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Simulation of Melting Process of a Phase Change Material (PCM) using ANSYS (Fluent)

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Abstract - *This paper represents the numerical study and simulation of melting of a Phase Change Material for thermal energy storage. The melting of a rectangular PCM domain with its left side exposed to constant heat flux and other three sides insulated is simulated using ANSYS (Fluent) 15.0 software. The assumptions, equations used in numerical modelling and the specifications of the software are also discussed in the paper. The contours of liquid fraction, density, temperature and velocity of particles of PCM at regular intervals of 30min are represented for a total melting time of 240min (4 hours). The contours help in determining the change in shape and motion of melting interface with increase in time. The change in the melting fraction with time is also discussed, which tells us about the percentage of melted PCM at different instants of time.*

Key Words: Phase Change Materials, GHGs, Thermal Energy Storage, Latent Heat Storage, CFD etc.

1. INTRODUCTION

In the modern world with improved lifestyle the energy demands of human beings have increased. We all know that our conventional energy resources (fossil fuels) are limited in quantity and are being used up at higher rate. [1] The use of fossil fuels such as coal, petroleum poses a large number of problems due to their high cost, emission of greenhouse gases (GHGs) and oil security. [2] So it becomes important to conserve these fossil fuels and to protect our environment from the harmful effects of environmental pollution. We all know that most of our fossil fuels are used in power plants and transportation sector, which are not much efficient in terms of energy use. There are huge amount of energy losses in these systems. Most of these energy losses are in the form of heat loss. If we take the example of an automobile about 30-40% of the energy produced by burning fuel is lost as waste heat, which reduces the range of automobile. Also we have HVAC systems in our automobile. A heating system of about 5kW is used in i-miEV of MITSUBISHI Motors. [3] This excess need of energy reduces the driving range of such vehicles by about 10-65%. [2] So it becomes important to do the proper thermal management of such systems to increase their efficiency which can help us in achieving our goal of conserving fossil fuels and protecting the environment. The use of thermal energy storage (TES) systems is an emerging technology used nowadays for thermal management. These systems are designed to store thermal energy. This can be done with various modes such as by storing it as sensible heat, latent heat and thermochemical process. [4] The latent heat storage (LHS) system makes the use of Phase Change Materials (PCMs) for thermal energy storage. [5]

1.1 Phase Change Materials (PCMs)

PCMs are the materials which are used for storing latent heat energy. These are the materials which changes its one state to another when heat energy is supplied or extracted away from them. [6] They can change from solid to liquid state by absorbing latent heat of fusion and vice versa or they can change their state from liquid to gaseous by absorbing latent heat to vaporization and vice versa or they can change their state from solid to gaseous by absorbing latent heat of sublimation and vice versa at constant temperature. The solid to liquid phase change mode is most widely used for LHS. [7] The fig -1 shows the phenomenon of phase change for solid to liquid phase change mode. The shaded region shows the total heat energy stored during phase change of a material from solid to liquid. The total energy stored is the sum of sensible heat in solid state, latent heat during phase change at constant temperature and sensible heat in liquid state.

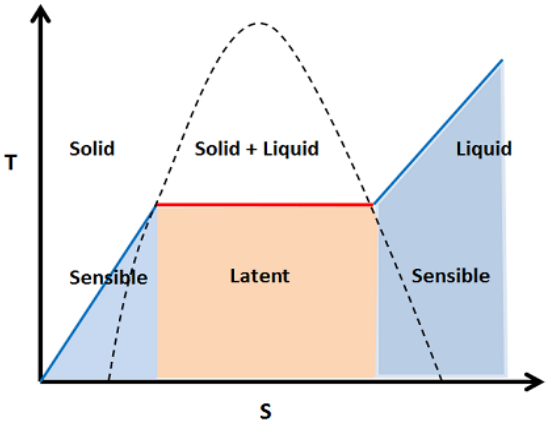

Fig -1: Heat stored during phase change of material

A large variety of PCMs are available in the market. These are classified as organic PCMs, inorganic PCMs and eutectics. [7], [8] in our numerical study Paraffin wax is used as PCM. The properties of paraffin wax are given in the Table -1.

