Enthalpy Porosity Method for CFD Simulation of Natural Convection Phenomenon for Phase Change Problems in the Molten Pool and its Importance during Melting of Solids

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Abstract

Shielded transportation casks are commonly used for the transportation and storage of radioactive waste materials. Design approval of such casks by the regulatory authority is subject to its demonstration of compliance with a thermal test (among other tests) Due to exposure of cask to fire in thermal test /actual conditions, there is a possibility of melting of the shielding material (lead) used for the cask and need to evaluate extent of melting. Conduction based codes have been used extensively for modeling the melting process in such casks. Conventionally, for modeling melting, these codes employ effective specific heat methods, heat flow methods or enthalpy formulation where the energy equation employs a fixed grid (fully solid or fully liquid) philosophy. Both the solid and liquid regions of the phase change material are treated as a single continuous phase having identical density and the effect of natural convection in liquid phase is neglected. But in actual case there will be natural convection in the molten region and there is possibility of more melting in upper region. This paper intends to bring out the effect of neglecting natural convection phenomena for thermal analysis of such casks by considering a validation problem reported in open literature.

Nomenclature

A	Porosity function for momentum equations	L	Latent heat of melting (J/Kg)
c_p	Specific heat (J/kg-K)	s	Liquid fraction
h	Sensible enthalpy (J/kg)	t	Time (s)
ΔH	Latent content of enthalpy (J/kg)	T	Temperature (K)
k	Thermal conductivity (W/m-K)	u, v	Velocity components in x and y directions

Greek symbol

β	Liquid fraction
ρ	Density (kg/m^3)
η	Large number
μ	Molecular viscosity (Kg/m-s)

Subscripts

solidus	Solid region
liquidus	Liquid region
ref	Reference
S_h	Enthalpy source term

1.0 Introduction

Shielded transportation casks are commonly used for the transportation of radioactive waste materials/spent fuel. A typical radioactive material transportation cask consists of a rectangular shaped box with an inner cavity to store the radioactive material for transportation. In order to minimize the radiation dose to the public domain, lead sandwiched between two stainless steel liners provides the necessary shielding. The cask contains radioactive material which is a source of internal heat generation due to decay of radioactive products. Besides decay heat generation in the radioactive material, there is also small amount of heat generated in the lead due to gamma attenuation. The cask has to maintain its structural integrity under normal and accidental (fire) conditions. Design approval of such casks by the regulatory authority [1] is subject to its demonstration of compliance with a thermal test (among other tests), which consists of exposure of the cask to hydrocarbon fuel/air fire on all sides with a flame temperature of about 800°C for a period of 30 minutes. During the fire test, the radiative flux from the fire is incident on the outer surface of the cask, which will cause rapid heating of the various inner elements of the cask, which may cause melting of the shielding material i.e. lead. The melting of lead can cause loss of shielding capability due to relocation of molten lead in lower region, thus creating space in the top region. The molten lead may come out in case of mechanical seal failure due to high temperature and radiation dose may leak into the public domain. Therefore, it is of utmost importance to calculate the amount of lead melted during the fire test so as to assess the loss of shielding. The confirmation of design compliance mentioned above is generally shown by carrying out detailed steady-state and transient thermal analysis of the cask which involves solving the basic transient 3-D conduction equation (ignoring natural convection) for the appropriate radiative and convective boundary conditions. However, ignoring the natural (buoyancy driven) convection because of the density gradients in the molten pool of the lead may lead to a significant error in the predictions of both the extent of melting of lead and of the pattern of melt front propagation during the transients. Not much literature is available for thermal analysis of transportation casks involving natural convection in the molten pool. This is due to the fact that numerical simulation of convective flow and heat transfer in presence of phase change is a challenging task because the heat transfer is coupled with the turbulent flow field in 3D in a global domain where the pure solid and the pure liquid phases are separated by an ever-changing interface. Because of the complex geometry of the cask, at first, a simple problem reported in open literature has been considered for demonstrating the effect of natural convection during melting of lead. This present paper briefly describes the numerical model and the effect of neglecting natural convection phenomena for thermal analysis of transportation casks.

