic object can vary strongly with the conditions under which it is burned if its melt viscosity generates considerable flow. Zhang et al. [5-6] studied the effect of melting behavior on upward flame spread of thermoplastic materials when subjected to small ignition. They found that the melting behavior of thermoplastic polymers significantly affects their burning behavior, particularly in upward flame spread. This melting can result in a pool-like fire for polymer linings installed in a wall configuration. It was observed that the size of the flame from the pool fire controlled the flame spread on the panel, and also that flame height from the pool was a function of pool area, resulting from molten polymer flow from the vertical sheet. Xie et al. [7] experimentally studied the melting and flowing behavior of thermoplastics combustion with a T-shape trough. The results show that the softening and clinging of the thermoplastic sheets plays a considerable role during their vertical burning process.

Although several researches have been made on fire behavior of polymeric material involving melting, deforming, and dropping, it still lacks fundamental observation in order to understand detailed phenomena of melting, deforming, and dropping during fire. Reason could be found in

difficulty in experiment. Since all phenomena combines together, it is hard to extract and observe each role such as melting, deforming, and dripping, simplification is first necessary. Therefore it is strongly recommended to simplify the problem and study fundamental behavior of melting, deforming, and dropping under various potential conditions by using parametric numerical research. One of well known standard test is shown in [29]. They simplified sample as rectangular and investigated melting, deforming and dropping process during fire. However, since shape of sample is very simple, it is hard to apply itself to engineering field or industry. It is necessary to investigate and apply those problem into real engineering field.

### **1.1.3 Wire combustion**

One of special combustion case which involves melting, deforming, and dropping phenomena is combustion over insulated electric wire. It has been investigated as an important fire safety issue in connection with a variety of aspects of fires in building and automated facilities, such as factories, power plants, etc. According to reported statistics, fires involving electrical wiring account for 13,000 fires and \$ 0.5 billion in property loss during a year in USA [8] and account for 3 % (971 cases) of all fires in Japan [9]. It is desirable to prevent fires through an accurate understanding of their causes. Therefore, model introduced in this thesis is applied to melting, deforming, and dropping process which happen in insulated electric wire without combustion process.

Over the past few decades, a series of experimental studies on combustion over the electric wires has been conducted, providing a rich database [10-13]. Bakhman explained that the metal rod in the wire could play an important role to determine the combustion process of the electric wire [14-15]. Umemura et al., revealed, by the numerical approach, that the thermal interaction between the metal rod and surrounded insulated matter (mainly polymeric materials) is a leading key process in understanding the fire character of the wire [16]. Nakamura et al. investigated pressure effect on flame spread over electric wire in enclosed vacuum chamber, elucidating that the flame spread rate increases with decreasing pressure[17], and suggesting that two distinctive modes (flame-driven and wire-driven modes) are spread-dependent controlling factors [18]. In particular, Nakamura et al. reported that

molten PE significantly deformed and eventually dropped from the bulk of the insulation during the spreading event under the low pressure condition as shown schematically in Fig. 1.2 [19]. It shows the magnified still image of spreading flame over the specially-designed “model” wire (polyethylene-coated on the several kinds of metal wires. For details, see above references). During the combustion event, the coated polymer liquefies to form large molten ball, and then decomposes to produce fuel gas released into the atmosphere. As notified clearly, it includes complex phenomena associated with the formation of molten layer; e.g., deformation of outer shape, bubble formation and its internal motion in the molten polymer etc. Moreover, it has also been found that the size of molten polymer gradually increased during the flame spread over the wire under the limit condition. As a result of the size growth, "falls-off" of molten layer is frequently observed. The timing of the dropping off of PE was not random, but rather was periodic, and the frequency depended on the applied environmental conditions such as the type of burning materials. Importantly, this observation on significant PE-deformation concerns two major problems involved in predicting the associated fire hazard. One is the non-steadiness of the spreading rate owing to the continuous change of the size of the molten PE caused by frequent accumulation and dropping off [19]. This is important in fire science because one needs to determine whether the spread rate over the electric wire, as one representative of multi-layered combustibles, can be considered as the system eigenvalue or not. All the previous works, which define flame spread rate, suggest that the flame spread event is steady problem [20-21]. The second is the enlargement of fire damage, not limited to the region around the cable but also extending to the space underneath owing to the dropping of the PE. Therefore, as similar with general thermoplastic material which exposed to the fire, understanding the enlargement of fire damage caused by melting and dynamic behavior of polymeric material is an important issue for establishing better safety strategies to prevent the growth of fire.

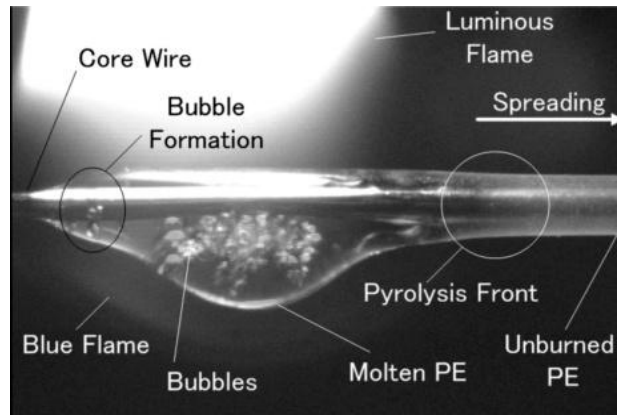


Figure 1.2 Typical observation of flame spreading over polyethylene (PE) coated electric wire [19]

## 1.2 Objective and scope

The objective of this study is to establish simplified numerical model for melting, deforming, and dropping process during fire. Figure 1.3 shows flow chart for sequential modeling for combustion process which involves melting, deforming, and dropping process. However, it is very hard to establish whole model to predict all phenomena involving fire even though it is simplified. Reason could be summarized following. First, three phases (solid, liquid, and gas phase) are necessary to be solved simultaneously. Second, melting and gasification process as phase transition are necessary to be modeled accurately. Third, accuracy of tracking free surface should be guaranteed. Fourth, huge computational costs are necessary in order to consider all phenomena. Therefore, it is also valuable to consider the most fundamental case that involves melting, deforming, and dropping process under analogical condition with fire without combustion process.

In this thesis, we only focus on the melting, deforming, and dropping process subjected to external heat source which is given as similar condition with fire by doing numerical parametric research. Thus, scope of thesis is bounded from modeling 1 to 4 in Fig. 1.3. In order to achieve this objective, the fundamental conservation equations (for mass, momentum and energy) are solved with Volume of Fluid method (VOF) [49] and Enthalpy-Porosity [72-73]. The 3-D configuration of polymer coated wire surrounded by air is simplified as 2-D PCM attached on the metal plate surrounded by air. This study could cover moveable external thermal input-induced melting, deforming and dropping

phenomena of the polymeric material attached on the metal plate associated with thermocapillary convection. This study could partially cover the gasification associated with above-mentioned phenomena. The modeling for reaction will be reported in the future work.

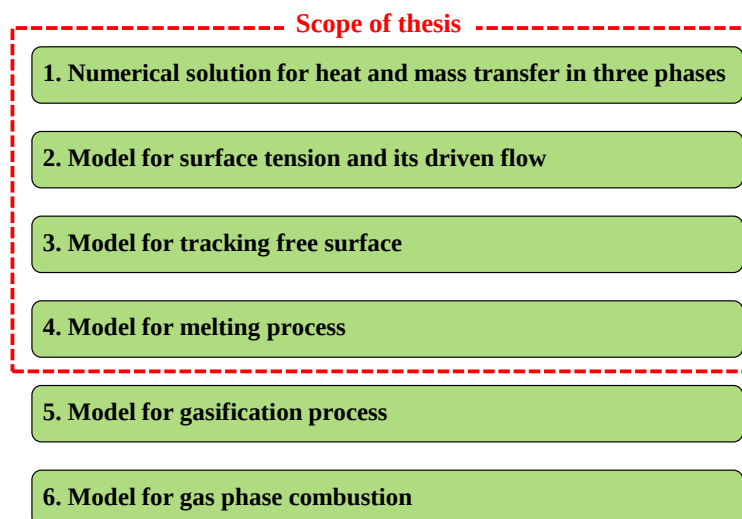


Figure 1.3 Flow chart of sequential modeling for combustion process involving melting, deforming, and dropping process and scope of current thesis

## 1.3 Numerical approach

Polymeric material does “melt” and “evaporate” during the fire event. Those phase change play a role in flame spreading because it is directly connected in heat transfer and generation of fuel. The shape of liquefied polymer freely modifies and sometimes tremendously deforms, thus, the precise tracking of the liquid-gas interface is one of important task since the major chemical reaction at interface should govern the overall gasification rate [22-23], ie., gas-phase combustion behavior. Unfortunately, it is hard to track the complete history of melting and deforming of polymeric material with combustion process in experiment, numerical observation is required. In fact, International Collaborative Project to Evaluate Fire Models for Nuclear Power Plant Applications (ICFMP) assessed and validated fire simulation codes for cable fire scenarios in nuclear power plant [24]. However, all models presented in [24] are predicting flame spread rate, focusing on developing the pyrolysis model without considering melting process. Only a few numerical attempts have been made

on this subject because of the complexity of the numerical modeling representing the melting and dynamic behavior simultaneously. Zheng et al. [25-27], numerically investigated diffusion flame over a solid surface and the associated melting effect, showing that an increase of Stefan number increases the flame spread rate and the size of the flame. However, their focus was limited to the energy change caused by melting under a flat surface with constant density, and no consideration of fluid motion was made, either inside or on the molten surface. Schiller et al. [28] and Di Blasi [22-23] simulated flame spread over liquid fuel with the inclusion of surface tension effects, and revealed that considerable motion near the gasifying surface ahead of flame is initiated by thermo-capillary flow. Obviously this study of liquid combustion did not involve melting. Most recently, Butler et al. [29] and Oñate et al. [30] successfully simulated the time-dependent behavior of melt flow and gasification of polymeric materials exposed to radiant heating using the Particle Finite Element Method (PFEM). Their numerical results revealed that PFEM can calculate both melting and dynamic motion of polymers. However, their simulation did not include a precise analysis of heat transfer associated with melting.

### **1.3.1 Numerical model under the multiphase framework**

In order to solve melting, deforming, and dropping process under analogous condition with fire, we need to introduce numerical calculation based on multi-phase framework because tracking the interface and phase changes are inherently associated in the problem.

#### **1.3.1.1 Tracking melting front**

In the past, a few analytical methods of tracking melting front offered an exact solution [85]. Even though they were mathematically robust, applicable ranges of solution are limited to one-dimensional cases of an infinite or semi-infinite region with simple initial and boundary conditions and constant thermal properties. Therefore, treatments were extended to numerical analyses with finite difference and finite element methods. Particularly, because of their simplicity in formulation, finite difference method (FDM) is still used for a wide range of industrial processes. The essential feature of FDM is that the latent heat absorption or release is accounted for in the governing energy equation by defining

either a total enthalpy [31-34] or a specific heat capacity [35]. Consequently, the numerical analysis can be carried out on a space grid that remains fixed throughout the calculation, the so-called fixed grid method [36]. In contrast to the variable grid method, domain or coordinate transformation does not require proving a low computational cost. One of approaches in the fixed grid method, enthalpy method taking account of latent heat evolution, is applied in our calculation. A major advantage of the enthalpy method is that it can calculate the melting with convection in transient region between solid and liquid by the simple concept of porosity [37]. In other words, the combined Enthalpy-Porosity method can accommodate the zero velocity condition which is required as a liquid region turns to solid. Mathematical treatment of this method is very simple, and has a wide range of application such as energy storage systems and casting processes [38-40]. By using this method, we can include the effect of latent heat of melting and track the position of the melting front.

### **1.3.1.2 Tracking liquid-gas interface**

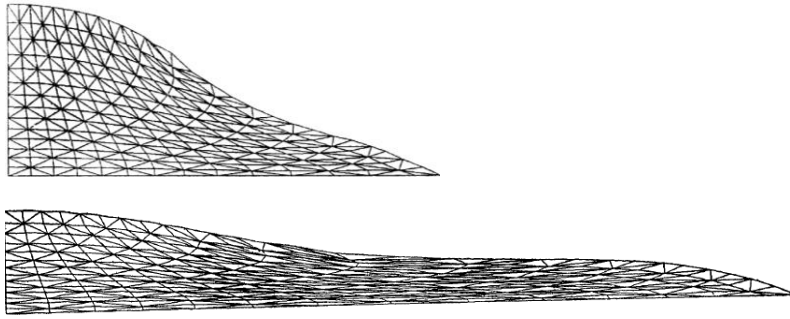
Existing methods for the computation of free surfaces and fluid interfaces can be classified into two groups [41], namely:

- interface tracking methods,
- interface capturing methods.

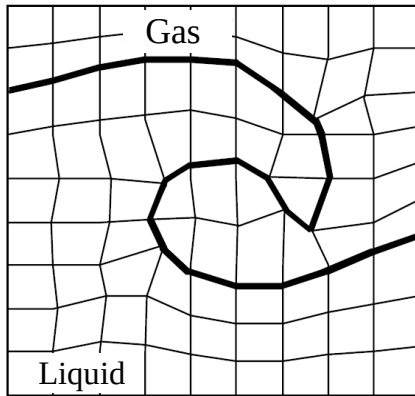
#### **1.3.1.2.1 Interface tracking method**

As shown in Fig. 1.4, interface tracking methods has two types; moving grid and body-fitting method. Moving grid method solves for the flow within the liquid region only, the free surface being placed at the boundary of the computational domain, whereas, body-fitting method solves for the flow within two phases, the free surface being placed at inside of computational grids by associating the interface with a set of nodal points. The motion of the free surface in both methods is accounted by a coordinate transformation which maps the motion of the interface so that system maintains sharp interfaces for which the exact position is known during the calculation [42]. Various techniques for moving grid and for body-fitting method to attach the interface to a mesh surface have been developed [43-45]. These methods are implemented mainly to reduce computer storage needed for the interface markers, and

ensure a sharp interface. However, if the interface is experienced the high distortion, a new mesh needs to be generated in order to prevent both grid singularities and highly skewed grid. For this reason, these methods are limited to interfaces which are not subjected to large deformations [46], so that the special treatment in order to deal with interfaces which are exposed to large deformations or stretching. For instance, numerical results on the collapse of a liquid column show that such large deformations may occur even in an early stage of the computation [46]. To maintain a well defined mesh it would therefore be necessary to re-mesh continuously, which brings with it yet more complexities.



(a)



(b)

Figure 1. 4 Example of time-dependent liquid behavior simulated by (a) moving grid and (b) body-fitting method

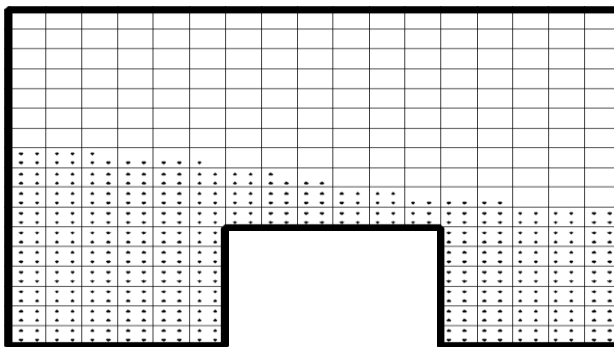
#### 1.3.1.2.2 Interface capturing method

The Interface capturing methods avoid the grid-related problems associated with interface tracking

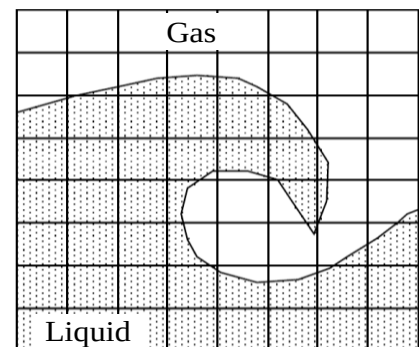
methods by employing a fixed grid and by defining the location of the liquid and gas regions in the fixed grid. In a fixed grid system, the interface can potentially occupy any position, and its position is determined by capturing the fraction of near-interface cell that is partially filled. Interface capturing methods typically discretize the computational domain into non-overlapping cells which are then designated, depending on whether the cell contains all liquid, all gas, or the interface. The cells must be designated at each time step to reflect the new interface configuration.

#### a. The marker and cell method (MAC)

The numerical schemes, which first introduced the interface capturing idea, was the marker and cell (MAC) method proposed by Harlow and Welch [47], conceptual description is shown in Fig. 1.5 (a). In this method, the location of interface is identified by placing discrete, mass-less “marker particles” in one phase and convecting them according to the instantaneous velocity field, while a cell with no markers are considered to be empty [47]. The particles are only used to distinguish phases and do not participate directly in the calculation. The MAC method is readily expandable to three-dimensional computations and also can deal complex phenomena such as wave problem [48]. However, in three-dimensional calculation, a significant increase in computational effort is necessary because a large number of particles should be necessary to track the motion satisfactory with solving the governing equation for flow.



(a) The MAC method



(b) Advanced interface capturing method

Figure 1. 5 Example of interface capturing methods [48]

## **b. Volume of fluid (VOF) and level set (LS) method**

Two of the most popular versions of interface capturing methods are the volume of fluid (VOF) [49] and the level-set (LS) method [50]. In the VOF method, a scalar field quantity is introduced and advected *on* the grid. The fluid interface is located where the volume fraction experiences a sharp change. The LS method is similar to the VOF method in the sense that a scalar field quantity detects the presence of either one of the multi phases, and is advected *on* a grid [51]. However, by using LS approach the field quantity is *not* interpreted as a fluid volume fraction, but as a distance to the interface which itself corresponds to an isovalue manifold of the level-set function. In LS method, a continuous function known as a LS function is applied over the whole computational domain. By using LS method, the interface is defined at which LS function has the value of zero, the signed distance function is set to make a distinction between phases. Numerous researches have been paid attention to develop level-set method in order to get better accuracy and efficiency. Chang et al. [52] proposed a level-set formulation to compute an incompressible two-phase flow with a free surface including the effect of surface tension. They found that spatial derivative discretized by a 4th order central difference scheme was more accurate and less diffusive than Essentially Non-Oscillatory (ENO) scheme. However, ENO scheme was more robust in case of a large density ratio. Sussman et al. presented an improved LS method which is coupled with variable density projection method [53], and coupled the LS method to the adaptive projection method. Quecedo and Pastor [54] show a level-set method to solve two-phase flows using the finite element method. Yue, Lin and Patel [55] presented a numerical method that coupled the incompressible Navier-Stokes equations with the LS method in a curvilinear coordinate system. Kohno and Tanahashi [56] developed a novel numerical scheme by coupling the LS method with adaptive mesh refinement in order to analyze moving interfaces, reporting that the computational time could be reduced by at least 50% as compare with previous LS method. Olsson and Kreiss [57] presented a mass conservative LS method by use of an artificial compression step to make sure that the interface keeps its thickness and shape, and found that mass conservation was significantly improved as compare with conventional LS method. Deshpande and Zimmerman [58] proposed a unique approach to simulate mass transfer across a moving droplet with LS method. They proposed a new algorithm for computing the mass transfer across a moving droplet

by adopting a two stage approach where the convection-diffusion equations for mass transfer were decoupled from the governing equations of the LS methodology. With this formulation, they could accurately infer the mass transfer coefficients without using any empirical correlations. Nagrath et al. [59] presented a novel stabilized finite element method employing a combination of the ghost fluid and the LS method for studying the hydrodynamics of the implosion and rebound of a small air bubble in water. Gibou et al. [60] proposed a LS sharp interface method for two-phase flows with phase change. Where, sharp interface is captured by a ghost fluid method. Tangui Ménard and Berlemont [61] presented a method devoted to reactive interface simulations with emphasis on vaporization.

In summary, it can be said that LS methods proposed so far represent a viable solution to use in modeling of two-phase flows. They are easy to implement in 3D and can precisely compute the curvature and normal to the interface. However, their main drawback as standalone methods comes from the fact that they are not conservative and physically incorrect loss or gain of mass occurs. Moreover, they are quite expensive in term of CPU usage due to the need to re-initialize the level set function after each time step.

As another type of interface capturing method, the volume of fluid method (VOF), which is introduced by Hirt and Nichols [49], is widely used in the computation of two phase-flows due to its advantage in conserving mass. In VOF, scalar indicator function between zero and one known as the volume fraction,  $\alpha$ , is used to distinguish the phases. The intermediate value in computational cell indicates the presence of interface, while the value of zero and one indicates the complete phase. By solving the advection equation of volume fraction,  $\alpha$ , the position of interface changes according to the time. In order to avoid the numerical diffusion, Youngs [62] introduced a Piecewise Linear Interpolation Calculation (PLIC) method to calculate the flux in a geometrical way for the transport of the volume fraction  $\alpha$ . The results obtained were in good agreement with both experiments and other Lagrangian methods. PLIC method was tested to confirm the ability to track the interface accurately, and revealing that PLIC method has good agreement as compare with experiment. Brackbill et al. [63] proposes a continuum surface force (CSF) method in order to model the surface tension force under interface capturing method such as VOF. To do so, surface tension force is specified as a volumetric source term in the momentum equation. Kothe et al. [64] presented algorithms for tracking interfaces

with VOF methods applying PLIC to calculate the flux of volume fraction, and to account for the surface tension force, CSF model is applied. The numerical results they obtained confirmed the accuracy of their algorithm. Jeong and Yang [65] have adapted the VOF method for the finite element analysis of transient fluid flow with a free surface. Chen and Li [66] introduced VOF combined with a semi-implicit algorithm and higher-order advection scheme which is appropriate for two-phase flows with high density ratios. Rider and Kothe [67] reported second order spatial accuracy algorithm for VOF. Gueyffier et al. [68] proposed a numerical scheme based on the VOF method which uses a piece-linear interface calculation in a 3D domain. Ginzburg and Wittum [69] have introduced spline surface reconstruction, and found that spline surface reconstruction considerably reduced the parasitic currents in VOF models, even if they are based on regular grids. Meier, Yadigaroglu and Smith [70] presented interface curvature determined by least square fitting of reference data with VOF, its result shows spurious currents 2 orders of magnitude smaller than the original CSF model. Lorstad and Fuchs [71] introduced a combination of Youngs's method [62] together with the direction split technique of Rudman [65] for VOF.

## 1.4 Strategy in this thesis

In order to propose acceptable model for melting, deforming, and dropping process in similar condition with fire, multiphase-based numerical approach is used. First, we consider the most fundamental case, namely, no species and chemical reaction are taken into account and only heat and mass transfers play a major role in dynamic motion and melting. The problem then becomes a phenomenon of pure melting and dynamic motion without flaming. In this regard, the governing equations can only consist of the fundamental conservation equations (for mass, momentum and energy) under a multi-phase framework. We employ the Enthalpy-Porosity [72-73] and Volume of Fluid method (VOF) [49] in order to model the melting and dynamic motion of molten matter suspended by a metal plate. This simplified geometry provides a physically similar analogy of the wire combustion case [116].

Based on aforementioned numerical strategy, general observations on melting and dynamic behavior

of PCM are summarized in chapter 4. Effect of inclusion of thermocapillary convection is discussed in chapter 5 by adapting the source-based tangential force driven by surface tension, which linearly depends on the temperature, into previous model. With additional considering of moving heat flux as external thermal input into the numerical model, the dynamic effect on melting speed is investigated in chapter 6. Two types of gasification model, namely, thermal driven and concentration driven mass source, are adapted into model, and the qualitative results are given in appendices A. All processes are globally described in Fig.1.6. This study is done with commercial software (FLUENT 12.0) based on the finite volume method [74].

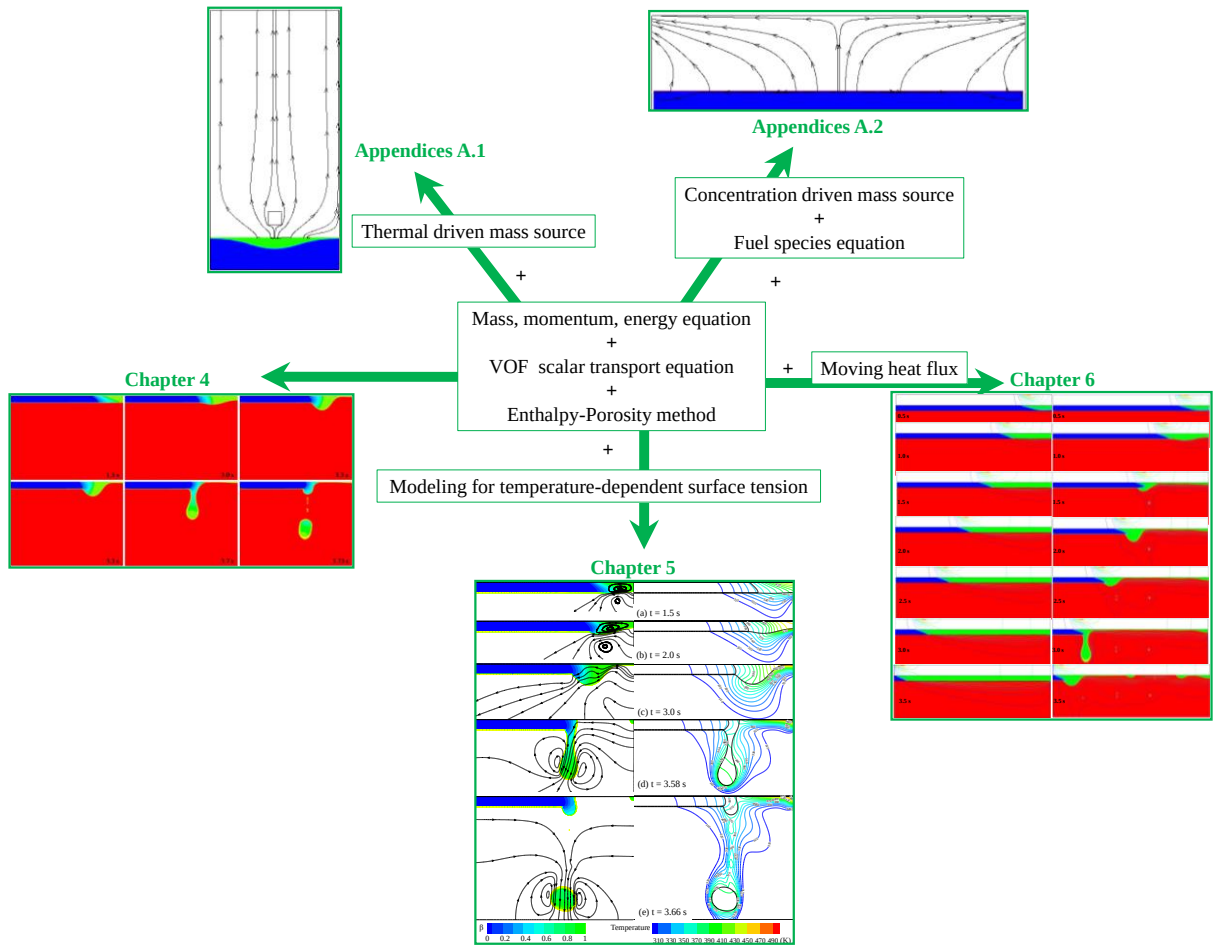


Figure 1.6 Flow description for whole process of this thesis

# Chapter 2

## Mathematical formulation and numerical detail

### 2.1 Mathematical formulation

#### 2.1.1 Local instantaneous governing equations for bulk

Let  $\Phi(x, t)$  be a representative of dependent variable, e.g. a fluid property being transported within a spatial-temporal domain. The rate of change of  $\Phi(x, t)$  in time within an arbitrary control volume  $V$  is generally constituted from different contributions that are either volume or surface sources. In order to describes rate of change of  $\Phi$ , the general integral balance can be written as

$$\frac{d}{dt} \int_V \rho \Phi dV = - \oint_S \mathbf{n} \cdot \mathbb{J} dS + \int_V \rho \varphi dV \quad (2-1)$$

Here,  $\rho$ ,  $\mathbb{J}$ ,  $\varphi$  and  $\mathbf{n}$  stand for density, diffusive flux, body source of quantity  $\Phi$  and normal vector across the bounding control surface  $S$ , respectively. Subscript  $V$  and  $S$ , respectively, represent the volume and surface area. This balance equation states that the time rate of change of  $\rho\Phi$  in the control volume is equal to the flux through  $S$  plus the body source. When the Eq. (2-1) is continuous such Jacobian transformation between material coordinate and spatial coordinate, differential form of the balance equation can be obtained. To do so, the Reynolds transport theorem as

$$\frac{d}{dt} \int_V \Phi dV = \int_V \frac{\partial \Phi}{\partial t} dV + \oint_S \Phi \mathbf{v} \cdot \mathbf{n} dS \quad (2-2)$$

and Gauss' theorem as

$$\begin{aligned} \int_V \nabla \cdot \mathbb{J} dV &= \oint_S \mathbf{n} \cdot \mathbb{J} dS, \\ \int_V \nabla \mathbb{J} dV &= \oint_S \mathbf{n} \mathbb{J} dS \end{aligned} \quad (2-3)$$

are used to define. Thus, the general integral balance for rate of change of  $\Phi$  can be described as

$$\int_V \frac{\partial \rho \Phi}{\partial t} dV + \int_V \nabla \cdot (\rho \mathbf{v} \Phi) dV = - \int_V \nabla \cdot \mathbb{J} dV + \int_V \rho \varphi dV \quad (2-4)$$

Eventually we obtain a differential balance equation

$$\frac{\partial \rho \Phi}{\partial t} + \nabla \cdot (\rho \mathbf{v} \Phi) = - \nabla \cdot \mathbb{J} + \rho \varphi. \quad (2-5)$$

In LHS, the first term and second term are the rate of change of the quantity,  $\Phi$ , per unit volume and the rate of convection per unit volume, respectively. In RHS, the first and second term are, respectively, surface flux and the volume source. Based on this transport equation, we can obtain the general conservation equation for mass, momentum and energy. The conservation of mass can be expressed in a differential form by introducing

$$\Phi = 1, \quad \mathbb{J} = 0, \quad \varphi = 0, \quad (2-6)$$

then, we obtain mass balance equation from general balance equation as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0. \quad (2-7)$$

The conservation of momentum can be obtained from Eq. (2-5) by setting

$$\Phi = \mathbf{v}, \quad \mathbb{J} = \mathbb{T} = p\mathbb{I} + \mathbb{D} = p\mathbb{I} + 2\mu\mathbb{S} \quad \varphi = \mathbf{f} = \rho\mathbf{g}. \quad (2-8)$$

Here,  $\mathbb{T}$ ,  $p$ ,  $\mathbb{I}$ ,  $\mathbb{D}$ ,  $\mu$ ,  $\mathbb{S}$ ,  $\mathbf{f}$  and  $\mathbf{g}$  are the surface stress tensor, pressure, unit tensor, viscous stress, viscosity, rate of strain tensor ( $\mathbb{S} = \frac{1}{2}(\nabla \mathbf{v}) + \frac{1}{2}(\nabla \mathbf{v})^T$ ), gravitational force and gravity acceleration, respectively. Hence, we can obtain momentum balance equation from general balance Eq. (2-5) as

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) = - \nabla p + \nabla \cdot \left( \mu (\nabla \mathbf{v} + \nabla \mathbf{v}^T) \right) + \rho \mathbf{g}. \quad (2-9)$$

In the same way, the conservation of energy can be described by introducing

$$\Phi = e + \frac{\|\mathbf{v}\|^2}{2}, \quad \mathbb{J} = \mathbf{q} - \mathbb{T} \cdot \mathbf{v}, \quad \varphi = \mathbf{q} \cdot \mathbf{v} + \frac{Q}{\rho}. \quad (2-10)$$

Here,  $e$ ,  $\mathbf{q}$  and  $Q$  represent the internal energy, heat flux and the body heating, respectively. By substituting Eq. (2-10) to (2-5) we have the balance equation for energy as

$$\frac{\partial \rho(e + \frac{\|v^2\|}{2})}{\partial t} + \nabla \cdot (\rho(e + \frac{\|v^2\|}{2})\mathbf{v}) = -\nabla \cdot \mathbf{q} + \nabla \cdot (\mathbb{T} \cdot \mathbf{v}) + \rho \mathbf{g} \cdot \mathbf{v} + Q. \quad (2-11)$$

Dotting the momentum equation by the velocity, we obtain

$$\frac{\partial(\rho \frac{\|v^2\|}{2})}{\partial t} + \nabla \cdot (\rho \frac{\|v^2\|}{2} \mathbf{v}) = -\mathbf{v} \nabla p + \mathbf{v} \cdot (\nabla \cdot \mathbb{D}) + \rho \mathbf{v} \cdot \mathbf{g}. \quad (2-12)$$

For a symmetrical stress tensor

$$\mathbb{D} : \nabla \mathbf{v} \equiv (\mathbb{D} \cdot \nabla) \cdot \mathbf{v} = \nabla \cdot (\mathbb{D} \cdot \mathbf{v}) - \mathbf{v} \cdot (\nabla \cdot \mathbb{D}) \quad (2-13)$$

is valid. Thus, velocity-dotted momentum equation becomes

$$\frac{\partial(\rho \frac{\|v^2\|}{2})}{\partial t} + \nabla \cdot (\rho \frac{\|v^2\|}{2} \mathbf{v}) = -\mathbf{v} \nabla p + \nabla \cdot (\mathbb{D} \cdot \mathbf{v}) - \mathbb{D} : \nabla \mathbf{v} + \rho \mathbf{v} \cdot \mathbf{g}. \quad (2-14)$$

By subtracting Eq. (2-14) into the Eq. (2-11), we obtain the internal energy equation as

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot (\rho e \mathbf{v}) = -\nabla \cdot \mathbf{q} - p \nabla \cdot \mathbf{v} + \mathbb{D} : \nabla \mathbf{v} + Q. \quad (2-15)$$

Here, we assumed that the heat flux is proportional to the gradient of the temperature, following Fourier's law of heat conduction,  $\mathbf{q} = -k \nabla T$ . Here,  $k$  is thermal conductivity. Thus, Eq. (2-15) can be simplified as

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot (\rho e \mathbf{v}) = -\nabla \cdot (k \nabla T) - p \nabla \cdot \mathbf{v} + \mathbb{D} : \nabla \mathbf{v} + Q. \quad (2-16)$$

Substituting  $e = h - p / \rho$  energy equation becomes

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho h \mathbf{v}) = -\nabla \cdot (k \nabla T) + \mathbb{D} : \nabla \mathbf{v} + \frac{Dp}{Dt} + Q. \quad (2-17)$$

Where  $h$  is enthalpy. For simplicity, the net rate of work done by compressibility and viscous heating is ignored, also body heating (e.g., radiation, electric or magnetic heating) is not considered. Then, Eq. (2-17) becomes

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho h \mathbf{v}) = -\nabla \cdot (k \nabla T). \quad (2-18)$$

### 2.1.2 Volume averaging and one field formulation

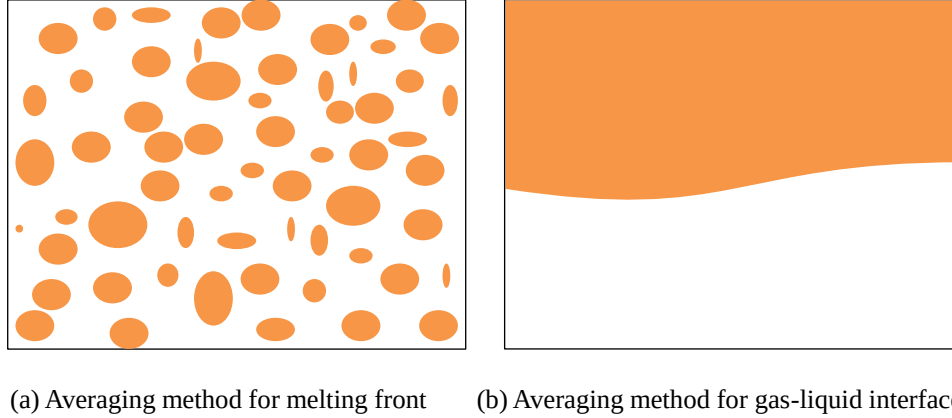


Figure 2.1 Schematic descriptions for different types of spatial distribution for concept of volume averaging methods

In multi-phase flows, the presence of interfacial surfaces introduces great difficulties in the mathematical and physical formulation of the problem. From mathematical and physical point of view, a multi-phase flow can be considered as a field that is subdivided into single-phase regions with moving boundaries between the phases. For single-phase region, field equations (e.g., the equation for mass, momentum, energy, etc.) and constitutive equations are well established in continuum mechanics. Thus, the differential balance can hold for each sub-region. However, it cannot be applied to the set of sub-regions because of the presence of the interface which violates the condition of continuity. It is necessary to find a way to solve the field with interfacial discontinuities. As it is well described by [75], [76], and [77], volume averaging process is one of the efficient way to solve field equations with interfacial discontinuities. We can get appropriate field equations with jump conditions which arise at interface. Figure 2.1 shows different spatial distribution in a control volume so that different type of volume averaging is required. Figure 2.1 (a) shows volume of one phase which is randomly filled in volume of another phase with different sizes. In contrast, Fig. 2.1 (b) shows volume of one phase which is exactly separated by critical line from another phase. Figure 2.1 (a) can explain the melting front (liquid-solid interface) of metallic alloy or polymeric material. In contrast with the

melting process of a pure solid, a metallic alloy or a polymeric material undergoes melting with thick phasic interface so that there is no sharp interface; rather, a certain transient region between solid and liquid appears. In metallic alloy, such thick intermediate state of phase between solid and liquid is called “mushy”. When we look at inside such transient region microscopically, quite complicated distribution appears due to the presence of intermediate state material between solid and liquid state (e.g., metallic alloy contains different types of dendrite in mushy zone). Thus, it is difficult to resolve the melting problem in macroscopic point of view due to presence of such complicated microscopic spatial distribution, volume averaging technique is necessary to account all physics raised from micro structure. Figure 2.1 (b) can be used in order to explain volume averaging for liquid-gas interface. Two phases are bounded by interface. Thus, relatively simple averaging can hold the problem which will be explained in section 2.1.2.1.

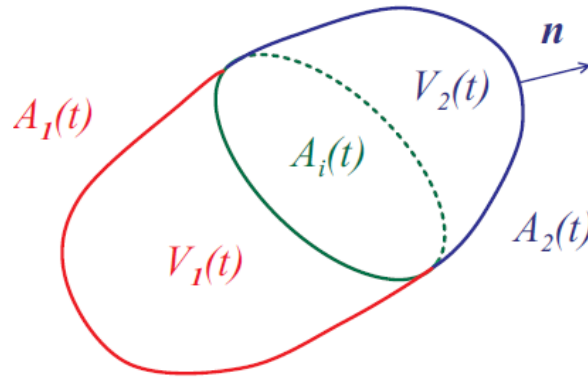


Figure 2.2 Schematic description for two phase bounded by surface  $A_i(t)$

### 2.1.2.1 Volume averaging for gas and liquid phase

When we consider that computational domain is divided by surface  $A_i(t)$ , it has two bulk phase ( $V_1(t)$  and  $V_2(t)$ ) and bounding surface  $A_i(t)$ . If position of bounded surface  $A_i(t)$  is fixed, displacement velocity is not required, but if surface  $A_i(t)$  is freely moving, this displacement velocity is needed to be considered. To understand displacement velocity, derivation of integral theorem based on Leibniz rule

is introduced as

$$\frac{d}{dt} \int_{V(t)} \Phi dV = \int_{V(t)} \frac{\partial \Phi}{\partial t} dV + \int_{A(t)} \Phi \mathbf{v}_s \cdot \mathbf{n}_\Sigma dA \quad (2-19)$$

Here  $\mathbf{v}_s$  is displacement velocity vector,  $\mathbf{n}_\Sigma$  is interfacial normal vector directing outward. Using Leibniz rule, we can consider how material volume can be changed to arbitrary volume.

For material volume,  $V_m(t)$ , surrounded by area  $A$ , Eq. (2-19) can be changed as

$$\frac{d}{dt} \int_{V_m(t)} \Phi dV = \int_{V_m(t)} \frac{\partial \Phi}{\partial t} dV + \int_{A_m(t)} \Phi \mathbf{v} \cdot \mathbf{n}_\Sigma dA \quad (2-20)$$

with assuming that the displacement velocity,  $\mathbf{v}_s$ , is same with liquid velocity,  $\mathbf{v}$ .

For arbitrary volume  $V(t)$ , which coincides with material volume, surrounded by area  $A$ , Eq. (2-19) can be changed as

$$\frac{d}{dt} \int_{V(t)} \Phi dV = \int_{V(t)} \frac{\partial \Phi}{\partial t} dV + \int_{A(t)} \Phi \mathbf{v}_s \cdot \mathbf{n}_\Sigma dA \quad (2-21)$$

Therefore, we can consider all arbitrary volumes  $V(t)$  which coincides with material volume as

$$\frac{d}{dt} \int_{V_m(t)} \Phi dV = \frac{d}{dt} \int_{V(t)} \Phi dV + \int_{A(t)} \Phi (\mathbf{v} - \mathbf{v}_s) \cdot \mathbf{n}_\Sigma dA \quad (2-22)$$

According to the Eq. (19-22), we can conclude that  $\mathbf{v}_s \cdot \mathbf{n} = 0$  if volume is fixed in coordinate, and

$\mathbf{v}_s \cdot \mathbf{n}_\Sigma = \mathbf{v} \cdot \mathbf{n}_\Sigma$  if volume is material volume.

By use of this rule mass conservation equation for one bulk phase with bounded surface  $A_i(t)$  can be written as,

$$\begin{aligned} \frac{d}{dt} \int_{V_m(t)} \rho dV &= \frac{d}{dt} \int_{V(t)} \rho dV + \int_{A(t)} \rho (\mathbf{v} - \mathbf{v}_s) \cdot \mathbf{n}_\Sigma dA = 0 \\ \Rightarrow \frac{d}{dt} \int_{V(t)} \rho dV &= - \int_{A(t)} \rho (\mathbf{v} - \mathbf{v}_s) \cdot \mathbf{n}_\Sigma dA. \end{aligned} \quad (2-23)$$

Hence, above mass balance equation exactly represents that time variation of the mass equals the net mass flow rate entering in the volume  $V(t)$ .

Recall the original two phase problem that has two volumes ( $V_1(t)$  and  $V_2(t)$ ) and bounding surface  $A_i(t)$ . First consider whole domain with fixed volume,  $V(t)$  and area,  $A(t)$ , then integral form of mass

conservation is

$$\frac{d}{dt} \int_{V(t)} \rho dV = - \int_{A(t)} \rho \mathbf{v} \cdot \mathbf{n}_\Sigma dA, \quad (2-24)$$

and split contributions from each volume of  $V_1(t)$  and  $V_2(t)$ , then mass conservation equation is separated as

$$\frac{d}{dt} \int_{V_1(t)} \rho_1 dV + \frac{d}{dt} \int_{V_2(t)} \rho_2 dV = - \int_{A_1(t)} \rho_1 \mathbf{v}_1 \cdot \mathbf{n}_{\Sigma_1} dA - \int_{A_2(t)} \rho_2 \mathbf{v}_2 \cdot \mathbf{n}_{\Sigma_2} dA \quad (2-25)$$

Here, first term in LHS of  $V_1(t)$  is

$$\frac{d}{dt} \int_{V_1(t)} \rho_1 dV = \int_{V_1(t)} \frac{\partial \rho_1}{\partial t} dV + \int_{A_1(t)} \rho_1 \mathbf{v}_i \cdot \mathbf{n}_{\Sigma_1} dA, \quad (2-26)$$

for volume of  $V_2(t)$  is

$$\frac{d}{dt} \int_{V_2(t)} \rho_2 dV = \int_{V_2(t)} \frac{\partial \rho_2}{\partial t} dV + \int_{A_2(t)} \rho_2 \mathbf{v}_i \cdot \mathbf{n}_{\Sigma_2} dA. \quad (2-27)$$

By use of Gauss theorem, RHS first term for  $V_1(t)$  and  $V_2(t)$  becomes,

$$\int_{A_1(t)} \rho_1 \mathbf{v}_1 \cdot \mathbf{n}_{\Sigma_1} dA = \int_{V_1(t)} \nabla \cdot (\rho_1 \mathbf{v}_1) dV - \int_{A_1(t)} \rho_1 \mathbf{v}_1 \cdot \mathbf{n}_{\Sigma_1} dA \quad (2-28)$$

and

$$\int_{A_2(t)} \rho_2 \mathbf{v}_2 \cdot \mathbf{n}_{\Sigma_2} dA = \int_{V_2(t)} \nabla \cdot (\rho_2 \mathbf{v}_2) dV - \int_{A_2(t)} \rho_2 \mathbf{v}_2 \cdot \mathbf{n}_{\Sigma_2} dA. \quad (2-29)$$

Eventually, mass conservation equation for each phase becomes

$$\int_{V_k(t)} \left( \frac{\partial \rho_k}{\partial t} + \nabla \cdot (\rho_k \mathbf{v}_k) \right) dV = - \int_{A_k(t)} \rho_k (\mathbf{v}_k - \mathbf{v}_i) \cdot \mathbf{n}_{\Sigma_k} dA. \quad (2-30)$$

where, subscript  $k$  denotes phases. First term in volume integral represents the mass conservation equation for bulk in each phases and second term in surface integral indicates the mass jump which appear at the interface between each phase. Thus, we can separate mass conservation equation for bulk phase as

$$\frac{\partial \rho_k}{\partial t} + \nabla \cdot (\rho_k \mathbf{v}_k) = 0 \quad (2-31)$$

and mass jump equation for interface as

$$\rho_k(\mathbf{v}_k - \mathbf{v}_i) \cdot \mathbf{n}_{\Sigma k} = 0. \quad (2-32)$$

Here,  $\mathbf{v}_i \cdot \mathbf{n}_{\Sigma k}$  is the normal velocity of the interface itself. If there is no phase change, mass jump equation becomes zero.