Table -1: Thermo-physical properties of Paraffin Wax

Property	Value
Density (kg/m³)	870 at T= 300K 780 at T= 340K
Specific heat (J/kgK)	2900
Thermal conductivity (W/mK)	0.24 at T= 300K 0.22 at T= 340K
Viscosity (Ns/m²)	0.0057933
Latent heat (J/kg)	190000
Solidus temperature (K)	331
Liquidus temperature (K)	331.8

2. NUMERICAL MODEL

The melting and solidification model of ANSYS (Fluent) 15.0 software was used for modelling and simulation of the melting of PCM. ANSYS Fluent uses enthalpy porosity method for modelling the solidification and melting process. [9] In this method the melting interface is not tracked explicitly. A quantity named as liquid fraction (fraction of cell volume which is in liquid form) is associated with each cell in the PCM domain. Based on enthalpy balance the liquid fraction is calculated after each iteration. In this method phase change interface is shown as a mushy zone in which the value of liquid fraction changes from 0 to 1. Mushy zone is like a pseudo (porous zone) whose porosity decreases from 1 to 0. When the material solidifies the porosity becomes 0 and the velocity drops to zero in that zone. [9], [10]

2.1 Assumptions

The assumptions made during the numerical modelling are:

1. Melting is transient and assumed to be 2-D phenomenon.
2. The motion of PCM in liquid state is incompressible, non-Newtonian and turbulent.
3. The density, viscosity and thermal conductivity of the PCM vary as piecewise linear.
4. Viscous heating and volume expansion is ignored.
5. No heat generation within the PCM.

2.2 Energy equations

The energy equations solved in ANSYS (Fluent) model are:

$$\frac{\partial(\rho H)}{\partial t} + \nabla.(\rho \vec{v} H) = \nabla.(k \nabla T) + S$$

Where 'H' is the enthalpy, 'ρ' is the density, 'v' is the velocity of fluid and 'S' is the source term.

The enthalpy 'H' is calculated as the sum of sensible and latent heat.

$$H = h + \Delta H$$

Where 'h' is the sensible enthalpy at a point at a given instant of time; 'ΔH' is the latent heat.

$$h = h_{ref} + \int_{T_{ref}}^{T} c_p dT$$

Where h_{ref} is the reference enthalpy, T_{ref} is the reference temperature and c_p is the specific heat at constant pressure of PCM.

$$\Delta H = \beta L$$

Where β is the value of liquid fraction and L is the latent heat of PCM. The value of latent heat is zero when material is solid (β=0) and L when material is liquid (β=1).

$$\beta = 0 \quad \text{if } T < T_{solidus}$$

$$\beta = 1 \quad \text{if } T > T_{liquidus}$$

$$\beta = \frac{T - T_{solidus}}{T_{liquidus} - T_{solidus}} \quad \text{if } T_{solidus} < T < T_{liquidus}$$

Where $T_{solidus}$ and $T_{liquidus}$ are the properties of the material. [9], [10], [11]

2.3 Model Description

A geometric model of the PCM domain used for simulation is shown in the Fig -2. The PCM domain is a 2-D planer rectangular domain of length 100mm and height 150mm. The boundary condition for the PCM domain is as follows: The top, right and bottom sides of the PCM domain are perfectly insulated i.e. q"=0 W/m². The left side of the PCM domain is having constant heat flux boundary condition i.e. q"=2500 W/m².

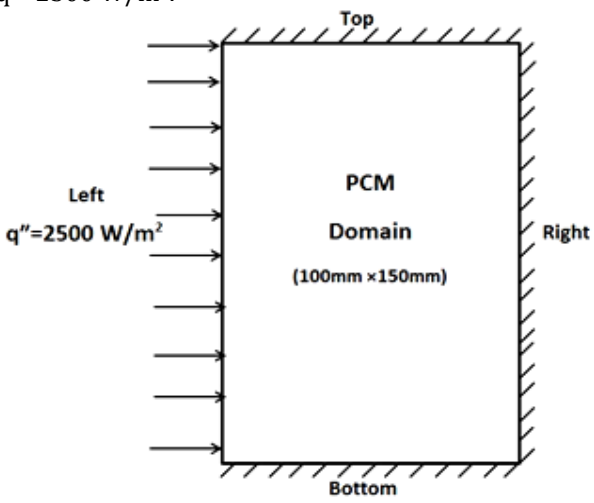

Fig -2: Schematic diagram of the model

2.4 Mesh generation and simulation approach

The problem is solved by finite volume method using ANSYS (Fluent) 15.0 software. The selection of mesh size is an

important step during the pre-processing. The meshed model shown in Fig -3 consists of 9576 nodes and 9375 elements.