2.0 Numerical Modeling

For studying the effect of natural convection during melting, a validation problem reported in open literature is considered [2]. The problem considered consists of a 2-D cavity filled with

phase change material (i.e. Gallium) insulated on top and bottom sides (Fig. 1). The left face is maintained at a higher temperature than the melting point of the material and the right face is maintained at a lower temperature than the melting point of the material. Melting experiments were performed [2] in a rectangular test cell with dimensions of 8.89 cm in width, 4.5 cm in height and 3.81 cm in depth. To model the phase change phenomenon, **enthalpy-porosity technique** [3] has been employed; the density variations in the liquid region are modeled using Boussiniesq approximation to account for the natural convection in the melted region.

2.1 Enthalpy Porosity technique

In considering the phase change of a metal/alloy, three distinct regions are present: a solid region, a totally liquid region, and a mushy region consisting of liquid dispersed among solid dendrites. To model such a phase change, the basic conservation equations have to be solved throughout the calculation domain. For enthalpy-porosity technique, the melt interface is not tracked explicitly. Instead, a quantity called liquid fraction, which indicates the fraction of the cell volume that is in liquid form, is associated with each cell in the domain. The liquid fraction is computed at each iteration, based on an enthalpy balance. The mushy zone is a region in which the liquid fraction lies between 0 and 1. The mushy zone is modeled as a pseudo porous medium in which the porosity increases from 0 to 1 as the material liquidities. Porosity decreases to zero for the solid region and hence the velocities also drop to zero.

2.2 Governing equations

The energy equation can be written in terms of the sensible enthalpy follows:

$$\frac{\partial(\rho h)}{\partial t}+\frac{\partial(\rho u h)}{\partial x}+\frac{\partial(\rho v h)}{\partial y}=\frac{\partial}{\partial x}(\alpha\frac{\partial h}{\partial x})+\frac{\partial}{\partial y}(\alpha\frac{\partial h}{\partial y})+S_h \tag{1}$$

where $h=\int_{T_{ref}}^{T} c_p dT$ is the sensible enthalpy, α is (k/c_p), and S_h is the source term.

The momentum and the continuity equation are written as:

u-momentum eq:

$$\frac{\partial(\rho u)}{\partial t}+\frac{\partial(\rho u u)}{\partial x}+\frac{\partial(\rho v u)}{\partial y}=\frac{\partial}{\partial x}(\mu\frac{\partial u}{\partial x})+\frac{\partial}{\partial y}(\mu\frac{\partial u}{\partial y})-\frac{\partial p}{\partial x}+A u \tag{2}$$

v-momentum eq:

$$\frac{\partial(\rho v)}{\partial t}+\frac{\partial(\rho u v)}{\partial x}+\frac{\partial(\rho v v)}{\partial y}=\frac{\partial}{\partial x}(\mu\frac{\partial v}{\partial x})+\frac{\partial}{\partial y}(\mu\frac{\partial v}{\partial y})-\frac{\partial p}{\partial y}+A v+S_b \tag{3}$$

Continuity eq:

$$\frac{\partial\rho}{\partial t}+\frac{\partial(\rho u)}{\partial x}+\frac{\partial(\rho v)}{\partial y})=0 \tag{4}$$

where u, v are the velocities in x and y direction respectively, p is pressure , μ is the viscosity and ρ is the density. Assuming the Boussinesq treatment to be valid, we have

$$S_b = \frac{\rho_{ref} g\beta(h - h_{ref})}{c_p} \tag{5}$$

where β is a thermal expansion coefficient and h_{ref} and ρ_{ref} are reference values of enthalpy and density respectively. The function of parameter A in the momentum equations will be discussed below.