As same manner introduced in mass conservation equation for two phases, momentum equation can be also similar form by use of Leibniz rule and Gauss theorem as

$$\begin{aligned} & \int_{V_k(t)} \left( \frac{\partial \rho_k \mathbf{v}_k}{\partial t} + \nabla \cdot (\rho_k \mathbf{v}_k \mathbf{v}_k) + \nabla p_k - \mu (\nabla \mathbf{v}_k + \nabla \mathbf{v}_k^T) - \rho_k \mathbf{g} \right) dV \\ &= - \int_{A_i(t)} \rho_k \mathbf{v}_k (\mathbf{v}_k - \mathbf{v}_i) \cdot \mathbf{n}_{\Sigma k} dA + \int_{A_i(t)} \nabla p_k \cdot \mathbf{n}_{\Sigma k} dA - \int_{A_i(t)} \mu (\nabla \mathbf{v}_k + \nabla \mathbf{v}_k^T) \cdot \mathbf{n}_{\Sigma k} dA + \int_{A_i(t)} (-\nabla_\Sigma \sigma^T + \sigma \kappa_c \mathbf{n}_\Sigma) \cdot \mathbf{n}_{\Sigma k} dA. \end{aligned} \quad (2-33)$$

Thus, momentum balance equation for bulk can be taken as

$$\frac{\partial \rho_k \mathbf{v}_k}{\partial t} + \nabla \cdot (\rho_k \mathbf{v}_k \mathbf{v}_k) + \nabla p_k - \mu (\nabla \mathbf{v}_k + \nabla \mathbf{v}_k^T) - \rho_k \mathbf{g} = 0 \quad (2-34)$$

and momentum jump equation for the stress at the interface can be separated as

$$\rho_k \mathbf{v}_k (\mathbf{v}_k - \mathbf{v}_i) \cdot \mathbf{n}_{\Sigma k} + \nabla p_k \cdot \mathbf{n}_{\Sigma k} - \mu (\nabla \mathbf{v} + \nabla \mathbf{v}^T)_k \cdot \mathbf{n}_{\Sigma k} - \nabla_\Sigma \sigma^T + \sigma \kappa_c \mathbf{n}_\Sigma = 0. \quad (2-35)$$

Here RHS term is the surface tension force and  $\sigma$  is the surface tension coefficient,  $\kappa_c$  is the curvature.

Volume averaged energy equation for two phases also can be defined by Leibniz rule and Gauss theorem as

$$\begin{aligned} & \sum_{k=1}^2 \int_{V_k(t)} \left( \frac{\partial (\rho_k h_k)}{\partial t} + \nabla \cdot (\rho_k h_k \mathbf{v}_k) - \nabla \cdot (k_k \nabla T_k) \right) dV - \int_{A_i(t)} \rho_k h_k (\mathbf{v}_k - \mathbf{v}_i) \cdot \mathbf{n}_{\Sigma k} dA \\ & - \int_{A_i(t)} k_k \nabla T_k \cdot \mathbf{n}_{\Sigma k} dA = 0. \end{aligned} \quad (2-36)$$

Energy equation for two phases can be separated as

$$\frac{\partial (\rho_k h_k)}{\partial t} + \nabla \cdot (\rho_k h_k \mathbf{v}_k) - \nabla \cdot (k_k \nabla T_k) = 0 \quad (2-37)$$

for bulk, and

$$\rho_k h_k (\mathbf{v}_k - \mathbf{v}_i) \cdot \mathbf{n}_{\Sigma k} - k_k \nabla T_k \cdot \mathbf{n}_{\Sigma k} = 0 \quad (2-38)$$

for interfacial energy jump equation.

### 2.1.2.2 Volume averaging for liquid and solid phase

In order to account for the melting process, we roughly introduced the volume averaging concept how to do for melt front in Fig. 2.1. Detail derivation is following;

Ni and Beckermann [78] derived the appropriate governing equation by use of a local volume averaged model of the two phase solid and liquid region. To derive the local volume averaged governing equation, ‘representative elementary volume’, (REV), was introduced. In REV, microscopic balances on the transport of enthalpy in the distinct solid and liquid fractions are contained. According to integrating the equations over the given REV, assuming a constant temperature and small local velocity fluctuation, averaged equations are obtained.

$$\begin{aligned} \frac{\partial}{\partial t}(\beta_s H_s) + \nabla \cdot (\beta_s H_s \mathbf{v}_s) &= \nabla \cdot (\beta_s k_s \nabla T) - S_s \\ \frac{\partial}{\partial t}(\beta_l H_l) + \nabla \cdot (\beta_l H_l \mathbf{v}_l) &= \nabla \cdot (\beta_l k_l \nabla T) + S_l \quad \text{where } \beta_s + \beta_l = 1 \end{aligned} \quad (2-39)$$

Here  $\beta$  is liquid volume fraction,  $H$  is specific enthalpy,  $\mathbf{v}$  is velocity,  $k$  is thermal conductivity,  $T$  is temperature and  $S$  is interfacial source term. Subscript  $s$  and  $l$  are solid and liquid state respectively. Specific enthalpy of solid and liquid for unit volume can be defined as

$$H_s = \int_{T_{ref}}^T \rho_s c_{p,s} dT, \quad H_l = \int_{T_{ref}}^T \rho_l c_{p,l} dT + \rho_l L \quad (2-40)$$

Here  $c_p$  is specific heat at constant pressure,  $L$  is the latent heat of melting. It is convenient to combine two energy equations by adding them together to attain a single energy equation in order to adapt it in one field formulation. We should introduce the mixture enthalpy  $H$  and mixture thermal conductivity  $k$  as following:

$$\begin{aligned} H &= \beta_s H_s + \beta_l H_l = \beta_s \int_{T_{ref}}^T \rho_s c_{p,s} dT + \beta_l \int_{T_{ref}}^T \rho_l c_{p,l} dT + \beta_l \rho_l L, \\ k &= (1 - \beta_l) k_s + \beta_l k_l. \end{aligned} \quad (2-41)$$

Then, by using the mixture enthalpy  $H$ , transient term in LHS of Eq. (2-39) can be changed to

$$\frac{\partial H}{\partial t} = \left\{ \rho(1 - \beta_l) c_{p,s} + \rho \beta_l c_{p,l} \right\} \frac{\partial T}{\partial t} + \left\{ \rho(c_{p,l} - c_{p,s})(T - T_{ref}) + \rho L \right\} \frac{\partial \beta_l}{\partial t} \quad (2-42)$$

Eventually, combined energy equation becomes

$$\left\{ \rho(1-\beta_l)c_{p,s} + \rho\beta_l c_{p,l} \right\} \frac{\partial T}{\partial t} + \left\{ \rho(c_{p,l} - c_{p,s})(T - T_{ref}) + \rho L \right\} \frac{\partial \beta_l}{\partial t} + \nabla \cdot (\beta_s H_s \mathbf{v}_s + \beta_l H_l \mathbf{v}_l) = \nabla \cdot (k \nabla T) \quad (2-43)$$

Where, defining  $c_p$  as mixture specific heat is

$$c_p = c_{p,s}(1-\beta_l) + c_{p,l}\beta_l \quad (2-44)$$

Equation is then changed to

$$\rho c_p \frac{\partial T}{\partial t} + \left\{ \rho(c_{p,l} - c_{p,s})(T - T_{ref}) + \rho L \right\} \frac{\partial \beta_l}{\partial t} + \nabla \cdot (\beta_s H_s \mathbf{v}_s + \beta_l H_l \mathbf{v}_l) = \nabla \cdot (k \nabla T) \quad (2-45)$$

Considering the fact that velocity in the solid is zero and substituting enthalpy for liquid, equations becomes

$$\begin{aligned} & \rho c_p \frac{\partial T}{\partial t} + \left\{ \rho(c_{p,l} - c_{p,s})(T - T_{ref}) + \rho L \right\} \frac{\partial \beta_l}{\partial t} + \nabla \cdot (\beta_l H_l \mathbf{v}_l) = \nabla \cdot (k \nabla T) \\ & \rightarrow \rho c_p \frac{\partial T}{\partial t} + \nabla \cdot (\beta_l H_l \mathbf{v}_l) = \nabla \cdot (k \nabla T) - \left\{ \rho(c_{p,l} - c_{p,s})(T - T_{ref}) + \rho L \right\} \frac{\partial \beta_l}{\partial t} \\ & \rightarrow \rho c_p \frac{\partial T}{\partial t} + \nabla \cdot \left\{ \beta_l \left( \int_{T_{ref}}^T \rho_l c_{p,l} dT \right) \mathbf{v}_l \right\} = \nabla \cdot (k \nabla T) - \nabla \cdot (\beta_l \rho_l L \mathbf{v}_l) \\ & - \left\{ \rho(c_{p,l} - c_{p,s})(T - T_{ref}) + \rho L \right\} \frac{\partial \beta_l}{\partial t} \end{aligned} \quad (2-46)$$

As next, combine the transient terms each other, also convection terms as well, then reformulating it from temperature form to enthalpy form. We can get the energy equation transformed into the following equation:

$$\frac{\partial(h + \beta L)}{\partial t} + \nabla \cdot \mathbf{v}(h + \beta L) = \nabla \cdot (k \nabla T). \quad (2-47)$$

Hereafter, we use  $H$ , which is called as enthalpy in condensed phase, instead of  $h + \beta L$  by defining  $H = h + \beta L$ . Eventually, we get volume averaged conservation equation with appropriate jump condition for mass, momentum and energy for two phases and it is summarized in table.

Table 2.1 Balance equation for bulk and interface

|          | For bulk                                                                                                                                                                                            | For interface                                                                                                                                                                                                                                                                       |
|----------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Mass     | $\frac{\partial \rho_k}{\partial t} + \nabla \cdot (\rho_k \mathbf{v}_k) = 0$ (2-48)                                                                                                                | $\rho_k (\mathbf{v}_k - \mathbf{v}_i) \cdot \mathbf{n}_{\Sigma k} = 0$ (2-51)                                                                                                                                                                                                       |
| Momentum | $\frac{\partial \rho_k \mathbf{v}_k}{\partial t} + \nabla \cdot (\rho_k \mathbf{v}_k \mathbf{v}_k) + \nabla p_k - \mu (\nabla \mathbf{v}_k + \nabla \mathbf{v}_k^T) - \rho_k \mathbf{g} = 0$ (2-49) | $\rho_k \mathbf{v}_k (\mathbf{v}_k - \mathbf{v}_i) \cdot \mathbf{n}_{\Sigma k} + \nabla p_k \cdot \mathbf{n}_{\Sigma k} - \mu (\nabla \mathbf{v} + \nabla \mathbf{v}^T)_k \cdot \mathbf{n}_{\Sigma k} - \nabla_{\Sigma} \sigma^T + \sigma \kappa_e \mathbf{n}_{\Sigma} = 0.$ (2-52) |
| Energy   | $\frac{\partial (\rho_k H_k)}{\partial t} + \nabla \cdot (\rho_k H_k \mathbf{v}_k) - \nabla \cdot (k_k \nabla T_k) = 0$ (2-50)                                                                      | $\rho_k c_{p,k} T_k (\mathbf{v}_k - \mathbf{v}_i) \cdot \mathbf{n}_{\Sigma k} = k_k \nabla T_k \cdot \mathbf{n}_{\Sigma k}$ (2-53)                                                                                                                                                  |

### 2.1.2.3 One field formulation

In contrast to the volume averaged governing equations and jump condition which couple the solutions at the interface, it is possible to write one set of governing equations for the whole domain which contains phases with interface without jump conditions [79]. When multiphase flow is simulated by solving a single set of equations for the whole flow field, it is necessary to account for differences in the material properties of the different fluids and to add appropriate interface terms for interfacial phenomena, such as surface tension. The various phases are treated as one fluid with variable material properties that change abruptly at the phase boundary. To do so, we need two processes, namely, (1) phase indicator function that recognizes where bulk phase is and (2) jump condition that is treated as a part of solutions. Particularly, to account jump condition as an extra term in inner solution, it is necessary to add singular terms (later, all jump conditions required to be added in solutions are multiplied with  $\nabla \alpha$  which is treated as singular function) to the equations. These singular terms are the counterpart of the jump conditions, and it can be shown that both formulations are equivalent. Firstly, to distinguish between the two phases in the subsequent one-field formulation, the phase indicator function

$$\alpha = \begin{cases} 1 = \text{phase 1,} \\ 0 < \alpha < 1 = \text{the cell contains the interface,} \\ 0 = \text{phase 2.} \end{cases} \quad (2-54)$$

is applied by averaging quantity  $\Phi$  in a control volume  $V$ . Averaging process is not needed in the interior of the bulk, hence we only look at control volumes that contains the interface.

As the phase specific average of quantities  $\Phi_k$  in a control volume  $V$ , we define

$$\langle \Phi_k \rangle := \frac{1}{|V_k|} \int_{V_k} \Phi dn = \frac{1}{|V_k|} \int_V \alpha_k \Phi dn, \quad (2-55)$$

where subscript  $k$  denotes the each phase,  $V_k$  is interfacial volume in each phase  $k$  in the control volume  $V$ .

As the volume specific average of quantities  $\Phi_k$  in a control volume  $V$ , we define

$$\bar{\Phi}_k := \frac{1}{|V|} \int_V \alpha \Phi dn = \frac{|V_k|}{|V|} \langle \Phi_k \rangle = \alpha_k \langle \Phi_k \rangle \quad (2-56)$$

Below, we drop the time and space variables for simplicity. For the phase specific averages, the relations

$$\begin{aligned} \frac{\partial \bar{\Phi}_k}{\partial t} &= \alpha_k \left\langle \frac{\partial \Phi_k}{\partial t} \right\rangle = \frac{\partial \langle \alpha_k \Phi_k \rangle}{\partial t} - \frac{1}{|V|} \int_{V_i} \Phi_k \mathbf{v}_{\Sigma k} \cdot \mathbf{n}_{\Sigma} dA \\ \nabla \bar{\Phi}_k &= \alpha_k \langle \nabla \Phi_k \rangle = \nabla \alpha_k \langle \bar{\Phi}_k \rangle + \frac{1}{|V|} \int_{V_i} \Phi_k \mathbf{n}_{\Sigma k} dA \\ \nabla \cdot \bar{\Phi}_k &= \alpha_k \nabla \cdot \langle \bar{\Phi}_k \rangle = \nabla \cdot (\alpha_k \langle \bar{\Phi}_k \rangle) + \frac{1}{|V|} \int_{V_i} \Phi_k \cdot \mathbf{n}_{\Sigma k} dA \end{aligned} \quad (2-57)$$

hold, where  $\mathbf{n}_{\Sigma k}$  is the outward unit normal.

With  $\Phi_k=1$ , we obtain following from second volume specific average in Eq. (2-57). as

$$\nabla \alpha_k = -\frac{1}{|V|} \int_{V_i} \mathbf{n}_{\Sigma} dA. \quad (2-58)$$

$\nabla \alpha_k$  is called interface area density, is useful expression for the gradient of the volume fraction field because jump condition can be counted as volumetric source term with multiplying it. Applying the Eq. (2-58) to the liquid and gas phase, we get the two sets of averaged balance equations. Summation of the equation for two phases in a control volume intersected by the interface can result in the set of one

field equation.

By use of one-field equation, mass, momentum and energy equation can be re-described as

$$\alpha_k \left\langle \frac{\partial \rho_k}{\partial t} \right\rangle + \alpha_k \nabla \cdot \langle \rho_k \mathbf{v}_k \rangle = 0 \quad (2-59)$$

$$\alpha_k \left\langle \frac{\partial \rho_k \mathbf{v}_k}{\partial t} \right\rangle + \alpha_k \nabla \cdot \langle \rho_k \mathbf{v}_k \otimes \mathbf{v}_k \rangle + \alpha_k \nabla \langle p_k \rangle - \alpha_k \nabla \cdot \langle \mu (\nabla \mathbf{v}_k + \nabla \mathbf{v}_k^T) \rangle - \rho_k \mathbf{g} = 0 \quad (2-60)$$

$$\alpha_k \left\langle \frac{\partial (\rho_k H_k)}{\partial t} \right\rangle + \alpha_k \nabla \cdot \langle \rho_k H_k \mathbf{v}_k \rangle - \alpha_k \nabla \cdot \langle k_k \nabla T_k \rangle = 0 \quad (2-61)$$

with jump condition, and recall the phase indicator function (Eq. (2-54)), then we can eventually get the general governing equation for mass, momentum and energy as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (2-62)$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) + \nabla p - \nabla \cdot \mu (\nabla \mathbf{v} + \nabla \mathbf{v}^T) - \rho \mathbf{g} = 0 \quad (2-63)$$

$$\frac{\partial (\rho H)}{\partial t} + \nabla \cdot (\rho H \mathbf{v}) - \nabla \cdot (k \nabla T) = 0 \quad (2-64)$$

with jump condition. The material properties attain phase dependent values determined by

$$\begin{aligned} \rho &= \alpha_1 \rho_1 + (1 - \alpha_1) \rho_2, \quad \mu = \alpha_1 \mu_1 + (1 - \alpha_1) \mu_2, \\ k &= \alpha_1 k_1 + (1 - \alpha_1) k_2, \quad c_p = \alpha_1 c_{p,1} + (1 - \alpha_1) c_{p,2}. \end{aligned} \quad (2-65)$$

Now, we recall the energy equation which is averaged for melting process (Eq. (2-47)) with assuming that (1) specific heat capacity in each phase does not change, and (2)  $\beta$  can hold the two phases (solid and liquid) as indicator function like  $\alpha$ , resulting energy equation then becomes

$$\frac{\partial (h + \beta L)}{\partial t} + \nabla \cdot ((h + \beta L) \mathbf{v}) = \nabla \cdot (k \nabla T) \quad (2-66)$$

with temperature dependent indicator function for melting front as

$$\beta = \begin{cases} 0 & \text{if } T < T_{\text{solidus}}, \\ 1 & \text{if } T > T_{\text{liquidus}}, \\ (T - T_{\text{solidus}}) / (T_{\text{liquidus}} - T_{\text{solidus}}) & \text{if } T_{\text{solidus}} < T < T_{\text{liquidus}}, \end{cases} \quad (2-67)$$

where,  $T_{\text{solidus}}$  and  $T_{\text{liquidus}}$  are the solidus and liquidus temperatures respectively.

In order to get general balance equation for melting, deforming and dropping process, let us first

assume that there is no phase change in between liquid and gas phase. Then,  $\rho_k(\mathbf{v}_k - \mathbf{v}_i) \cdot \mathbf{n}_{\Sigma k} = 0$ .

Thus, jump condition for mass and energy disappear, only remain jump condition is momentum as

$$(p\mathbf{I})_k \cdot \mathbf{n}_{\Sigma k} - \mu(\nabla \mathbf{v} + \nabla \mathbf{v}^T)_k \cdot \mathbf{n}_{\Sigma k} = \nabla_{\Sigma} \sigma^T + \sigma \kappa_c \mathbf{n}_{\Sigma}. \quad (2-68)$$

Therefore, final equations for melting, deforming and dropping process can be drawn as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (2-69)$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) + \nabla p - \nabla \cdot \mu(\nabla \mathbf{v} + \nabla \mathbf{v}^T) - \rho \mathbf{g}, \quad \|\nabla_{\Sigma} \sigma^T + \sigma \kappa_c \mathbf{n}_{\Sigma}\| = 0 \quad (2-70)$$

$$\frac{\partial(\rho H)}{\partial t} + \nabla \cdot (\rho H \mathbf{v}) - \nabla \cdot (k \nabla T) = 0 \quad (2-71)$$

The jump quantity can be implicitly accounted for the balance equation with surface quantities acting as source term at the interface. The only surface quantity in the model described above is the surface tension force. This is incorporated in the discretized form as a body force via the interfacial delta function which is related to the phase indicator by means of

$$\delta_{\Sigma} = \|\nabla \alpha\| \quad (2-72)$$

The resulting momentum balance equation then reads as

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) + \nabla p - \nabla \cdot \mu(\nabla \mathbf{v} + \nabla \mathbf{v}^T) - \rho \mathbf{g} + (\nabla_{\Sigma} \sigma^T + \sigma \kappa_c \mathbf{n}_{\Sigma}) \delta_{\Sigma} = 0. \quad (2-73)$$

It is solved for the gas, liquid and mushy regions according to the one-field assumption under the volume averaging framework [75]. To do so, we assume that the velocity and mixture pressure is shared in each phase. Here, we assume that the columnar and equiaxed dendrite in the transient region in between solid and liquid are homogeneously distributed and are shrunk or dissipated from the macroscopic points of view. This implies that the transient zone is porous medium filled with liquid by an up-scaling procedure. Given these restrictions, the microscopic momentum equation becomes a macroscopic equation with an additional sink term,  $S_M$  as last term in Eq. (2-73), where

$$S_M = -A_{mush} \frac{(1 - \beta)^2}{(\beta^3 + \varepsilon)} \mathbf{v}. \quad (2-74)$$

Here,  $A_{mush}$  is a constant ( $1.0 \times 10^6$  (kg/(m<sup>3</sup>s))) accounting for the mushy region morphology.  $\varepsilon$  is a represented small value (0.001) introduced to prevent the numerical singularity at  $\beta = 0$ .  $\beta$  is the

fraction of liquid in the cell, which behaves effectively as a porous media [72]. Mathematically, this  $\mathbf{S}_M$  term arises from the dissipative interfacial stress during volume the averaging process [78], and is modelled as a momentum sink term using a knowledge of the permeability of the porous medium [80]. Diverse modelling to deal with such a permeability tensor has been studied in research on porous media [81-83]. In this study we represent it as a type of Carman-Kozeny permeability tensor [84]. As described in [78], the basic principle underlying the force  $S_M$  relates to a gradual increase in velocity from zero in the solid to a finite value in the liquid over the cells that are undergoing a phase change. Thus when  $\beta = 1$  the sink term becomes zero, and the general momentum equation is solved for the liquid, but when  $\beta \neq 1$  the permeability tensor dominates over the transient, convective and diffusive term, and the momentum equation becomes identical to the so-called Carman-Kozeny equation. Eventually momentum equation evolving melting and surface tension force are

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) + \nabla p - \nabla \cdot \mu (\nabla \mathbf{v} + \nabla \mathbf{v}^T) - \rho \mathbf{g} + (\nabla_\Sigma \sigma^T + \sigma \kappa_c \mathbf{n}_\Sigma) \delta_\Sigma - A_{mush} \frac{(1-\beta)^2}{(\beta^3 + \varepsilon)} \mathbf{v} = 0. \quad (2-75)$$

### 2.1.3 Gasification modeling

#### 2.1.3.1 Thermally defined gasification

In order to define gasification, recall the mass jump condition which is

$$\|\rho(\mathbf{v} - \mathbf{v}_\Sigma)\| \cdot \mathbf{n}_{\Sigma, g-l} = 0 \quad (2-76)$$

Hereafter subscript  $g$ ,  $l$  and  $g-l$  denotes gas, liquid and gas-liquid interface, respectively. It means that flow is not across the liquid-gas interface so that the normal velocity of bulk phase at the gas-liquid interface is considered to be equal to the normal velocity of the gas-liquid interface itself (i.e., there is no phase change, namely, gasification). Assuming no slip at the gas-liquid interface, the jump conditions at the liquid-gas interface can be simplified as:

$$\|\mathbf{v}_g\| \cdot \mathbf{n}_{\Sigma, g-l} = \|\mathbf{v}_l\| \cdot \mathbf{n}_{\Sigma, g-l} = \|\mathbf{v}_\Sigma\| \cdot \mathbf{n}_{\Sigma, g-l} \quad (2-77)$$

However, if we consider gasification, mass jump should be counted so that it is necessary to model the

appropriate mass source that is exactly same with left term in Eq. (2-76). Therefore, gasification mass source  $\dot{m}$  is defined as

$$\dot{m} = \|\rho(\mathbf{v} - \mathbf{v}_\Sigma)\| \cdot \mathbf{n}_{\Sigma, g-l}, \quad (2-78)$$

and then, we first used mass jump caused by energy jump. To do so, we need to introduce latent heat of gasification which is defined as  $L_v = (c_{p,g} - c_{p,l})T$  and recall the energy jump condition as

$$\|\rho c_p T(\mathbf{v} - \mathbf{v}_\Sigma)\| \cdot \mathbf{n}_{\Sigma, g-l} = -\|k \nabla T\| \cdot \mathbf{n}_{\Sigma, g-l} \quad (2-79)$$

and then let's decompose it as the liquid and gas parts by use of definition of latent heat of gasification and phasic material properties:

$$\begin{aligned} \|\rho c_p T(\mathbf{v} - \mathbf{v}_\Sigma)\| \cdot \mathbf{n}_{\Sigma, g-l} &= -\|k \nabla T\| \cdot \mathbf{n}_{\Sigma, g-l} \\ \rightarrow \|\rho_g c_{p,g} T(\mathbf{v} - \mathbf{v}_\Sigma) - \rho_l c_{p,l} T(\mathbf{v} - \mathbf{v}_\Sigma)\| \cdot \mathbf{n}_{\Sigma, g-l} &= -\|k_g \nabla T\| \cdot \mathbf{n}_{\Sigma, g-l} + \|k_l \nabla T\| \cdot \mathbf{n}_{\Sigma, g-l} \\ \rightarrow \|L_v(\rho_g - \rho_l)(\mathbf{v} - \mathbf{v}_\Sigma)\| \cdot \mathbf{n}_{\Sigma, g-l} &= -\|(k_g - k_l) \nabla T\| \cdot \mathbf{n}_{\Sigma, g-l}. \end{aligned} \quad (2-80)$$

Eventually the energy jump condition for gasification is given. By using this, mass jump condition could be derived as follows

$$\|(\rho_g - \rho_l)(\mathbf{v} - \mathbf{v}_\Sigma)\| \cdot \mathbf{n}_{\Sigma, g-l} = -\frac{\|(k_g - k_l) \nabla T\| \cdot \mathbf{n}_{\Sigma, g-l}}{L_v}. \quad (2-81)$$

Left hand side represents decomposed mass jump at the gas-liquid interface. Thus mass source  $\dot{m}$  could be modeled by

$$\dot{m} = -\frac{\|(k_g - k_l) \nabla T\| \cdot \mathbf{n}_{\Sigma, g-l}}{L_v}. \quad (2-82)$$

### 2.1.3.2 Concentration driven gasification

For the modeling of the evaporation mass flux, the gas phase is considered to be a binary system consisting of fuel and oxygen. The definition of the mass flux (Eq. (2-78)) makes

$$\dot{m}' = \|\rho_F(\mathbf{v}_F - \mathbf{v}_\Sigma)\| \cdot \mathbf{n}_\Sigma = \|\rho_F(\mathbf{v}_{MG} - \mathbf{v}_\Sigma)\| \cdot \mathbf{n}_\Sigma + \|\rho_F(\mathbf{v}_F - \mathbf{v}_{MG})\| \cdot \mathbf{n}_\Sigma \quad (2-83)$$

Here, subscript F and MG stands for fuel and mixture binary gas, respectively. Introducing

the mass fraction of vapor  $Y_F = \frac{\rho_F}{\rho_{MG}}$  gives

$$\dot{m}' = \|Y_F \rho_{MG} (\mathbf{v}_{MG} - \mathbf{v}_\Sigma)\| \cdot \mathbf{n}_\Sigma + \|\rho_F (\mathbf{v}_F - \mathbf{v}_{MG})\| \cdot \mathbf{n}_\Sigma = \left\| Y_F \sum_{k=F, Ox} \dot{m}'_k \right\| - \|\rho_{MG} D_{Bin} \nabla Y_F\| \cdot \mathbf{n}_\Sigma. \quad (2-84)$$

In the first term of Eq. (2-82),  $\|\rho_{MG} (\mathbf{v}_{MG} - \mathbf{v}_\Sigma)\| \cdot \mathbf{n}_\Sigma$  is the mass flux of the mixture phase at the interface, which can be expressed by the sum of the mass fluxes of its components, vapor and the inert gas. The latter is assumed to be stagnant at the interface due to negligible effect of gas absorption, i.e  $\mathbf{v}_L = \mathbf{v}_\Sigma$ , where the subscript  $L$  denotes the liquid, so that the total flux of the mixture is equal to the fuel flux. The second term in Eq. (2-84) is the mass flux due to relative velocity between vapor and inert gas and can be modeled by the Fick's law. Here,  $D_{bin}$  is the diffusion coefficient between fuel and oxygen. We hence obtain

$$\dot{m}' = Y_F \dot{m}' - \rho_{MG} D_{Bin} \nabla Y_F \cdot \mathbf{n}_\Sigma \quad (2-85)$$

The final expression is

$$\dot{m}' = \frac{\rho_{MG} D_{bin}}{1 - Y_F} \nabla Y_F \cdot \mathbf{n}_\Sigma \quad (2-86)$$

In order to get the mass fraction of fuel,  $Y_F$ , species equation for it is needed to solve. To do so, one needs to start the transport equation of one component  $i$  in a multicomponent gas mixture as

$$\frac{\partial(\rho_{p,i})}{\partial t} + \nabla \cdot (\rho_{p,i} \mathbf{v}) = \nabla \cdot [\rho D \nabla (\frac{\rho_{p,i}}{\rho})] + \dot{m}' \quad (2-87)$$

Here  $\rho_{p,i}$  is partial density,  $\rho$  is mixture density. Let recall the definition of volume fraction,  $\alpha$ , and partial density  $\rho_{p,i}$  as

$$\alpha_i = \frac{V_i}{V}, \rho_{p,i} = \frac{m_i}{V} = \frac{\rho_i V_i}{V} = \frac{\rho_i \alpha_i V}{V} = \rho_i \alpha_i \approx \rho Y_i \quad (2-88)$$

Then, transport equation of one component (Eq. (2-87)) can be

$$\frac{\partial(\rho_i \alpha_i)}{\partial t} + \nabla \cdot (\rho_i \alpha_i \mathbf{v}) = \nabla \cdot [\rho D \nabla (\frac{\rho_i \alpha_i}{\rho})] + \dot{m}' \quad (2-89)$$

Based on Eq. (2-89), we can separate the species equation for fuel and liquid as

$$\frac{\partial(\rho_F \alpha_F)}{\partial t} + \nabla \cdot (\rho_F \alpha_F \mathbf{v}) = \nabla \cdot [\rho_{MG} D \nabla (\frac{\rho_F \alpha_F}{\rho_{MG}})] + \dot{m}' \quad (2-90)$$

and

$$\frac{\partial(\rho_L \alpha_L)}{\partial t} + \nabla \cdot (\rho_L \alpha_L \mathbf{v}) = \nabla \cdot [\rho_L D \nabla (\frac{\rho_L \alpha_L}{\rho_L})] + \dot{m}' \quad (2-91)$$

Where, liquid does not have diffusion itself because it is mono-liquid, then Eq. (2-91) becomes

$$\frac{\partial(\alpha_L)}{\partial t} + \nabla \cdot (\alpha_L \mathbf{v}) = \frac{\dot{m}'}{\rho_L} \quad (2-92)$$

Thus, species equation for fuel can be written as

$$\frac{\partial(\rho_F \alpha_F)}{\partial t} + \nabla \cdot (\rho_F \alpha_F \mathbf{v}) = \nabla \cdot [\rho_{MG} D \nabla (\frac{\rho_F \alpha_F}{\rho_{MG}})] + \dot{m}' \quad (2-93)$$

or

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho Y_i \mathbf{v}) = \nabla \cdot [\rho D \nabla (Y_i)] + \dot{m}' \quad (2-94)$$

#### 2.1.4 Material properties

Material properties are phase-dependent values, determined by phase indicator function,  $\alpha$ , and temperature dependent liquid fraction,  $\beta$ , as

$$\begin{aligned} \rho &= \alpha_{PCM} \rho_{PCM} + \alpha_g \rho_g, \quad \mu = \alpha_{PCM} \mu_{PCM} + \alpha_g \mu_g, \\ k &= \alpha_{PCM} k_{PCM} + \alpha_g k_g, \quad c_p = \alpha_{PCM} c_{p,PCM} + \alpha_g c_{p,g}. \end{aligned} \quad (2-95)$$

Where,

$$\begin{aligned} \rho_{PCM} &= \rho_{S-PCM} + \beta(\rho_{S-PCM} - \rho_{L-PCM}), \quad \mu_{PCM} = \mu_{L-PCM}, \\ k_{PCM} &= k_{S-PCM} + \beta(k_{S-PCM} - k_{L-PCM}), \quad c_p = c_{p,S-PCM} + \beta(c_{p,S-PCM} - c_{p,L-PCM}). \end{aligned} \quad (2-96)$$

Thus, one can be simplify as

$$\begin{aligned} \rho &= \alpha_{PCM} (\rho_{S-PCM} + \beta(\rho_{S-PCM} - \rho_{L-PCM})) + \alpha_g \rho_g, \\ \mu &= \alpha_{PCM} \mu_{PCM} + \alpha_g \mu_g, \\ k &= \alpha_{PCM} (k_{S-PCM} + \beta(k_{S-PCM} - k_{L-PCM})) + \alpha_g k_g, \\ c_p &= \alpha_{PCM} (c_{p,S-PCM} + \beta(c_{p,S-PCM} - c_{p,L-PCM})) + \alpha_g c_{p,g}. \end{aligned} \quad (2-97)$$

## 2.2 Discretization and numerical details

### 2.2.1 Discretization

We used a collocated finite volume so that integral form in conservative form is solved as [74]

$$\int_V \frac{\partial \rho \Phi}{\partial t} + \int_V \nabla \cdot (\rho \mathbf{u} \Phi) = 0 \quad (2-98)$$

Time integration is performed by a first-order implicit Euler method incorporating a variable time stepping by a first order Euler discretization. For the convective term, the Green-Gauss theorem is applied and the volume integral is transformed into a surface integral. FLUENT uses a mid-point rule integration of the surface integral which has second-order accuracy. The discretization of the convective term is done using a second-order upwind scheme, and the diffusive term in the equations is evaluated using a central-differencing scheme. The pressure field is not known a priori and must be obtained as part of the solution. Here the SIMPLE scheme was used for pressure-velocity coupling. Since FLUENT uses a collocated grid where pressure and velocity are stored at cell-centers, an interpolation procedure is needed to interpolate the pressure face values from the cell-center values. PRESTO (the Pressure Staggering Option) was used to interpolate the pressure at the face from the cell-center values. The pressure-based approach was selected for our calculation due to the low speed incompressible flow characteristics. The pressure field is determined by solving a pressure correction equation obtained from the continuity and momentum equations (called the projection method). The algorithm is illustrated in Fig. 2.3.

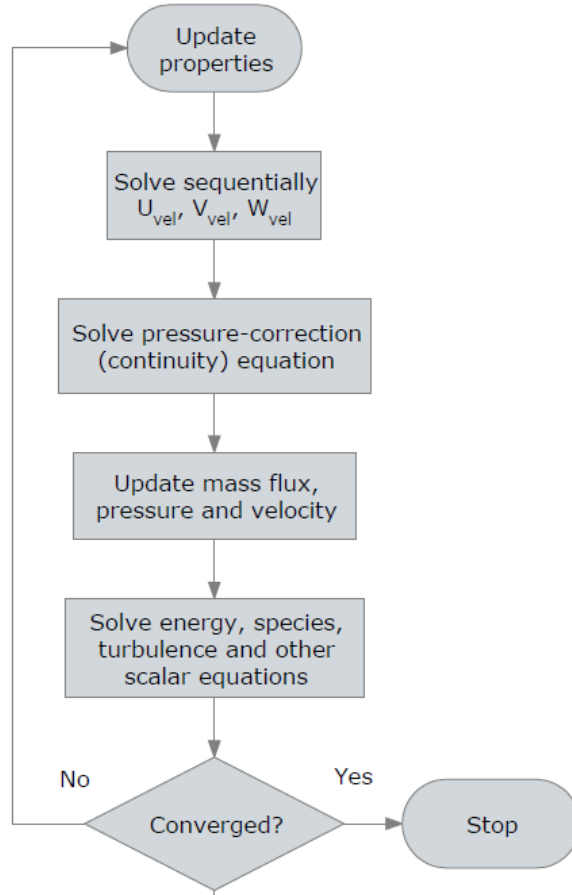


Figure 2.3 Flowchart for calculation process [74]

### 2.2.2 Numerical detail for Volume of Fluid (VOF) method

The function  $\alpha$  varies between the constant value one in full cells to zero in empty cells, while mixed cells with an intermediate value of  $\alpha$  define the transition region where the interface is localized. In grid cells,  $\alpha$  is associated as

$$\alpha_{i,j} \Delta x \Delta y = \text{volume of fluid in cell}(i,j) . \quad (2-99)$$

$\alpha$  is defined as

$$\alpha_{i,j} = \begin{cases} 1 = \text{liquid} \\ 0 < \alpha_{i,j} < 1 = \text{partial liquid} , \\ 0 = \text{gas} \end{cases} \quad (2-100)$$

here  $\alpha$  is volume fraction ,  $\Delta x$  and  $\Delta y$  is grid spacing.

In this regards, we can say

$$\alpha_{i,j}\Delta x\Delta y \approx \iint_{i,j \text{ cell}} \alpha_{i,j} dx dy. \quad (2-101)$$

Above volume fraction function  $\alpha$  is passively advected with the flow. Hence,  $\alpha$  satisfies the advection equation,

$$\frac{\partial \alpha}{\partial t} + \mathbf{v} \cdot \nabla \alpha = 0 \quad (2-102)$$

If flow is incompressible, velocity vector  $\mathbf{v}$  satisfies continuity equation

$$\nabla \cdot \mathbf{v} = 0 \quad (2-103)$$

By multiplying the equation with  $\alpha$  and adding this to the advection equation, advection equation for  $\alpha$  becomes

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{v}) = 0 \quad (2-104)$$

which means that conservation of volume to be equal to the conservation of mass in incompressible flow.

Integration of volume equation requires the evaluation of volume fluxes at each cell face. This flux represents the volume of constituent passing through a face during the current time step. Sum of all volume fluxes must be equal to the total volume flux. For example, east face of cell is

$$\sum dV_{i+1/2,j} = V_{i+1/2,j} = (\Delta t \cdot \mathbf{v}_{i+1/2,j}) \times \mathbf{A}_{i+1/2,j} \quad (2-105)$$

where  $\mathbf{v}$  is velocity field and  $\mathbf{A}$  is the edge area vector.

Based on the face velocity at the east face of the cell, control volume shown in Eq. (2-105) can be calculated. As shown in Fig. 2.4, fluid will be fluxed into the neighbor cell which can be calculated as

$$\alpha_e \mathbf{v}_e = \mathbf{v}_{i+1/2,j} = \frac{V_{i+1/2,j}}{\Delta t \times \Delta y}. \quad (2-106)$$

Thus, by use of discretization, equation could be

$$\begin{aligned}
& \frac{(\alpha^{n+1} - \alpha^n) \Delta x \Delta y}{\Delta t} + \sum_i (\alpha \mathbf{v} A)_i = 0 \\
& \rightarrow \frac{(\alpha^{n+1} - \alpha^n) \Delta x \Delta y}{\Delta t} + (\alpha_e \mathbf{v}_e A_e - \alpha_w \mathbf{v}_w A_w) + (\alpha_n \mathbf{v}_n A_n - \alpha_s \mathbf{v}_s A_s) = 0 \\
& \rightarrow \frac{(\alpha^{n+1} - \alpha^n) \Delta x \Delta y}{\Delta t} + (\alpha_e \mathbf{v}_e - \alpha_w \mathbf{v}_w) \Delta y + (\alpha_n \mathbf{v}_n - \alpha_s \mathbf{v}_s) \Delta x = 0 \\
& \rightarrow \alpha^{n+1} = \alpha^n + (\alpha_w \mathbf{v}_w - \alpha_e \mathbf{v}_e) \frac{\Delta t}{\Delta x} + (\alpha_s \mathbf{v}_s - \alpha_n \mathbf{v}_n) \frac{\Delta t}{\Delta y}
\end{aligned} \tag{2-107}$$

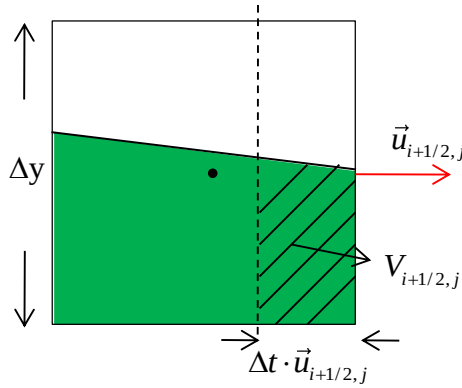


Figure 2.4 Schematic description of a computational cell for flux calculation

Youngs et al. [62] have shown that gradient  $\alpha$  can be taken to point the direction normal to the approximate interface by using linear polynomial as

$$\frac{\partial \alpha}{\partial x} = \frac{\alpha_E - \alpha_W}{2}, \quad \frac{\partial \alpha}{\partial y} = \frac{\alpha_N - \alpha_S}{2} \tag{2-108}$$

Here, the approximated values of  $\alpha$  in the E, W, N, and S control volumes are calculated as

$$\begin{aligned}
\alpha_E &= \frac{1}{2+\eta} (\alpha_{i+1,j-1} + \eta \alpha_{i+1,j} + \alpha_{i+1,j+1}) \\
\alpha_W &= \frac{1}{2+\eta} (\alpha_{i-1,j-1} + \eta \alpha_{i-1,j} + \alpha_{i-1,j+1}) \\
\alpha_N &= \frac{1}{2+\eta} (\alpha_{i-1,j+1} + \eta \alpha_{i+1,j+1} + \alpha_{i+1,j+1}) \\
\alpha_S &= \frac{1}{2+\eta} (\alpha_{i-1,j-1} + \eta \alpha_{i,j-1} + \alpha_{i+1,j-1})
\end{aligned} \tag{2-109}$$

Geometrical distribution of  $\alpha_{i,j}$  surrounded neighbor cells are shown in Fig. 2.5.

|            |            |            |
|------------|------------|------------|
| $i-1, j+1$ | $\alpha_N$ | $i+1, j+1$ |
| $\alpha_W$ | $i, j$     | $\alpha_E$ |
| $i-1, j-1$ | $\alpha_S$ | $i+1, j-1$ |

Figure 2.5 Schematic description for  $\alpha_{i,j}$  distribution with surrounded cells

Where,  $\eta$  is free parameter, we choose  $\eta = 2$ . Therefore, if reconstruct the interfacial curve with consideration of volume fraction ( $y=kx+b$ ), the slope of the approximated interface,  $k$  is

$$k = \frac{\partial \alpha / \partial x}{\partial \alpha / \partial y}. \quad (2-110)$$

Eventually we can get the slope of linear interfacial line.

Thus,  $n_x$  and  $n_y$  components of the unit normal vector  $\mathbf{n}$  are

$$\begin{aligned} n_x &= -\frac{\partial \alpha / \partial x}{\sqrt{(\partial \alpha / \partial x)^2 + (\partial \alpha / \partial y)^2}} \\ n_y &= -\frac{\partial \alpha / \partial y}{\sqrt{(\partial \alpha / \partial x)^2 + (\partial \alpha / \partial y)^2}}. \end{aligned} \quad (2-111)$$

We need to guess the distance between line interface and cell center, which is schematically shown in Fig. 2.5. Let me set this distance is  $L$ , and is defined by

$$\begin{aligned} L_1 &= |\mathbf{n}_x \cdot \Delta x + \mathbf{n}_y \cdot \Delta y|, L_2 = |-\mathbf{n}_x \cdot \Delta x + \mathbf{n}_y \cdot \Delta y| \\ \text{maximum } L &= 0.5 \times \text{Max}(L_1, L_2). \end{aligned} \quad (2-112)$$

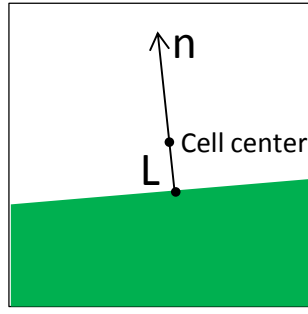


Figure 2.6 Schematic description of calculating the distance between line interface and cell center

Eventually, to estimate the linear interface, we got the slope of line and length, between cell center and interface, by use of normal vector.

As simply say, it is all for process of VOF method.

1. Give initial distribution of volume fraction
2. When velocity is solved in governing equation, we can take each face velocity (E, W, N, S), and then is given to solve how much volume is advected.
3. By use of guessed volume, slope of interface,  $k$  and distance,  $L$ , is estimated. Eventually linear curve is generated. and then interpolation to smooth the interface is done by use of linear curve.