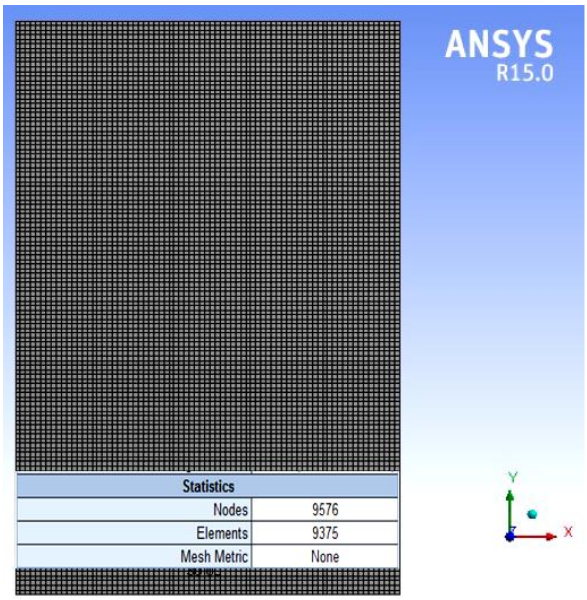

Fig -3: Schematic diagram of the meshed PCM domain

Convective terms in momentum equations are discretized using second order upwind interpolation scheme. Convective terms in energy equations are discretized using first order upwind interpolation scheme. The coupling between pressure and velocity is done by SIMPLE algorithm and PRESTO is adopted for pressure interpolation. The calculations are performed using a default commercial CFD code in ANSYS (Fluent) 15.0. Convergence is obtained when the residual of the energy, momentum and continuity equations are reduced to less than 10^{-10}, 10^{-8} and 10^{-5} respectively. The time step is set as 0.1s. The number of iterations per time step is set as 10. The simulation was performed on 2.4GHz Intel Core i3 processor with 4 GB RAM.

3. RESULTS AND DISCUSSIONS

The numerical study of melting of paraffin wax in a rectangular domain of size 100mm×150mm with constant heat flux heating from the left side of the domain and other three sides are perfectly insulated. The results of the simulation were recorded at regular intervals of 30 minutes for a complete melting cycle of 240 minutes (4 hours). Those results are represented as contours of liquid fraction, temperature, density and velocity.

3.1 Contours of liquid fraction

Fig -4 represents the variation of liquid fraction with time. We can easily examine the shape and motion of melting interface as the time passes. The red color represents the condition when material is completely liquid (β=1) and blue color represents the condition material is completely solid (β=0). The mushy zone represents the melting front; it separates the liquid and solid region. We can observe that at the initial stages time=0-30 min of melting process the melting interface is almost parallel to the left wall, which indicates that in early stages the heat transfer is mainly by conduction. As the time elapsed to 60 minutes the liquid PCM having higher temperature and lower density rises up and then moves downward and this continues for a large number of cycles. It can also be seen that it takes around 60 minutes to melt the top layer of the PCM chamber. It takes around 120 minutes to melt half of the PCM in the PCM chamber.