2.3 Source Terms

In using a fixed-grid approach for the analysis of melting and solidification systems, a main difficulty is in accounting for mass and heat transfer conditions in the vicinity of the phase change. The basic approach for overcoming this problem is to define appropriate volume source terms for the governing equations. In the enthalpy-porosity approach, the latent heat is accounted for by defining source term in the energy equation [3]:

$$S_h = \frac{\partial(\rho\Delta H)}{\partial t} + \frac{\partial(\rho\Delta H)}{\partial x} + \frac{\partial(\rho\Delta H)}{\partial y} \tag{6}$$

where ΔH is the latent heat content and is function of temperature.
The latent heat content can also be written in terms of the latent heat of the material, (L) as:

$$\Delta H = sL \tag{7}$$

where s is the liquid fraction and can be defined for the temperature between solidus and liquidus temperature as:

$$s = \frac{T - T_{solidus}}{T_{liquidus} - T_{solidus}} \text{ with } T_{solidus} < T < T_{liquidus} \tag{8}$$

Liquid fraction for the temperature in liquidus and solidus region can be given as

$s = 0$ if $T < T_{solidus}$

$s = 1$ if $T > T_{liquidus}$

The condition that all velocities in solid regions are zero is accounted for in the enthalpy-porosity approach by appropriately defining the parameter A in equations (2) and (3). The basic principle is to gradually reduce the velocities from a finite value in the liquid to zero in the full solid. In order to achieve this behaviour, an appropriate definition of A is given as [3]:

$$A = -\eta \frac{(1-s)^2}{s^3+b} \quad (9)$$

where b is a small computational number (0.001) to avoid division by zero and η is a very large number (10^9) [4].
It should be mentioned that although any convenient model may be acceptable for extinguishing velocities in solidifying cells in isothermal phase change systems, it is desirable that the method chosen allows a smooth, gradual transition rather than a step change in the velocity. Step changes in the momentum equation source term tend to retard numerical convergence and may even lead to divergence.

3.0 Solution Methodology

For studying the effect of natural convection during melting, two cases have been studied: Case 1 involves effect of natural convection while Case 2 is solved without considering the density variations in the melted (liquid) region so as to make buoyancy (natural convection) effects inactive. The geometry considered is a 2-D cavity of dimensions 89 mm (L) x 45 mm (H) filled with phase change material i.e. Gallium insulated on top and bottom sides (Fig.1) for which experimental results are available.The left face is maintained at the temperature of 311.3 K which is higher than the melting point of the material (302.78 K) and the right face is maintained at a temperature of 301.3 K which is lower than the melting point of the material. The density variations in the liquid region are modeled using Boussiniesq approximation to account for the natural convection in the melted region. The transient analysis was carried out by using appropriate source terms in commercial multiphysics code COMSOL 4.0 [5].

In the present version of COMSOL (version 4.0), direct modeling of melting/solidification cannot be done , hence to model the same, enthalpy porosity technique has been employed with suitable source terms in COMSOL 4.0 [5]. The physical data used in the problem has been taken from [3] and is listed below:

Reference Density, ρ_{ref}	6095 $Kg.m^{-3}$
Reference Temperature, T_{ref}	29.78 °C
Volumetric Thermal Expansion Coeff.	1.2×10^{-4} K^{-1}
Thermal Conductivity, k	32.0 $W.m^{-1}.K^{-1}$
Melting point, T_m	29.78 °C
Latent Heat of Melting, L	80160 $J.Kg^{-1}$
Specific Heat, c_p	381.5 $J.Kg^{-1}K^{-1}$
Dynamic Viscosity, μ	1.81×10^{-3} $Kg.m^{-1}.s^{-1}$
Prandtl number, Pr	2.16×10^{-2}
Solidus temperature, $T_{solidus}$	29.78 °C
Liquidus temperature, $T_{liquidus}$	30.28 °C

Sufficient number of cells (5000) have been considered and checked for mesh independence test. A time step of 0.01 seconds has been used for the calculations. Computational time for 19 minutes transient is approx. 26 hours on a Intel Xeon 8 core machine.