Thus, we need to iteratively calculate the above process in order to get the time-dependent moving volume. Such sequence is schematically shown in Fig. 2.7.

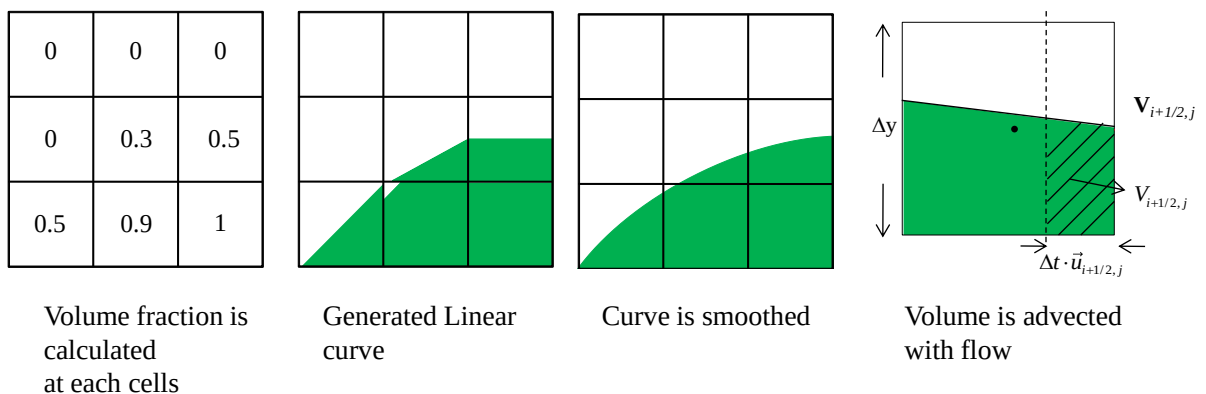


Figure 2.7 Schematic descriptions of VOF method to get the advected new volume

### 2.2.3 Calculation of Surface tension modeling

The surface tension force is a force which acts on the interface between the two fluids. The surface tension force per area can be expressed as [63]

$$F_s = \sigma \kappa \mathbf{n} \quad (2-112)$$

Where  $\sigma$  is the surface tension coefficient,  $\kappa$  is the curvature of the interface and  $\mathbf{n}$  is the interface normal pointing into the air. When surface tension coefficient  $\sigma$  is constant, 2-D curvature is defined as

$$\kappa = \frac{1}{R} \quad (2-113)$$

Where  $R$  is the local radius of curvature of the interface.

#### 2.2.3.1 Continuum surface force

To implement the surface tension force as numerically, we used the continuum surface force (CSF) method which is introduced by Brakbill et. al [63]. The method describes both the curvature estimation and the smoothing of the surface tension over a few cell widths near the interface. The curvature is calculated from a smoothed colour function field  $\alpha$ . Since the surface force is calculated from the smoothed colour function field, no surface force was generated to counteract the forming of the folds.

Let  $\mathbf{n} = \nabla \tilde{\alpha}$ , a normal vector which is not normalized, pointing into a gas. According to the [59], the curvature can be expressed as

$$\kappa = -\nabla \cdot \frac{\mathbf{n}}{|\mathbf{n}|} \quad (2-115)$$

The expression of curvature is rewritten by use of the quotient rule

$$\begin{aligned}
\kappa &= -\nabla \cdot \frac{\mathbf{n}}{|\mathbf{n}|} \\
&= -\left( \frac{\partial}{\partial x} \frac{n_x}{|\mathbf{n}|} + \frac{\partial}{\partial y} \frac{n_y}{|\mathbf{n}|} \right) \\
&= -\left( \frac{1}{|\mathbf{n}|^2} \left( |\mathbf{n}| \frac{\partial n_x}{\partial x} - n_x \frac{\partial |\mathbf{n}|}{\partial x} \right) + \frac{1}{|\mathbf{n}|^2} \left( |\mathbf{n}| \frac{\partial n_y}{\partial y} - n_y \frac{\partial |\mathbf{n}|}{\partial y} \right) \right) \\
&= -\frac{1}{|\mathbf{n}|^2} \left( |\mathbf{n}| \frac{\partial n_x}{\partial x} - n_x \frac{\partial |\mathbf{n}|}{\partial x} + |\mathbf{n}| \frac{\partial n_y}{\partial y} - n_y \frac{\partial |\mathbf{n}|}{\partial y} \right) \\
&= -\frac{1}{|\mathbf{n}|^2} \left( |\mathbf{n}| \left( \frac{\partial n_x}{\partial x} + \frac{\partial n_y}{\partial y} \right) - \left( n_x \frac{\partial |\mathbf{n}|}{\partial x} + n_y \frac{\partial |\mathbf{n}|}{\partial y} \right) \right) \\
&= -\frac{1}{|\mathbf{n}|^2} (|\mathbf{n}| \nabla \cdot \mathbf{n} - \mathbf{n} \cdot \nabla |\mathbf{n}|) \\
&= -\frac{1}{|\mathbf{n}|} \left( \left( \frac{\mathbf{n}}{|\mathbf{n}|} \cdot \nabla \right) |\mathbf{n}| - (\nabla \cdot \mathbf{n}) \right)
\end{aligned} \tag{2-116}$$

First, the vertex-centered normals  $n_{i+1/2, j+1/2}$  are found by averaging two central differences:

$$\begin{aligned}
n_{i+1/2, j+1/2} &= \frac{1}{2} \left( \frac{\partial \tilde{f}}{\partial x_{i+1/2, j}} + \frac{\partial \tilde{f}}{\partial x_{i+1/2, j+1/2}} \right) \\
&= \frac{1}{2} \left( \frac{\tilde{f}_{i+1, j} - \tilde{f}_{i, j}}{\Delta x} + \frac{\tilde{f}_{i+1, j+1} - \tilde{f}_{i, j+1}}{\Delta x} \right) \\
&= \frac{\tilde{f}_{i+1, j} + \tilde{f}_{i+1, j+1} - \tilde{f}_{i, j} - \tilde{f}_{i, j+1}}{2\Delta x} \\
n_{i+1/2, j+1/2} &= \frac{\tilde{f}_{i, j+1} + \tilde{f}_{i+1, j+1} - \tilde{f}_{i, j} - \tilde{f}_{i+1, j}}{2\Delta x}
\end{aligned} \tag{2-117}$$

Cell-centered normal  $n_{i+j}$  are found by averaging the four surrounding vertex-centered normals;

$$n_{i, j} = \frac{1}{4} \left( n_{i+1/2, j+1/2} + n_{i+1/2, j-1/2} + n_{i-1/2, j+1/2} + n_{i-1/2, j-1/2} \right) \tag{2-118}$$

Let the magnitude of the normal be

$$|\mathbf{n}| = \sqrt{n_x^2 + n_y^2} \quad \text{and is defined in cell corners and centers.}$$

Then first term in RHS can be discretized as

$$\begin{aligned}
\left( \frac{\mathbf{n}}{|\mathbf{n}|} \cdot \nabla \right) |\mathbf{n}| &= \left( \frac{n_x}{|\mathbf{n}|} \right)_{i,j} \left( \frac{\partial |\mathbf{n}|}{\partial x} \right) + \left( \frac{n_y}{|\mathbf{n}|} \right)_{i,j} \left( \frac{\partial |\mathbf{n}|}{\partial y} \right) \\
&= \frac{n_{xi,j}}{|\mathbf{n}|} \left( \frac{|\mathbf{n}|_{xi+1/2,j+1/2} - |\mathbf{n}|_{xi-1/2,j+1/2} + |\mathbf{n}|_{xi+1/2,j-1/2} - |\mathbf{n}|_{xi-1/2,j-1/2}}{2\Delta x} \right) \\
&+ \frac{n_{yi,j}}{|\mathbf{n}|} \left( \frac{|\mathbf{n}|_{yi+1/2,j+1/2} - |\mathbf{n}|_{yi-1/2,j+1/2} + |\mathbf{n}|_{yi+1/2,j-1/2} - |\mathbf{n}|_{yi-1/2,j-1/2}}{2\Delta y} \right)
\end{aligned} \tag{2-119}$$

and second term in RHS is discretized as

$$\begin{aligned}
\left( \frac{\mathbf{n}}{|\mathbf{n}|} \cdot \nabla \right) |\mathbf{n}| &= \left( \frac{n_x}{|\mathbf{n}|} \right)_{i,j} \left( \frac{\partial |\mathbf{n}|}{\partial x} \right) + \left( \frac{n_y}{|\mathbf{n}|} \right)_{i,j} \left( \frac{\partial |\mathbf{n}|}{\partial y} \right) \\
&= \frac{n_{xi,j}}{|\mathbf{n}|} \left( \frac{|\mathbf{n}|_{xi+1/2,j+1/2} - |\mathbf{n}|_{xi-1/2,j+1/2} + |\mathbf{n}|_{xi+1/2,j-1/2} - |\mathbf{n}|_{xi-1/2,j-1/2}}{2\Delta x} \right) \\
&+ \frac{n_{yi,j}}{|\mathbf{n}|} \left( \frac{|\mathbf{n}|_{yi+1/2,j+1/2} - |\mathbf{n}|_{yi-1/2,j+1/2} + |\mathbf{n}|_{yi+1/2,j-1/2} - |\mathbf{n}|_{yi-1/2,j-1/2}}{2\Delta y} \right)
\end{aligned} \tag{2-120}$$

$$\begin{aligned}
(\nabla \cdot \mathbf{n})_{i,j} &= \left( \frac{\partial n_x}{\partial x} \right) + \left( \frac{\partial n_y}{\partial y} \right) \\
&= \frac{n_{xi+1/2,j+1/2} - n_{xi-1/2,j+1/2} + n_{xi+1/2,j-1/2} - n_{xi-1/2,j-1/2}}{2\Delta x} \\
&+ \frac{n_{yi+1/2,j+1/2} - n_{yi-1/2,j+1/2} + n_{yi+1/2,j-1/2} - n_{yi-1/2,j-1/2}}{2\Delta y}
\end{aligned}$$

Thus, the curvature can be calculated at cell centers in the vicinity of the interface.

## 2.2.4 Numerical modeling of melting

The essential feature of the basic enthalpy method is that the evolution of the latent heat is accounted by the enthalpy as well as the relationship between the enthalpy and temperature. The relationship between the enthalpy and temperature can be defined in terms of the latent heat release characteristics of the phase change material. This relationship is usually assumed to be a linear

function for non-isothermal phase change problem. Figure 2.8 shows the enthalpy–temperature curves for general case. The enthalpy as a function of temperature is given by Eq. (2-67), and numerical smoothing is done at the non linear corner.

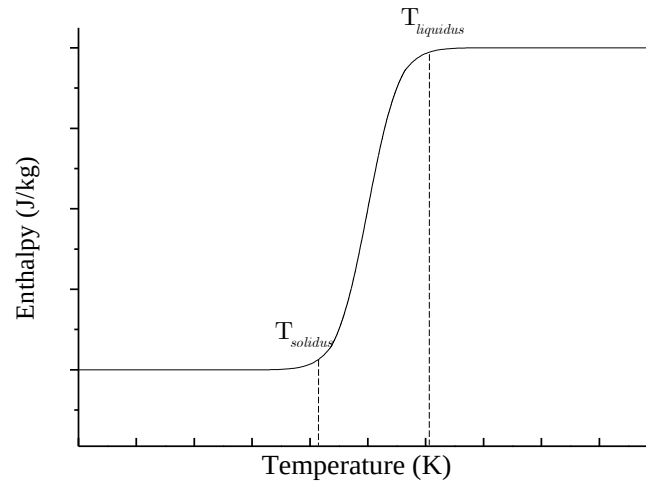


Figure 2.8 Temperature-dependent enthalpy distribution

The enthalpy–temperature curve is employed in Fluent as enthalpy method. However, when problem is needed to solve melting and gas phase species transport together, default enthalpy method cannot be used. Enthalpy method employed in Fluent is designed for the problem involving multi-component melting or solidification which needs to solve species transport between each component in liquid phase. Thus, species transport equation employed in Fluent only works for liquid phase's species, not the species in gas phase when it turns on in Fluent. In fact, implementing species equation to Fluent by user-defined subroutine is more difficult than implementing enthalpy model when gasification is needed to solved. Therefore, it is better to model the enthalpy method by user-subroutine function to the Fluent when gasification is considered. Following shows two types of functions which defines relation between enthalpy and temperature, and is tested.

#### 2.2.4.1. Sinusoidal function

Firstly, temperature-dependent specific latent heat function is given in order to account the melting process. Figure 2.9 shows two types of specific latent heat function, where, red line shows box shaped

constant latent heat and black line shows sinusoidal distribution of the specific latent heat. In order to make consistency, latent heat of melting bounded inside of two lines (integrated area), black and red, are given as same. The phase change takes place within a defined temperature interval  $\Delta T_m$ . If the temperature change of an element  $\Delta T = T_{is} - T_{is}^{pre}$  intersects with this phase change interval during one time step, the latent heat has to be partly released as a heat source according to the amount of intersection. The specific latent heat to be applied is calculated by the integral over the intersected temperature region. However, this simple formulation was observed to be numerical unstable because of the sudden onset of the source term when the temperature first reaches the phase change interval. Therefore a sinusoidal distribution of the temperature against specific latent heat was chosen in such a way, that the integral over the whole temperature interval equals the latent heat equation, Eq. (2-117), shows the sinusoidal function as

$$c_{p,L} = \frac{L_m}{\Delta T_m} \left[ 1 - \cos \left( 2\pi \frac{T - T_m + 0.5\Delta T_m}{\Delta T_m} \right) \right] \quad (2-121)$$

here,

$L_m$  = latent heat of melting (J/kg)=180 kJ/kg,

$\Delta T_m$  = Range of temperature between solidus and liquidus (K),

$T_{solidus} = 350 \text{ K}$ ,  $T_{liquidus} = 400 \text{ K}$ ,  $\Delta T_m = (T_{liquidus} - T_{solidus} = 50 \text{ K})$ .

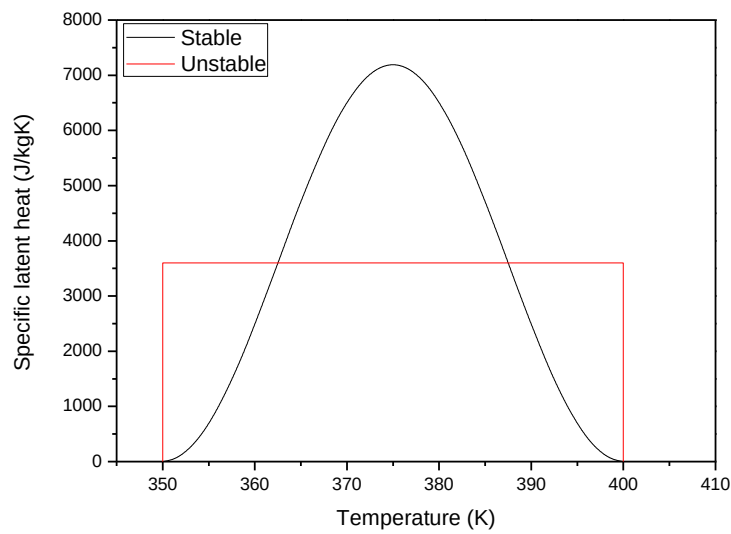


Figure 2.9 Temperature-dependent specific latent heat distribution

Since the specific latent heat to be applied is included as source term by the integral over the intersected temperature region, Eq. (2-121) becomes

$$\begin{aligned}
& \int_{T_{is}^{pre}}^{T_{is}} \frac{L_m}{\Delta T_m} \left[ 1 - \cos \left( 2\pi \frac{T - T_m + \frac{\Delta T_m}{2}}{\Delta T_m} \right) \right] dT \\
&= \frac{L_m}{\Delta T_m} \left[ T + \frac{\Delta T_m}{2\pi} \sin \left( 2\pi \frac{T - T_m + \frac{\Delta T_m}{2}}{\Delta T_m} \right) \right]_{T_{is}^{pre}}^{T_{is}} \\
&= \frac{L_m}{\Delta T_m} \left[ T_{is} - T_{is}^{pre} + \frac{\Delta T_m}{2\pi} \cdot \sin \left( 2\pi \frac{T_{is} - T_m + \frac{\Delta T_m}{2}}{\Delta T_m} \right) - \frac{\Delta T_m}{2\pi} \cdot \sin \left( 2\pi \frac{T_{is}^{pre} - T_m + \frac{\Delta T_m}{2}}{\Delta T_m} \right) \right].
\end{aligned} \tag{2-122}$$

Within the intersection interval  $\Delta T$ , the heat source is calculated by the integral of Eq. (2-121), divided by the current time step size. Further the expression has to be multiplied by the volume fraction. Then, source type enthalpy equation arise as

$$S_h = \frac{L_m \alpha}{\Delta T_m \Delta t} \left[ T_{is} - T_{is}^{pre} - \frac{\Delta T_m}{2\pi} \left( \sin \left( 2\pi \frac{T_{is} - T_m + \frac{\Delta T_m}{2}}{\Delta T_m} \right) - \sin \left( 2\pi \frac{T_{is}^{pre} - T_m + \frac{\Delta T_m}{2}}{\Delta T_m} \right) \right) \right]. \tag{2-123}$$

This integrated source term is implemented in energy equation.

#### 2.2.4.2. Sigmoid function

As similar with sinusoidal function, discretized form of specific latent heat is given as respect to temperature by sigmoid function;

$$\begin{aligned}
c_{p,L} &= \frac{L_m \cdot A}{e^{-A(T-T_f)} + e^{-A(T-T_f)} + 2} = \frac{L_m \cdot A \cdot e^{-A(T-T_f)}}{e^{-2A(T-T_f)} + 1 + 2e^{-A(T-T_f)}} \\
&= \frac{L_m \cdot A \cdot e^{-A(T-T_f)}}{1 + 2 \cdot 1 \cdot e^{-A(T-T_f)} + (e^{-A(T-T_f)})^2} = \frac{L_m \cdot A \cdot e^{-A(T-T_f)}}{(1 + e^{-A(T-T_f)})^2}.
\end{aligned} \tag{2-124}$$

taking integration over time interval

$$\int_{T_{is}}^{T_{is}^{n+1}} c_{p,L} dT = \int_{T_{is}}^{T_{is}^{n+1}} \frac{L_m \cdot A \cdot e^{-A(T-T_f)}}{(1 + e^{-A(T-T_f)})^2} dT = \left[ \frac{L_m}{(1 + e^{-A(T-T_f)})} \right]_{T_{is}}^{T_{is}^{n+1}} \quad (2-125)$$

$$= \frac{L_m}{(1 + e^{-A(T_{is}^{n+1}-T_f)})} - \frac{L_m}{(1 + e^{-A(T_{is}-T_f)})}$$

And multiply with  $\frac{\alpha}{\Delta t}$ , to make the function form as source, then :

$$S_h = -\frac{L_m \alpha}{\Delta t c_p} \left[ \frac{1}{1 + e^{-a(T_{is}^{n+1}-T_f)}} - \frac{1}{1 + e^{-a(T_{is}^n-T_f)}} \right] \quad (2-126)$$

Eventually, integrated source term (Eq. (2-125)) is implemented in energy equation.

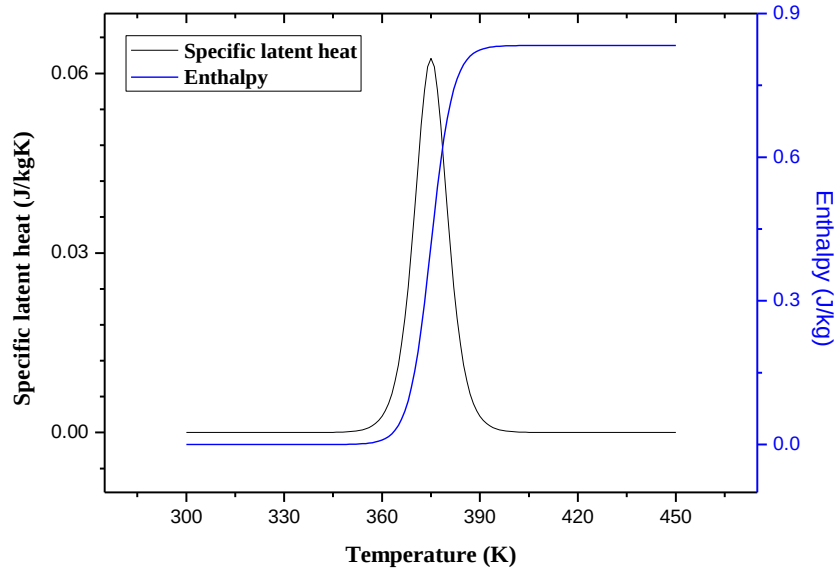


Figure 2.10 Temperature-dependent specific latent heat and enthalpy distribution

These two types of function (sinusoidal and sigmoid function) listed in section 2.2.4.1 and 2.2.4.2 was implemented as source term in User Defined Function (UDF) in order to take account for the latent heat of melting appropriately when we solve the problem involving gas phase species transport with melting process. As compare with results obtained by default enthalpy method in Fluent, result achieved from sigmoid function shows better accuracy than that from sinusoidal function. Its results will be shown in chapter 3.

## Chapter 3 Validation

In this section, we show general case of melting and of free surface problem as validation against the current numerical model. In general, melting problem calculating melting phase front is often called moving boundary or Stefan problem. To solve such problem calculation method has been developed as (1) analytical solution for the 1-D cases of an infinite or semi-infinite region with simple initial and boundary condition and constant thermal properties in closed form and (2) numerical solution for moving phase front at which displacement rate is controlled by the latent heat lost or absorbed at the boundary. Especially melting can be numerically calculated by use of different method (i.e. fixed grid, adaptive mesh (moving mesh)). However fixed grid method is recently popular because it can be applicable for both of mushy (see the explanation for mushy in section 2.1.2) and isothermal phase change problem. In present study, Enthalpy method, one of representative way as fixed grid method, is used and is validated with (1) analytical solution obtained by Nuemman [85] and (2) numerical solution obtained from the effective heat capacity method under fixed grid method [27].

### 3.1 Comparison of Enthalpy method with 1D effective heat capacity method and 1D analytical solution (Neumann's solution)

#### 3.1.1 1D analytical solution

Current model, the enthalpy method, is validated by comparing the simulations of well known stefan's one-dimensional phase change problem with the analytical solution [85]. The analytical solution derived by Neumann (so-called Neumann's analytical solution) is a solution for temperature and phase front in semi-infinite one dimensional domain (0 to  $\infty$ ) shown in Fig. 3.1. System is initially in the solid phase at temperature  $T_0 < T_{SL}$ . Higher temperature,  $T_1$ , than melting temperature is imposed on right side, and then the solid begins to melt as time progresses.

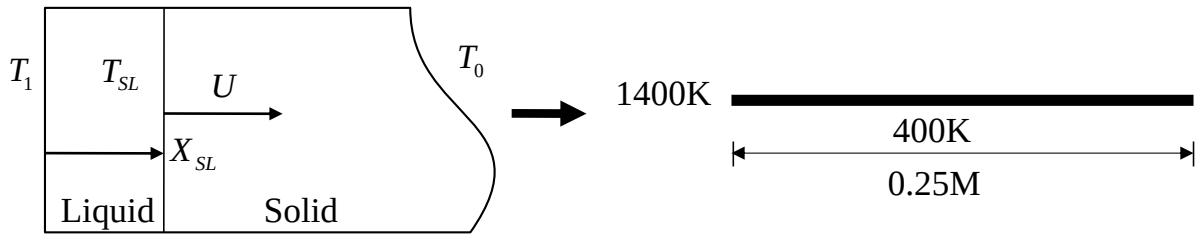


Figure 3.1 Schematics of 1-D melting phase change problem

Properties of system are used as copper and are shown in Table 1.

Table 3.1 Physical properties of copper

| Parameter              | Symbol    | Value              | Units             |
|------------------------|-----------|--------------------|-------------------|
| Copper (solid phase)   |           |                    |                   |
| Density                | $\rho_s$  | 8920               | kg/m <sup>3</sup> |
| Thermal conductivity   | $k_s$     | 365                | W/(m K)           |
| Specific heat          | $c_{p,s}$ | 435                | J/(kg K)          |
| Latent heat of melting | $L$       | $2.05 \times 10^5$ | J/kg              |
| Melting temperature    | $T_m$     | 500                | K                 |
| Copper (liquid phase)  |           |                    |                   |
| Density                | $\rho_l$  | 8920               | kg/m <sup>3</sup> |
| Thermal conductivity   | $k_l$     | 174                | W/(m K)           |
| Specific heat          | $c_{p,l}$ | 494.5              | J/(kg K)          |

The problem initially has two distinct regions (solid & liquid), hence, equation is based on the equation of transient conduction as

$$\frac{1}{\alpha_L} \frac{\partial T_L}{\partial t} = \frac{\partial^2 T_L}{\partial x^2}, \quad 0 \leq x < X_{LS} \quad (3-1)$$

$$\frac{1}{\alpha_S} \frac{\partial T_S}{\partial t} = \frac{\partial^2 T_S}{\partial x^2}, \quad X_{LS} \leq x < \infty \quad (3-2)$$

where,  $X_{SL}$ ,  $\alpha_S$ ,  $\alpha_L$  are position of interface, thermal diffusivity of solid and of liquid respectively.

The initial and boundary condition are

$$T_S(x, t=0) = T_0, \quad (3-3)$$

$$T_L(x=0, t) = T_1, \quad (3-4)$$

$$T_S(x \rightarrow \infty, t) = T_0, \quad (3-5)$$

$$T_L(x = X_{SL}, t) = T_{SL}, \quad (3-6)$$

$$T_S(x = X_{SL}, t) = T_{SL}, \quad (3-7)$$

$$-k_L \left. \frac{\partial T_L}{\partial x} \right|_{x=X_{SL}} + k_L \left. \frac{\partial T_L}{\partial x} \right|_{x=X_{SL}} = \rho h_{SL} \frac{dX_{SL}}{dt}. \quad (3-8)$$

To get the non-dimensional form of equation, let us introduce on-dimensional liquid and solid temperature as

$$\bar{T}_L = \frac{T_L - T_1}{T_{SL} - T_0}, \quad \bar{T}_S = \frac{T_S - T_1}{T_{SL} - T_0}. \quad (3-9)$$

By use of PDEs for these temperatures, Eq. (3-1) and (3-2) becomes

$$\bar{T}_L'' + 2\eta_L \bar{T}_L' = 0, \quad (3-10)$$

$$\bar{T}_S'' + 2\eta_S \bar{T}_S' = 0. \quad (3-11)$$

Appropriate boundary condition is then

$$\bar{T}_L(\eta_L = 0) = 0, \quad (3-12)$$

$$\bar{T}_L(\eta_L = \eta_{SL}) = 1, \quad (3-13)$$

$$\bar{T}_S(\eta_S = \beta\eta_{SL}) = 1, \quad (3-14)$$

$$\bar{T}_s(\eta_s \rightarrow \infty) = 0. \quad (3-15)$$

Here,  $\eta_s$  and  $\eta_L$  are respectively non-dimensional position of solid and liquid side interface and  $\eta_{SL}$  is solution of non-dimensional position of interface, which is defined as

$$\eta_{SL} = \frac{X_{SL}}{2\sqrt{\alpha_L t}} \quad (3-16)$$

and  $\beta$  is arbitrary value defined by

$$\beta = \sqrt{\frac{\alpha_L}{\alpha_s}}. \quad (3-17)$$

To get non-dimensional form for temperature, let's use non-dimensional position of interface and then following procedure written in [85], we can get

$$\bar{T}_L = \frac{\text{erf}(\eta_L)}{\text{erf}(\eta_{SL})}, \quad (3-18)$$

$$\bar{T}_s = \frac{1 - \text{erf}(\eta_s)}{1 - \text{erf}(\eta_{SL})}. \quad (3-19)$$

The interface speed is given by  $U = dX_{SL} / dt$ , so by using Eq. (3-16) the interface speed is

$$U = \sqrt{\frac{\alpha_L}{t_s}} \eta_{SL}. \quad (3-20)$$

To get the value of  $\eta_{SL}$ , recall the boundary condition shown in Eq. (3-8), then the liquid phase temperature derivative is given by

$$\left. \frac{\partial T_L}{\partial x} \right|_{X_{SL}} = (T_{SL} - T_L) \left. \frac{d\bar{T}_L}{d\eta_L} \right|_{X_{SL}} \cdot \frac{1}{2\sqrt{\alpha_L t}}. \quad (3-21)$$

And likewise for the solid phase as well. Performing operation on equation for boundary condition at interface (shown in Eq. (3-8)) and simplifying, then resulting non-dimensional form of equation is

$$\left. \frac{\partial \bar{T}_L}{\partial \eta_L} \right|_{\eta_{SL}} - \frac{k_s \sqrt{\alpha_L} (T_{SL} - T_0)}{k_L \sqrt{\alpha_s} (T_1 - T_{SL})} \left. \frac{d\bar{T}_s}{d\eta_s} \right|_{\beta \eta_{SL}} = 2 \frac{h_{SL}}{c_{p,L} (T_1 - T_{SL})} \eta_{SL}. \quad (3-22)$$

Now use the solution of non dimensional temperature (Eq. (3-18) and (3-19)), to evaluation derivatives, then

$$\bar{T}'_L(\eta_{SL}) = \frac{2}{\sqrt{\pi}} \frac{\exp(-\eta_{SL}^2)}{\text{erf}(\eta_{SL})}, \quad (3-23)$$

$$\bar{T}'(\beta\eta_{SL}) = -\frac{2}{\sqrt{\pi}} \frac{\exp(-(\beta\eta_{SL})^2)}{1 - \text{erf}(\beta\eta_{SL})}. \quad (3-24)$$

and replace Eq. (3-22) by Eq. (3-23) and (3-24) with introducing graphical solution, then we obtain

$$\frac{\exp(-\eta_{SL}^2)}{\text{erf}(\eta_{SL})} - \frac{k_s \sqrt{\alpha_L} (T_{SL} - T_0)}{k_L \sqrt{\alpha_S} (T_1 - T_{SL})} \frac{\exp(-(\beta\eta_{SL})^2)}{1 - \text{erf}(\beta\eta_{SL})} = \sqrt{\pi} \frac{h_{SL}}{c_{p,L} (T_1 - T_{SL})} \eta_{SL}. \quad (3-25)$$

By use of this equation we can get the non-dimensional phase interface,  $\eta_{SL}$ , and it can be used in Eq. (3-16) to get real position interface according to appropriate material properties (Table 3.1). First solving Eq. (3-25), we get  $\eta_{SL} = 0.73$ . Then dimensional position of interface is  $X_{SL} = 0.92\sqrt{t}$ . By using information in terms of position of interface, we get time dependent  $X_{SL}$  from 0 s to 30 s as shown in Fig 3.2

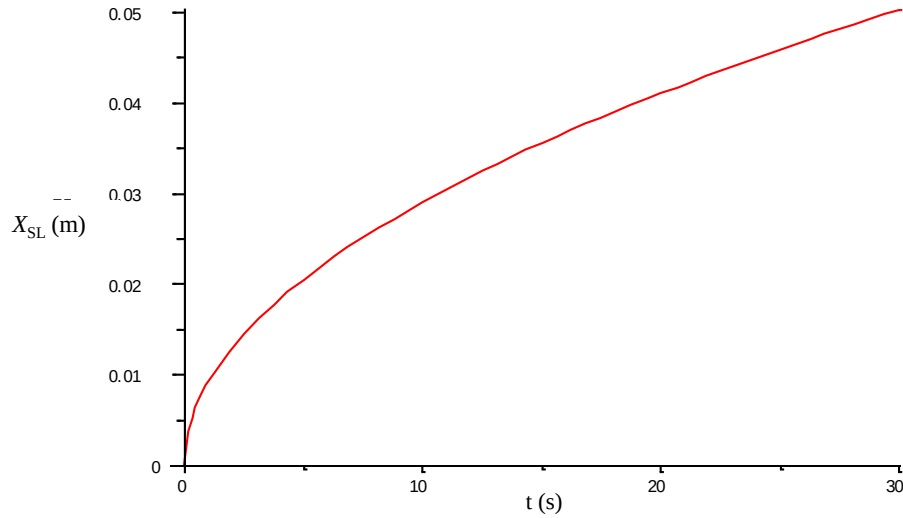


Figure 3.2 Position of interface with respect to time

And also, by use of Eq. (3-9), we can get equation for liquid and solid state temperature. Eventually that equation can be solved with information of boundary condition and position of interface

$$T_L = T_1 + (T_{SL} - T_1) \frac{\text{erf}(\eta_L)}{\text{erf}(\eta_{SL})} \rightarrow T_L = 1400 - 1287 \times \text{erf}\left(\frac{7.9 \times 10^8 x}{\sqrt{t}}\right) \quad (3-26)$$

$$T_s = T_0 + (T_{SL} - T_0) \frac{1 - \text{erf}(\eta_s)}{1 - \text{erf}(\beta\eta_{SL})} \rightarrow T_s = 598.9 - 198.9 \times \text{erf}\left(\frac{51.5x}{\sqrt{t}}\right) \quad (3-27)$$

with considering thermal boundary condition as

$$T = T_s \text{ (when } T > T_{SL}), T = T_{SL} \text{ (when } T = T_{SL}), T = T_L \text{ (when } T < T_{SL}). \quad (3-28)$$

Left one in Fig. 3.3 shows temperature profile obtained from Eq. (3-26) and (3-27) at  $t=30.0$  s, here intersection point stands for position of interface. Based on thermal boundary condition (shown in Eq. (3-28)), temperature profile at right side could be achieved according to intersection point.

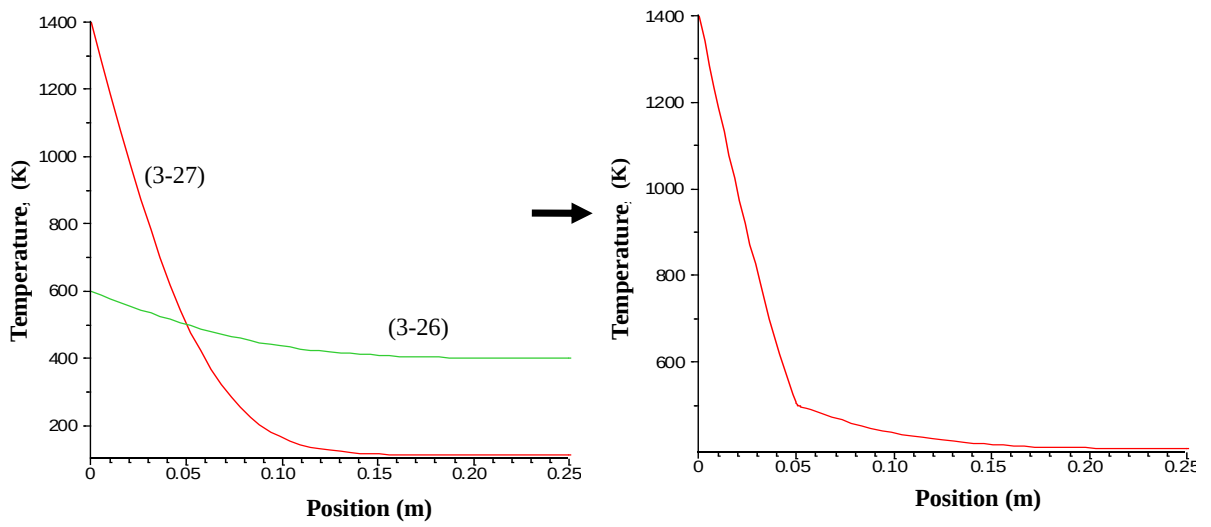


Figure 3.3 Analytical solution of temperature profile

Eventually, we get position of interface (Fig. 3.2) and temperature profile (Fig. 3.3) by use of analytical way.

### 3.1.2 1-D Enthalpy method

Even though analytical methods were mathematically robust, applicable ranges of solution are limited to one-dimensional cases of an infinite or semi-infinite region with simple initial and boundary conditions and constant thermal properties. Therefore treatments were extended to numerical analyses with finite difference and finite element methods. Particularly, because of their simplicity in formulation, finite difference methods are still used for a wide range of industrial processes. The

essential feature of finite difference methods is that the latent heat absorption or release is accounted for in the governing energy equation by defining either a total enthalpy [33-34, 36] or a specific heat capacity [35]. Consequently, the numerical solution can be carried out on a space grid that remains fixed throughout the calculation, the so-called fixed grid method [37]. In contrast to the variable grid method, domain or coordinate transformation is not required, implying a low computational cost. Therefore, above analytical solution will be compare with numerical solution obtained from enthalpy method and effective heat capacity method. One of approaches in the fixed grid method, enthalpy method taking account of latent heat evolution, is applied in our calculation. Equation of enthalpy method, which is already described in equation part, is used to calculate 1-D melting problem as same condition (Fig. 3.1) with analytical solution. Material properties are used same with Table. 3.1, and we get the time dependent position of interface as well as temperature profile at  $t=30$  s, which is shown in Fig. 3.4.

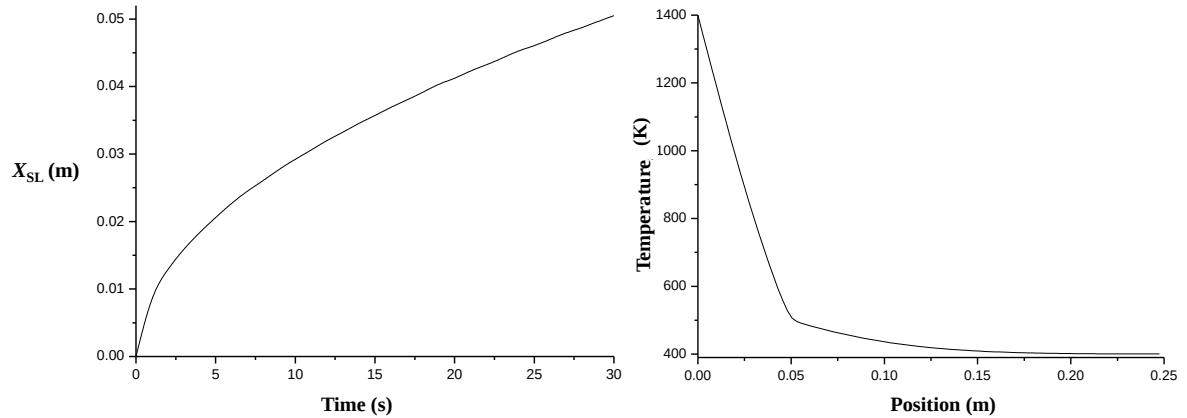


Figure 3.4 Time-dependent position of interface and temperature profile obtained at 3 s by using 1-D enthalpy method

### 3.1.3 Effective heat capacity method

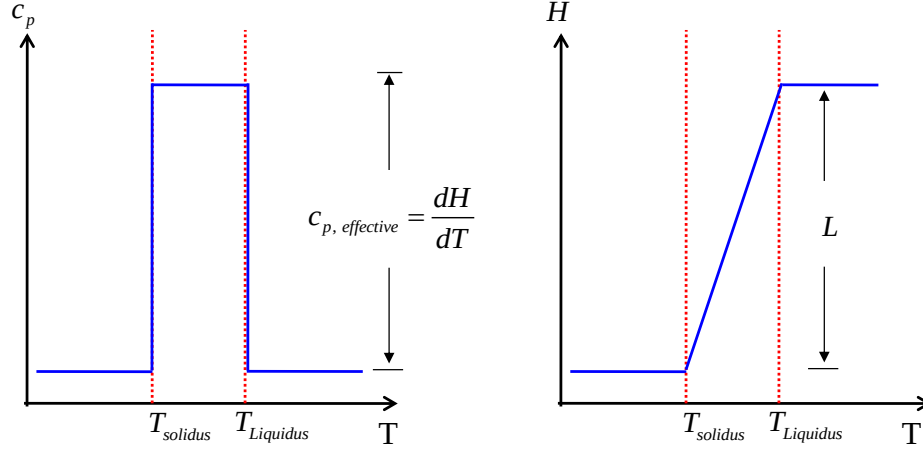


Figure 3.5 Relationship of heat capacity or derivative of heat capacity against temperature

Figure 3.5 briefly shows relationship of heat capacity against temperature and of enthalpy against temperature for melting with mushy region. Here, the effective heat capacity,  $c_{p, effective}$ , is defined as the slope of enthalpy-temperature curve [35] and is directly proportional to the stored and released energy during the phase change [39]. In this method, the latent heat is accounted by increasing the heat capacity of the material in between solidus and liquefying temperature. Therefore, definition of the effective heat capacity is given as

$$c_{p, effective} = \begin{cases} \left( \frac{c_{p,s} + c_{p,l}}{\Delta T} \right) & \text{if } T < T_{solidus} \\ 2 \left( \frac{c_{p,s} + c_{p,l}}{\Delta T} \right) + \frac{\int_{T_{solidus}}^{T_{liquidus}} c(T) dT + L}{\Delta T} & \text{if } T > T_{liquidus} \\ c_{p, interface} = \frac{\int_{T_{solidus}}^{T_{liquidus}} c(T) dT + L}{\Delta T} & \text{if } T_{solidus} < T < T_{liquidus} \end{cases} \quad (3-28)$$

Here,  $c_{p,l}$ ,  $c_{p,s}$  and  $c_{p, interface}$  are specific heat capacity at liquid state, solid state and interface

respectively.  $T_{solidus}$ ,  $T_{liquidus}$  and  $\Delta T$  are respectively solidus temperature, liquefying temperature and temperature range between solidus and liquefying temperature. Unlike enthalpy method, heat capacity method is solved in temperature form of energy equation to directly get the temperature.

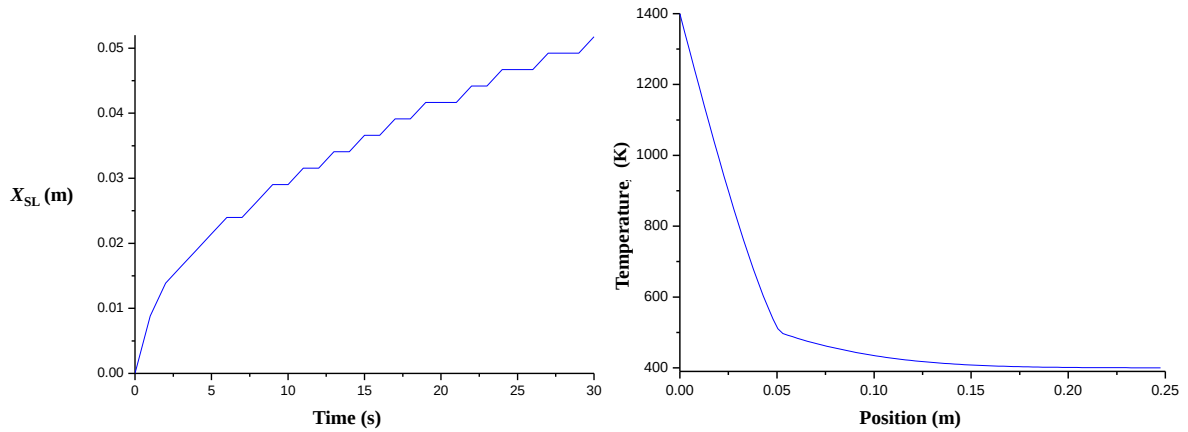


Figure 3.6 Time-dependent position of interface and temperature profile obtained at 3 s by using 1D effective heat capacity method

As results calculated from 1-D effective heat capacity method, time dependent position of interface and temperature distribution at  $t = 30.0$  s are shown together in Fig. 3.6. Position of interface  $X_{SL}$  shows stair shape of profile with increase of time. It may happen due to numerical error caused by abrupt jump of heat capacity vicinity of mushy zone.

### 3.1.4 Comparison of results obtained from three method (Nuemann's solution, enthalpy method, effective heat capacity method)

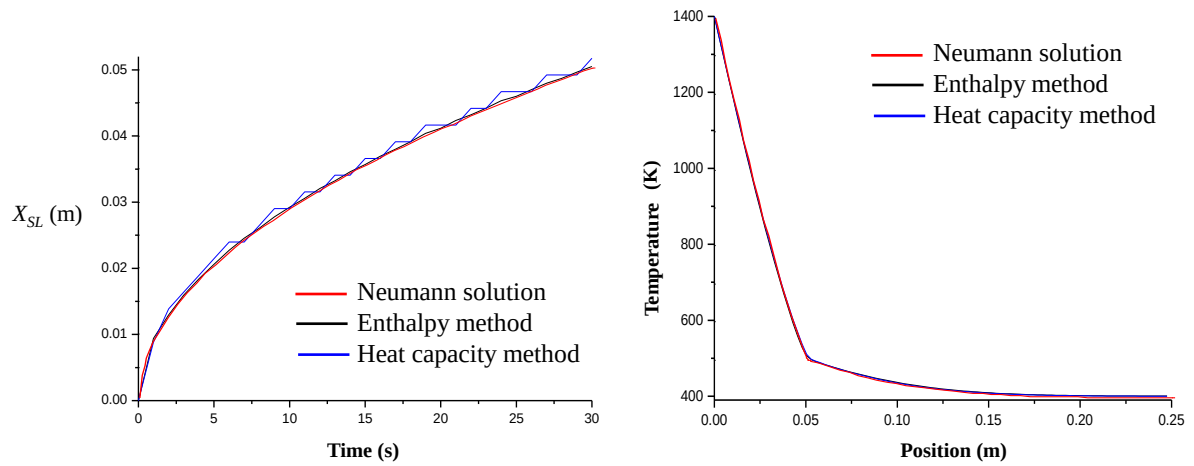


Figure 3. 7 Time-dependent position of melting front and temperature distribution at 30.0 s

Based on result obtained from analytical solution and different numerical method (enthalpy method effective heat capacity method, time dependent position of melting front and temperature distribution at 30 s was superimposed in Fig. 3.7. Temperature profile obtained from Neumann solution, enthalpy method and effective heat capacity method shows good agreement, but time dependent position of melt front achieved from effective heat capacity method, which shows oscillated pattern, has discrepancy in comparison with analytical solution. However, both results came from enthalpy method shows good agreement.