4.0 Results and Discussions

The computational mesh considered is shown in Fig.2.The melt fronts obtained at various times have been compared with experimental results [1] and are shown in Fig. 3. It is observed that both the qualitative behaviour and acute morphology of the experimental melt fronts have been realistically obtained in the numerical study. Excellent agreement exists between the computed and experimental melt front positions, and small discrepancies between the measured and calculated results may be attributed to factors such as (a) anisotropic thermal conductivity of gallium, (b) three dimensional effects in the experimental apparatus. Fig. 4 shows the melt front location at different times. Fig. 5 shows the velocity vector plots at the end of 5 and 19 minutes transient. Fig.6 shows the comparison for the melt fronts determined by present numerical study for both the cases (i.e. Case 1 and Case 2). It may be noted from the figure that by neglecting natural convection, not only lesser amount of melting is predicted but also the shape of melt front is totally different. From this it can be concluded that solving melting/solidification problems without considering natural convection may not give accurate results.

5.0 Conclusions

Commercial Multiphysics code COMSOL 4.0 has been used to model phase change problems considering natural convection with the help of user defined source terms incorporating **Enthalpy-Porosity technique**. An important conclusion drawn from the present study is that conduction analysis alone (neglecting natural convection) is not adequate to accurately model the phase change problems. The future studies will involve to model the actual cask geometry considering natural convection with the help of enthalpy porosity technique.

5.0 References

[1] Code for Safety in Transport of Radioactive Materials, AERB Code No. SC/TR-1, 1986, Page 46

[2] Gau, C. and Viskanta, R., 1986, "Melting and Solidification of a Pure Metal on a Vertical Wall,"*Journal of Heat Transfer – Transactions of the ASME*, Vol. 108, pp. 174~181.

[3] Brent, A. D., Voller, V. R. and Reid, K. J., 1988, "Enthalpy-Porosity Technique for ModelingConvection-Diffusion Phase hange: Application to the Melting of a Pure Metal, " *Numerical Heat Transfer*, Vol. 13, pp. 297~318.

[4] Viswanath, R. and Jaluria, Y., 1993, "A Comparison of Different Solution Methodologies forMelting and Solidification Problems, " *Numerical Heat Transfer Part B - Fundamentals* , Vol. 24,pp. 77~105.

[5] COMSOL 4.0 User Manual.

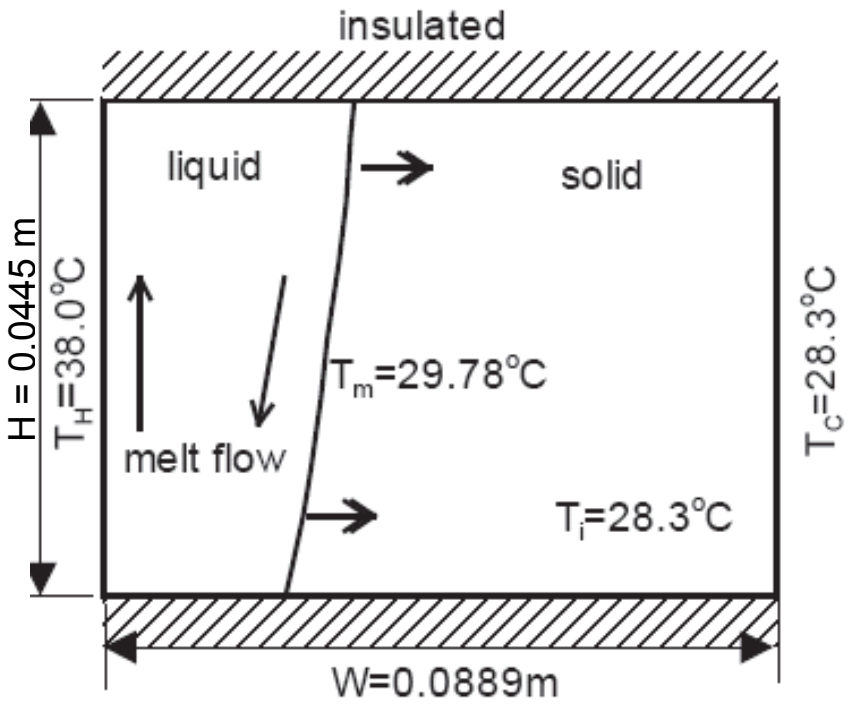

Fig. 1: Simple Schematic showing the configuration of cavity considered for melting analysis

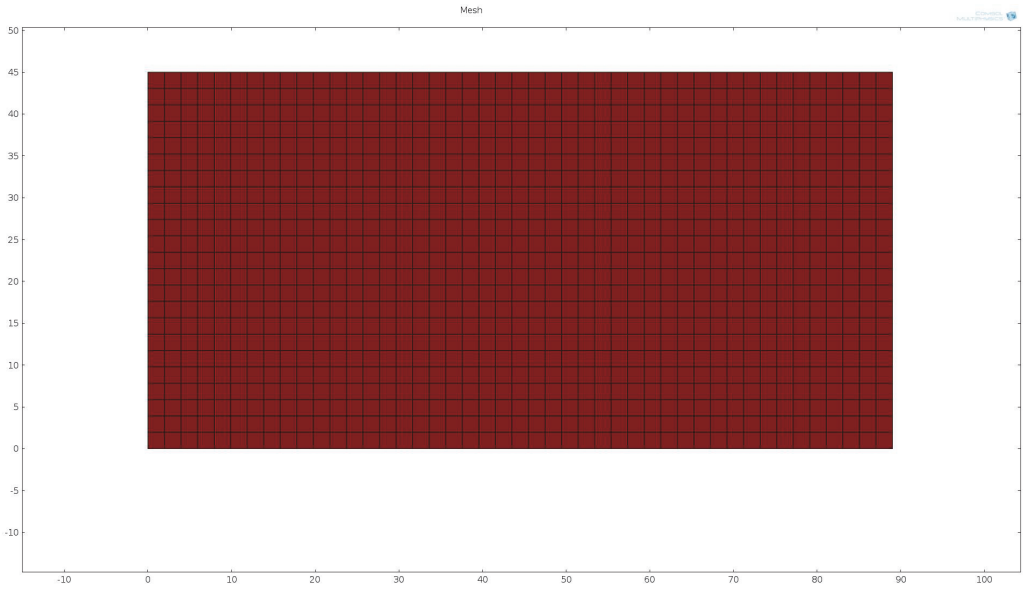

Fig. 2 : Computational Mesh used in COMSOL

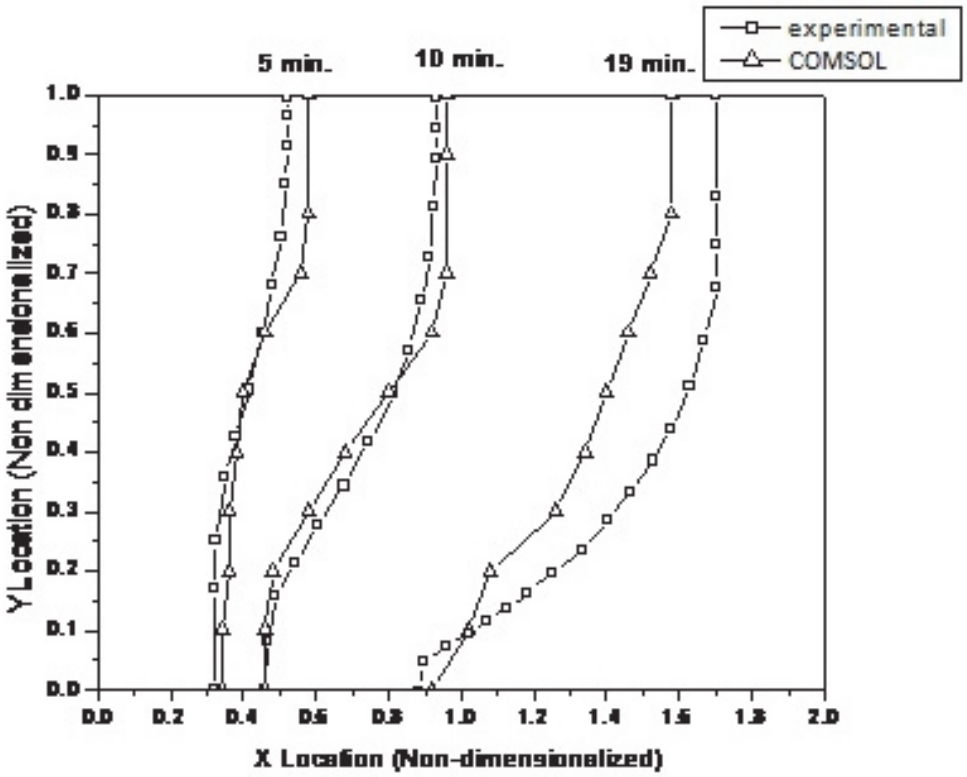

Fig. 3 : Comparison between experimental and predicted melt-fronts at different times