## 3.2 2D Enthalpy-porosity method for gallium melting

1-D calculation in section 3.1 shows that enthalpy method is better to use in order to predict the time-dependent melting front as compare with heat capacity method. Therefore, we choose enthalpy method to predict the melting process, and extend it to 2-D problem. Thus, it is necessary to test the 2-D enthalpy method. Our target is to check the accuracy of 2-D enthalpy method in predicting the position of melting front and fluid motion in molten area.

Simple 2D melting problem of gallium in a cavity by the use of Enthalpy-Porosity method was solved and compared with experimental results. Figure 3.8 shows the schematic illustration of the physical configuration of gallium melting. Solid gallium occupies the whole domain,  $T_H = 311$  K is heated wall temperature, and  $T_C = 301.3$  K is cold wall temperature. The boundaries of the top and bottom surfaces are insulated walls. The width  $W = 8.89$  cm and the height  $H = 6.35$  cm, respectively. Normal gravity is applied in the downward. Details of the applied material properties and information on the experimental setup are described in Brent's work [37].

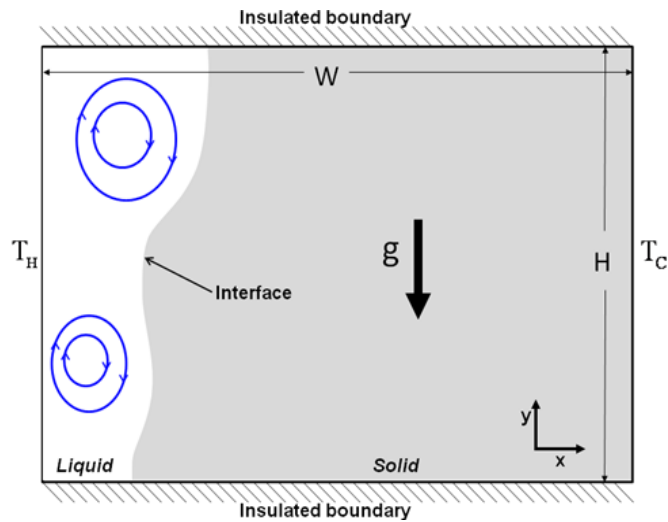


Figure 3.8 Schematic of gallium melting

Once the calculation is started, the solid gallium melts. Fig. 3.8 shows the shape and location of the solid-liquid interface at several times during the melting process. The black and red lines indicate the experimental [37] and calculated data obtained from current model respectively. Before a time of 2.0 minutes, the shape of the interface is nearly flat because convection is still weak and melting is driven by conduction. After 2.0 minutes, the interface becomes wavy due to the circular flow inside the molten region. The position of the melt front near the top surface in the calculation before a time of 12.5 minutes is over-estimated compared to experiment, and after 19.0 minutes, it is underestimated. However the overall trend shows good agreement with experiment and we can safely say that our model and code are fairly validated to track the melting boundary satisfactorily.

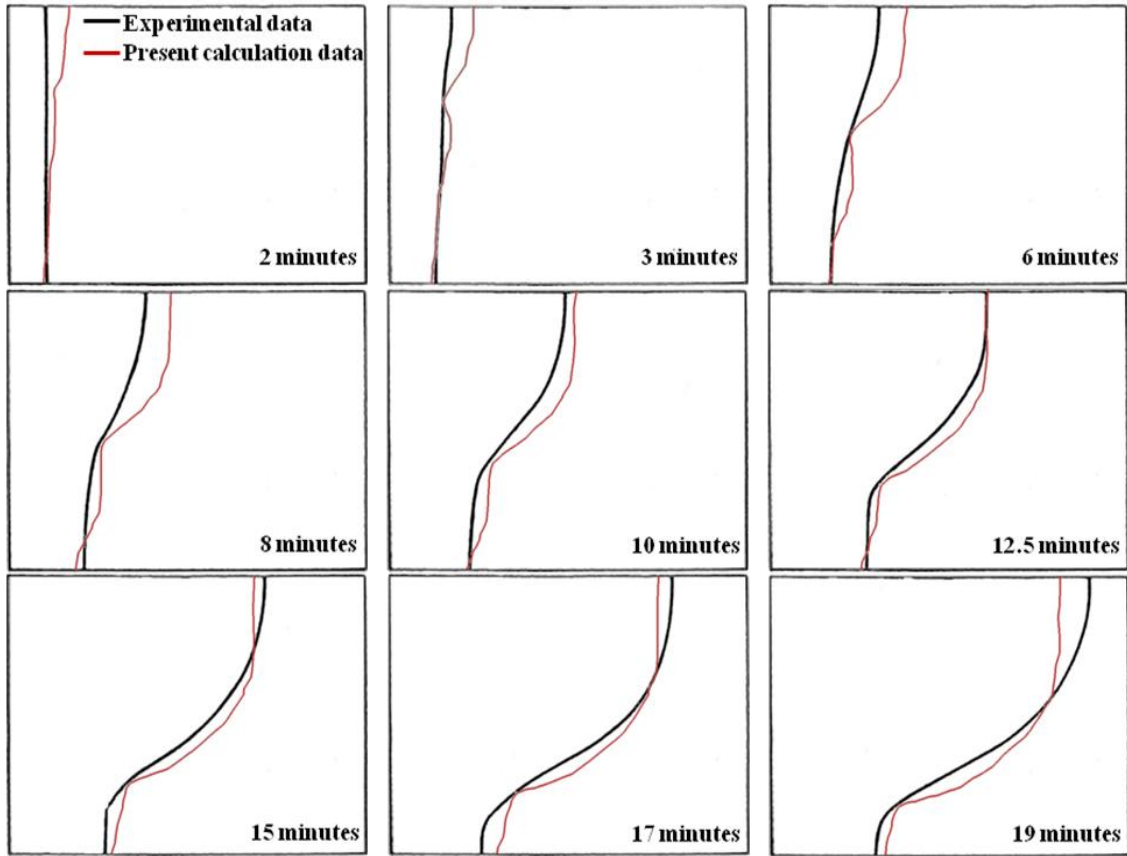


Figure 3.9 Comparison of experiment [37] and current numerical model: position of melt front with time

It is well known that a key point in the calculation of melting is the exact interface position between the solid and liquid phases. But in case of a convection-driven melting problem, such exact prediction is difficult due to the complex convection flow inside the liquid. For this reason, numerical studies for convection flow inside molten liquids need to pay more attention. One of example was shown in Nouredine's work [86]. In his report, he tried to resolve the controversy over tin and gallium melting in a rectangular cavity heated from one side. He presented flow pattern inside of a cavity by using many types of calculation method and code, but eventually he concluded that we could not beg the question in terms of how many circular cell in a cavity is contained, in other words, only data providing reliability is position of melting front. Figure 3.10 shows circular cell as flow pattern inside of a gallium cavity taken by (a) Nouredine's work [86] and taken by (b) our model.

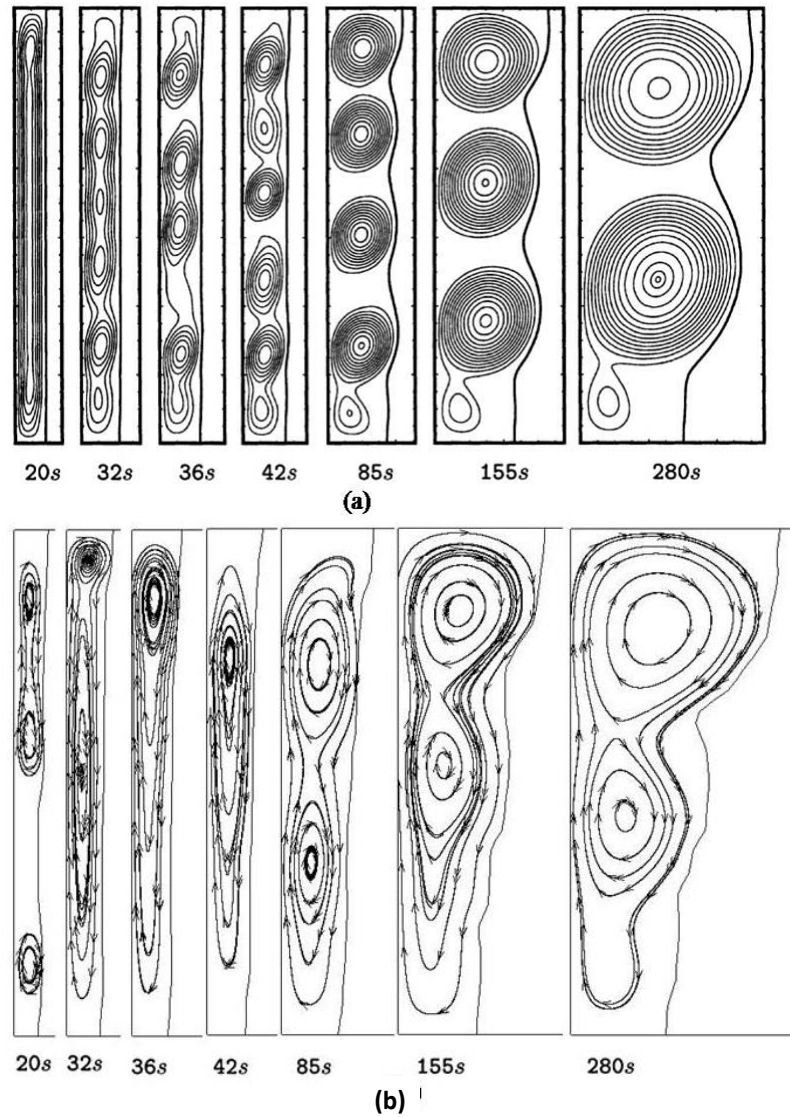


Figure 3.10 Flow pattern with streamline and position of melting front over time in a gallium cavity obtained from (a) Nouredine's work [86] and (b) calculation

In Nouredine's work [86] circular cell was not shown in beginning, but at 32.0 s, small circular cells are generated with increase of molten gallium area, and then are merged each other, eventually two large cells dominates flow inside a cavity. But in our simulation, three cells are initially generated and then two big circular cells are remained. It means that small circular cells are not well predicted in our simulation as compare with Nouredine's work. However, following both Fig. 3.9 and 3.10, it was figured out that position of melting front is well predicted as compare with experimental data even though such small circular cells are not well predicted in our simulation. It means that, even though such small circular cells appear when precise calculation is performed, circular cells are not

dominating factor to modify the position of melting front. Since we focus on the appropriate method to predict the position of melting front, we can say our results are qualitatively validated.

### **3.3 Validation of sigmoid function**

In the last of chapter 2, we introduced two functions (sinusoidal and sigmoid function) in order to take into account for the melting problem which simultaneously happens with gas phase species transport. These two functions are necessary to be validated so that it is validated with 2-D gallium melting case which has exactly same condition introduced in section 3.2. As compare with results shown in experiment [37] and obtained by default enthalpy method in Fluent, results achieved from sinusoidal and sigmoid function show almost same accuracy in terms of time-dependent position of melting front. Therefore, result obtained by sigmoid function is only shown here.

Figure 3.11 shows position of melting front with respect to time. Dot and solid black line is taken from experiment [37] and calculation [86], red line represents the position of melting front calculated by default enthalpy method in Fluent, blue line is achieved by sigmoid function implemented by UDF into Fluent. It shows that position of melting front calculated from sigmoid function is overestimated as compare with experimental data before 17.0 minute. However, results obtained by sigmoid function show more accurate position of melting front than numerical data taken from [86] and default enthalpy method in Fluent. Therefore, we concluded that sigmoid function has reasonable accuracy.

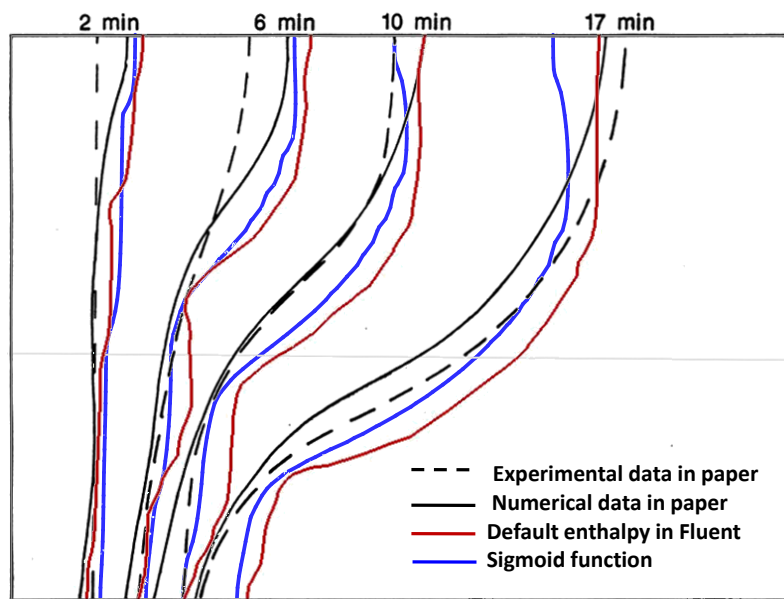


Figure 3.11 Comparison of experiment [37], numerical results obtained by default enthalpy method in Fluent and sigmoid function employed by UDF: position of melt front with time

### 3.4 Validation of tracking liquid-gas interface (pendant drop)

In this study, interface tracking plays a big role to achieve the accuracy of calculation (e.g., tracking melting front and free surface). Both are equally important because melting phase change and deformation of PCM-air interface simultaneously occur in reality [19]. As mentioned, we use Enthalpy-porosity method and VOF method to track the melting front and PCM-air interface, respectively. From section 3.1-4, we performed the validations for melting process by use different method including enthalpy method, concluding that even though small internal circular motion is not well captured, enthalpy method has qualitative accuracy at tracking melting front. Hence, it is also required to validate the VOF method in order to achieve reliability in prediction of PCM-air interface. To do so, we examine the pendent dropping problem which is most well-known calculation example for tracking liquid-gas interface [89]. Case of pendent drop is good case for validation of this study because it essentially has dropping process which we would like to simulate. Figure 3.12 shows schematic and computational domain of a drop formation [91]. The 2-D computational domain consists of water and air. The total horizontal and vertical lengths are 5.0 and 25.0 cm respectively, and the diameter of inlet is 1 cm. The liquid drop is formed into a quiescent supported by a constant flow rate  $Q$ . Drop suppose to be suspended at a nozzle and tend to grow when surface force can be against gravity. However, the liquid breaks as drops from the tip of the nozzle under its own weight when surface force cannot be against gravity [90]. Time-dependent drop was calculated by using VOF method and results are validated in Fig. 3.13. Left figure in each time shown in Fig. 3.13 is drop formation obtained from experiment [91] and right figure is calculated drop by use of VOF method included in our model. Figure 3.13 shows good agreement in prediction of time-dependent position of drop. However, tiny drop (so-called satellite drop) between water drop and water suspended from nozzle inlet is not well captured in calculation as compare with experimental results. According to the investigation of Grimm et al [43], expensive computational cost is essentially necessary to capture the satellite droplet due to the fact that a satellite droplet is typically very small and possess a very less than 1 % of that of the detached drop. VOF method employed in current study is under the fixed grid, which means that grid resolution should be fine enough. Thus, according to the validation of pendent

drop problem, we can conclude that VOF method is depend on the grid resolution when we observe the small scale problem (i.e. satellite droplet). However, VOF method can appropriately predict the dropping time when our concern is to the main dropping phenomena.

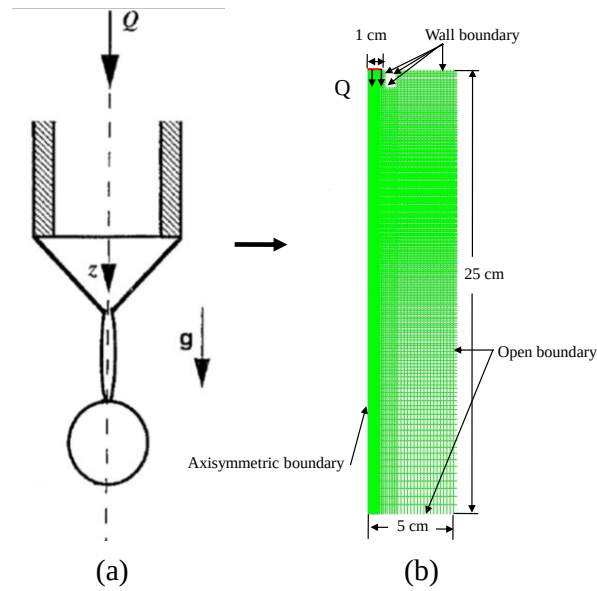


Figure 3.12 Schematic and computational domain of a drop formation supported from a constant flow rate under gravity [91]

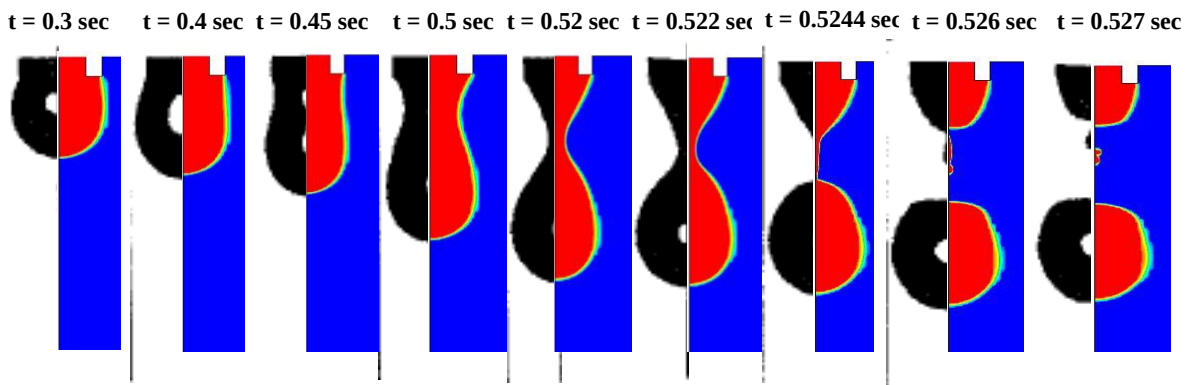


Figure 3.13 Time sequence of drop formation during its pinch-off process under normal gravity of  $9.81 \text{ m/s}^2$  (left: experimental results obtained from [91], right: calculation results obtained from VOF method)

# Chapter 4

## Melting and dropping of a phase change material (PCM)

### 4.1 Numerical model, initial and boundary conditions

The physical configuration is schematically illustrated in Fig. 4.1. The 2-D computational domain consists of copper, PCM and air. The total horizontal and vertical lengths are 8.0 and 7.0 cm, respectively, and the thickness of the PCM is 5 mm. A normal downward gravity field is considered (with corresponding gravitational acceleration of  $9.81 \text{ m/s}^2$ ). A localized external thermal input at temperature 500 K is placed on the top surface of the copper to initiate melting of the PCM, and the temperature 300 K is used over the whole domain as the initial thermal condition. The melting process evolves with an increase of the local temperature in the PCM. As the volume of molten PCM increases, the liquid-gas interface starts to become severely deformed, and PCM is eventually detached from the main part of the molten PCM owing to gravity drag. We assumed that the solid is homogeneously distributed in the mushy region. Except for interfacial volumetric source term as a jump condition, several additional conditions at interfaces are necessary to solve mathematically. For flow condition, the quiescent environment is initially given in whole domain. No slip boundary condition is applied on all boundaries of copper as well as left and right side of PCM. All boundaries of air except for PCM-air interface are treated as open boundaries. For flow condition at phasic interface, first we assume that there is no flow in solid phase as well as vicinity of solid surface so that there is no flow jump across the solid-liquid and solid-gas interface. Thus, zero velocity is imposed on solid-gas and solid-liquid interface. Since no phase change occurs at the gas-liquid interfaces, no flow exists across there. Thus

the interfacial normal velocity is equal to normal velocity of liquid phases at the gas-liquid interface. For point where a molten PCM/air interface meets a copper surface, we assume that the contact angle is 90 degree, which could exclude any adhesion effect (i.e., the interface is normal to the adjacent wall). Adiabatic condition is given on left and right side of PCM, and also given on whole boundary of copper except for copper-PCM interface. The temperature is assumed to be continuous at the gas-liquid and gas-solid interface. Two-side heat balance (so-called conjugated heat transfer condition) is considered at the solid-liquid interface as  $k_{copper}(\partial T_{copper} / \partial n) = k_{PCM}(\partial T_{PCM} / \partial n)$ .

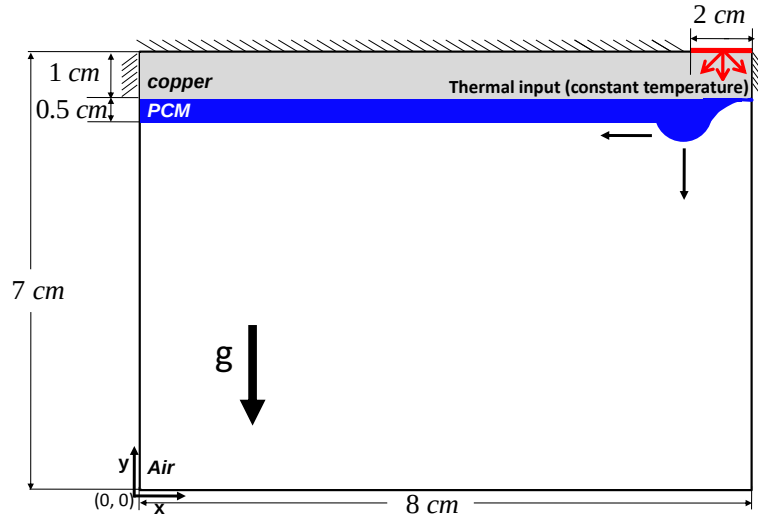


Figure 4.1 Schematic illustration of the computational domain

Material properties are phase-dependent values, determined by phase indicator function,  $\alpha$ , and temperature dependent liquid fraction,  $\beta$ , as shown in Table 4.1.

Table 4.1 Physical properties used in the present calculation

| Parameter                   | Symbol     | Value                  | Units             |
|-----------------------------|------------|------------------------|-------------------|
| <b>Air (gas phase)</b>      |            |                        |                   |
| Density                     | $\rho_g$   | 1.225                  | kg/m <sup>3</sup> |
| Thermal conductivity        | $k_g$      | 0.0242                 | W/(m K)           |
| Specific heat               | $c_{p, g}$ | 1006.43                | J/(kg K)          |
| Viscosity                   | $\mu_g$    | $1.789 \times 10^{-5}$ | kg/(m s)          |
| <b>Copper (solid phase)</b> |            |                        |                   |
| Density                     | $\rho_c$   | 8978                   | kg/m <sup>3</sup> |
| Thermal conductivity        | $k_c$      | 387.6                  | W/(m K)           |
| Specific heat               | $c_{p, c}$ | 381                    | J/(kg K)          |
| <b>PCM (solid phase)</b>    |            |                        |                   |
| Density                     | $\rho_s$   | 980                    | kg/m <sup>3</sup> |
| Thermal conductivity        | $k_s$      | 24                     | W/(m K)           |
| Specific heat               | $c_{p, s}$ | 1360                   | J/(kg K)          |
| Latent heat of melting      | $L$        | $1.8 \times 10^5$      | J/kg              |
| Melting temperature         | $T_m$      | 400                    | K                 |
| <b>PCM (liquid phase)</b>   |            |                        |                   |
| Density                     | $\rho_l$   | 900                    | kg/m <sup>3</sup> |
| Thermal conductivity        | $k_l$      | 15                     | W/(m K)           |

|                            |           |     |          |
|----------------------------|-----------|-----|----------|
| Specific heat              | $c_{p,l}$ | 680 | J/(kg K) |
| Viscosity                  | $\mu_l$   | 0.1 | kg/(m s) |
| Solidification temperature | $T_s$     | 350 | K        |

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## 4.2 Overall behavior of time-dependent melting and dropping process

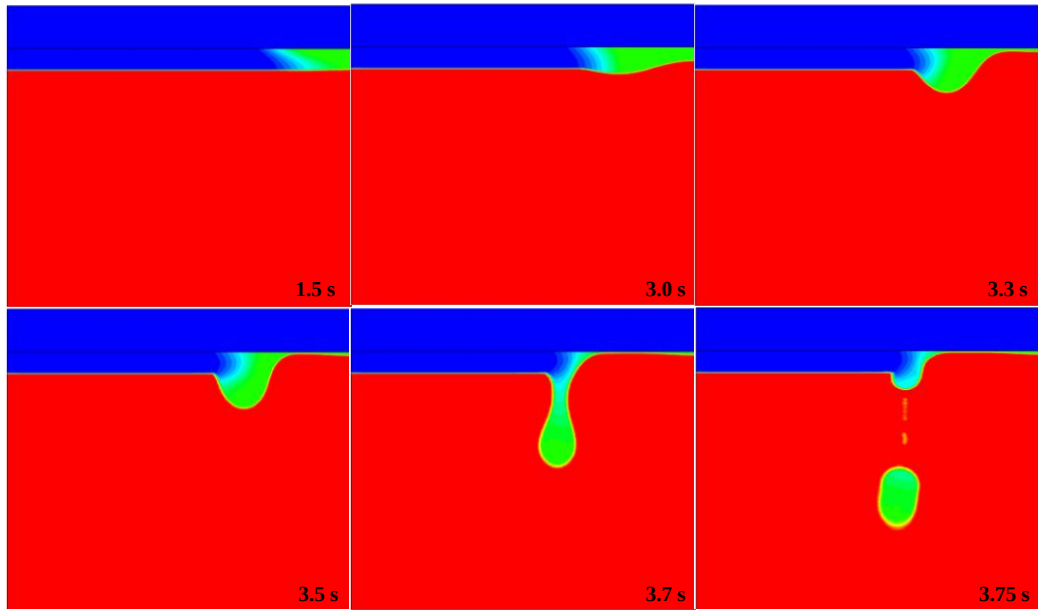


Figure 4.2 Time-sequence of  $(\alpha + \beta) / 2$  distribution with respect to time

Figure 4.2 shows a scalar distribution,  $(\alpha + \beta) / 2$ , to visualize the overall process of the melting and dropping. The white, red, green and blue colors correspond to computational cells filled with copper, air, molten PCM and solid PCM, respectively. This figure clearly shows how the PCM is melting, growing and dropping. The PCM starts to melt with the appearance of a mushy region on the upper-right side, and melting proceeds after that. At around 2.8 s, the interface between the molten PCM and the air tends to deform with increase of volume of the molten region, and because of this deformation the volume of molten PCM on the right is forced to move left. At the same time, molten

PCM starts to grow in size, resulting in a pinching of the fluid neck between the main and suspended PCM. Eventually, generated molten PCM is detached from the main part, and soon disappears from computational domain. At 3.75 s, a liquid spot between the detached and cone-shaped molten PCM is maintained along the un-melted (solid) part. According to Fig. 4.2, it is difficult to distinguish whether the spot is a satellite droplet [87] or a thin line representing a point of singularity in the diameter [88-90], because typically a satellite droplet is very small (e.g., possessing a volume less than 1% of that of the detached molten matter [91]) and also a point of singularity (e.g., a micro-thread) that approaches its limiting size of the order of  $1\ \mu\text{m}$  [92]. To simulate such satellite droplets or points of singularity satisfactorily, the fixed grid resolution should be fine enough. Because our interest in this chapter is limited to the pre-dropping process, the details of the tiny secondary droplet and the point of singularity should not be discussed.

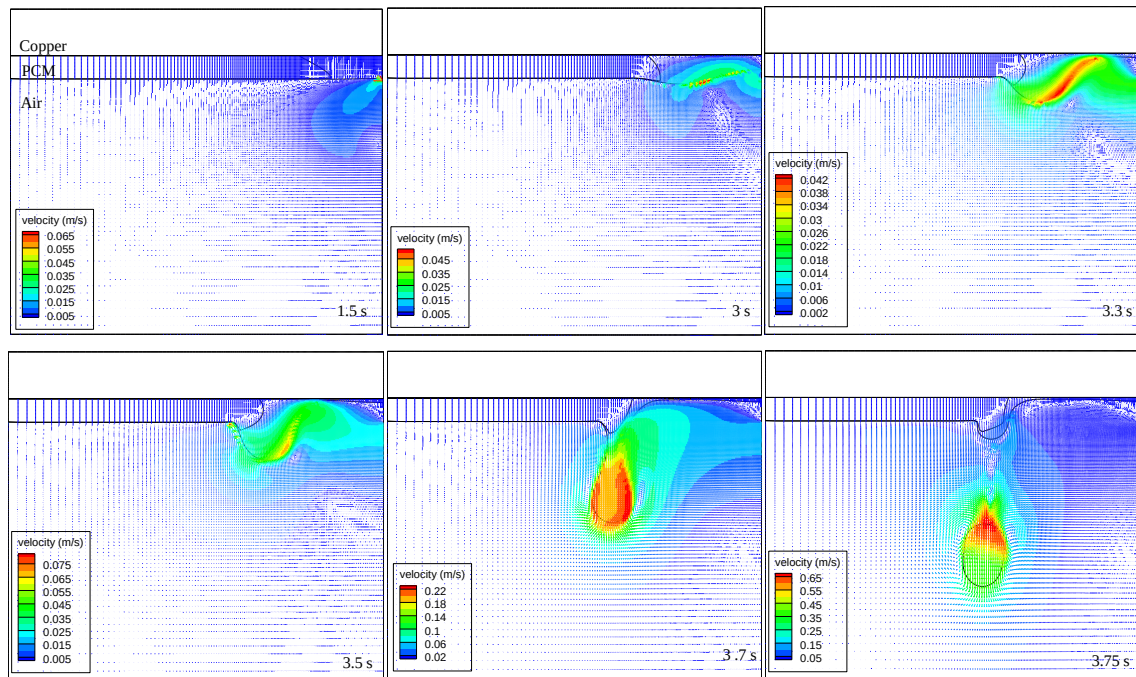


Figure 4.3 Velocity distributions with respect to time

In order to see dynamic behavior precisely, the velocity vectors over time is depicted in Fig.4.3, where the color represents the magnitude of the velocity. Once deformation is initiated, relatively

high velocity is generated near the PCM-air interface. When molten PCM starts to drop, maximum velocity (around 65 cm/s) is observed and air flow around dropping molten PCM shows vortical motion.

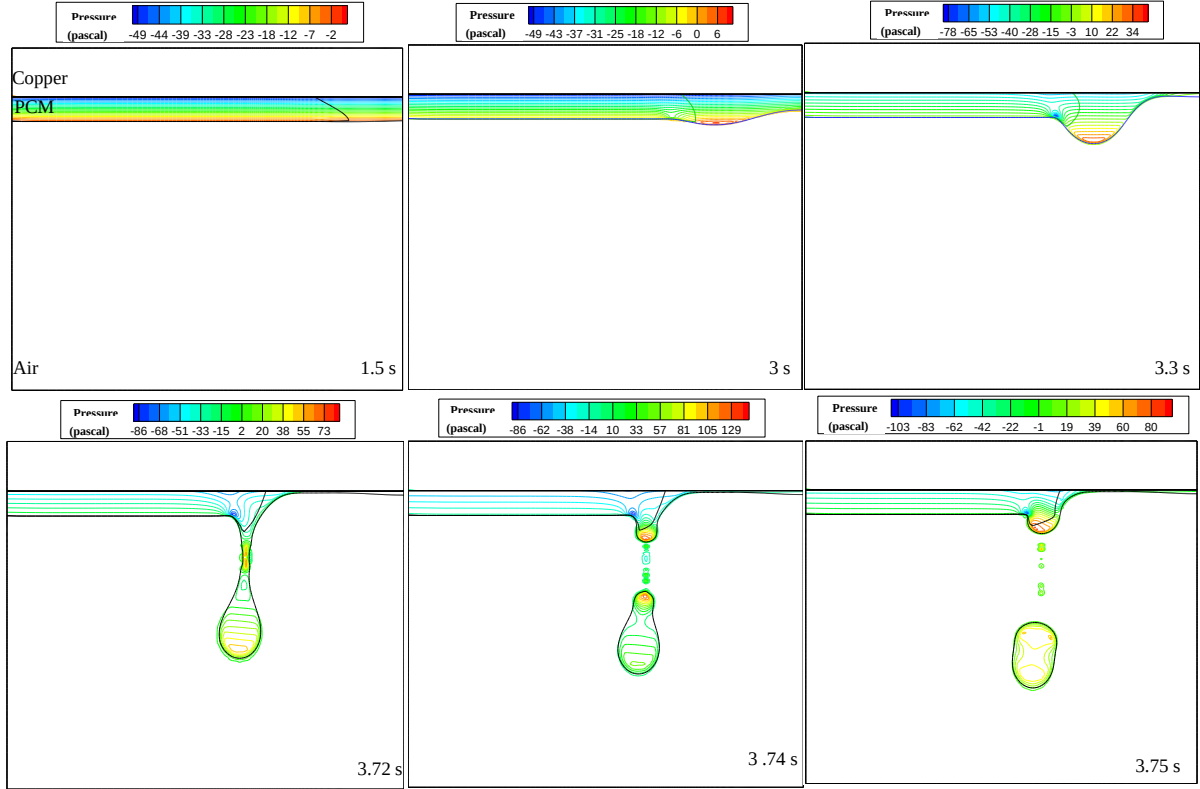


Figure 4.4 Pressure distributions with respect to time

Figure 4.4 shows pressure distribution at time of 1.5, 3, 3.3, 3.72, 3.74 and 3.75 s. High pressure appears at neck when neck of molten PCM becomes thin ( $t = 3.72$  s), and is separated to main molten PCM attached on solid PCM and detached molten PCM ( $t = 3.74$  s). Thus recoils occur due to pressure variation and the surface contracts to reduce its surface energy. It leads that tip of molten PCM attached on solid PCM recoils back to the upward direction and tip of detached molten PCM curls up. It is almost similar with phenomenon of necking and pinch-off of pendant drop (see [89]).

Figure 4.5 shows the temperature distribution at a different time as that of Fig. 4.2. The position of the melting front and the liquid-gas interface are approximated by  $\beta = 0.5$  and  $\alpha = 0.5$ , respectively. Heat generated from the external thermal input diffuses by conduction first through the copper and is

absorbed in the PCM to initiate the melting, and is then released to the ambient air. Following the deformation of the free surface triggered by a volume increase of the molten area, the temperature profile also becomes distorted. In particular, the temperature profile tends to spread out as molten PCM drops off.

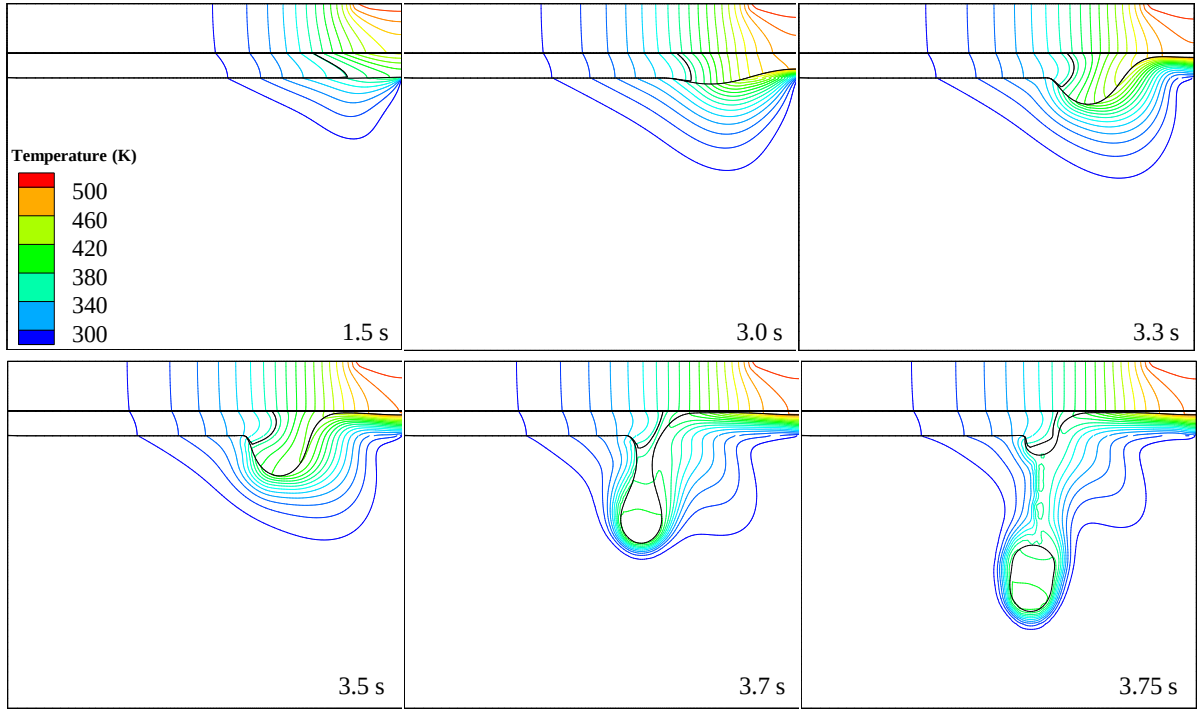


Figure 4.5 Temperature distributions with respect to time

In order to observe the energy field precisely, the temperature profile at the interface between copper-PCM over time and time-dependent area-weighted enthalpy in copper is depicted in Fig.4.6. Left and right vertical axis is area-weighted enthalpy in copper and temperature at copper-PCM interface, respectively. The upper and bottom horizontal axis are time and distance, respectively. Here, are-weighted enthalpy  $h_A$  is defined as  $h_A = \frac{1}{A} \int h dA$ , and an area  $A$  of copper and PCM is determined by initial area of copper ( $8 \text{ cm}^2$ ) and initial area of PCM ( $4 \text{ cm}^2$ ), respectively. Hereafter, all definitions of are-weighted enthalpy is following as same definition of  $h_A$  in this thesis.

According to enthalpy profile, one can be seen that heat is accumulated with time, but rate of

increase of enthalpy becomes slow. It could be seen in interfacial temperature as well. With increase of time, temperature profile becomes broaden, but rate of increase of temperature becomes slower.

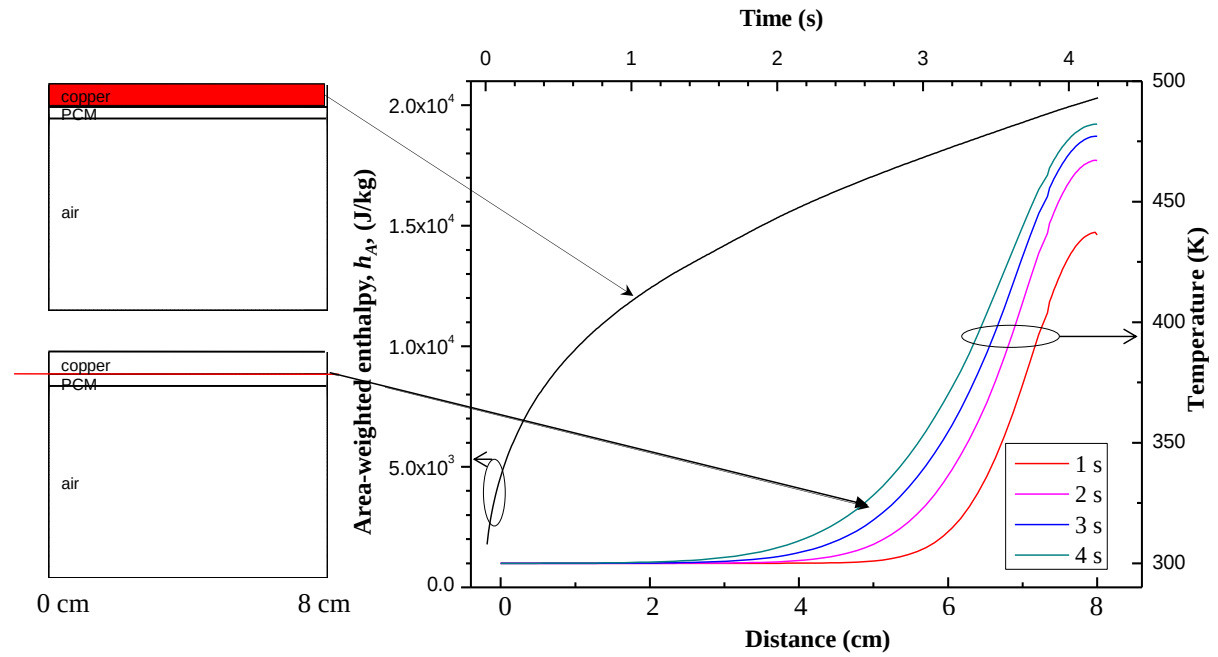


Figure 4.6 Area-weighted enthalpy of copper with respect to time and temperature distribution of  $x$  direction at interface between copper and PCM according to different time (1.0, 2.0, 3.0 and 4.0 s)

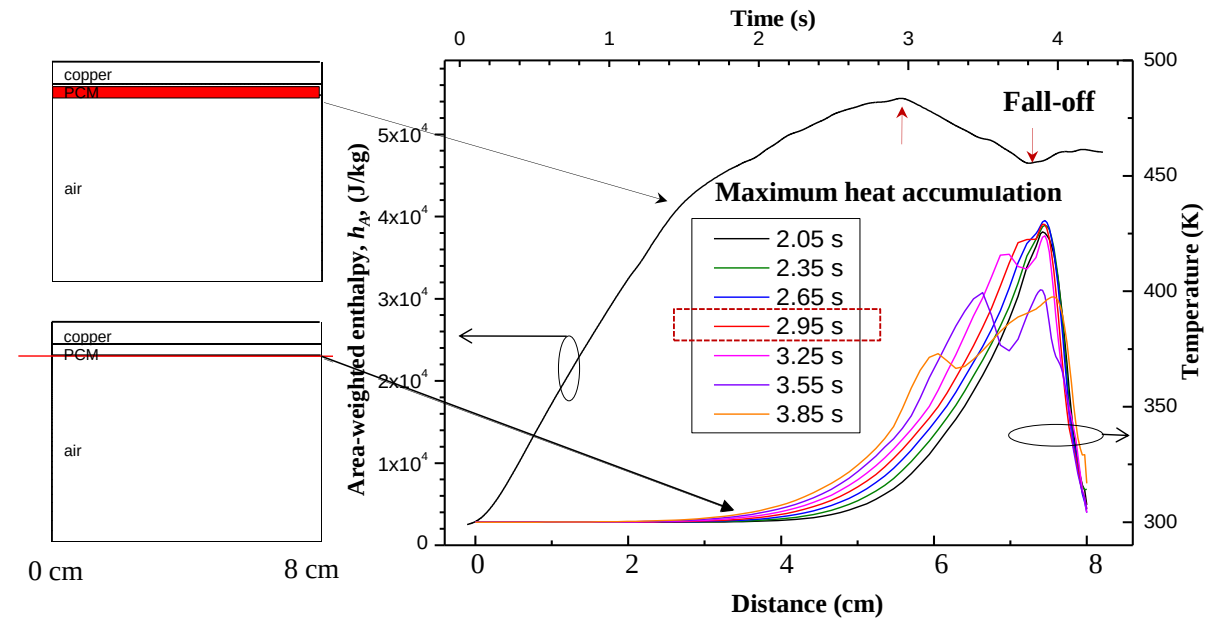


Figure 4.7 Area-weighted enthalpy of PCM with respect to time and temperature distribution of  $x$

direction at interface between PCM and air according to different time (2.05, 2.35, 2.65, 2.95, 3.25, 3.55 and 3.85 s)

Figure 4.7 shows area-weighted enthalpy in initial PCM area and temperature profile at interface between PCM and air. Being different from the case of copper-PCM interface, enthalpy profile shows two inflection points which are pointed as embedded red colored arrow. Here maximum enthalpy and temperature occur at 2.95 s. It means that heat accumulation becomes maximum in PCM and PCM-air interface at 2.95 s. At the same time, PCM starts to deform and accumulate the molten PCM like pendant shape. It reveals that PCM has maximum heat accumulation right before starting deformation. We can see the second inflection point which is turning point of enthalpy from decreasing curve to increasing curve at 3.9 s. It happens due to the fact that suspended PCM loses the molten PCM which accumulates certain heat during fall-off molten PCM. Therefore, PCM has minimum heat accumulation right after drop-off of molten PCM.