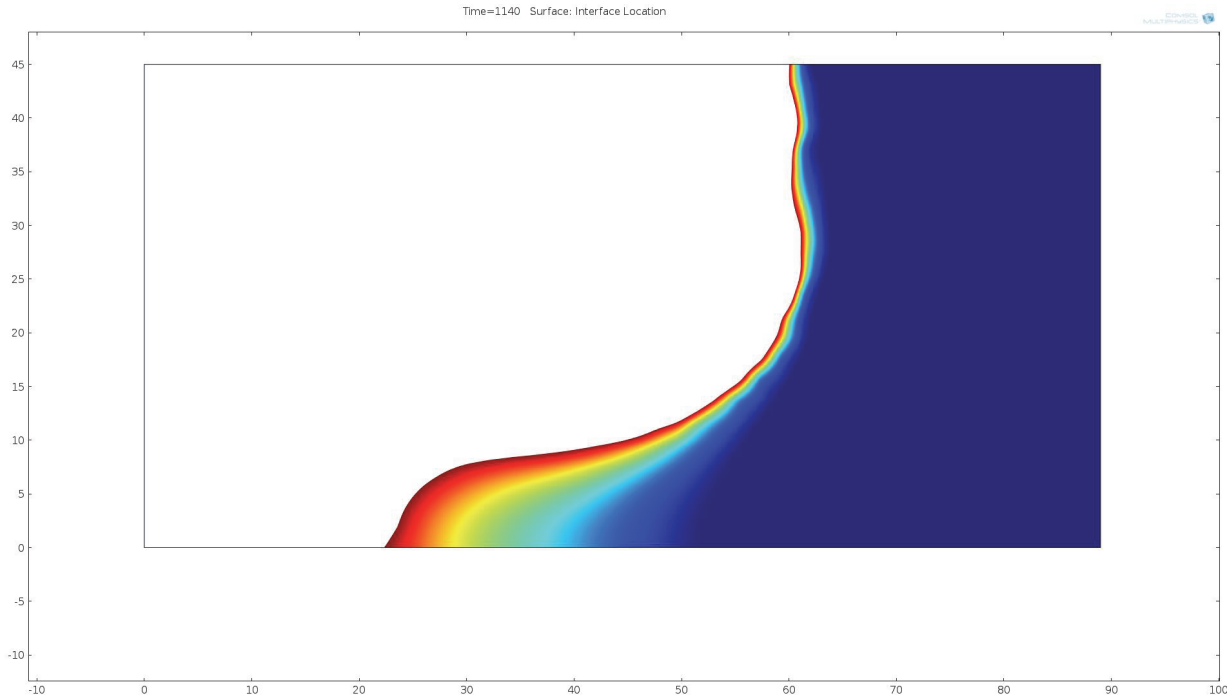

Fig. 4 : Predicted melt-front at the end of 19 minutes

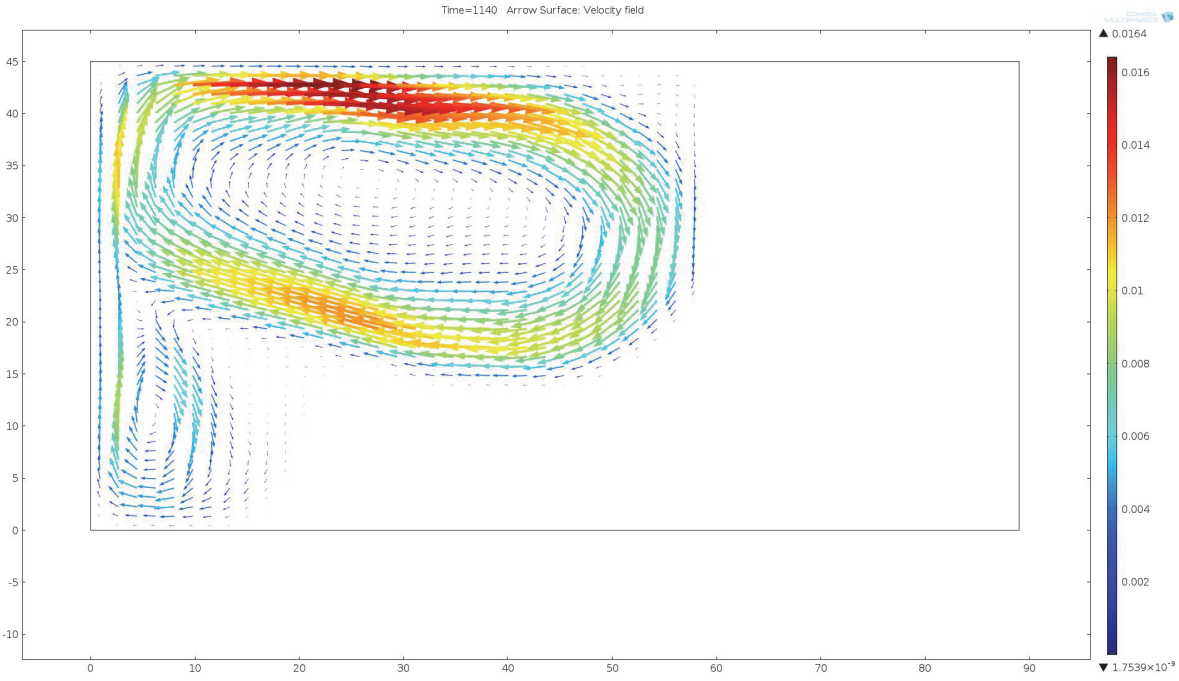

Fig.5 : Velocity Vector Plots at the end of 19 minutes

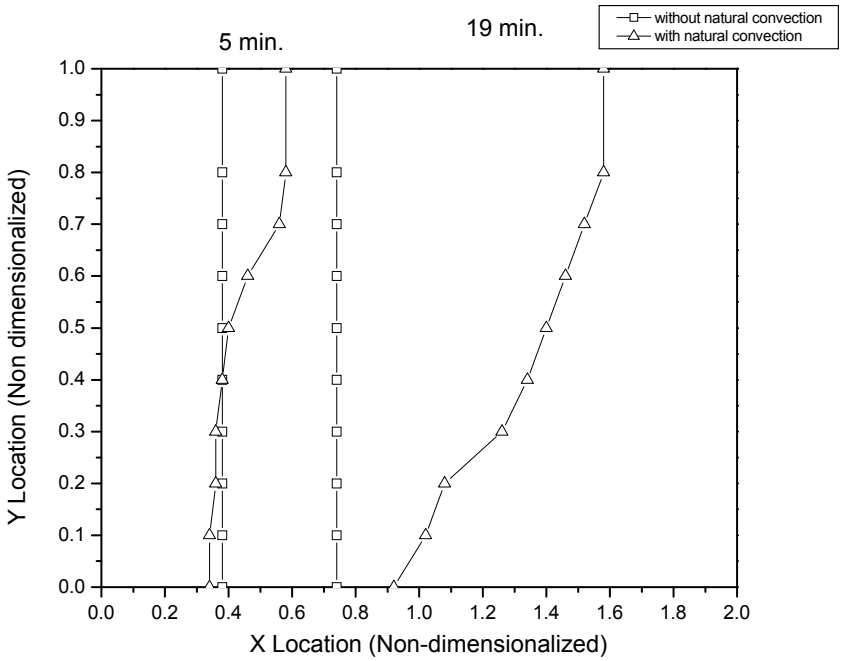

Fig. 6 : Comparison between predicted melt-fronts with and without natural convection