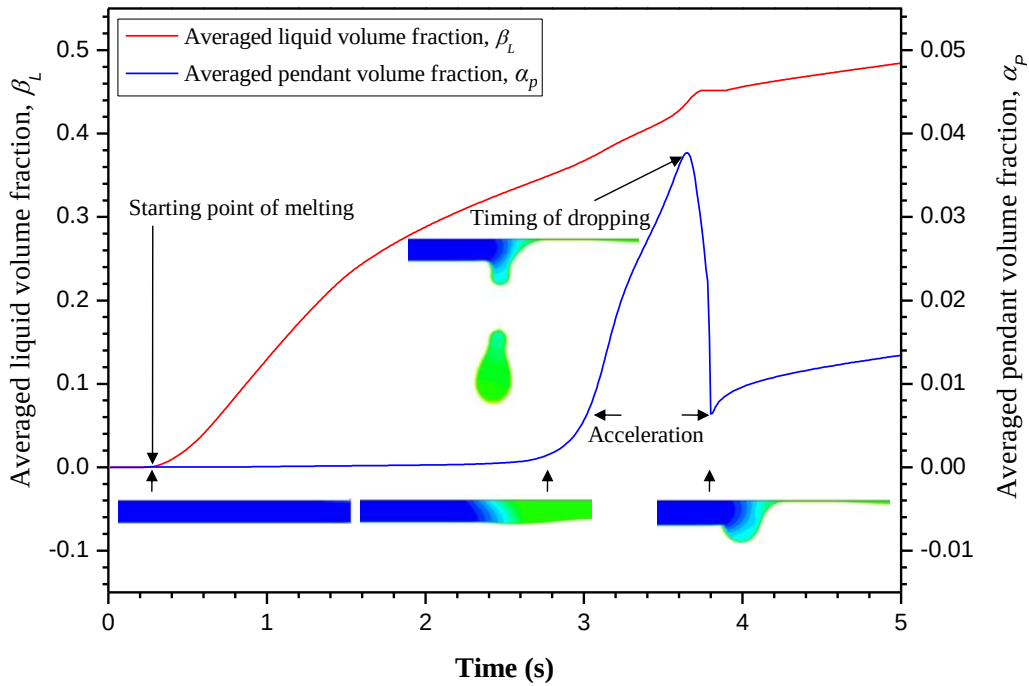


Figure 4.8 Time-dependent averaged liquid volume fraction of PCM and averaged pendant volume fraction of PCM

The volume increase of the molten and suspended, molten PCM are illustrated in Fig. 4.8. This figure depicts the time-dependent variation of the averaged pendant volume fraction and the averaged liquid volume fraction, defined as follows:

Averaged pendant volume fraction:

$$\alpha_p = V_{PA} / V_A, \quad (4-1)$$

Averaged liquid volume fraction:

$$\beta_L = 1 - V_{SP} / V_{TP}. \quad (4-2)$$

Here,  $V_{PA}$  is the volume of pendant and detached molten PCM in the initial volume of air,  $V_A$  is the initial volume of air,  $V_{SP}$  is the volume of the solid-state PCM, and  $V_{TP}$  is the total volume of PCM. The averaged pendant volume fraction ( $\alpha_p$ ) represents the volume of pendant or detached molten PCM generated, and is calculated by counting how much liquid volume is projected toward the air domain. More precisely, we calculate the volume of cells filled with liquid PCM inside the initially given total number of cells filled with gas, and then this quantity is divided by the initial volume of gas. The averaged liquid volume fraction ( $\beta_L$ ) represents how much PCM is melted in total volume of PCM. The averaged pendant volume fraction ( $\alpha_p$ ) first appears at 2.8 s, and the associated acceleration area is suddenly increased owing to a loss of equilibrium of the forces at the PCM-air interface. This volume fraction suddenly decreases from its maximum value around 3.75 s (as shown) while the suspended molten PCM is dropping. As can be seen from the distribution of the averaged liquid volume fraction ( $\beta_L$ ), melting initiates at around 0.3 s, and then continuously increases although the increment gradually becomes gentle. This “blending” feature arises from (1) the position of heat source being fixed at right upper side, and (2) the heat transferred from external thermal input not only being used to enhance the melting, but also being released into the air. Immediately before dropping of molten PCM at around 3.8 s,  $\beta_L$  locally increases, but after dropping-off it momentarily plateaus. This increase and momentarily plateau of  $\beta_L$  offers the key to an understanding of the role

of the dynamic motion effect on melting. In section 4.4. we will discuss this process in more detail.

### 4.3 Parametric research (different external thermal inputs, surface tension coefficients and melting temperatures)

Results concerning the general phenomena in heat transfer and dynamic behavior of PCM are investigated by examining the different surface tension and external thermal input. From the Fig. 4.9 to Fig. 4.16 shows the area-weighted enthalpy in copper and PCM, time-dependent averaged liquid volume fraction ( $\beta_L$ ) and averaged pendant volume fraction ( $\alpha_L$ ) over a range of Stefan numbers and external thermal inputs. From the Fig. 4.9 to Fig. 4.12, the Stefan number is defined as  $Ste = c_{p,l}(T_E - T_{Liquidus}) / L$ , where,  $T_E$  is the temperature of the external thermal input,  $T_{liquidus}$  is the temperature which solid state is changed to liquid,  $L$  is latent heat of melting. The range of the Stefan number is from  $Ste = 0.34$  to  $5.44$ .

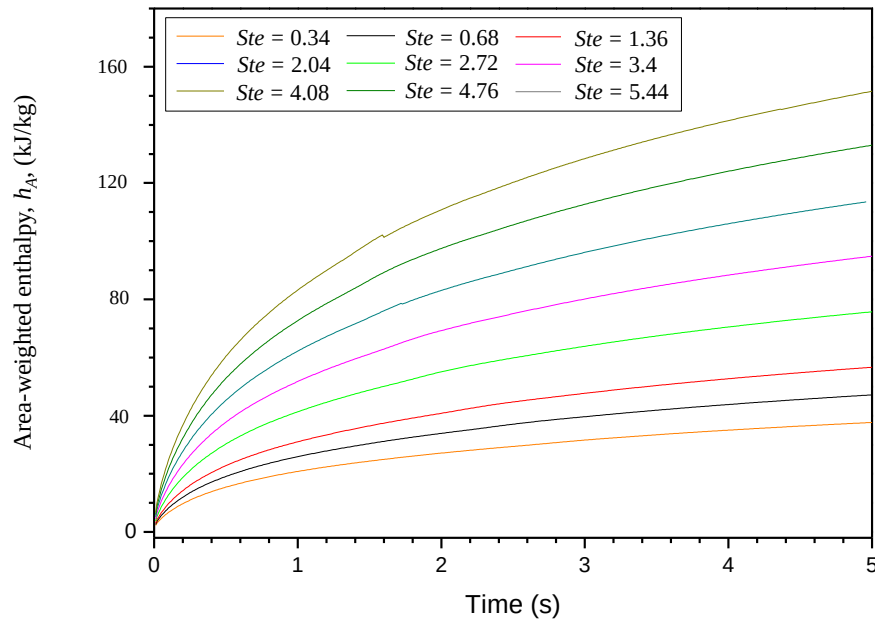


Figure 4.9 Area-weighted enthalpy of copper for various Stefan numbers with respect to time

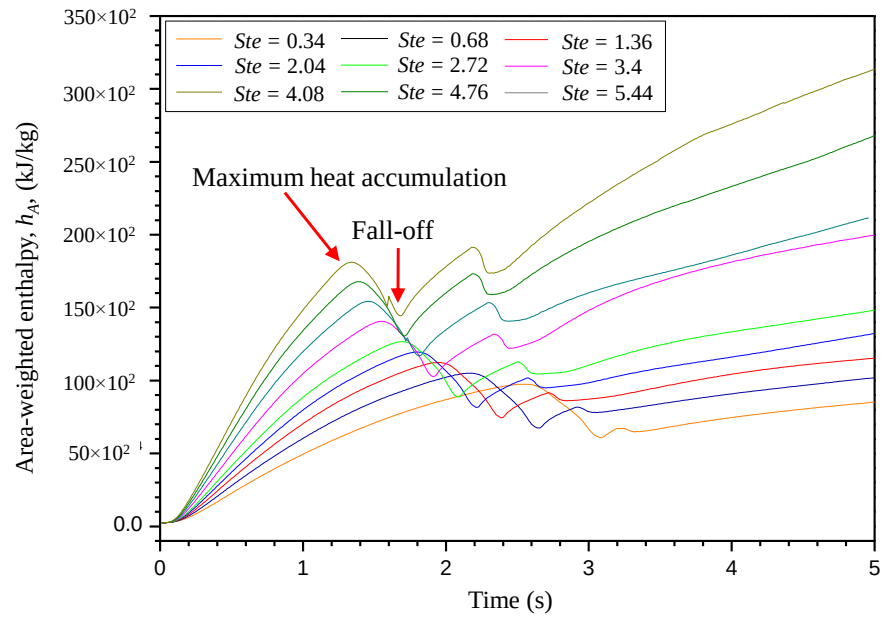


Figure 4.10 Area-weighted enthalpy of PCM for various Stefan numbers (Ste) with respect to time

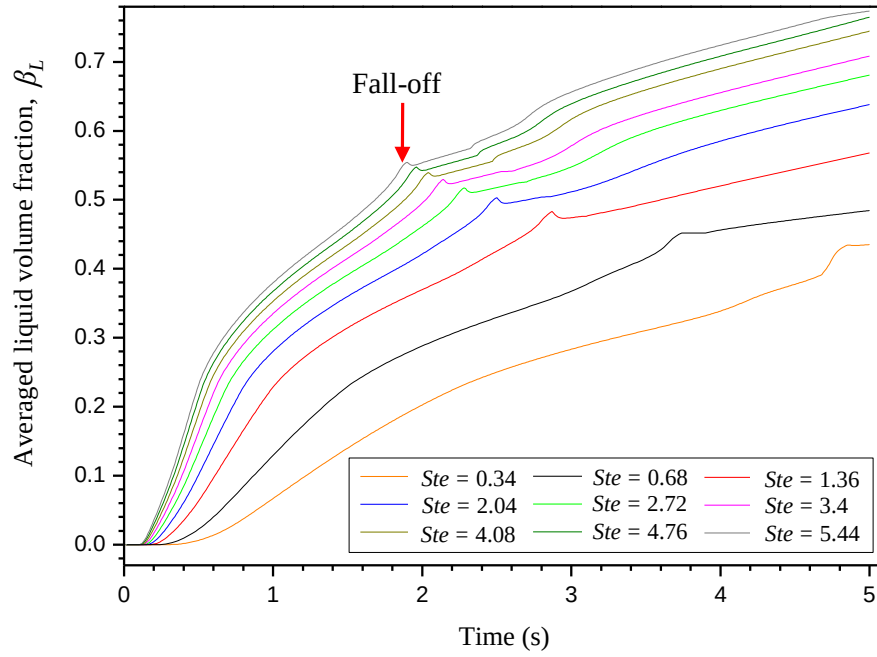


Figure 4.11 Time-dependent averaged liquid volume fraction distribution for various Stefan numbers at surface tension coefficient = 0.25

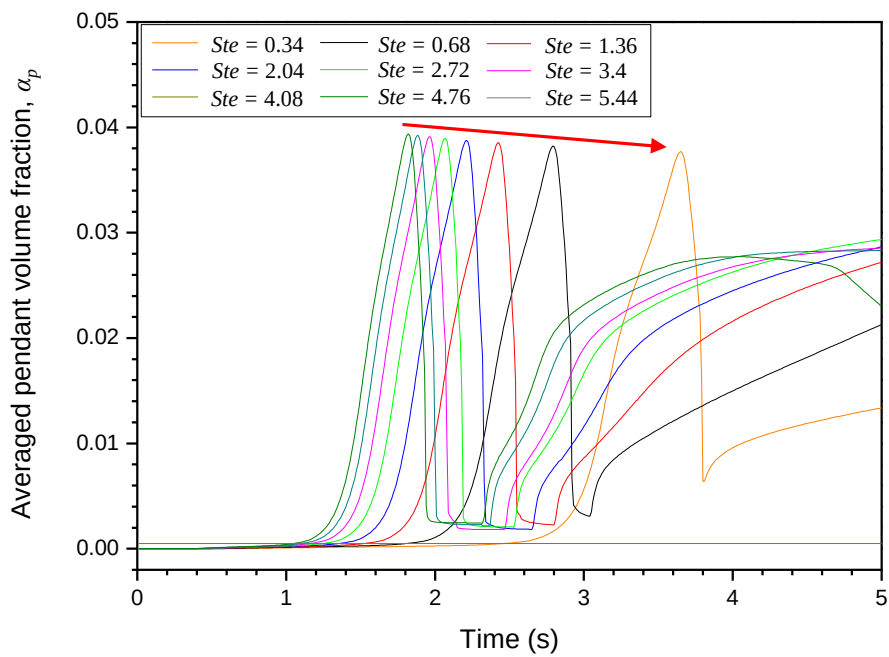


Figure 4.12 Time-dependent averaged pendant volume fraction distribution for various Stefan numbers at surface tension coefficient = 0.25

Since melting can happen very quickly under the combustion condition as compare with general slow melting process (e.g. ice melting, melting in thermal storage system), high Stefan number is considered as well. Figure 4.9 clearly shows that area-weighted enthalpy in copper monotonically increases with increase of Stefan number over time, while area-weighted enthalpy in PCM depicted in Fig. 4.10 shows more complicated time-dependent tendency. As pointed in Fig. 4.7, area-weighted enthalpy in PCM has two inflection points; maximum heat accumulation and fall-off points. With increase of Stefan number, area-weighted enthalpy in PCM is increased and both maximum heat accumulation and fall-off points are quickly experienced due to the increase of supporting heat from the thermal source. Figure 4.11 shows that  $\beta_L$  increases with increasing Stefan number. This trend is consistent with the results of Hirata [93] and Assis [94], showing that the larger the ratio of sensible heat to the latent heat of fusion of the material, the higher the melting rate. Hence, the volume of accumulated molten PCM should grow more quickly with increase of the Stefan number. Consequently, dropping is quickly experienced at high Stefan number. Figure 4.12 shows averaged pendent volume fraction. A size of pendent in high Stefan number is larger than that in small Stefan number. It caused by a fact that the high speed of melting supports more molten volume to pendent during the process of the growth of the pendent volume.

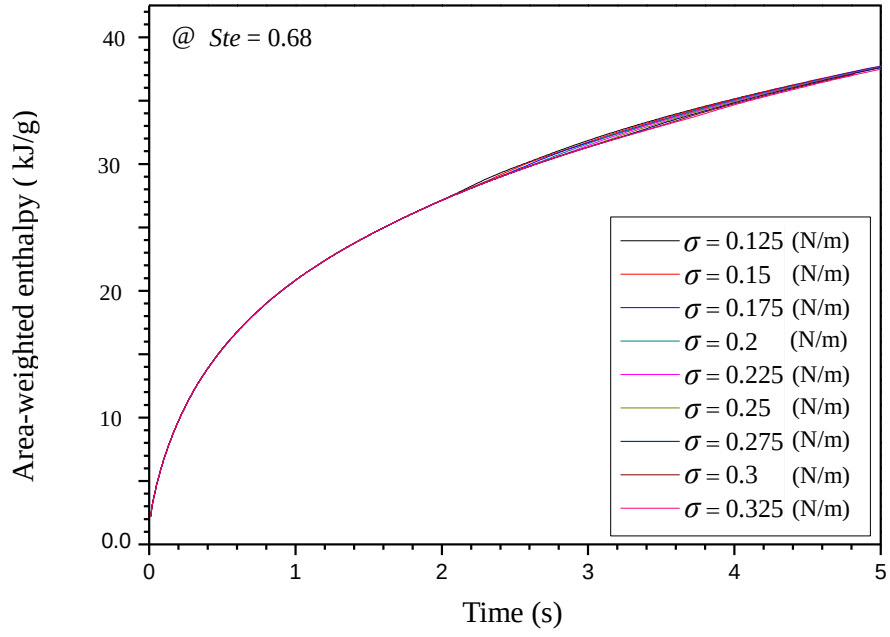


Figure 4.13 Area-weighted enthalpy of copper for various surface tension coefficients with respect to time at  $Ste = 0.68$

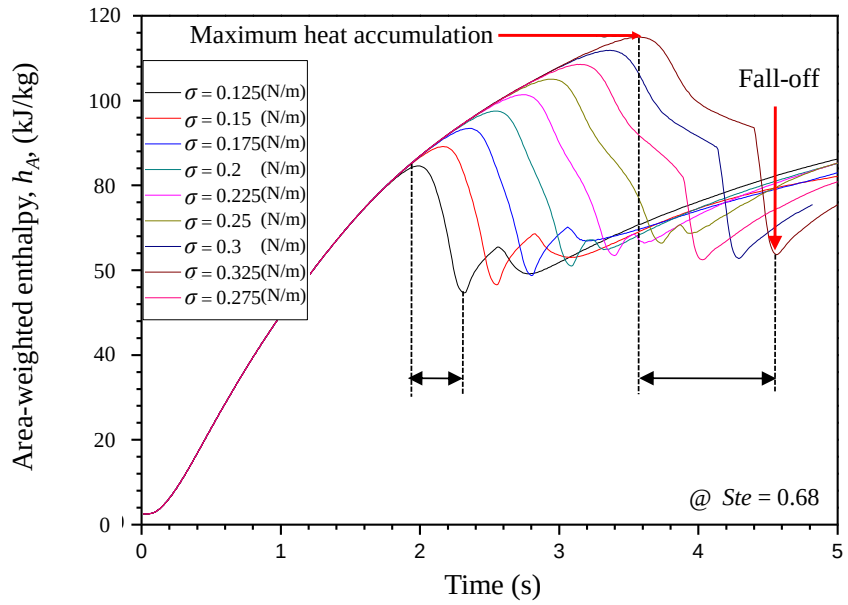


Figure 4.14 Area-weighted enthalpy of PCM for various surface tension coefficients with respect to time at  $Ste = 0.68$

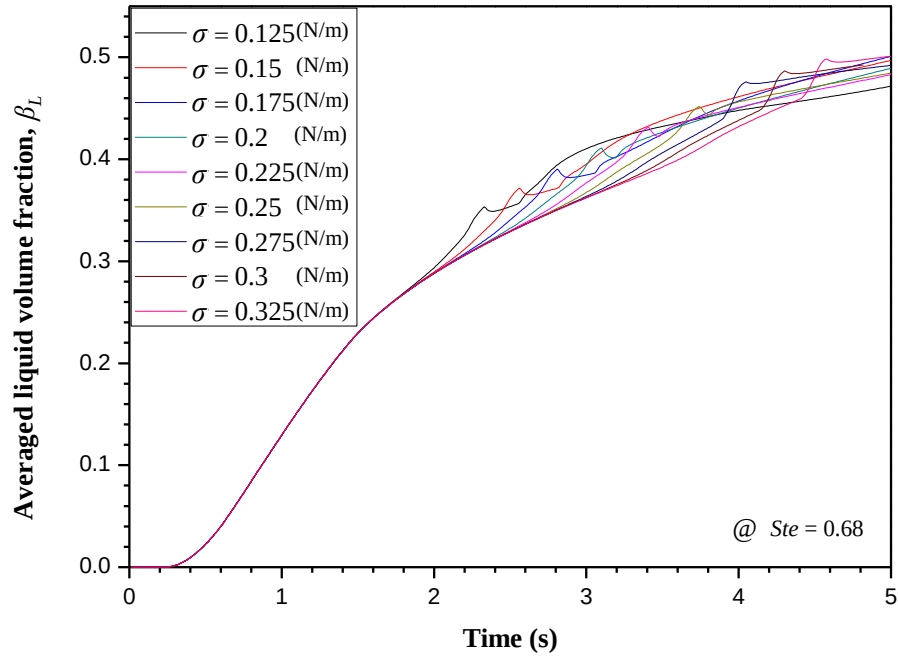


Figure 4.15 Time-dependent averaged liquid volume fraction distribution for various surface tension coefficients at  $Ste = 0.68$

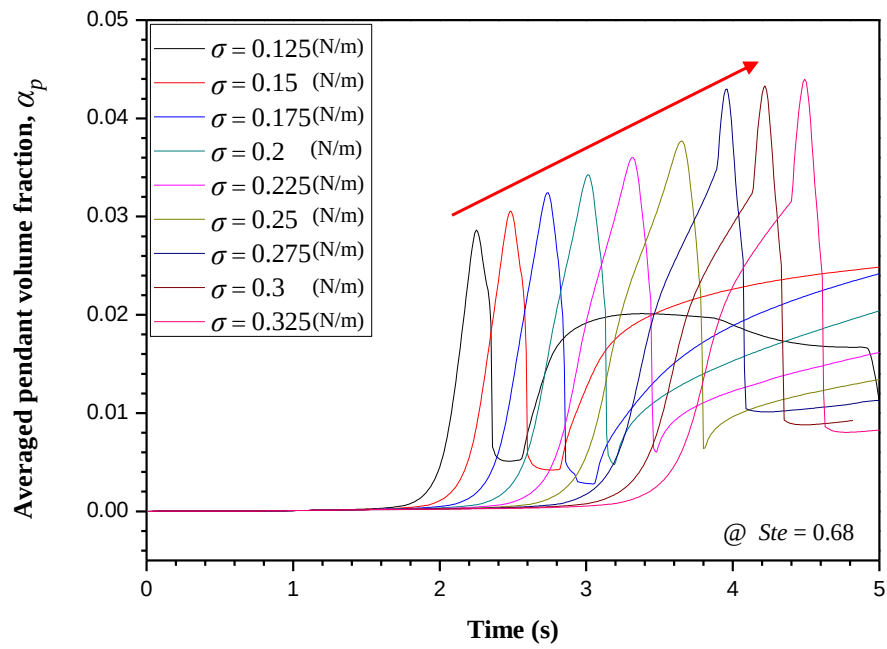


Figure 4.16 Time-dependent averaged pendant volume fraction distribution for various surface tension coefficients at  $Ste = 0.68$

Figure 4.13, which depicts area-weighted enthalpy in copper applied by different surface tension coefficients, shows almost constant enthalpy variation over time for all surface tension coefficients. However, area-weighted enthalpy in PCM depicted in Fig. 4.14 shows that maximum heat accumulation becomes large and time to reach its value is delayed when surface tension coefficient is increased. Moreover, one can see that high surface tension delays time of dropping from time of maximum heat accumulation. It means that molten PCM becomes hard to be dropping off even though molten PCM undergoes deforming of it. Averaged liquid volume fraction in Fig. 4.15 indicates that speed of melting is same even for different surface tension, but dropping time is delayed. As can be seen in Fig. 4.16, pendant volume increases with increase of surface tension coefficient because more surface tension gives more resistance force against gravity, so that pendant suspended along the copper can delay time to fall off and more volume can be stored in pendant.

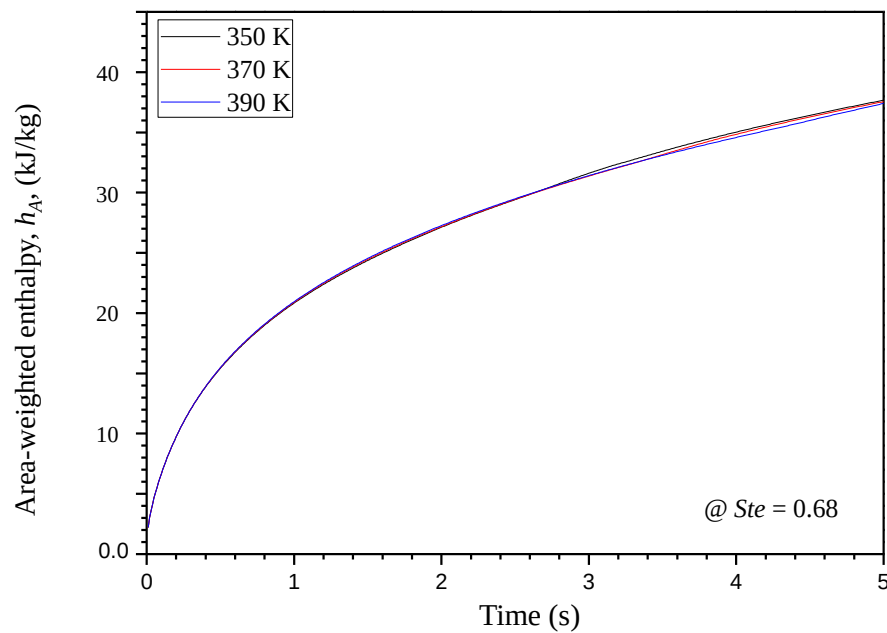


Figure 4.17 Area-weighted enthalpy of copper for various melting temperature with respect to time at  $Ste = 0.68$

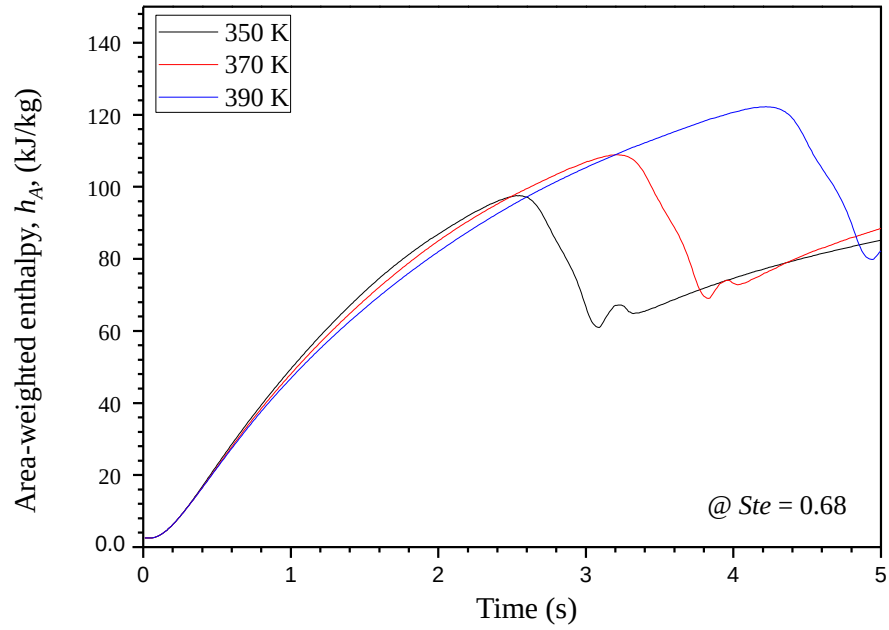


Figure 4.18 Area-weighted enthalpy of PCM for various melting temperature with respect to time at  $Ste = 0.68$

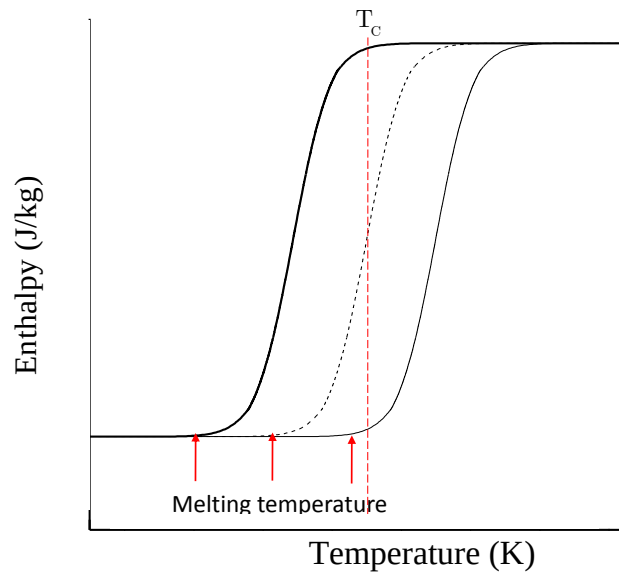


Figure 4.19 Schematic description for the relation between enthalpy and temperature for various melting temperature

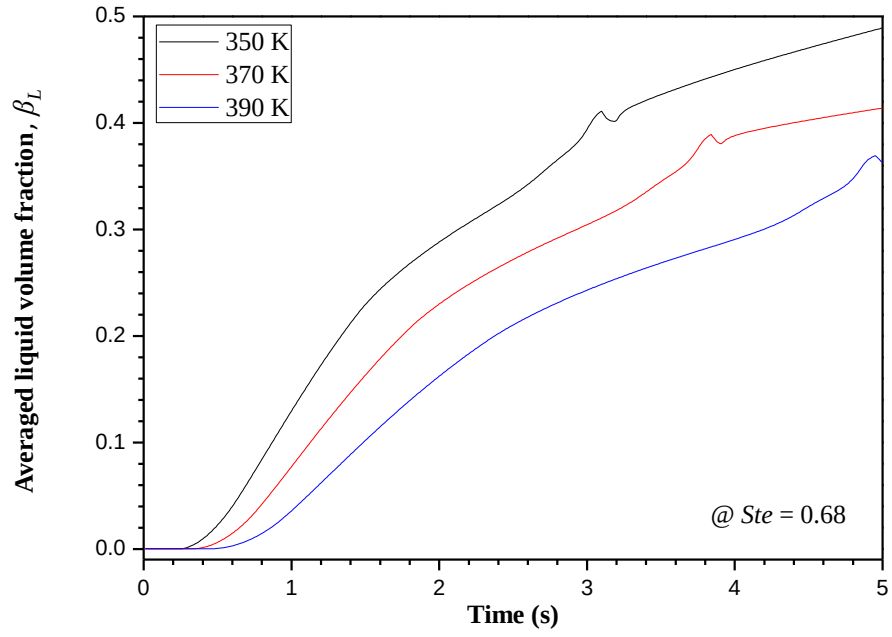


Figure 4.20 Time-dependent averaged liquid volume fraction distribution for various melting temperature at  $Ste = 0.68$

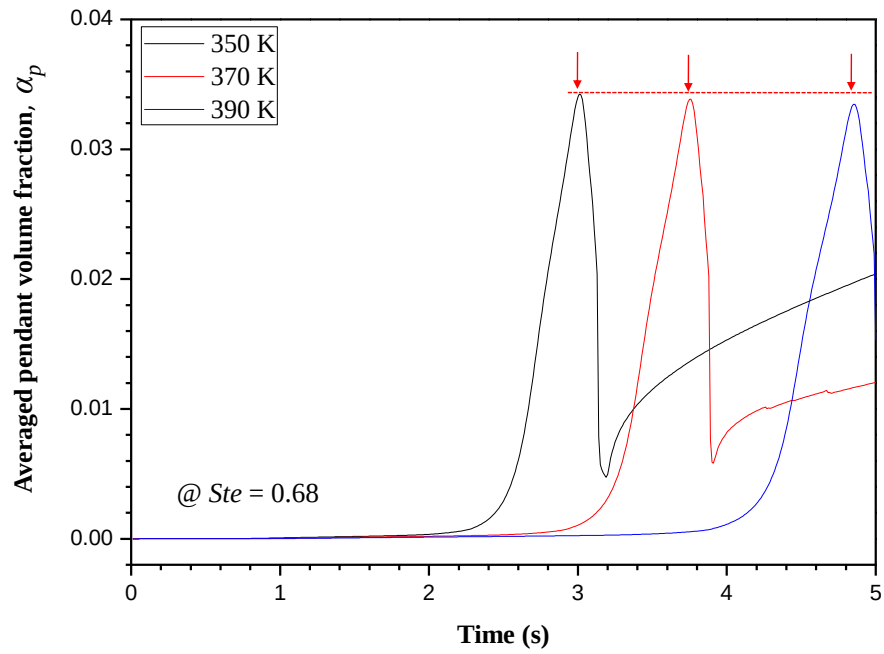
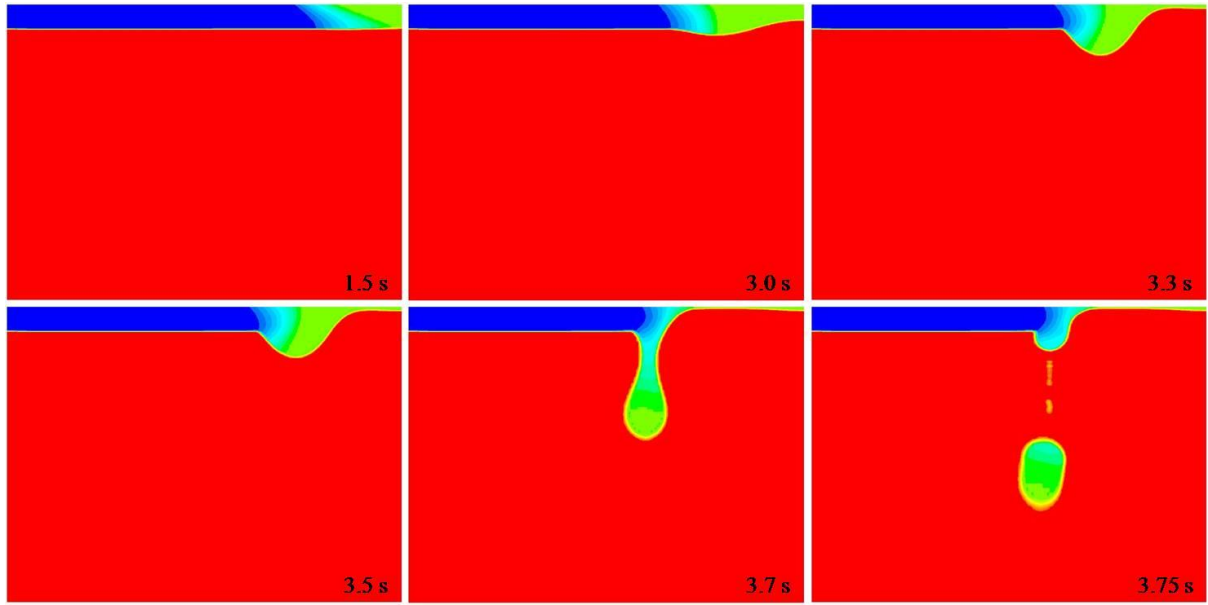


Figure 4.21 Time-dependent averaged pendant volume fraction distribution for various melting temperature at  $Ste = 0.68$

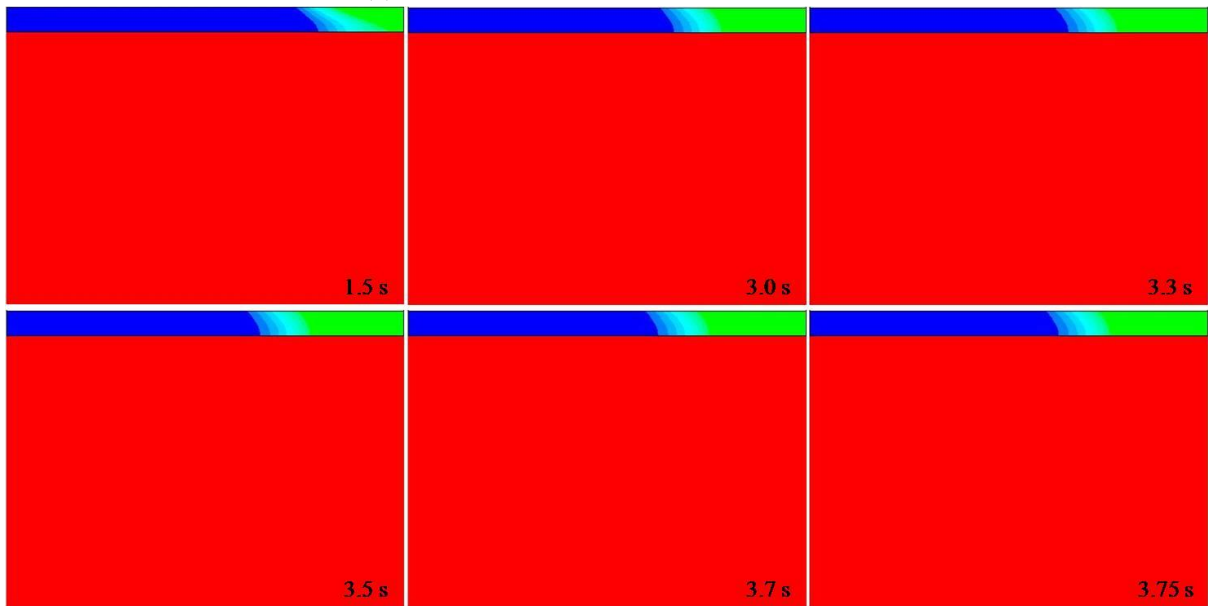
Figure 4.17, which depicts area-weighted enthalpy in copper applied by different melting temperature, shows negligible enthalpy changes over time. Unless heat does not directly concerned with copper, effect of melting temperature variation is insignificant on enthalpy change of copper. However, area-weighted enthalpy in PCM depicted in Fig. 4.18 shows that maximum heat accumulation becomes smaller and time to reach its value is faster when melting temperature decreases. It is caused by fact that low energy is required in case with low melting temperature to initiate melting process. Also, one can see that enthalpy in low melting temperature is bit higher than that in high melting temperature at the same time before it reaches maximum heat accumulation. As can be seen in Fig. 4.19, enthalpy of molten PCM with low melting temperature has higher value than that with high melting temperature at  $T_C$  when PCM undergoes melting process. Thus, low melting temperature-PCM that is already melted at  $T_C$  has higher enthalpy than high melting temperature-PCM that is not melted yet at  $T_C$ . Averaged liquid volume fraction in Fig. 4.20 shows increase of  $\beta_L$  with decrease of melting temperature due to low demand to initiate the melting. Thus, pendant volume fraction also quickly increases with decrease of melting temperature, eventually, dropping of pendant takes place earlier.

#### **4.4 Melting of a phase change material (PCM) enhanced by deformation of a liquid-gas interface**

Figure 4.22 depicts a scalar distribution,  $(\alpha + \beta) / 2$ , with and without consideration of deformable PCM-air interface in order to visualize difference of the melting and dropping process in each cases.



(a) Case with deformable PCM-air interface



(b) Case without deformable PCM-air interface

Figure 4.22 Distribution of  $(\alpha + \beta)/2$  with respect to time

Here only difference is whether deformation of PCM-air interface is considered or not. Thus, case (b) shows only the melting process initiated from external thermal input without motion of PCM-air interface while melting and deformation are simultaneously shown in case (a).

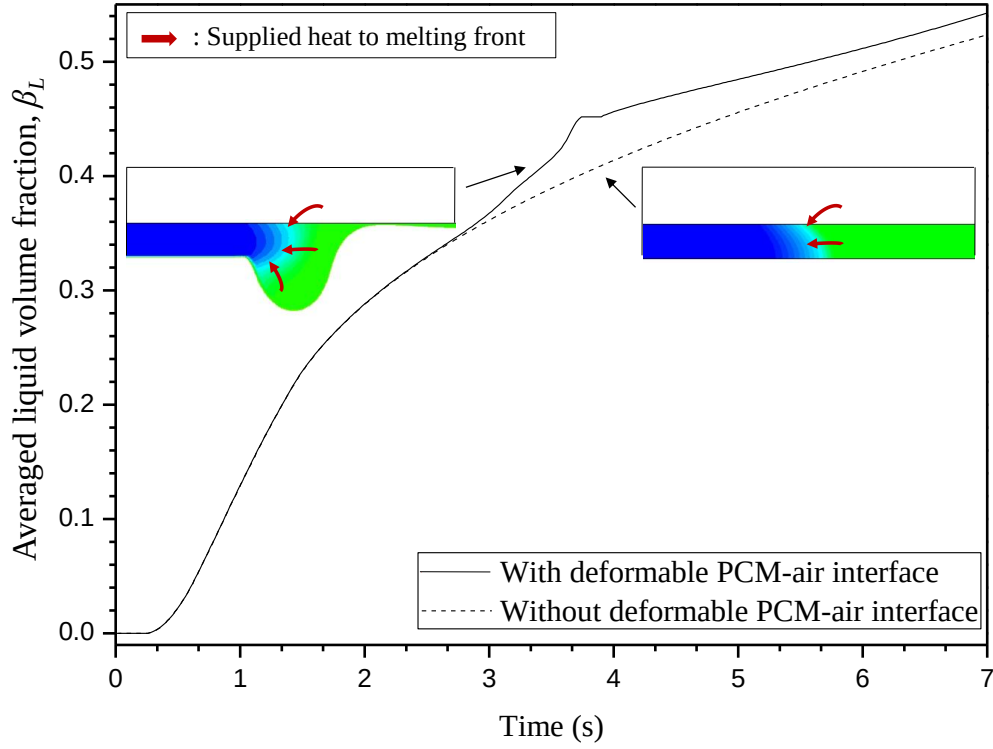


Figure 4.23 Time-dependent averaged liquid volume fraction distribution with and without deformable PCM-air interface

In order to get insight into effect of the abrupt dynamic motion on melting, we performed the simulation without deformation of molten matter: namely, the melting is assumed to occur without any local volume change of the molten PCM. In Fig. 4.23, the dashed line stands for the time-dependent variation of the liquid volume fraction for a fixed position of the PCM-air interface, and the solid line represents the case of a deformable interface. After a time of 2.8 s, coincident with the acceleration region shown with the averaged pendant volume fraction in Fig. 4.8, the deviation of the averaged liquid volume fraction ( $\beta_L$ ) is initiated with and without consideration of deformable PCM-air interface. Figure 4.23 shows the maximum deviation, at a time when the molten PCM starts to drop off. This means that the abrupt dynamic motion of the molten PCM locally enhances the melting. After the detachment of molten PCM, the deviation of  $\beta_L$  from the cases with and without deformable PCM-air interfaces decreases owing to the loss of molten PCM in which heat has accumulated.

#### 4.4.1 Heat transfer in case with and without deformable PCM-air interface during dynamic motion

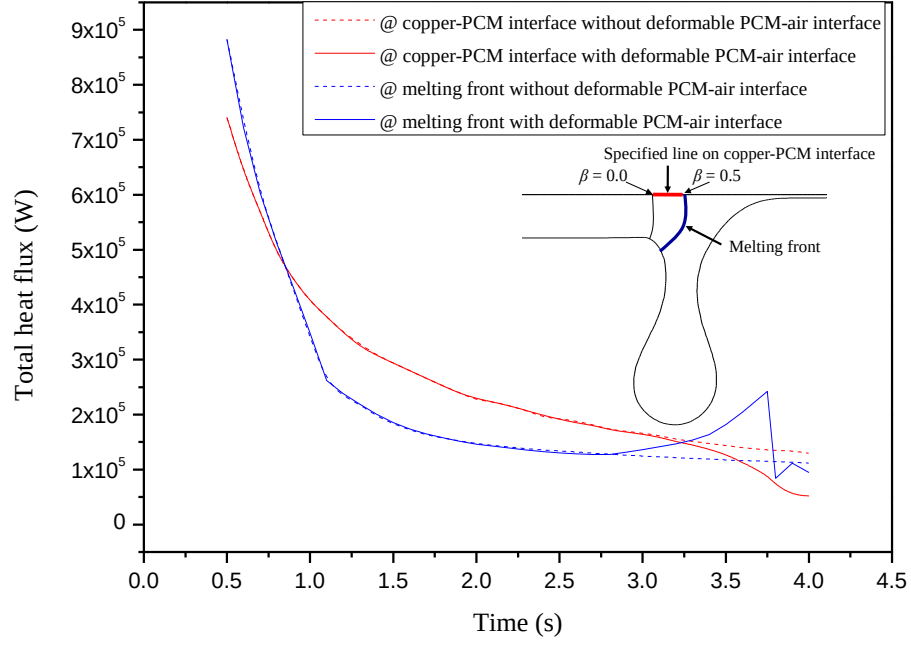


Figure 4.24 Time-dependent heat flux at copper-PCM interface (black) and melting front (blue) with and without deformable PCM-air interface

The local enhancement of melting by dynamic motion can be explained through the heat balance at the melting front and at the copper-PCM interface. In order to investigate this heat balance, the time-dependent total heat flux distributions at a specified line on the copper-PCM interface and at the melting front are shown in Fig. 4.24. The specified line is defined by a liquid fraction ranging from  $\beta = 0.0$  to  $\beta = 0.5$ . The red and blue colors stand for the heat flux at the copper-PCM interface and at the melting front, respectively. The solid and dashed lines correspond to cases with and without a deformable PCM-air interface, respectively. As can be seen in this figure, the total heat flux at different locations has the same order of magnitude, revealing that the total heat flux at both the specified line on the copper-PCM and the melting front have a significant effect on the melting rate. Keeping these facts in mind, when we look at the case of a non-deformable PCM-air interface (dashed

lines) after 0.9 s, the total heat flux at the specified line on the copper-PCM interface is always higher than that at the melting front. In other words, the heat transfer from the copper is relatively stronger than that from the melted PCM during the melting process after 0.9 s. In contrast, the case of a deformable PCM-air interface represented by solid lines in Fig. 4.24 shows that total heat flux at the melting front becomes higher than at the specified line after 3.2 s, which is identical to the moment of the onset of deformation. This indicates that the heat transfer from liquid PCM to the melting front is stronger than that from the copper during the deforming and dropping process. According to the time-dependent total heat flux distribution, the liquid fraction of deformable PCM-air interface becomes higher than that of the non-deformable interface after the onset of deformation.

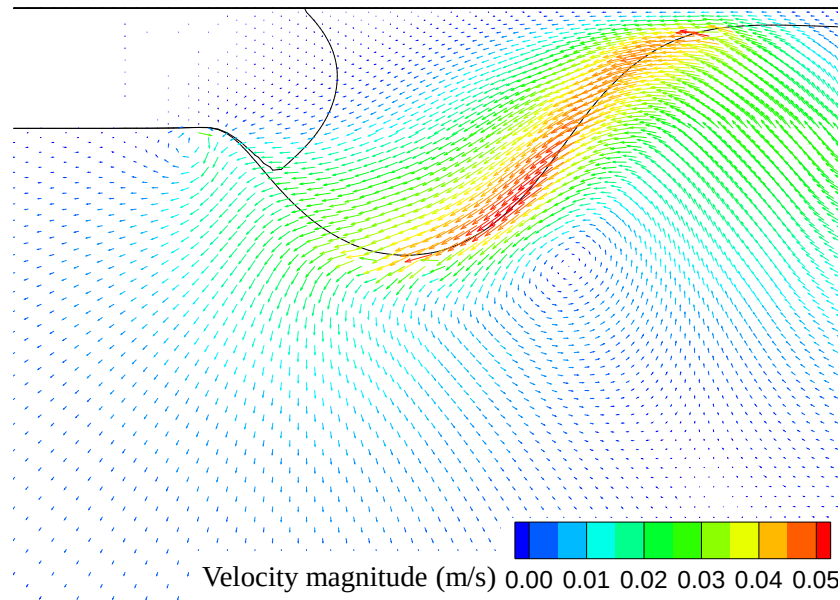


Figure 4.25 Velocity distribution inside molten PCM at 3.3 s

#### 4.4.2 Heat transfer through the copper-PCM interface

One can see from Fig. 4.24 that the total heat flux of the deformable PCM-air interface at the specified line on the copper-PCM interface (see the red solid line) decreases with time after 2.8 s as compared to that of the non-deformable case. This is caused by the heat transfer through the copper-PCM interface. Figure 4.25 depicts the velocity vectors around the deformed PCM at 3.3 s, where the

color represents the magnitude of the velocity. Although the maximum velocity appears along the PCM-air interface while the molten PCM is moving, we can clearly see that the amount of fluid motion inside the molten PCM is toward to melting front. Such fluid motion conveys heat and potentially enhances the melting. Figure 4.26 shows the surface heat flux along the copper-PCM interface in cases (a) with and (b) without the deformable PCM-air interface. The surface heat flux directed from the copper to PCM is defined as positive. Due to the fixed position of the thermal input, the surface heat flux tends to decrease in time both with and without a deformable PCM-air interface. However, as seen at 3.5 and 3.7 s, a negative heat flux, i.e. directed from PCM to the copper, is only found at the surface adjacent to the molten PCM. Such negative heat transfer is more clearly seen in Fig. 4.27, which shows the temperature distribution with and without the deformable PCM-air interface along the surface. The solid and dashed lines, respectively, represent a position corresponding to a vertical 1-mm distance from the copper-PCM interface to the copper and to the PCM at a time of 3.5 s. In the case without the deformable PCM-air interface, the conductive heat is always transferred from the copper to PCM, since the heat conduction from a localized thermal input through the copper is higher than that of the PCM. In contrast, the case with the deformable PCM-air interface shows a negative heat flux (see the range between 5.8 and 6.5 cm). Since the difference between these cases depends on whether the motion of PCM-air interface is considered, this proves that the negative heat flux is driven by the convection induced by the fluid motion of the molten PCM. In particular, the negative heat flux nearly disappears below 400 K, which corresponds to the melting temperature in this calculation. Even though flow could appear in the mushy region, its effect is not strong compared with the effect of the conduction from the copper to PCM. Thus the convective heat transfer, which can change the direction of heat transfer to work against conduction from the copper to PCM, only occurs in completely molten PCM. Consequently, Figs. 4.23, 4.24 and 4.25 reveal that the convective heat transfer in PCM induced by collapse of the PCM-air interface initiates the negative heat flux in the molten PCM, resulting in heat loss to the copper. This is directly reflected by the differences in heat flux on the specified line of the copper-PCM interface between these two cases, as shown in Fig. 4.22.

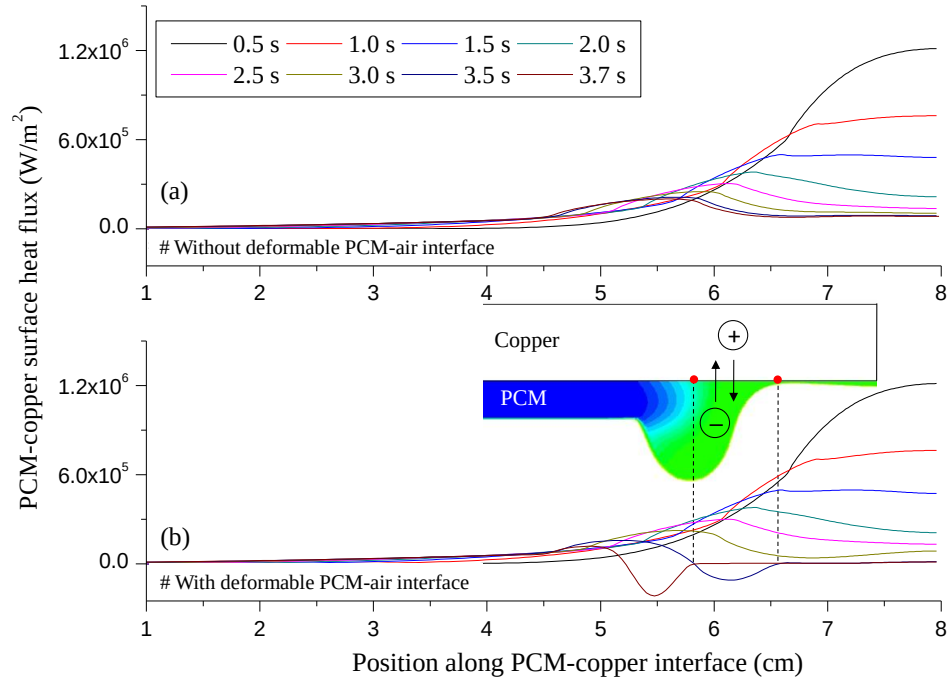


Figure 4.26 Surface heat flux distribution along copper-PCM interface for cases (a) without and (b) with considering deformable PCM-air interface over time

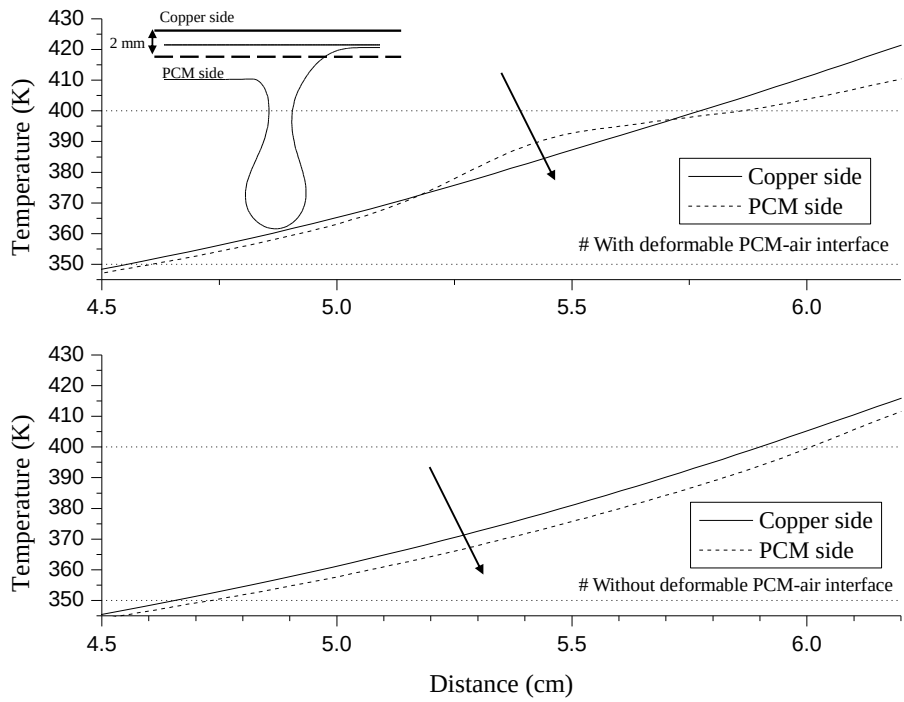


Figure 4.27 Temperature at a point which is 1 mm away from copper-PCM interface toward copper side (solid line) and PCM side (dashed line)

#### 4.4.3 Heat transfer through melting front

In Fig. 4.24, the total heat flux of the deformable PCM-air interface at the melting front increases from 2.8 s to 3.8 s compared to that of the non-deformable case. Such a sudden increase of heat flux might be caused by the following two effects. The first is the effect of the internal liquid convection inside the molten PCM initiated by the deforming and dropping process. As mentioned in 4.22, since the temperature of the bulk molten PCM is higher than that in the vicinity of the melting front, the fluid motion in the molten PCM can deliver the heat to sustain the high temperature gradient in the vicinity of the melting front while the molten PCM is moving and dropping. The second is the effect of length increase of melting front. Figure 4.28 shows the time-dependent length distribution of the melting front for the cases with (solid line) and without (dashed line) a deformable PCM-air interface. As shown in the inset in Fig. 4.28, the melting front first propagates left and downward. However, once the melting front reaches the PCM-gas interface, the melting front mainly propagates to the left while losing heat toward the air. Thus the length of the melting front increases sharply up to 1.1 s, and then decreases until the time of deformation, 2.8 s. After this time, the length of the melting front increases until the dropping of molten PCM, because the suspended molten PCM, which has a relatively high temperature compared to the solidus temperature (350 K), increases the contact area between solid and liquid PCM. Therefore, an increase of the length of the melting front gives a better chance of transferring heat from the suspended molten PCM to the melting front. One can also see at the inset in Fig. 4.28 that the angle  $\theta$  between the melting front and copper-PCM interface varies with respect to time. At 3.7 s, the angle  $\theta$  is large due to considerable heat transfer from molten PCM to the melting front, while the angle  $\theta$  is small at time of 1.1 s because melting is purely driven by the external thermal source. Therefore, we could expect how much a role the effect of deformation of PCM-air interface plays on melting process.

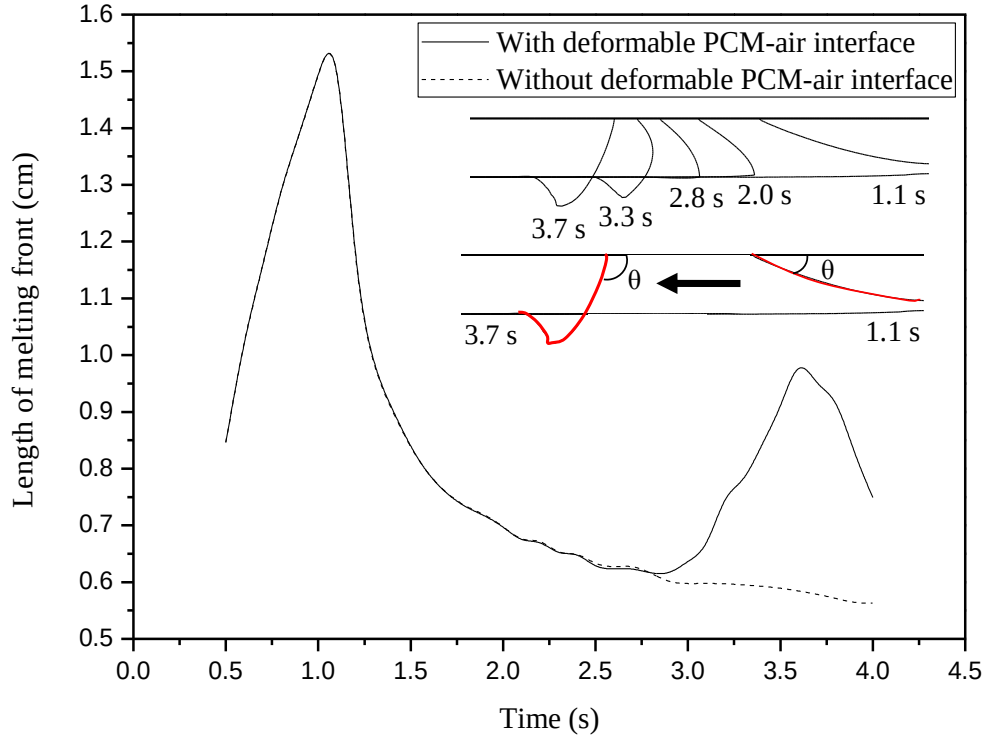


Figure 4.28 Time-dependent distribution of the length of the melting front with and without a deformable PCM-air interface

#### 4.4.4 Behavior of time-dependent liquid fraction for the various Stefan numbers and surface tension coefficients

Calculations were performed both in the cases with and without a deformable PCM-air interface for various Stefan numbers and surface tension coefficients. Figure 4.29 and 4.30 show the time-dependent distributions of the averaged liquid volume fraction ( $\beta_L$ ) for various Stefan numbers and surface tension coefficients, respectively. The solid and dashed lines, respectively, stand for the cases with and without a deformable PCM-air interface. Since melting can happen very quickly under the combustion condition as compare with general slow melting process (e.g. ice melting, melting in thermal storage system), high Stefan number is considered in Fig. 4.29. As expected, it is shown that  $\beta_L$  increases with increasing Stefan number in Fig. 4.29. This trend is consistent with the results of

Hirata [93] and Assis [94], showing that the larger the ratio of sensible heat to the latent heat of fusion of the material, the higher the melting rate. Hence, the volume of accumulated molten PCM should grow more quickly with increase of the Stefan number. Consequently, dropping is quickly experienced at high Stefan number.

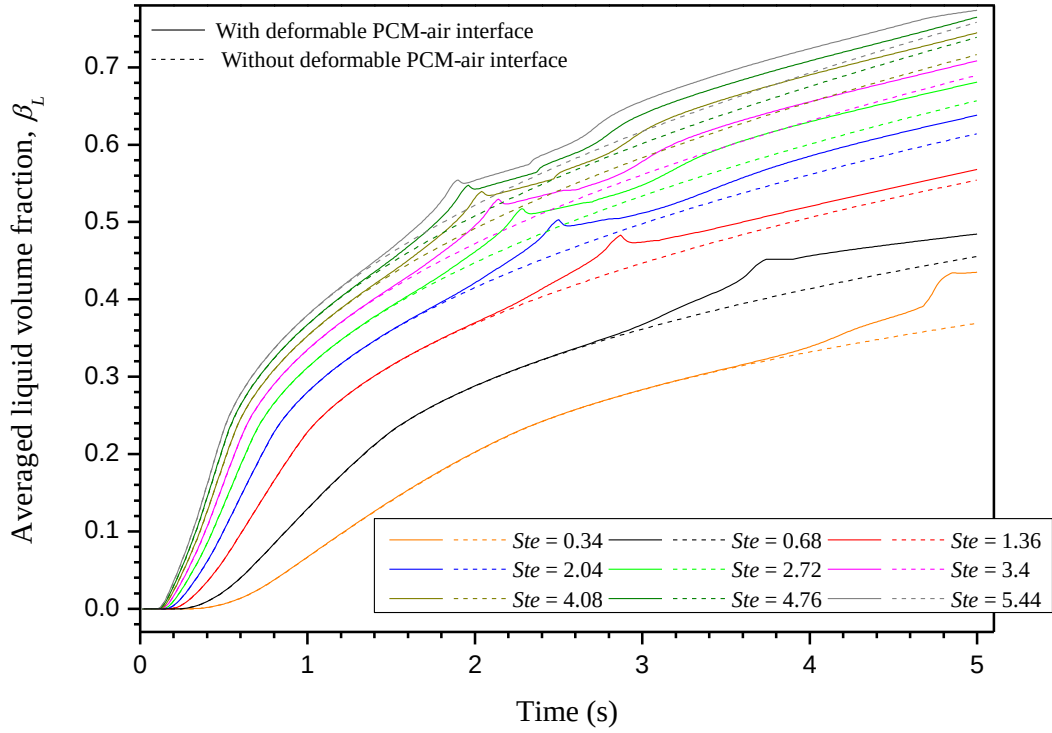


Figure 4.29 Time-dependent liquid fraction distribution for various Stefan numbers at surface tension coefficient = 0.25

Figure 4.30 clearly shows that a change in the averaged liquid volume fraction ( $\beta_L$ ) for the various surface tension coefficients only occurs when dynamic motion exists; since a higher surface tension creates a higher internal pressure, molten PCM can be suspended along the copper surface longer and more easily. A high surface tension coefficient evidently delays the dropping time, as can be seen in Fig. 4.31. We found in particular that  $\beta_L$  in case of a deformable PCM-air interface is always higher than that of non-deformable PCM-air interface over the chosen range of Stefan numbers and surface tension coefficients. Although after the molten PCM drops off several complicated physical processes

simultaneously appear and the heat balance at all interfaces is sharply changed, one can conclude from this study that abrupt dynamic motion always enhances the melting rate compared with the case of a non-deformable PCM-air interface. In general, we can conclude that a consideration of the dynamic motion effect associated with melting is highly desirable for better predictions of heat transfer at melting surfaces in order to understand the dropping timing.

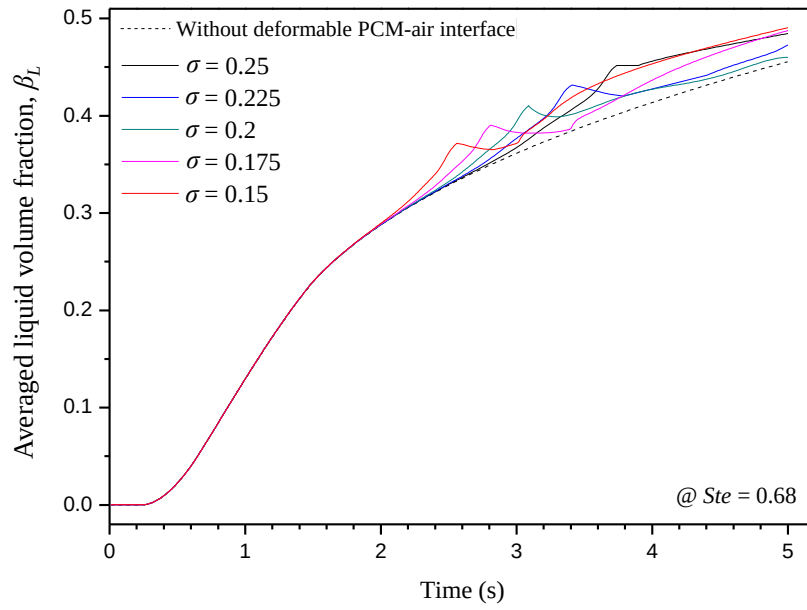


Figure 4.30 Time-dependent liquid fraction distribution for various surface tension coefficient at  $Ste = 0.68$

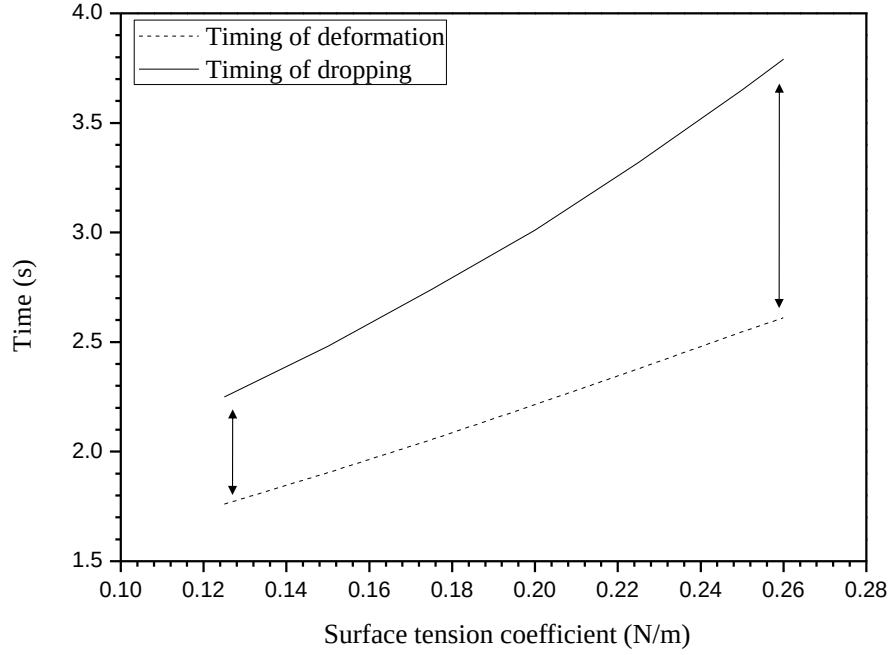


Figure 4.31 Time for deformation and dropping according to surface tension coefficient at  $Ste = 0.68$

#### 4.4.5 Effect of abrupt dynamic motion on melting rate for different Stefan number and surface tension

Results concerning the effect of abrupt dynamic motion on melting, in particular the difference of the averaged liquid volume fraction  $\Delta\beta_L$  between the cases of deformable and non-deformable PCM-air interface at the time of dropping of molten PCM, are shown in Fig. 4.32 over a range of Stefan numbers and surface tension coefficients. We expect  $\Delta\beta_L$  to arise purely from the effect of deforming and dropping of molten PCM. In Fig. 4.32,  $\Delta\beta_L$  is seen to become larger when the applied Stefan number is either small ( $< 2$ ) or large ( $> 5$ ). A large Stefan number results in an increase in the temperature gradient in molten PCM, an effect which contributes to further melting. This is consistent with the previous works [95-97]. In case of small Stefan number, the length of the melting front increases, as shown in Fig. 4.33. Even if conduction is not prominent, an increase of  $\Delta\beta_L$  results in an enhancement in the melting rate. Figure 4.32 also clearly shows that an increase in surface tension results in an increase in  $\Delta\beta_L$ , this is because, as explained in Section 4.4.4, a large surface tension results in a longer suspension time for the molten PCM. The length of the melting front therefore becomes larger, as can be seen in Fig. 4.33.

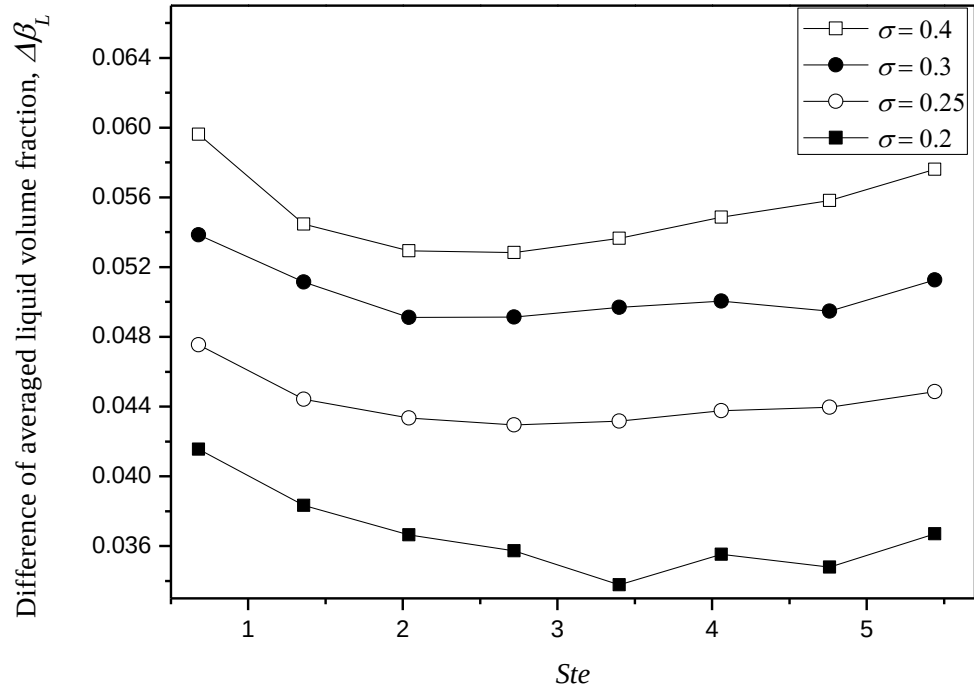


Figure 4.32 Deviation of averaged liquid volume fraction between cases of deformable and non-deformable PCM-air interface for various Stefan numbers and surface tension coefficients

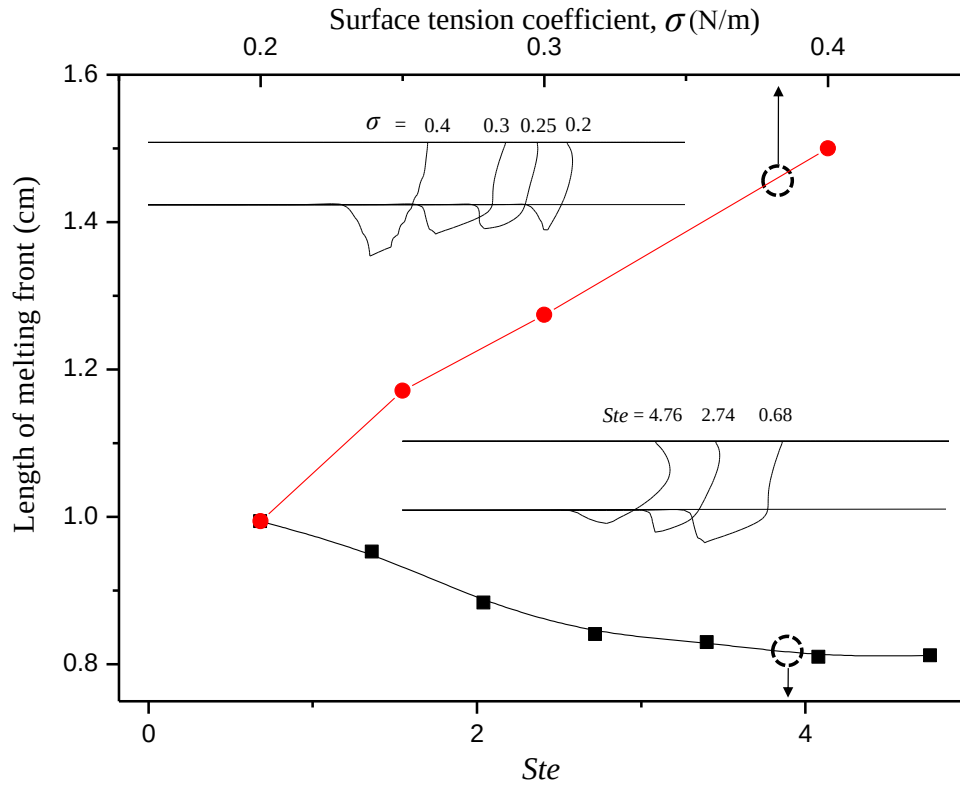


Figure 4.33 Length of melting front according to surface tension coefficient and Stefan number

## **Chapter 5**

# **Effect of thermocapillary convection on melting process of Phase Change Material subjected to local heating**

Thermocapillary motion is a flow in the viscous fluid arising from tangential motion of the interface driven by the difference of surface tension due to temperature gradient along the surface. Generally the surface tension has strong temperature dependency, therefore, the thermocapillary convection appears in non-uniform temperature field and its motion can be controlled by managing non-uniformity of temperature. Due to this unique feature, the thermocapillary convection always has potential to dominate the convective heat and mass transport when the large temperature difference exists in the system.

When buoyancy-driven flow exists in fluids under the presence of strong non-uniformity in temperature, the generated flow tends to relax the non-uniformity, resulting that the thermocapillary effect becomes weak accordingly. Oppositely, when the buoyancy-driven flow is suppressed (e.g., in microscale fluid flow) or reduced substantially (e.g., in microgravity) thermocapillary convection is often utilized as one of momentum source to drive the flow [98-100]. In order to understand its

fundamentals, many previous works focused on thermocapillary convection have been performed in simple rectangular cavity given by horizontally heated and cooled walls beside fluid [101-105]. As numerical point of view, Smith and Davis [106] analyzed thermocapillary flows in a rectangular cavity, showing disparate characteristics of oscillatory thermocapillary phenomena under the condition of flat surface (without any deformation). Sen and Davis [107], Sen [108], Nepomnyashchil et al. [109], and Mundrane et al. [110] had expanded numerical model to include the effect of deformation of free surface owing to oscillatory thermocapillary convection observed in experiments, and revealed that consideration of deformation of free surface is necessary to predict accurate flow field. Later, Kim and Kou [111], Roux et al. [112], Kim et al [113], and Wei et al. [114] numerically investigated the thermocapillary convection in melting process with consideration of deformation of free surface, and elucidated that melt volume was considerably affected by both thermocapillary convection and deformation of free surface. However, none of them revealed that the impact of thermocapillary effect on melting process itself.

The precise prediction of melting process is very important from view point of fire safety; for example, the fire of polymer-coated electric wire, which is shown in Fig. 1.2, is one typical case [19]. During the flame spreading event over the electric wire, the coated polymer receives substantial heat from the surrounding flame, and polymer undergoes melting and gasification, sometimes, molten polymer grows then eventually drops off. In particular, it was reported that core wire plays a thermodynamical role in the melting as well as burning of wire coating [15, 16]. Therefore, in order to understand/model the melting (and the following burning) processes of electric wire precisely, consideration of heat transfer through the conductive material (metal wire core) attached to the polymer is inevitable. Thus, a series of numerical simulation to examine the melting process of phase change material (PCM) subjected to local heating on the copper plate with deformable surface in 2-D system was investigated in chapter 4, as a one of simple model of the fire of the electric wire. It has been successfully ensured that the presence of internal fluid motion inside molten PCM could modify melting speed as well as the dropping-off timing. In the previous section, even though large temperature gradient around the melted polymer caused by surrounding flame was expected,

thermocapillary effect was not taken into account to avoid complexity. We must wonder the impact of thermocapillary convection on melting process precisely, which is still opened to the question.

In this chapter, we consider the time-dependent thermocapillary convection in the molten PCM during melting, deforming and dropping processes. Considered numerical model in the section is the same as the previous one, except for the inclusion of thermocapillary effect. Gravity as well as surface tension coefficient are treated as numerical parameters and varied to examine the effect of thermocapillary convection effectively. The fundamental conservation equations for mass, momentum and energy are solved with the Enthalpy-Porosity method and Volume of Fluid method as same with chapter 4. Additionally, effect of thermocapillary convection is needed to model as volumetric source term into momentum equation with surface tension force as inner solution, which is

$$\mathbf{F}_{ST} = \frac{\rho}{0.5(\rho_g + \rho_l)} [\sigma \kappa_c \mathbf{n}_s + (I - \mathbf{n}_s \otimes \mathbf{n}_s) \nabla_s \sigma^T] \delta_s \quad \text{where} \quad \mathbf{n}_s = \frac{\nabla \tilde{\alpha}}{|\nabla \tilde{\alpha}|}. \quad (5-1)$$

Here, all are same with surface tension force explained in chapter 4 except for the second term of RHS. It stands for the tangential force driven by surface tension due to temperature gradient;  $\nabla_s \sigma^T$ . Here,  $\nabla_s \sigma^T$  is considered to be linearly dependent on the temperature gradient as  $\nabla_s \sigma^T = (\partial \sigma / \partial T) \nabla_s T$ . According to Ref. [110], suggested value of the coefficient,  $\partial \sigma / \partial T$ , is  $-0.67 \times 10^{-3}$  [N/(m K)] for molten silicon. In fire of electric wire, temperature deviation along the interface ( $\nabla_s \sigma^T$ ) is expected to be several hundred Kelvin because temperature deviation is relaxed due to the presence of heat conductive matter; namely copper wire [116-117]. As stated, in this study, we choose 500 K (fixed value) of heat source to initiate the melting and subsequent deformation of PCM so that above-tangential force,  $\nabla_s \sigma^T$  (namely the source of thermocapillary convection), might be under-estimated. Therefore, we made the parametric study to modify the variation of temperature-dependent surface tension coefficient,  $\partial \sigma / \partial T$ , in order to magnify the thermocapillary effect. Figure 5.1 summarizes temperature-dependent surface tension coefficient. Here, five kinds of temperature dependency of  $\sigma$

are considered as numerical parameter as explained above (hereafter, they are referred as case 1 to case 5). If no special description is made, base case is case 5 to give maximum of  $\partial\sigma/\partial T$  in this study.

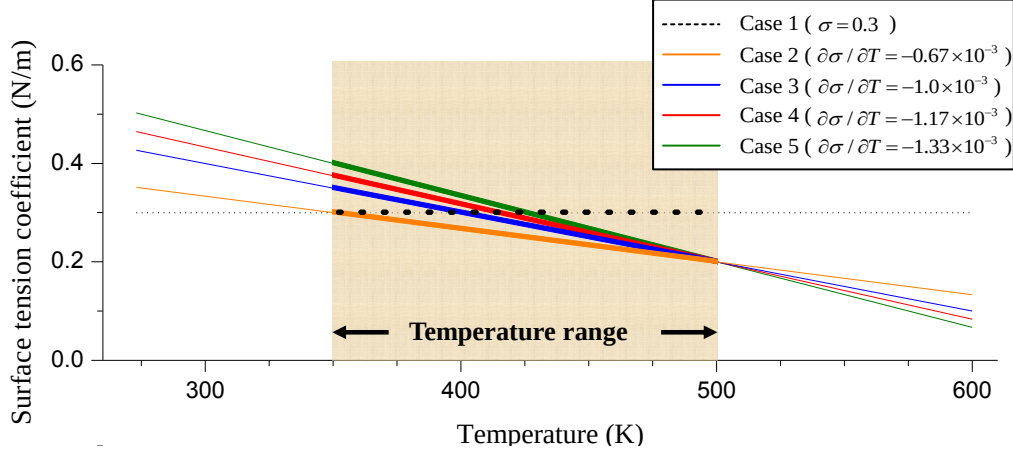


Figure 5.1 Schematic illustration of the temperature-dependent surface tension coefficient

## 5.1 Numerical model, initial and boundary conditions

The physical configuration is schematically illustrated in Fig. 5.2. Copper (as conductive matter) and PCM (as combustible-insulator) are placed on the top of 2-D numerical domain and the rest part is filled with air (as surrounding gas). In order to represent the heat flow toward the polymer through copper (conductor) satisfactory as noticed in the wire combustion, a localized external thermal input of 500 K is placed on the top surface of the copper to initiate melting of the PCM. We have studied the effect of the temperature of heat source (up to 1400 K) previously [116], and it has been revealed that melting and dropping processes are physically identical irrespective of the imposed temperature, although the dropping off timing is modified extensively. Since immediate melting and deformation is experienced when the high temperature is imposed as heat source, there would be less chance to observe the thermocapillary effect (we will discuss this in later). Selection of 500 K of heat source is simply due to better observation of thermocapillary effect in this study.

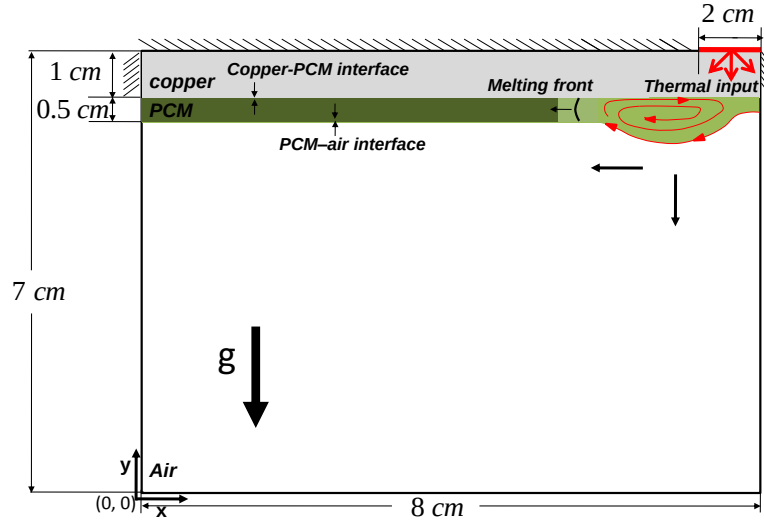


Figure 5.2 Schematic illustration of the computational domain

The temperature 300 K is used over the whole domain as the initial thermal condition. A normal downwardly-directed gravity (with corresponding gravitational acceleration  $9.81 \text{ m/s}^2$ ) and zero-gravity fields are considered in order to examine a role of thermocapillary convection. Since the strong temperature gradient in the molten PCM is expected in this system and thermocapillary convection is driven by the variation of surface tension caused by non-uniformity in temperature, effect of temperature sensitivity of surface tension is investigated as one of important numerical parameter in this section. As the molten volume is reached to its critical value to be suspended, molten PCM starts to deform severely, and is eventually detached from the main part of the molten PCM owing to gravity drag under normal gravity environment (of course no such thing occurs under zero-gravity case).

## 5.2 Results and discussion

In this section, we limit the discussion to thermocapillary convection of the molten PCM up to its first dripping off as a result of the growth, since quite complicated phenomena (i.e., re-solidification, tiny second dropping of molten PCM, and breaking molten PCM film on the copper surface etc.) appear after the first dropping.

### 5.2.1 Flow in molten PCM and temperature distribution under normal gravity

In Fig. 5.3, the time-sequence of distributions of liquid fraction,  $\beta$ , with streamlines (left) and temperature,  $T$ , (right) under normal gravity. In the right figure, the position of the melting front and the liquid-gas interface approximated by  $\beta = 0.05$  and  $\alpha = 0.5$ , respectively, are added by black line. It clearly shows thermocapillary convection in molten PCM before around 2.0 s. Since thickness of molten PCM is not large (0.5 cm) and high surface tension gradient due to varying temperature at the liquid-gas interface is given, thermocapillary convection inside the molten PCM could be held under the presence of buoyancy. However, once liquid-gas interface starts to deform due to increase of volume of the molten PCM after around 2.0 s, thermocapillary convection is masked, and gravitational force-driven flow dominates internal motion in the molten PCM.

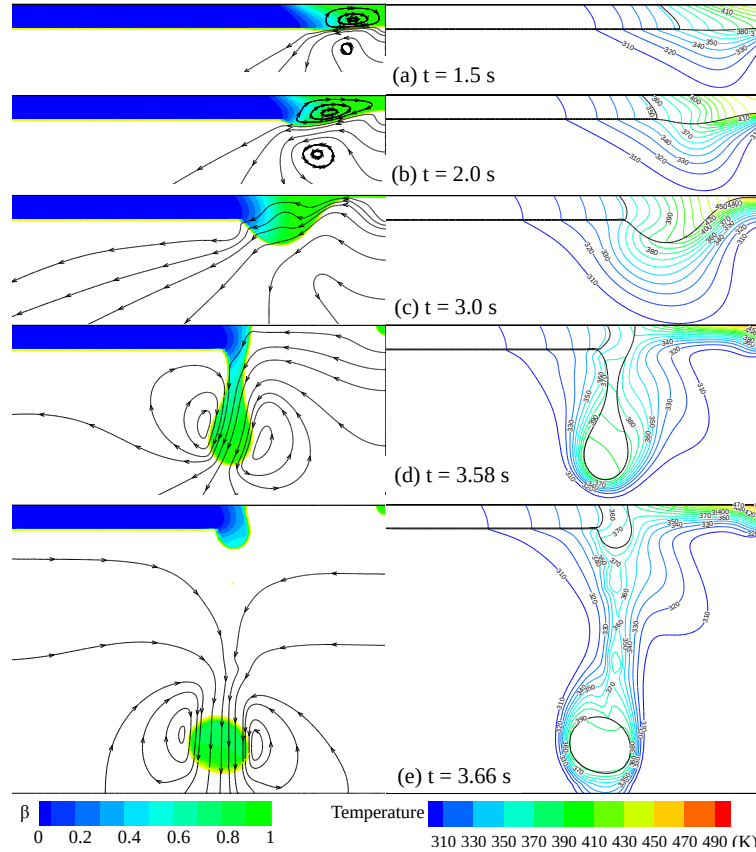


Figure 5.3 Time-sequence of distribution of streamline-superimposed liquid fraction  $\beta$  (from 0 to 1) and temperature (from 310 K to 490 K) under normal gravity with respect to time ((a)  $t = 1.5$  s, (b)  $t =$

2.0 s, (c)  $t = 3.0$  s, (d)  $t = 3.58$  s, (e)  $t = 3.66$  s) with  $\partial\sigma/\partial T = -1.33 \times 10^{-3}$  [N/(m K)]

### 5.2.2 Flow in molten PCM and temperature distribution under zero-gravity

Figure 5.4 shows the time-sequence of distributions of liquid fraction,  $\beta$ , with streamlines (left) and temperature,  $T$ , (right) under zero-gravity. Unlike normal gravity (see Fig. 5.3), thermocapillary convection appears and retain in molten PCM over whole time, and the size of vortical motion of flow grows in entire molten PCM. In particular, it is observed that liquid-gas interface is deformed by thermocapillary convection. Furthermore, thermocapillary convection affects temperature distribution as shown at right figure. Temperature distribution in air vicinity of liquid-gas interface is distorted toward same direction of surface flow induced by thermocapillary convection.

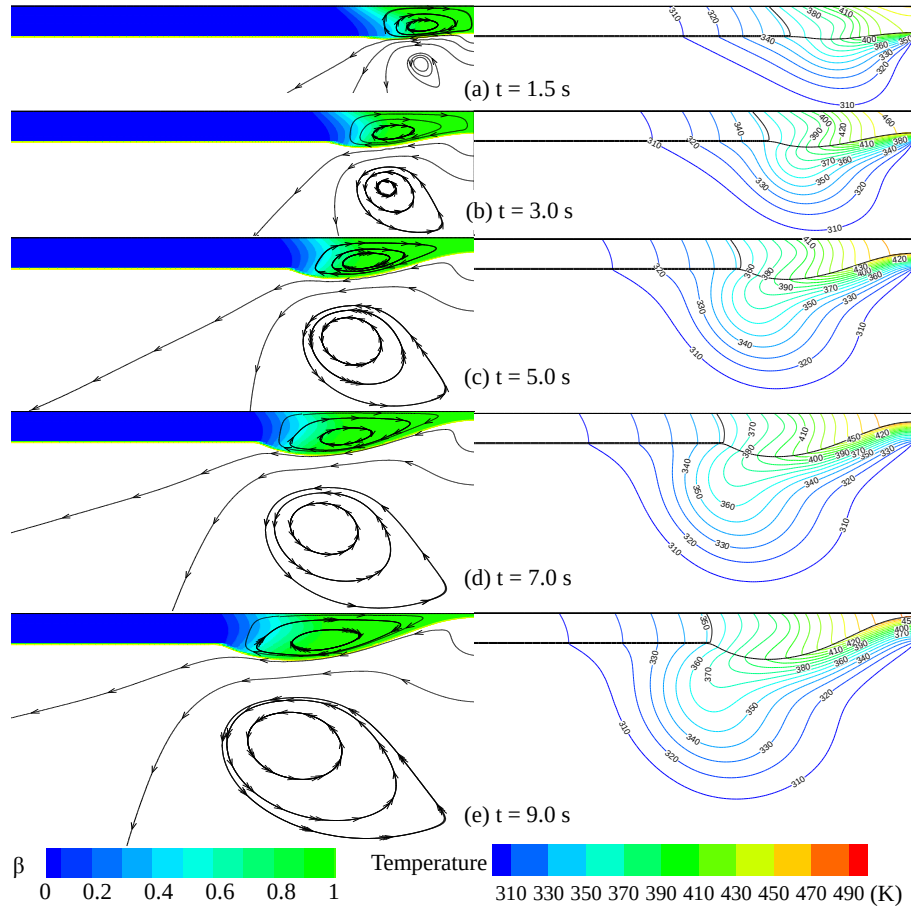


Figure 5.4 Time-sequence of distribution of  $\beta$  and temperature under zero-gravity with respect to time

((a)  $t = 1.5$  s, (b)  $t = 3.0$  s, (c)  $t = 5.0$  s, (d)  $t = 7.0$  s, (e)  $t = 9.0$  s) with  $\partial\sigma/\partial T = -1.33 \times 10^{-3}$  [N/(m K)]

### 5.2.3 Heat flux analysis

Figure 5.5 shows time-sequence of heat fluxes to un-melted PCM across the melting surface and the copper-PCM interface for the cases with/without consideration of thermocapillary effect (more precisely, comparison between case 1 and case 5). To focus on the thermocapillary effect on heat flux, only zero-gravity condition is considered. This figure clearly shows that the difference between two represented cases is pronounced at early stage ( $t < 2$ s) where the temperature distribution inside the molten PCM exists. The difference is minimized as the time goes by since the temperature distribution is relaxed due to the progress of melting. Importantly, the maximum heat flux gain due to the presence of thermocapillary effect is about 4.35 %. Thus it is expected that inclusion of thermocapillary effect in the model can increase the heat flux and accelerate the melting a bit, the speed does not change much. The time to reach the certain volume of molten PCM could be affected when the melting process is slow enough, because the volume of molten PCM is given by the integration of the melting speed in time so that the small difference of melting speed is accumulated.

Continuous reduction of the difference of heat flux of two cases in time is quite reasonable since the heat source in this system is fixed at the edge so that the melted length is monotonically increases as the melting progressed. However, in reality of fire, flame (heat source) moves with the melted front [19] so that such reduction might not be expected.

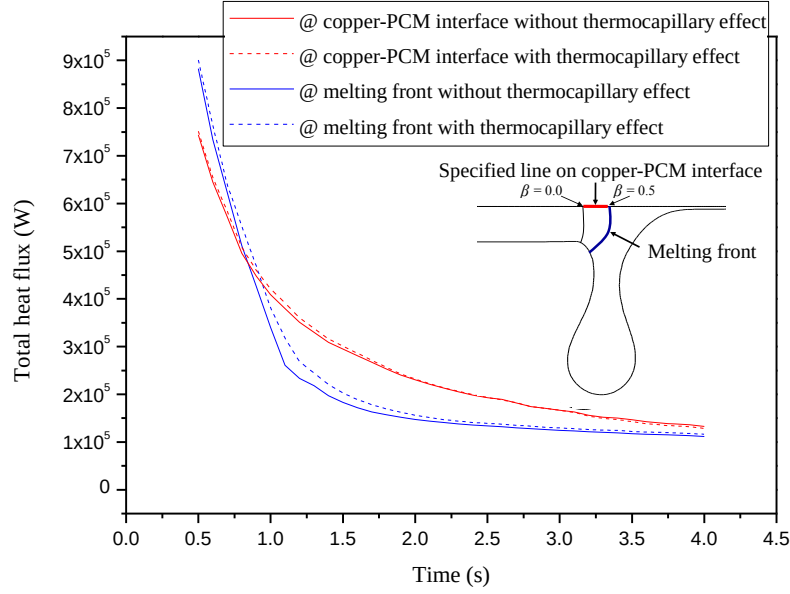


Figure 5.5 Time-dependent heat flux at copper-PCM interface (red) and melting front (blue) with/without thermocapillary effect in zero-gravity

#### 5.2.4 Time-variation of melting fraction and dropping-off timing

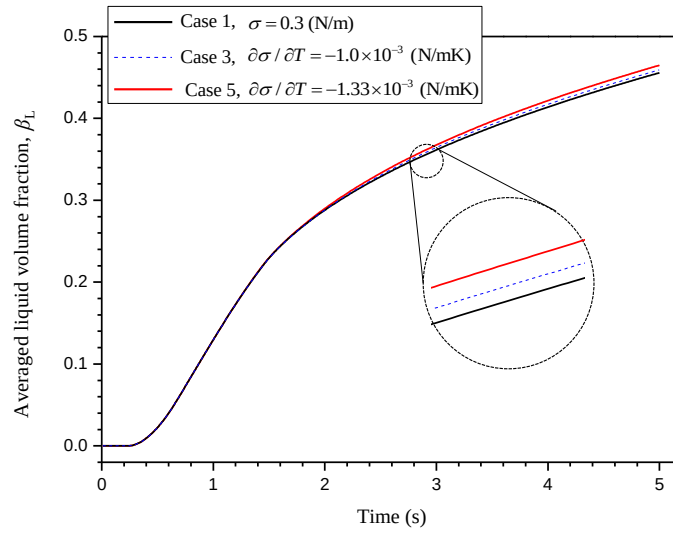
Figure 5.6 shows time-dependent averaged liquid volume fraction,  $\beta_L$ , for various pattern of surface tension coefficient (case 1 to case 5) under two different gravity conditions. Here,  $\beta_L$  represents how much PCM is melted in total volume of PCM, and is defined as

$$\text{Averaged liquid volume fraction: } \beta_L = 1 - V_{SP} / V_{TP}.$$

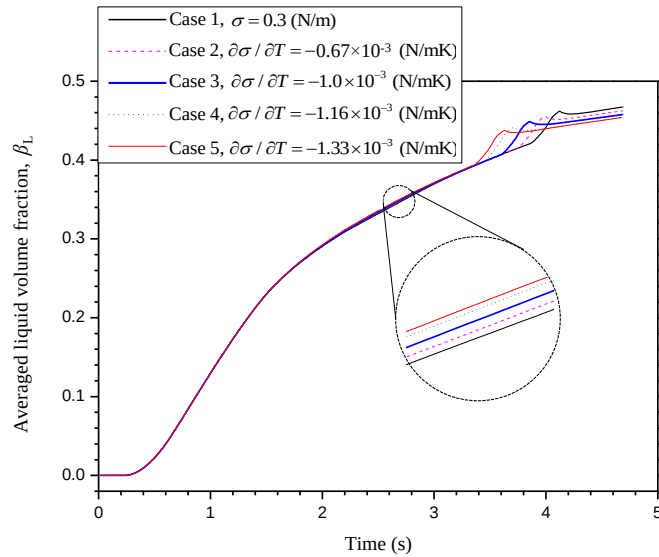
Here,  $V_{SP}$  is the volume of the solid-state PCM (un-melted volume of PCM) [m<sup>3</sup>] and  $V_{TP}$  is the initial total volume of PCM [m<sup>3</sup>], respectively.

Under zero-gravity condition,  $\beta_L$  increases with increasing temperature sensitivity of surface tension coefficient,  $\partial\sigma/\partial T$  [N/(m K)] as expected.  $\beta_L$  enhanced by effect of thermocapillary convection is not significant. For instance, deviation of  $\beta_L$  between constant surface tension coefficient,  $\sigma = 0.3$  [N/m], and varying surface tension coefficient of which  $\partial\sigma/\partial T = -1.33 \times 10^{-3}$  [N/(m K)] is 5 % at time of 3.0 s. Exactly the same trend is found under normal gravity condition (see Fig. 5.6(b)), although the deviation is further minimized. It becomes less than 2 % at time of 3.0 s, which is nearly half as compared to the zero-gravity case.

One can see from Fig. 5.6 that sudden increase and decrease of  $\beta_L$ , shown between time of 4.0 and 5.0 s, as a result of the strong deforming and time of the inflection point shown in Fig. 5.7 represents the moment of dropping-off of molten PCM [116]. Interestingly, increase of  $\partial\sigma/\partial T$  enhances time of dropping of molten PCM, although slightly enhancing  $\beta_L$ . Thus, it can be concluded that the inclusion of thermocapillary effect might be negligible for the precise prediction of melting speed, but it should be counted for the precise prediction of dropping-off timing.



(a) zero-gravity



(b) normal gravity

Figure 5.6 Time-dependent averaged liquid volume fraction distribution for various temperature-

dependent surface tension coefficients under (a) zero-gravity and (b) normal gravity

### 5.2.5 Geometric effect

In Sec. 5.2.2, under zero-gravity, deformation of molten PCM is generated due to thermocapillary convection. It is expected that this deformation can assist to hold the internal flow motion so as to increase the heat flux toward the un-melted PCM. Lastly, let us examine this point by considering the case of the gravity works in the opposite direction. Since gravity directs toward PCM, dropping-off of molten PCM is not expected, furthermore, gravity could suppress the deformation of PCM to reduce the thermocapillary effect.

Figure 5.7 shows time-sequence of  $\beta_L$  with  $\partial\sigma/\partial T = -1.33 \times 10^{-3}$  [N/(m K)] for three gravity cases ( $\mathbf{g} = -\mathbf{G}$ ,  $\mathbf{g} = 0$ ,  $\mathbf{g} = +\mathbf{G}$ ). In spite of small difference of  $\beta_L$  between zero and reverse gravity,  $\beta_L$  in zero-gravity condition is little higher than that in reverse gravity. It means that thermocapillary convection effect on melting is little higher in zero-gravity than in reverse gravity. However, when we look at difference of  $\beta_L$  between different directional gravity cases, it is shown that  $\beta_L$  under normal gravity is much higher than that of reverse gravity. In previous research [116], we observed that deforming and dropping-off of molten PCM locally increase  $\beta_L$  due to increase of heat transfer to melting front as compare with case which did not consider deformation model. Thus, difference of  $\beta_L$  in three cases (zero, normal and reverse gravity) can also be explained by deformation rate induced by the possible internal flow (i.e., thermocapillary convection and gravity-induced flow). Deformation and dropping-off caused by thermocapillary convection or gravity-driven flow are suppressed in reverse gravity whereas deformation occurs in zero-gravity. Thus,  $\beta_L$  in reverse gravity is smaller than that in zero-gravity. However, deformation in normal gravity is much larger than that in both zero and reverse gravity so that large  $\beta_L$  presents in normal gravity as compare with other cases.

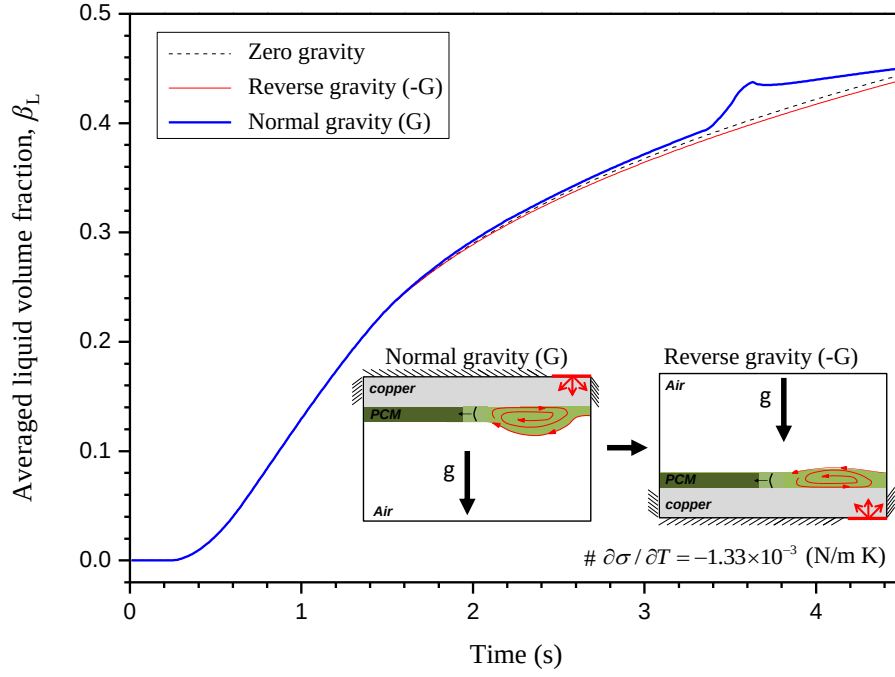


Figure 5.7 Time-sequence of averaged liquid volume fraction,  $\beta_L$ , with  $\partial\sigma/\partial T = -1.33 \times 10^{-3}$  [N/(m K)] for three gravity cases

### 5.3 Further discussion

Although thermocapillary effect was investigated in most preferable condition targeted at polymer coated electric wire exposed to a fire condition, sensitivity of other several factors, which is not considered in this study, is necessary to be discussed. Following is candidate which has potential to affect the thermocapillary motion.

(1) Gasification: Ratio between gasification and melting rate controls the volume of molten PCM. When gasification is higher than melting, volume of molten PCM decreases, deformation is suppressed. Thus, high gasification rate may increase the thermocapillary effect.

(2) Thickness: With increase of thickness, gravity-driven deformation is easily initiated. Thus, thermocapillary motion effect becomes insignificant.

(3) Temperature deviation along the PCM-air interface: If there is critical condition where temperature gradient exists with negligible gravity driven flow, thermocapillary effect becomes higher.

However, when high temperature is imposed to electric wire, melting speed becomes faster, molten volume quickly grows. Thus, although temperature gradient becomes higher, there is not enough time for thermocapillary motion to play a role, gravity-driven flow is dominant.

## **5.4 Concluding remarks**

Thermocapillary motion targeted at polymer-coated electric wire exposed to a fire condition was numerically modeled under a continuum mechanics for multiphase flow with melting phase change. Calculation was carried out by solving Navier-Stokes and energy with volume of fluid transport equation. The source-based tangential force driven by surface tension, which linearly depends on the temperature, was modeled in the previous-proposed model. Numerical parameters were selected in order to investigate the thermocapillary motion in effective way, and the following conclusions were drawn.

1. Effect of thermocapillary convection on melting of Phase Change Material (PCM) is found to be not so significant under the condition studied here. However, it should be taken into account if the precise prediction of dripping-off timing is desired.
2. Thermocapillary convection in molten Phase Change Material (PCM) only appears before deformation of liquid-gas interface, however, after that, gravitational force-driven flow dominates in molten Phase Change Material (PCM) under the condition studied here.

# Chapter 6 Moving heat flux

In previous section, numerical calculations have been performed by comparing the cases with/without deformation of the gas-liquid interface on a similar physical domain with experiment in order to understand pure effect of the dynamic behavior of molten polymers, although combustion was not considered. Through this research, it was found that the behavior of the molten polymer affects the melting speed during its growth and during dropping, and this dynamic effect on melting speed varied with different Stefan number and surface tension coefficient. However, investigation is necessary to be extended in order to get concrete conclusion as compare with wire combustion due to following reasons; (1) discussion was limited only to the case of a fixed position of the external thermal source even though in the combustion of electric wire, molten polymer is supported by heat from the moving flame. (2) Also, investigation is limited to phenomena till first dropping although multi-dropping could exist in real environment. (3) By giving fixed position of the external thermal source, melting speed tends to decrease according to time. This condition is not appropriate when effect of deformation and dropping on melting is target, because quantificational investigation is hard to be achieved. Considering altogether, we must wonder the impact of deforming and dropping of PCM on melting process supported by moving thermal source precisely, which is still opened to the question.

In this section, we numerically studied melting and deformation of polymeric material induced by a constant moving heat flux. As same with previous section, the polymer is also termed “Phase Change Material (PCM)”, and copper was selected as the core wire. The time-dependent melting and the behavior of the PCM are visualized together with the temperature distribution. The effect of the dynamic motion on the melting process with/without a deformable interface is discussed.

## 6.1 Numerical model

The physical configuration is schematically illustrated in Fig. 6.1. The 2-D computational domain

consists of copper, PCM and air. The total horizontal and vertical lengths are 15.0 and 5.0 cm respectively, and the thickness of the PCM is 0.5 cm. A normal downwardly-directed gravity field is considered with corresponding gravitational acceleration  $9.81 \text{ m/s}^2$ . The types, amount and speed of external thermal input is examined as shown in table 6.1.

Table 6.1 Various type of external thermal input

|        | Type                 | Amount                        | Speed  |
|--------|----------------------|-------------------------------|--------|
| Case 1 | Constant Temperature | 1000 K                        | 1 cm/s |
| Case 2 | Heat flux            | $1.5\text{e}^8 \text{ W/m}^2$ | 2 cm/s |
| Case 3 | Heat flux            | $1.5\text{e}^8 \text{ W/m}^2$ | 3 cm/s |
| Case 4 | Heat flux            | $1.5\text{e}^8 \text{ W/m}^2$ | 4 cm/s |

These external heat source moves from right to left, and is specified on the top surface of the copper with corresponding length of 2.0 cm. Temperature 300 K is used over the whole domain as the initial condition.

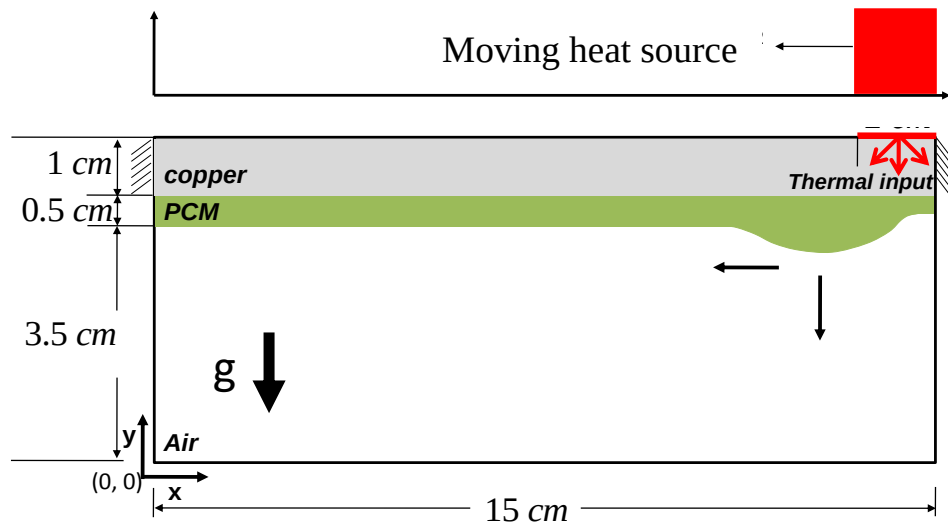
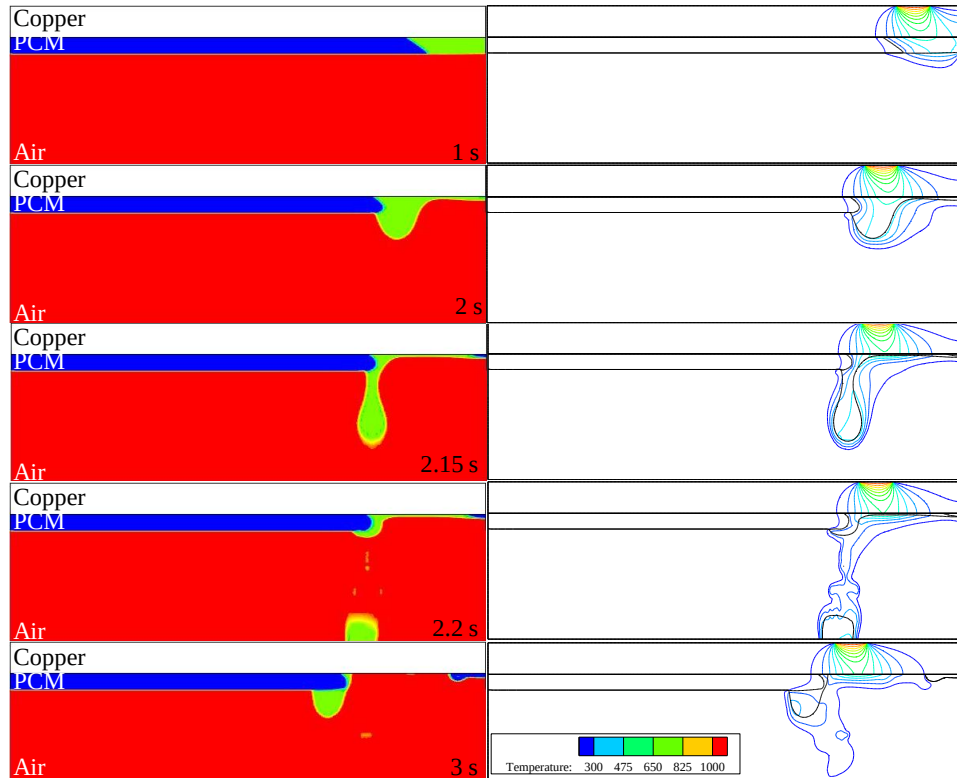
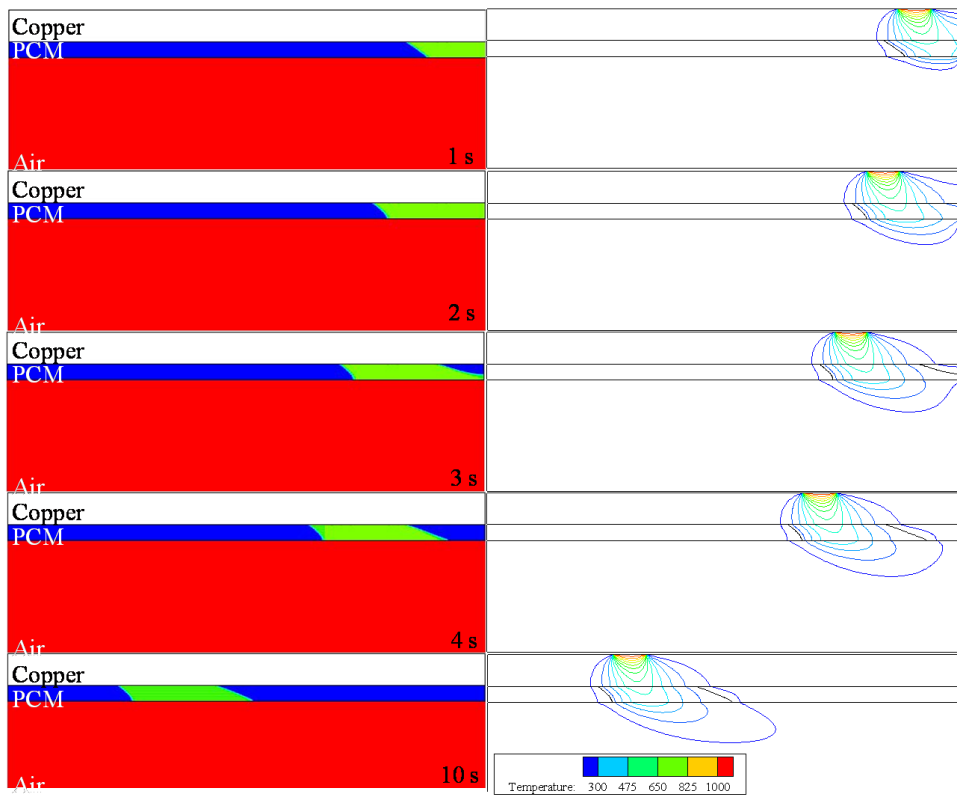


Figure 6.1 Schematic illustration of the computational setup



(a) Case with deformable PCM-air interface



(b) Case without deformable PCM-air interface

Figure 6.2 Distribution of  $(\alpha + \beta)/2$  on left and of temperature on right supported by moving heat

source defined by constant temperature over time (case 1)

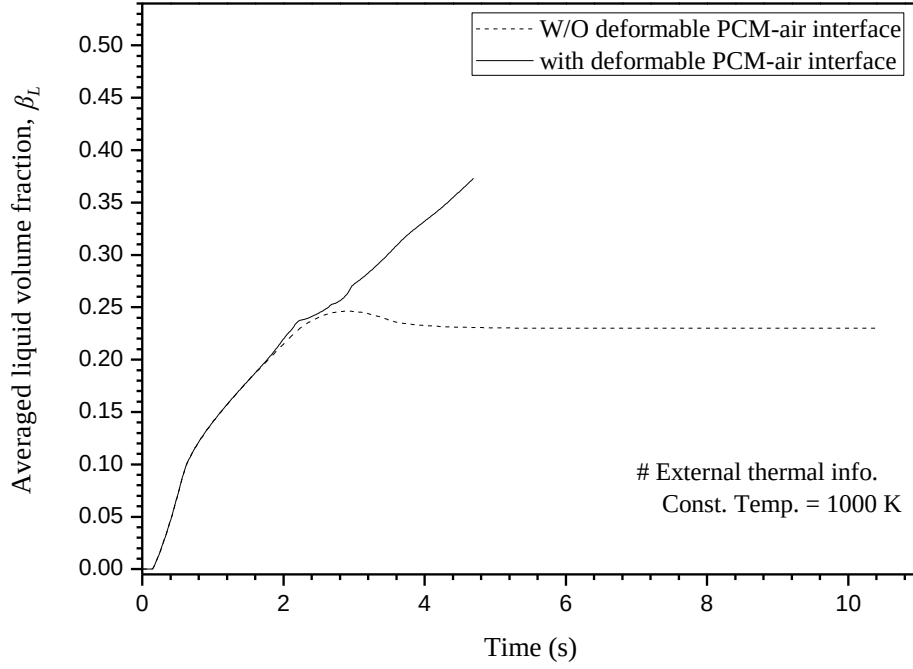


Figure 6.3 Time-dependent averaged liquid volume fraction with/without deformable PCM-air interface (case 1)

## 6.2 Results and discussions

Figure 6.2 shows the time-dependent distribution of the scalar quantity  $(\alpha+\beta)/2$  on the left and of the temperature on the right, thus, visualizing the overall process of the melting and the dynamic behavior supported by moving heat source of 1000 K (case 1). The white, red, green and blue colors correspond to computational cells filled with copper, air, molten PCM and solid PCM, respectively. For the given moving heat source, the growth of melting deformation and multi-dropping of PCM is clearly shown in case of a deformable PCM-air interface, whereas, deformation and dropping of PCM does not appear in the case without deformable PCM-air interface. When we look at the case without deformable PCM-air interface, one can be seen that melted region in PCM undergoes re-solidification. It is caused by fact that Dirichlet boundary condition as moving external thermal input does not satisfy the adiabatic condition on copper surface behind of melting front. Thus, it leads copper heated by moving heat source to be cooled down, and PCM loses the heat to the cooled copper. In order to help to understand, time-dependent averaged liquid volume fraction (same definition with that in Eq. 4.1)

with/without deformable PCM-air interface is shown in Fig. 6.3. Where, solid and dashed line is respectively the case with and without deformable PCM-air interface. Averaged liquid volume fraction in case with deformable PCM-air interface almost constantly increases over time, while that in case without deformable PCM-air interface does not increase, rather, becomes constant after around 3.4 s due to heat loss in PCM to copper. Since we are interested in effect of dynamic behavior of PCM on melting process itself, it is necessary to avoid other effects, except for dynamic behavior. Hence, adiabatic boundary condition is essentially necessary where moving heat source left.

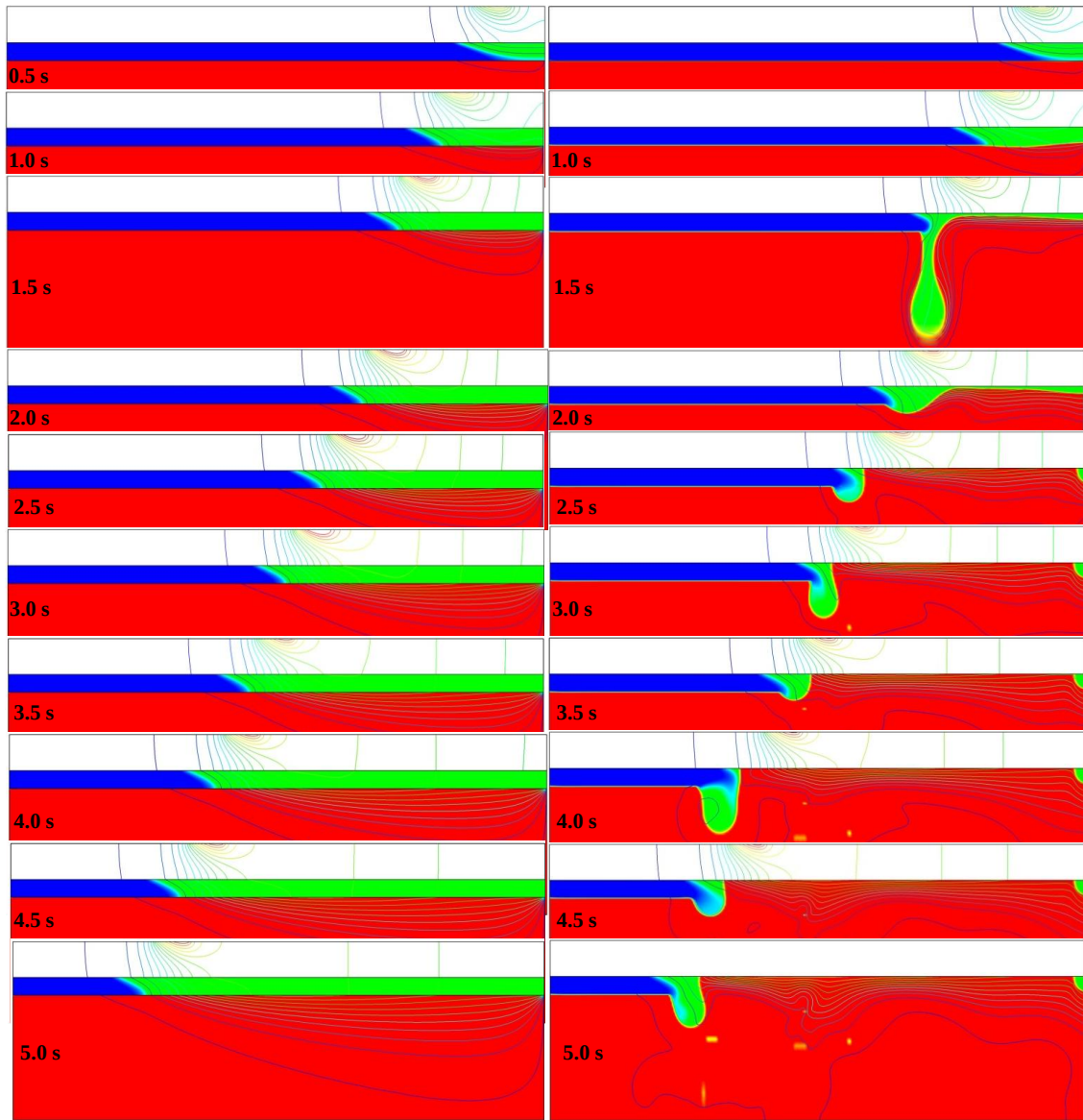


Figure 6.4 Time-dependent distribution of  $(\alpha + \beta)/2$  superimposed on the temperature profile in

case with (right) and without (left) deformable PCM-air interface by employing moving heat flux of  $150 \text{ MW/m}^2$  as speed of  $2 \text{ cm/s}$  (case 2)

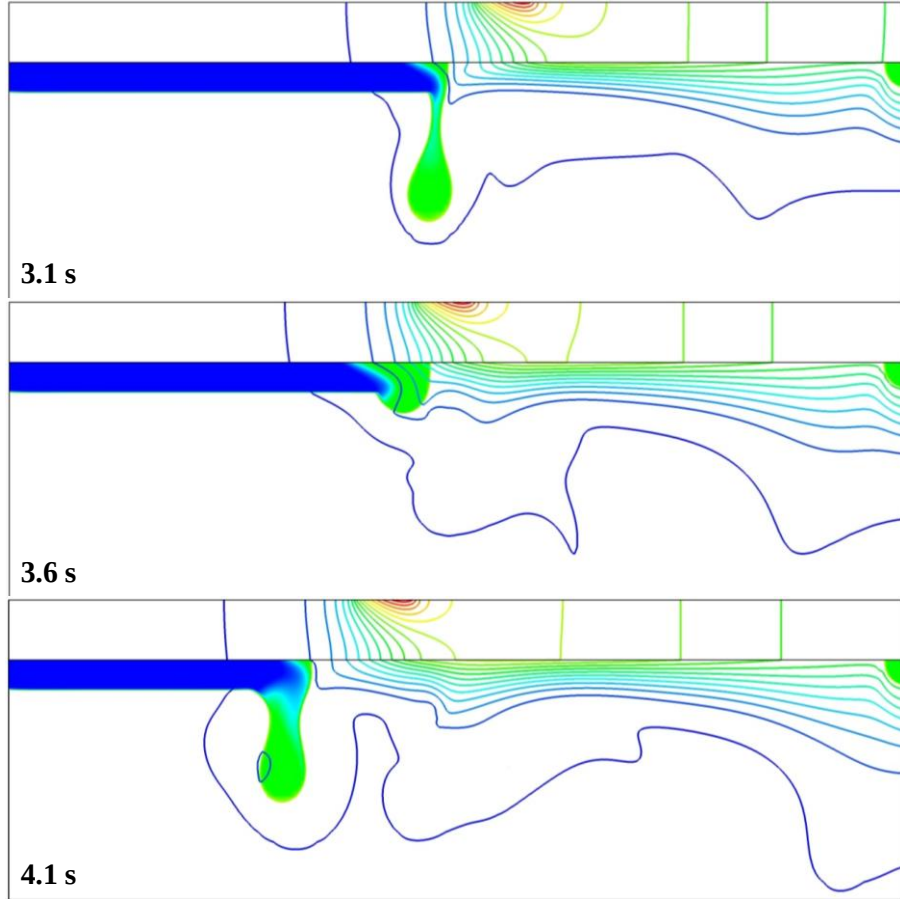


Figure 6.5 Distribution of  $(\alpha + \beta)/2$  superimposed on the temperature profile in case with deformable PCM-air interface by employing moving heat flux of  $150 \text{ MW/m}^2$  as speed of  $2 \text{ cm/s}$  over time (case 2)

Therefore, instead of constant temperature, heat flux boundary condition as external thermal heat source is used in order to give adiabatic boundary condition on moving heat source left area. Figure 6.4 shows the time-dependent distribution of the scalar quantity  $(\alpha + \beta)/2$  superimposed on the temperature profile in case with (right) and without (left) deformable PCM-air interface over time. The white, red, green and blue colors correspond to computational cells filled with copper, air, molten PCM and solid PCM, respectively. By giving moving heat flux boundary condition as external heat

source, heat is constantly supported from copper to PCM so that melting and deformation behavior of PCM continuously happens. Also, re-solidification in PCM does not occur because copper surface except for area of moving heat source is insulated. However, as can be seen in Fig. 6.5, the temperature profile shows that the speed of the moving heat flux is slower than that of the motion of the molten PCM. Since the molten polymer moves with the surrounding flame in the real case (see Fig.1.2), it is necessary to choose the same speed for the molten PCM as the moving heat flux in order to achieve consistency with experiment.

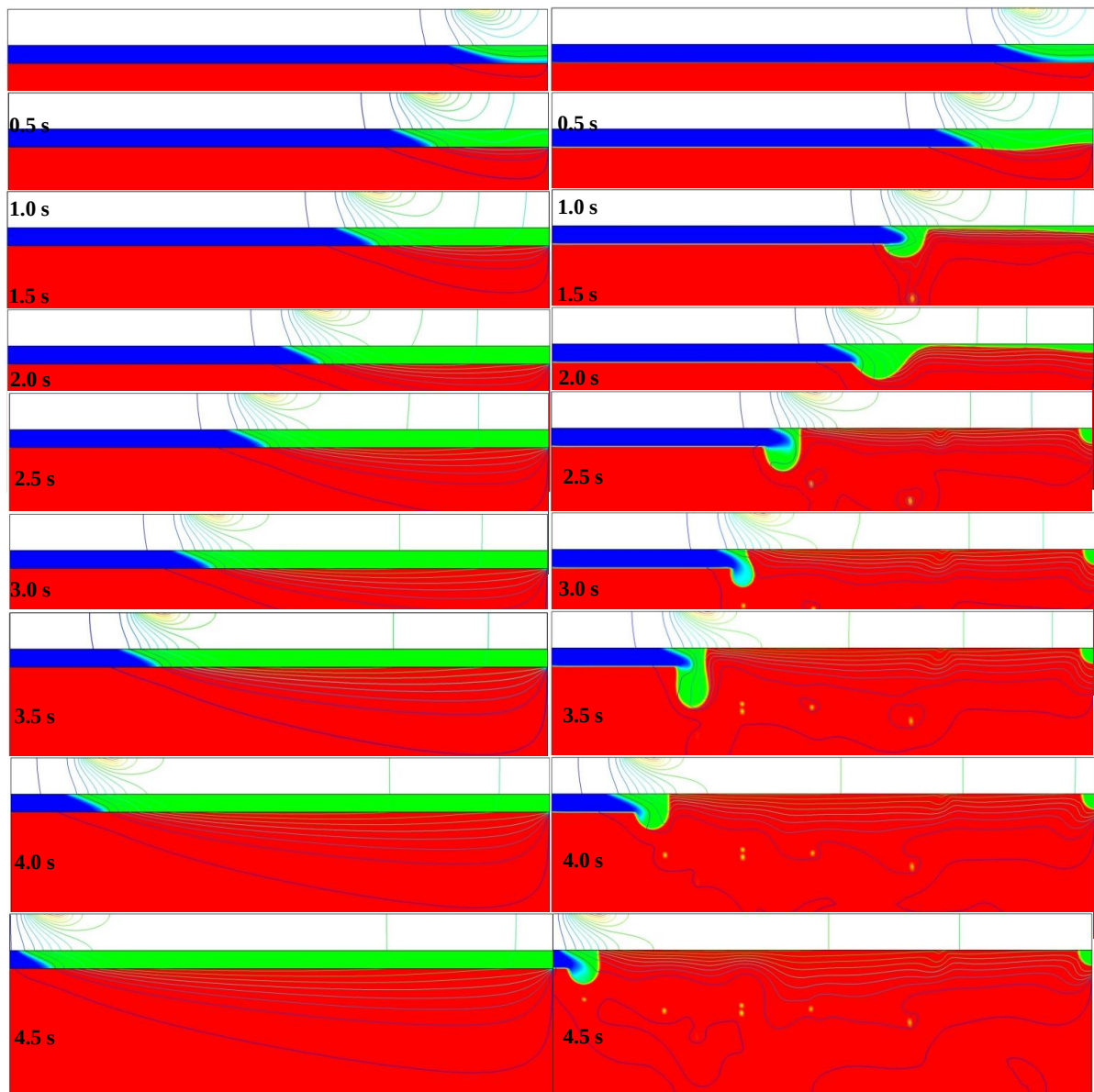


Figure 6.6 Time-dependent distribution of  $(\alpha + \beta)/2$  superimposed on the temperature profile in

case with (right) and without (left) deformable PCM-air interface by employing moving heat flux of  $150 \text{ MW/m}^2$  as speed of  $3 \text{ cm/s}$  (case 3)

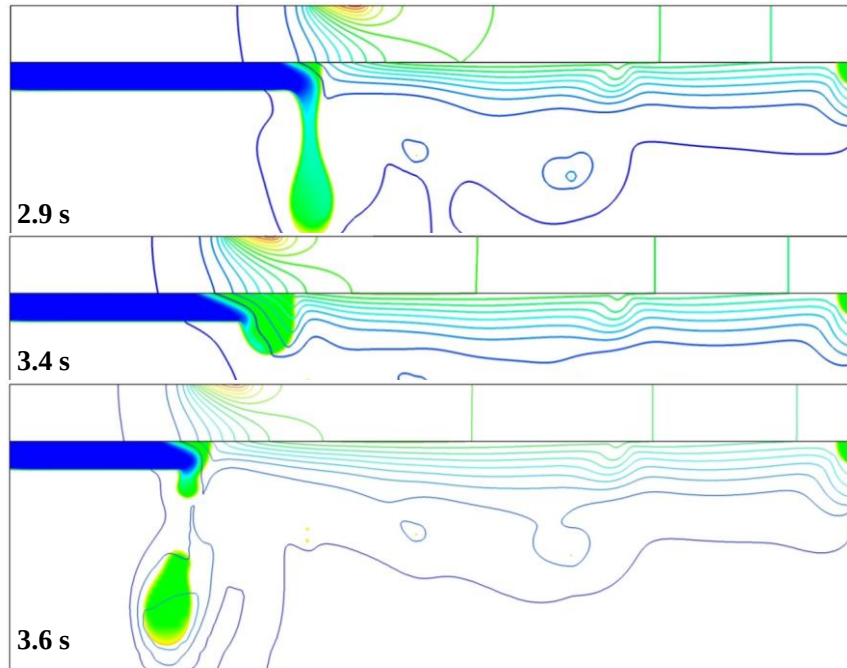


Figure 6.7 Distribution of  $(\alpha + \beta)/2$  superimposed on the temperature profile in case with deformable PCM-air interface by employing moving heat flux of  $150 \text{ MW/m}^2$  as speed of  $3 \text{ cm/s}$  over time (case 3)

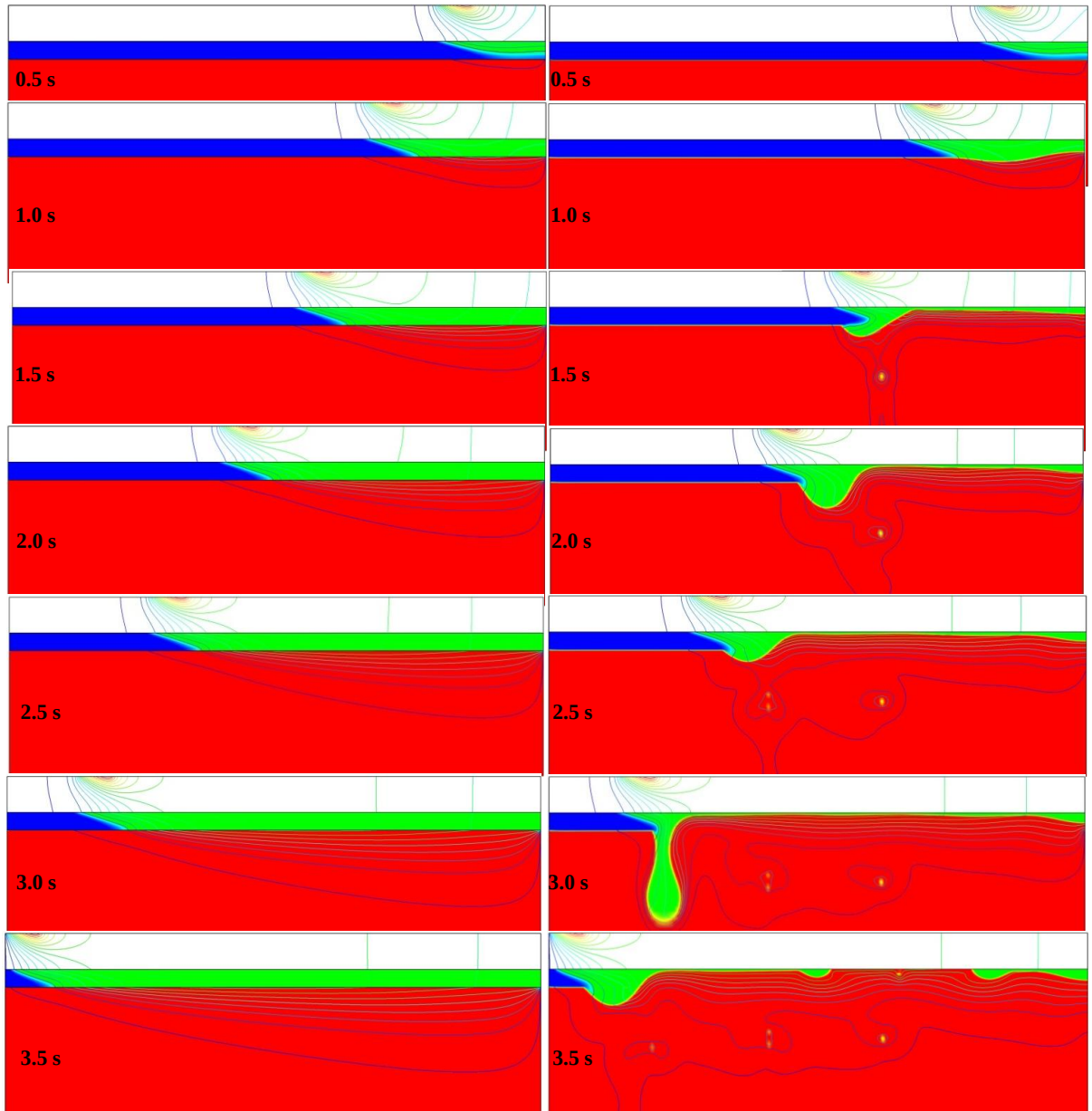


Figure 6.8 Time-dependent distribution of  $(\alpha + \beta)/2$  superimposed on the temperature profile in case with (right) and without (left) deformable PCM-air interface by employing moving heat flux of  $1.5e^8$

W/m<sup>2</sup> as speed of 4 cm/s (case 4)

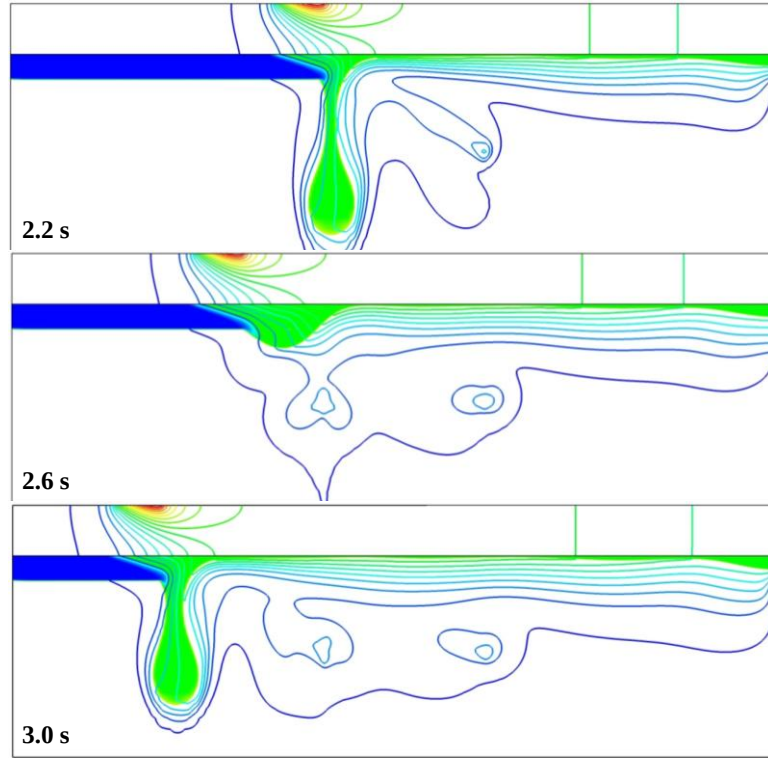


Figure 6.9 Distribution of  $(\alpha + \beta)/2$  superimposed on the temperature profile in case with deformable PCM-air interface by employing moving heat flux of 150 MW/m<sup>2</sup> as speed of 4 cm/s over time (case 4)

In order to find appropriate moving speed of external heat source, speed of 3 (Fig. 6.6-7) and 4 cm/s (Fig. 6.8-9) were evaluated. Figure 6.6 and 6.8 show overall time-dependent distribution of the scalar quantity  $(\alpha + \beta)/2$  superimposed on the temperature profile in case with (right) and without (left) deformable PCM-air interface over time. Figure 6.7 shows relative position between melting front and moving heat flux employing moving speed of 3 cm/s, in detail. When molten PCM is dropped, position of molten PCM is located at behind of heat flux (see 2.9 s and 3.6 s). However, during growth of molten PCM, position of heat flux becomes almost same with center of molten PCM (see 3.4 s). In other words, speed of melt front is not constant; rather, it is changed during beginning from growth till dropping of PCM. In contrast, Fig. 6.9, which employees moving speed of 4 cm/s, shows that position

of moving heat flux is always located in the front of melting front. It means that moving speed of 4 cm/s is always faster than the speed of melting front even though the speed of melting front locally changed during the process beginning of growth till dropping.

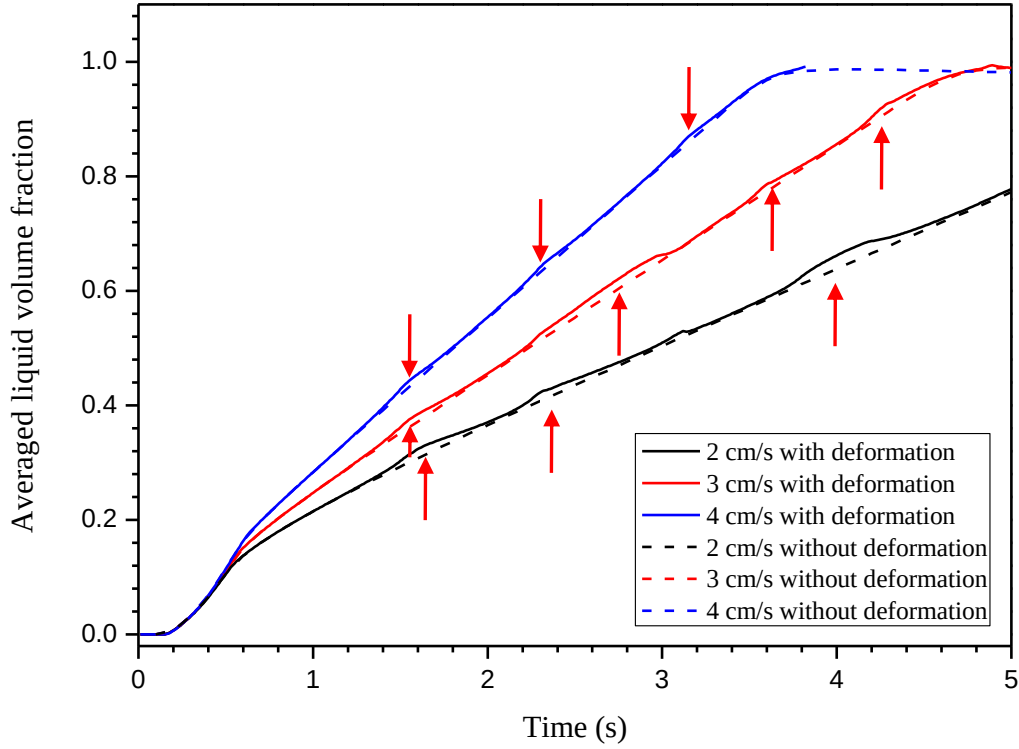


Figure 6.10 Time-dependent averaged liquid volume fraction with/without deformable PCM-air interface employing different moving speed of external heat sources (case 2-4)

Figure 6.10 shows the time-dependent averaged liquid volume fraction,  $\beta_L$ , in the cases with/without a deformable PCM-air interface employing different moving speed of external heat sources (2-4 cm/s). The dashed line stands for the fixed position of the PCM-air interface, and the solid line represents the case of a deformable interface. Since heat is transferred through the copper from the moving heat flux to the PCM,  $\beta_L$  exhibits a delay time around 0.2 s for initiation of melting. In the case of a non-deformable PCM-air interface,  $\beta_L$  is almost constant from the starting time to almost the end of the melting process. In contrast,  $\beta_L$  in the case of a deforming PCM-air interface locally increases and decreases at the time of dropping, indicated by the embedded arrows, repeating this behavior over the melting process. As discussed in section 4.4, such deviation is mainly induced by the deformation and

dropping of the PCM-air interface. More precisely, it is caused by considerable internal liquid motion in the PCM and by an increase of surface area of the melting front during the deformation and dropping processes. Therefore, it can be concluded that, for the above reasons, there is a change in  $\beta_L$  when periodic deformation and dropping of molten PCM arise from the presence of a moving heat source.

As discussed in section 4.4.3, shape of the melting front reveals that how much a role deformable PCM-air interface plays on melting process. With keep that in mind, when we look at the Fig. 6.11, we can figure out that the shape of melting front looks sharp and angle  $\theta$  defined in section 4.4.3 is small when speed of moving heat is fast. Especially, when speed of moving heat flux is 3 and 4 cm/s, the melting front is much sharper than speed of 2 cm/s. The deformation effect on melting speed is insignificant when moving speed of heat flux is dominating the melting speed. However, when the moving speed of heat flux is sufficiently low, effect of dynamic motion on melting becomes significant.

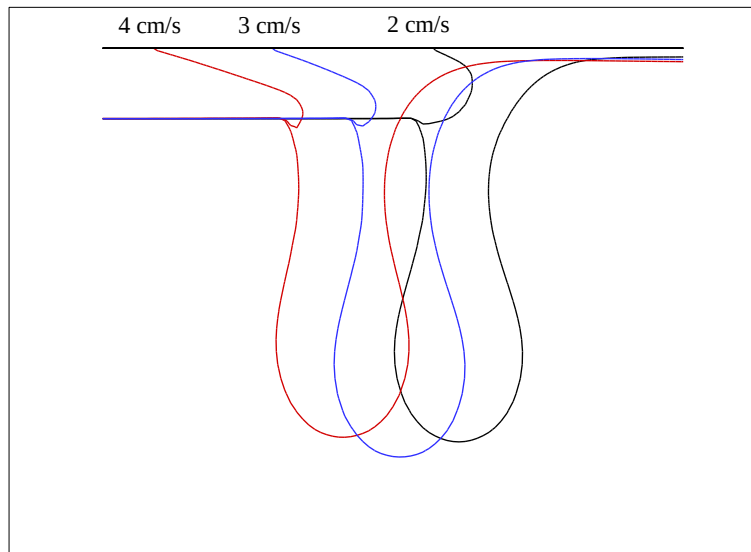


Figure 6.11 Time-dependent position of melting front for different moving speed of heat flux

# Chapter 7

## SUMMARY OF THESIS

In order to propose acceptable model for melting, deforming, and dropping process in analogous condition with fire, multiphase-based numerical approach is used. Numerical model is being developed as step-by-step. First, we consider a phenomenon of phase change associated with freely moving gas-liquid interface without flaming. In this regard, the governing equations can only consist of the fundamental conservation equations (for mass, momentum and energy) under a multi-phase framework. We employ the Enthalpy-Porosity [72-73] and Volume of Fluid method (VOF) [49] in order to model the melting and dynamic motion of molten matter suspended by a metal plate. This simplified geometry provides a physically similar analogy of the wire combustion case [116].

Based on aforementioned numerical strategy, the time-dependent melting and dropping processes involving three phases were studied in chapter 4. Melting and dynamic behavior of PCM (Phase Change Material) attached on metal plate is investigated by exploring various surface tension coefficients, external thermal inputs and melting temperatures. Pure effect of dynamic behavior of PCM is precisely investigated by comparing cases with/without deformation of gas-liquid interface on similar physical domain with experiment. Based on the observation in this chapter, the following conclusions can be drawn:

1. Dropping timing is modified by variation of surface tension coefficient, external thermal input and melting temperature.
2. Melting speed was modified by variation of melting temperature and external thermal input.
3. The deformable PCM-air interface enhances the melting from the time of deformation to that of dropping as compared with the case that of a non-deformable PCM-air interface.

4. The enhancement of the melting rate associated with a deformable PCM-air interface is mainly caused by (1) considerable internal liquid motion in the PCM triggered by surface fluid motion and (2) an increase of surface area of the melting front during the deforming and dropping processes.
5. Noticeable heat loss from the PCM to the copper is present while the deformed molten PCM undergoes dropping. This reduced the melting rate, but this as was relatively small effect compared to the enhanced melting rate owing to convection and the increase of surface area.
6. For varying surface tension coefficients and Stefan numbers, the melting rate in the case of a deformable PCM-air interface is always higher than that of a non-deformable PCM-air interface, suggesting that the inclusion of the deformation model is essential for a proper understanding and prediction of melting.
7. The effect of deformation alone, dependent of  $\Delta\beta_L$ , increased with (1) increase in surface tension owing to the increase of length of the melting front, and with (2) increase in Stefan number owing to an increase of the convection effect, and with (3) decrease of Stefan number due to an increase in length of the melting front.

We can conclude through this study that the VOF method coupled with the Enthalpy-Porosity method can deal with the dynamic behavior of multiphase flow involving phase transitions. Current numerical models thus have the potential to model combustion in multiphase conditions. In future, the dynamic contact angle, which is not considered in this study, could be included in the modeling because it is expected to play a role in wire combustion.

In chapter 5, thermocapillary motion targeted at polymer-coated electric wire exposed to a fire condition was numerically modeled under a continuum mechanics for multiphase flow with melting phase change. Calculation was carried out by solving Navier-Stokes and energy with volume of fluid transport equation. The source-based tangential force driven by surface tension, which linearly depends on the temperature, was implemented in the previous-proposed model. Numerical parameters were selected in order to investigate the thermocapillary motion in effective way, and the following conclusions were drawn.

1. Effect of thermocapillary convection on melting of Phase Change Material (PCM) is found to be not so significant under the condition studied here. However, it should be taken into account if the precise prediction of dripping-off timing is desired.

2. Thermocapillary convection in molten Phase Change Material (PCM) only appears before deformation of liquid-gas interface, however, after that, gravitational force-driven flow dominates in molten Phase Change Material (PCM).

In chapter 6, melting and deformation of polymeric material induced by a constant moving heat flux was investigated. The time-dependent melting and the behavior of the PCM are visualized together with the temperature distribution. The effect of the dynamic motion on the melting process with/without a deformable interface is discussed. As conclusion, following is drawn.

1. There is a change in averaged liquid volume fraction ,  $\beta_L$ , when periodic deformation and dropping of molten PCM arise from the presence of a moving heat source.
2. Deviation of averaged liquid volume fraction between with/without deformable PCM-air interface,  $\Delta\beta$ , becomes smaller when speed of moving heat flux becomes faster. It may be caused by fact that deformation effect on melting speed is insignificant when moving speed of heat flux is dominating the melting speed. However, when the moving speed of heat flux is sufficiently low (e.g., 2 cm/s), effect of dynamic motion on melting becomes significant.

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# Appendices

## A. Gasification

The actual process of evaporation can be treated using the analogy of heat and mass transfer for low mass transfer rates. However, industrial processes (high-temperature environment) can lead to high mass transfer rates where the mass transfer needs to be considered in another way. Mass transfer phenomena, defined as the molecular motion of constituents caused by a “driving force”, is very often encountered in nature and engineering systems. The most common driving force for mass transfer processes is the concentration gradient and temperature gradient. Thus, by use of these two driving force for mass transfer, mass source with the VOF method is tested.

VOF-based mass transfer has been considered by several authors. Chen et al. [118] incorporate evaporation in a VOF-based simulation of gas bubbles moving in a bounded viscous liquid. Their phase change model captures the volume change in the fluids due to mass transfer at the interface. Davidson and Rudman [119] present a VOF-based algorithm for the calculation of transport processes across deforming interfaces, using the analogy between heat and mass transfer. The algorithm is described assuming planar or axisymmetric flows and does not consider volume changes due to phase change. The calculation of heat transfer is separated for the two phases with respect to the enthalpy as transported quantity, while the temperature is treated as a single field based on an average in the interface cells. Nikolopoulos et al. [120] investigate the behavior of liquid droplets impinging onto a hot substrate using the VOF-method and adaptive mesh refinement. They are able to predict the levitation of the drops above the Leidenfrost temperature and to calculate parameters of the splashing process below the Leidenfrost point. Schlottke and Weigand [121] use the VOF method to simulate deformed evaporating droplets in high Reynolds number flows and can predict the global Sherwood number under droplet surface deformation. Kunkelmann and Stephan [122] developed a VOF-based model with adaptive mesh refinement for nucleate boiling, where a level-set extension is employed to reconstruct the sharp interface for a more accurate computation of the evaporation rate. Strotos et al.

[123] apply the VOF-method without the numerical reconstruction of the interface but with a local grid refinement technique to simulate multi-component droplet evaporation under forced convection in a hot environment. The model is validated with respect to evaporating time and droplet temperature. Ma and Bothe [124] apply the VOF-based evaporation and thermocapillary convection coupled with Ghost Fluid method. Here, they use two temperature approaches.

In this section, we attempt to adapt the two types of gasification model, namely thermal and concentration driven mass transfer, into previous model.

## A.1 Melting & gasification

Since, updating gasification model to previous model is essential in order to establish numerical model for wire combustion, we attempt to plug the slow gasification model to previous model. Implementation is done by User Define Function (UDF).

### A.1.1 Numerical model

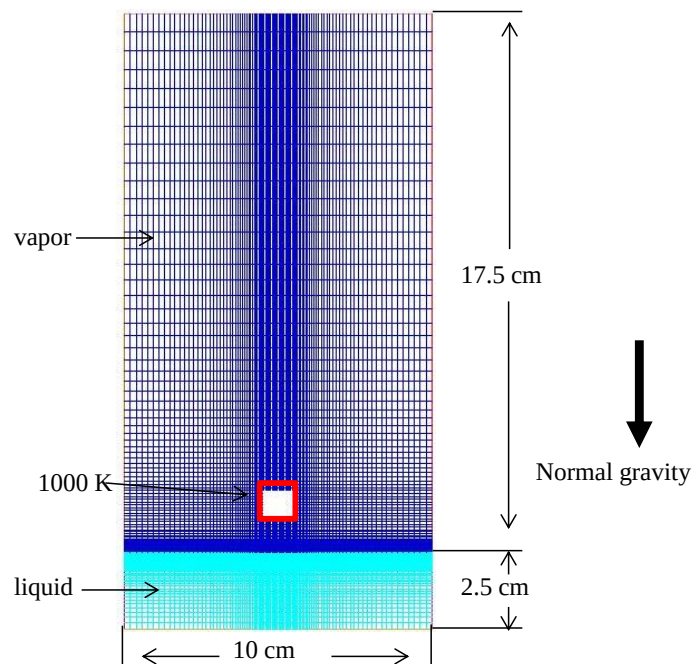


Figure A.1 Schematic illustration of the computational setup

The physical configuration for gasification is schematically illustrated in Fig. A.1. The 2-D computational domain consists of vapor, liquid and solid state of liquid. Here, solid state is artificially given in order to test modeling so that melting temperature is also chosen artificial value as 372.1 K. The total horizontal and vertical lengths are 10 and 20 cm respectively, and the height of the liquid from bottom is 2.5 cm. A normal downwardly-directed gravity field is considered (with corresponding gravitational acceleration  $9.81 \text{ m/s}^2$ ). A localized external thermal input at temperature 1000 K is placed in the middle of the vapor phase domain in order to heat and initiate melting and gasification of artificial solid state liquid, and the temperature 300 K is used over the whole domain as the initial thermal condition. The melting process evolves with an increase of the local temperature in the liquid. Once the local temperature in the liquid exceeds the designated gasification temperature, gasified vapor is initiated at the liquid-vapor interface with mass and volume losses in solid. For flow condition, the quiescent environment is initially given in whole domain. No slip boundary condition is applied on all boundaries of liquid. All boundaries of vapor except for liquid-vapor interface are treated as open boundaries. Adiabatic condition is given on left and right side of PCM. The temperature is assumed to be continuous at the gas-liquid and gas-solid interface. All properties used in the present calculation are summarized in Table A.1

Table A.1 Material properties used in calculation of melting and gasification

| Properties of material  | Gas phase                  | Liquid phase              |
|-------------------------|----------------------------|---------------------------|
| Density                 | 0.5542(kg/m <sup>3</sup> ) | 998.2(kg/m <sup>3</sup> ) |
| Specific heat           | 2014(J/kg-k)               | 4182(J/kg-k)              |
| Thermal conductivity    | 0.0261(w/m-k)              | 0.6(w/m-k)                |
| Viscosity               | 1.34e-5(kg/m-s)            | 0.001(kg/m-s)             |
| Evaporation temperature |                            | 373.15(K)                 |

|                            |               |
|----------------------------|---------------|
| Latent heat of evaporation | 100000 (J/kg) |
| Melting temperature        | 372.1 (K)     |
| Solidification temperature | 372 (K)       |
| Latent heat of melting     | 100000 (J/kg) |
| Surface tension            | 0.07 (N/m)    |

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### A.1.2. Numerical results

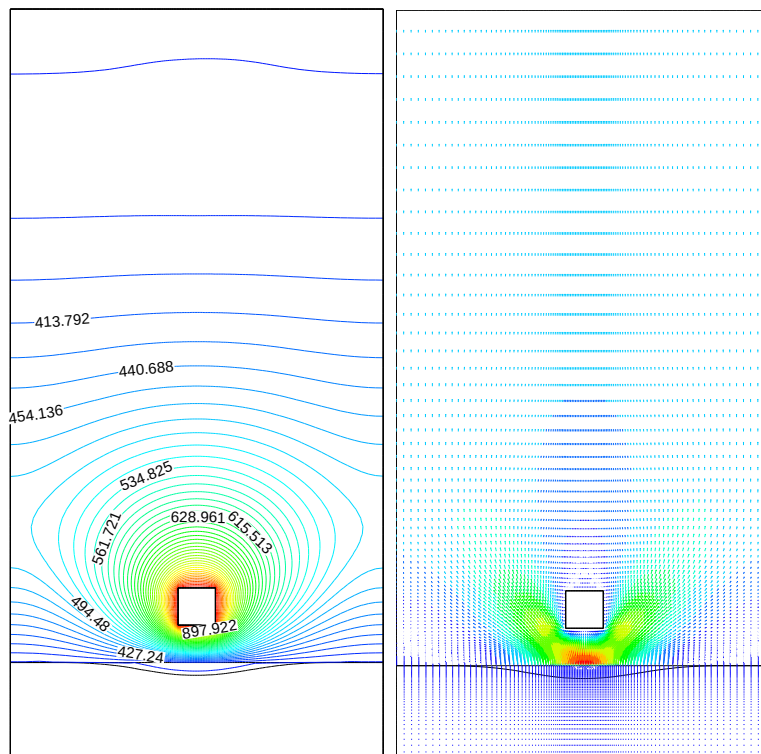


Figure A.2 Temperature (left) and velocity (right) distribution at 70 s

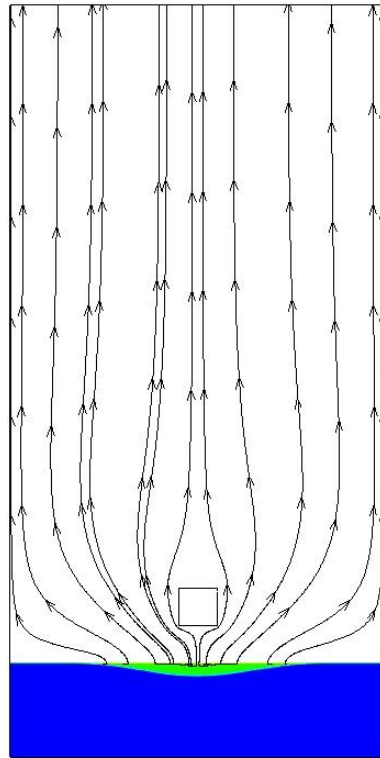


Figure A.3 Distribution of  $(\alpha + \beta) / 2$  superimposed on the streamline at 70 s

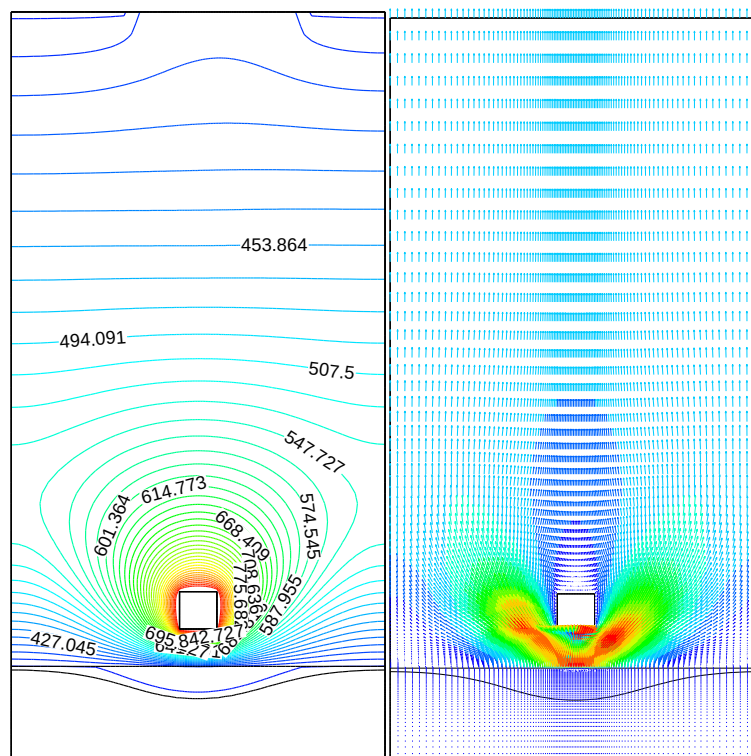


Figure A.4 Temperature (left) and velocity (right) distribution at 400 s

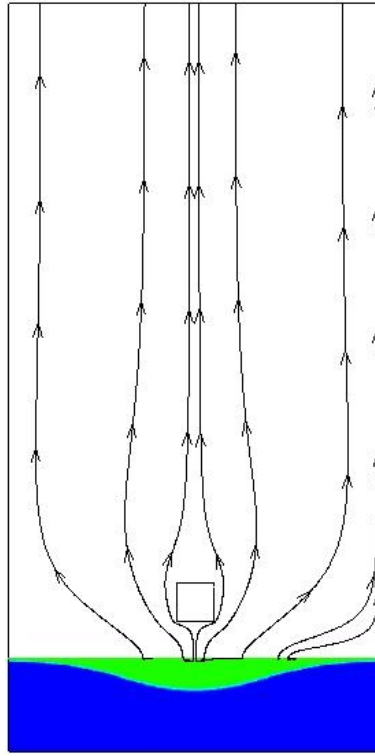
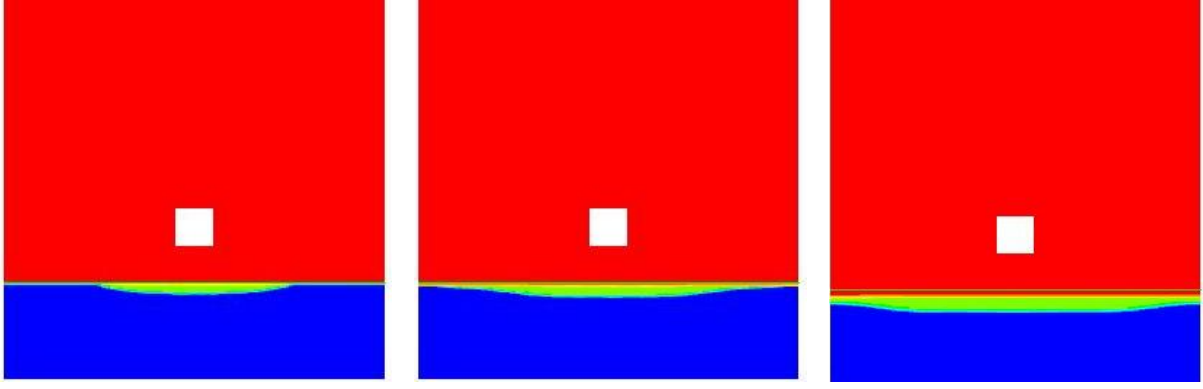
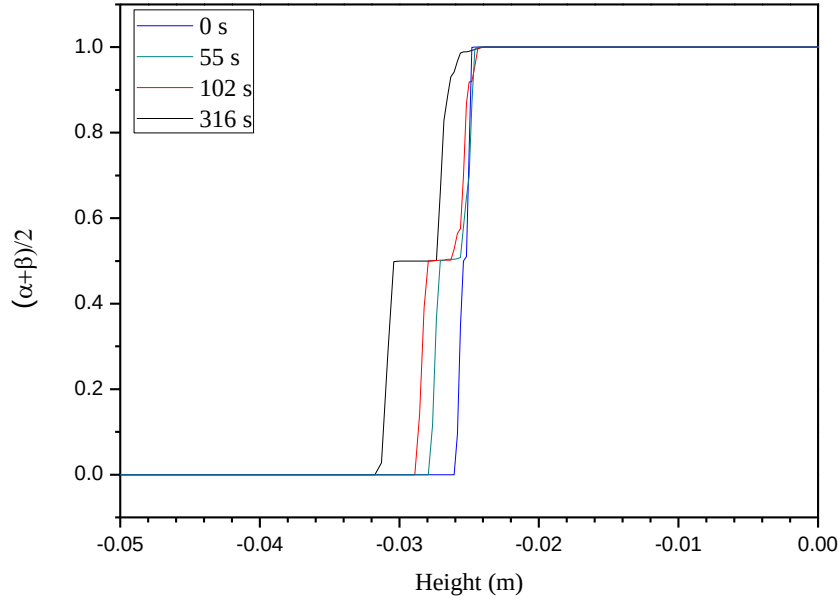


Figure A.5 Distribution of  $(\alpha + \beta) / 2$  superimposed on the streamline at 400 s

Figure A.2-5 shows the temperature, velocity vector profile and a scalar distribution,  $(\alpha + \beta) / 2$ , superimposed on the stream line at time of 70 (A.2-3) and 400 (A.4-5) s . Since mass source is based on slow mass transfer, we elapsed quite long time. In velocity vector profile, the color represents the magnitude of the velocity. Vapor gas is gradually heated by the imposed thermal source first and then that heat is transferred to the interface. Once temperature in solid is over the designated melting temperature, solid state undergoes melting process, liquid then starts to gasify. Since thermal input is located in the vapor, and boundary conditions at sides are treated as symmetric condition, gasified liquid flow from vapor-liquid surface is diverged at the thermal source, and then goes through the top boundary. With increase of time, system continuously undergoes both melting and gasification.



(a)



(b)

Figure A.6 Distribution of  $(\alpha + \beta)/2$  along the y direction over time variation as (a) color contour and (b) graph

A.6 shows Distribution of  $(\alpha + \beta)/2$  taken along the y axis at time of 0, 55, 102 and 316 s, as (a) color contour and (b) graph. Here,  $(\alpha + \beta)/2 = 0, 0.5$  and  $1$  stands for solid, liquid and gas state, respectively. As can be seen in Distribution of  $(\alpha + \beta)/2$  at time of 0 s, initial position of gas-liquid interface is located at height of  $-0.25$  m. As time goes by, melting front and liquid-gas interface move to the downward together. Particularly, melting front is located at around  $-0.03$  m, and liquid-gas interface located at around  $-0.032$  m at time of 316 s. One can see that each phase interfaces are sharp enough, not smeared out or broaden away even though those are moves with phase change.

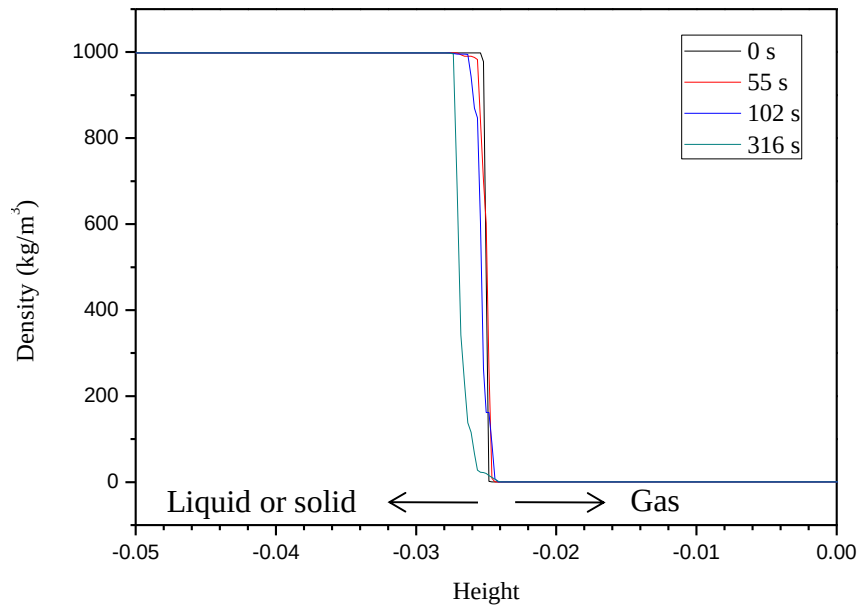


Figure A.7 Density distribution along the y direction over time variation

Such sharp interface can be also found in A. 7 which shows density distribution along the y direction over time variation. As similar with A. 6, we can see that density profile is sharply shifted toward the negative height due to the volume loses with increase of time. Therefore, we can safely say that modeling for melting and gasification under the volume of fluid framework is successfully done.

## A.2 Gasification defined by binary species transport without melting process

We tried to plug the species transport equation into the previous model because temperature gradient-based mass source is only applicable in slow mass transfer system (e.g., natural evaporation) so that it is not appropriate in fast mass transfer system such as combustion. Therefore, thermally defined mass source Eq. 2-82 is implemented into Navier-Stokes, energy equation coupled with VOF and Enthalpy-Porosity method. Additionally fuel species transport Eq. 2-94 shown in section 2.1.3.2 was solved in order to get the gasified fuel distribution.

### A.2.1 Numerical model

The physical configuration is schematically illustrated in Fig. A.8. The 2-D computational domain consists of liquid and fuel. The total horizontal and vertical lengths are 20 and 6 cm respectively, and the height of the liquid is 1 cm. A normal downwardly-directed gravity field is considered with corresponding gravitational acceleration  $9.81 \text{ m/s}^2$ . A radiation heat flux of 1000 K is imposed on the top surface, and the temperature 300 K is used over the whole domain as the initial thermal condition. Since the purpose to calculate this case is checking the numerical model and conforming whether model is working well in previous model or not, the melting process is excluded. Once the local temperature in the liquid exceeds the designated gasification temperature, gasified fuel is initiated at the liquid-gas interface with mass and volume losses. For flow condition, the quiescent environment is initially given in whole domain. No slip boundary condition is applied on all boundaries of liquid. Left and right boundaries of gas are treated as open boundaries. Adiabatic condition is given on left and right side of liquid. The temperature is assumed to be continuous at the gas-liquid and gas-solid interface. All properties used in the present calculation are summarized in Table A.2

Table A. 2 Material properties used in calculation of melting and gasification

| Properties of material | fuel | Water liquid |
|------------------------|------|--------------|
|------------------------|------|--------------|

|                            |                            |                           |
|----------------------------|----------------------------|---------------------------|
| Density                    | 0.5542(kg/m <sup>3</sup> ) | 998.2(kg/m <sup>3</sup> ) |
| Specific heat              | 2014(j/kg-k)               | 4182(j/kg-k)              |
| Thermal conductivity       | 0.0261(w/m-k)              | 0.6(w/m-k)                |
| Viscosity                  | 1.34e-5(kg/m-s)            | 0.001(kg/m-s)             |
| Evaporation temperature    |                            | 373.15(K)                 |
| Latent heat of evaporation |                            | 100000 (J/kg)             |
| Surface tension            |                            | 0.07 (n/m)                |

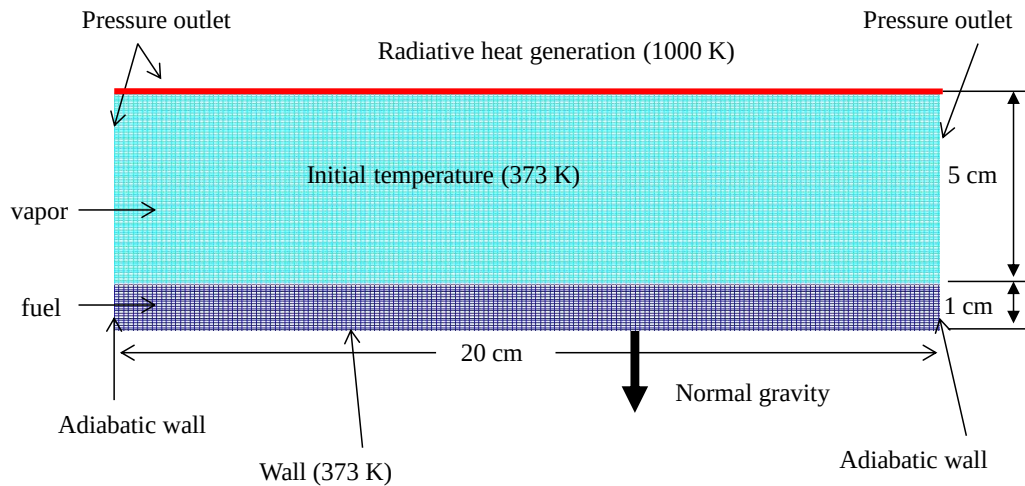


Figure A.8 Schematic illustration of the computational setup

### A.2.2. Numerical results

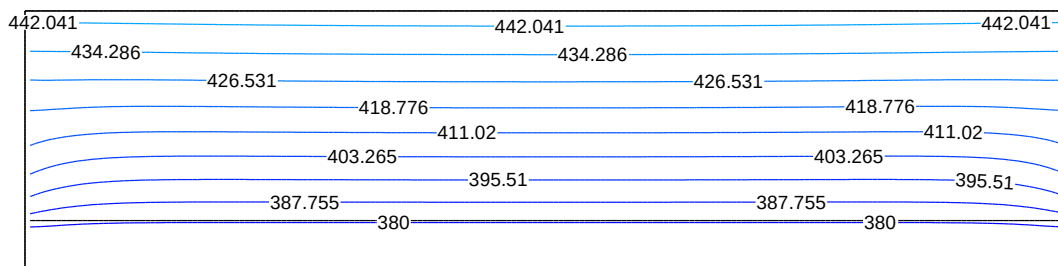


Figure A.9 Temperature distribution at 3 s

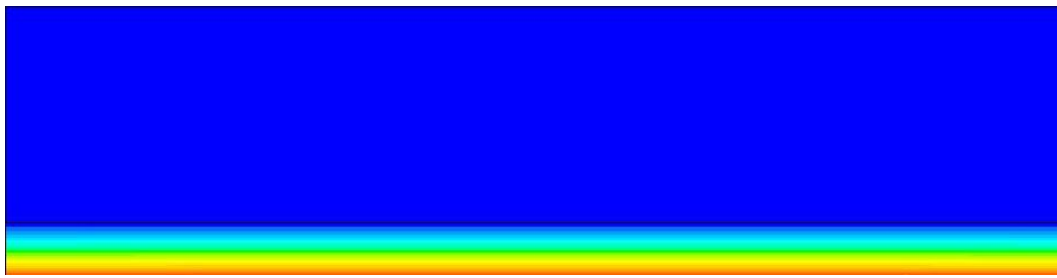


Figure A.10 Pressure distribution at 3 s

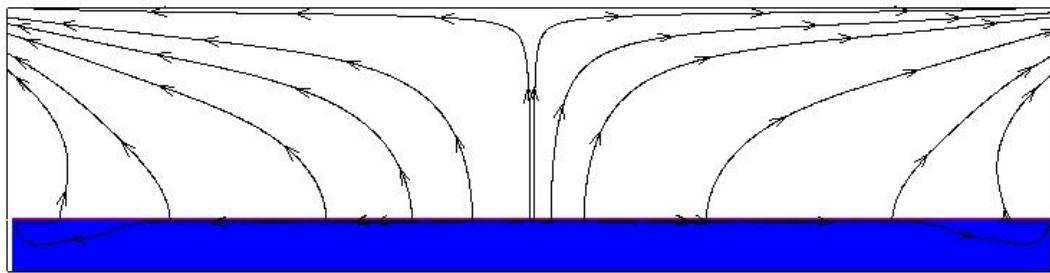


Figure A.11 Distribution of  $(\alpha + \beta) / 2$  superimposed on the streamline at 3 s

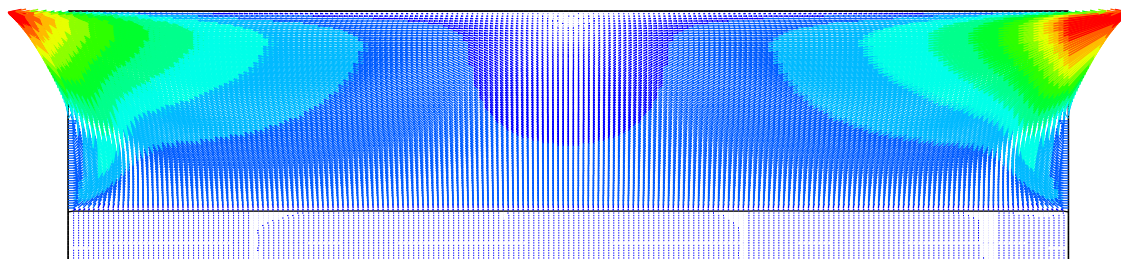


Figure A.12 Velocity distribution at 3 s



Figure A.13 Volume fraction,  $\alpha$ , distribution at 3 s

From Fig. A 9 to A 13, temperature, pressure, streamline, velocity vector and distribution of volume fraction,  $\alpha$ , at time of 3 s are shown. As increase of time, temperature in gas is heated up due to radiation heat transfer. When water liquid receives enough heat to generate the gas fuel, gasification is initiated. Figure A.11-12 clearly shows fuel velocity distribution during gasification. Since upper boundary is no slip condition and pressure outlet condition is imposed on the side boundary, flow generated from liquid-vapor interface as gasification flows out to the side boundaries. As can be seen in Fig.A.13, volume fraction distribution shows volume loss at time of 3 s. It reveals that current gasification model have capability to calculate the volume loss. Figure A.14 also shows volume fraction distribution along the y axis at time of 0 and 3 s. Here, initial position of interface is 0.01 m, but after time of 3 s, position of interface moves to the liquid side due to the loss of volume, as mention before.

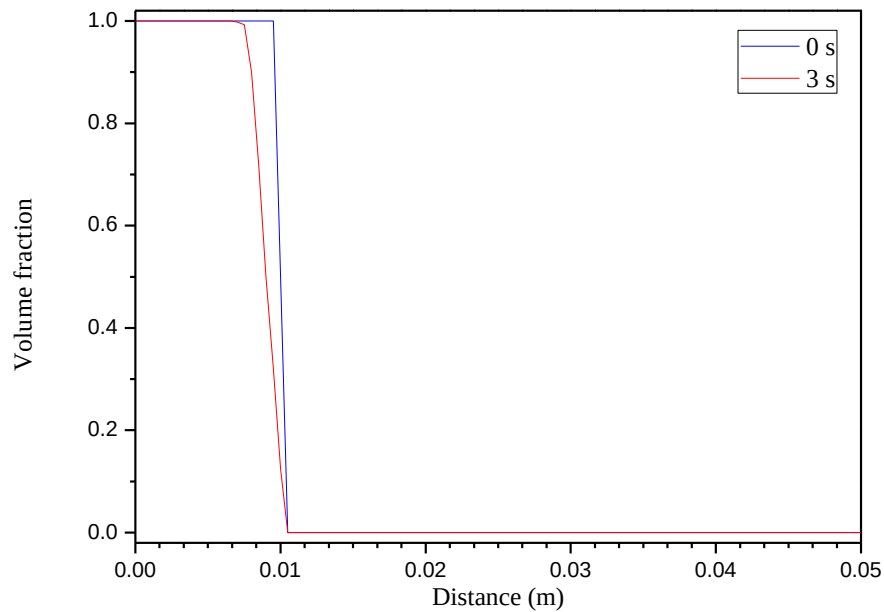


Figure A.14 Volume fraction,  $\alpha$ , distribution along the y axis at the center of x axis at 0 and 3 s

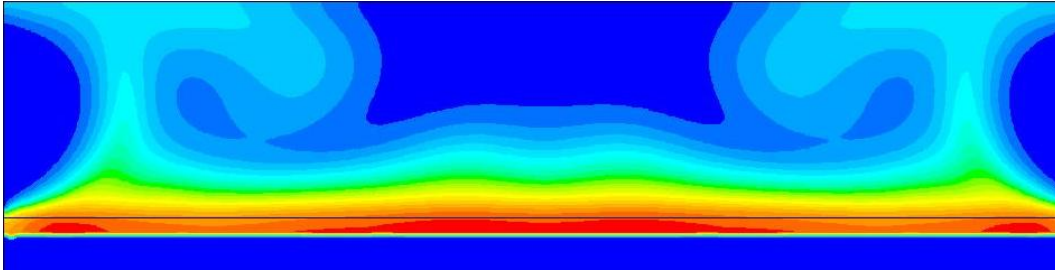


Figure A.15 Fuel mass fraction at 3 s

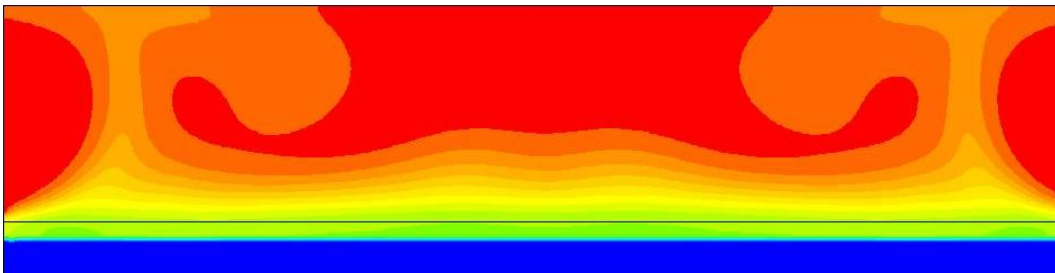


Figure A.16 Oxygen mass fraction at 3 s

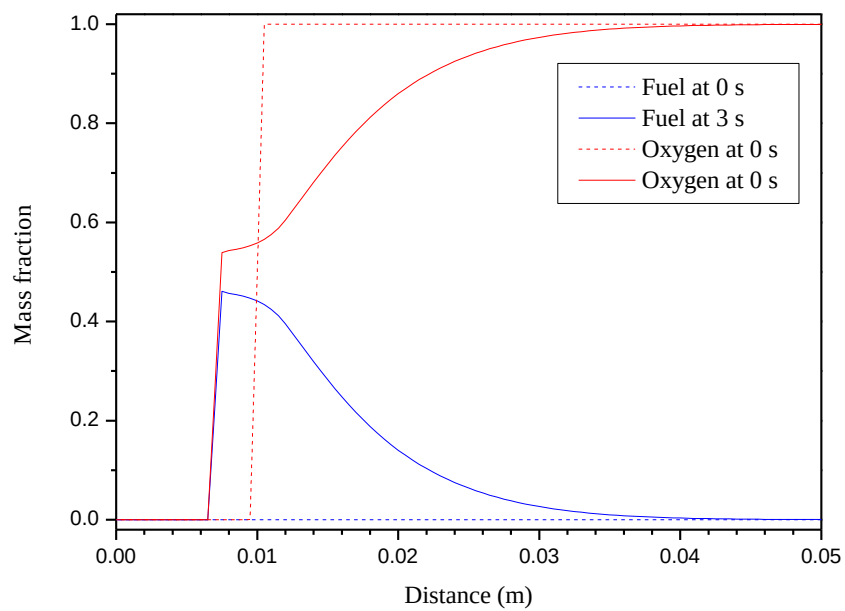


Figure A.17 Fuel and Oxygen mass fraction along the y axis at the center of x axis at 0 and 3 s

Figure A.15-16 shows fuel and oxygen mass fraction distribution at time of 3 s. Where, black line stands for the initial position of gasifying surface. Spatial distribution of both gases is well calculated. In particular, position of gasifying surface considerably shrunk as compare with original one. One can see in Fig. A.15 that interface keeps its sharpness as it is even though volume is shrunk.

It is more clearly seen in Fig.A.17 which shows the fuel and oxygen mass fraction along the y axis at the time of 0 and 3 s. Here, dot and solid line, respectively, represent time of 0 and 3 s, and red and blue line stands for the mass fraction of fuel and oxygen respectively. Since initially gas phase fully occupied by oxygen, fuel mass fraction was zero at time of 0 s. As fuel gas ejected to gas phase, fuel mass fraction increases. Simultaneously, oxygen mass fraction decreases as much as increase of fuel mass fraction. Note that interface between gas and liquid phase keeps its sharpness as it is. Thus, we can safely say that gasification caused by concentration gradient is well modeled into previous model although test case has quite simple geometrical configuration.