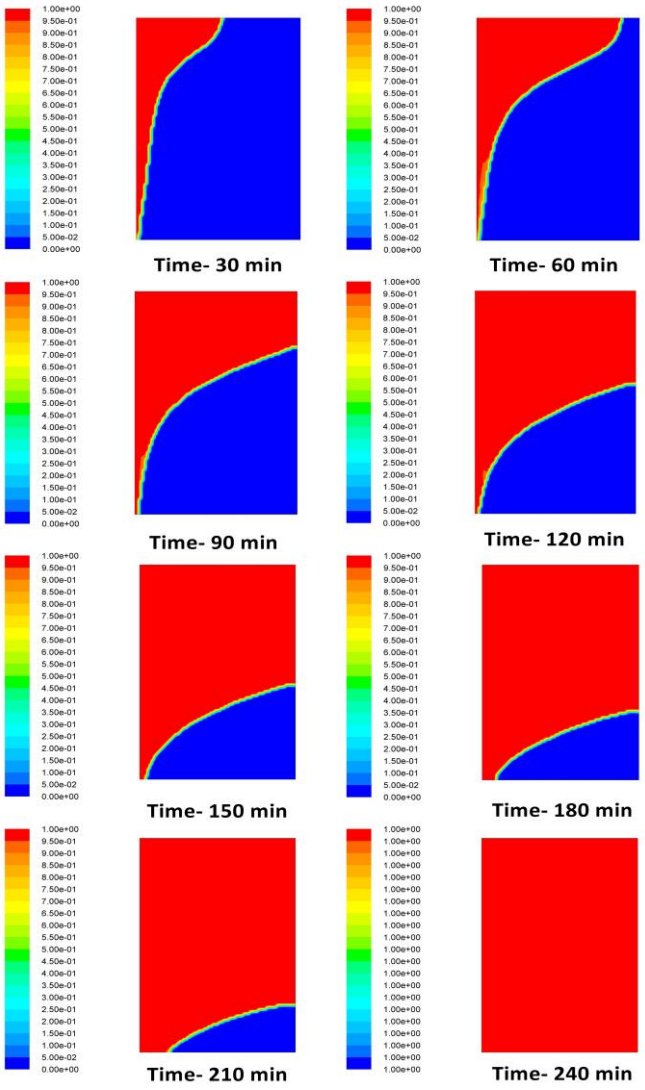

Fig -4 Contours of liquid fraction

Fig -5 shows the variation in the melting fraction (the percentage of the PCM which has been melted) with increase in time. We can see that at time=0min all the PCM in the domain is in solid state so the melting fraction is zero. As the time passes due to heating the PCM gets melted and the

value of melting fraction increase with time. The value of melting fraction is 17%, 32%, 44%, 59%, 71%, 80% and 86% for the melting time of 30, 60, 90, 120, 150, 180, and 210 minutes. At the end of the melting cycle i.e. after 240 minutes all the PCM in the PCM domain has been melted; giving a melting fraction of 100%. It is noticed that the rate of melting is almost same at the starting of the melting process and it increases in the middle and at the end of the melting process. Manar et al. [12] also simulated the melting of PCM using ANSYS (Fluent), Nabeel et al. [13] reviewed the melting behavior of various configurations and Abdullah et al. [14] investigated experimentally the melting of PCM with left wall as heating surface. The results given by them also show the similar melting behavior of PCM.

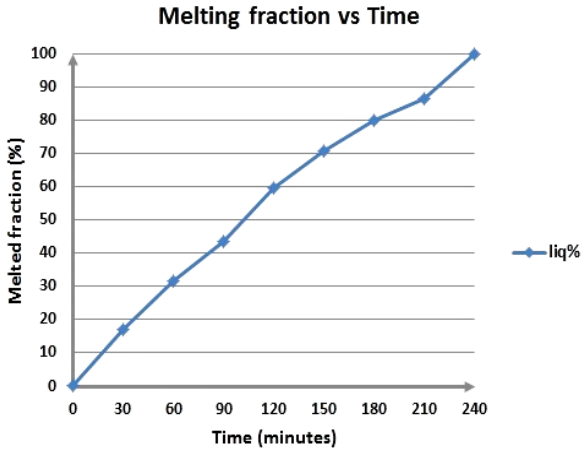

Fig -5 Variation of melting fraction with time

3.2 Contours of Temperature

Fig -6 represents the contours of temperature and the variation in temperature after regular interval of 30 minutes each. It can be analyzed from the figure that the maximum temperature achieved is 344K during the initial stage, 383K during the middle and 416K at the later stages of the melting process. I can also be observed from Fig -4 and Fig -6 that, when the temperature at any location in the PCM domain reaches 331K the PCM starts melting. The blue color shows the low temperature zone. The shape of this zone resembles to that of the solid PCM in the PCM domain as shown in the Fig – 4. There is a red zone developing in the PCM domain nearer to the left wall after 90min, and it gradually increases in size. This is because of the turbulence effects present in the liquid PCM. At the end of the melting process all the PCM is in liquid phase and the properties becomes constant so constant temperature zones have been developed which can be clearly seen in Fig -6 for Time =240 min.

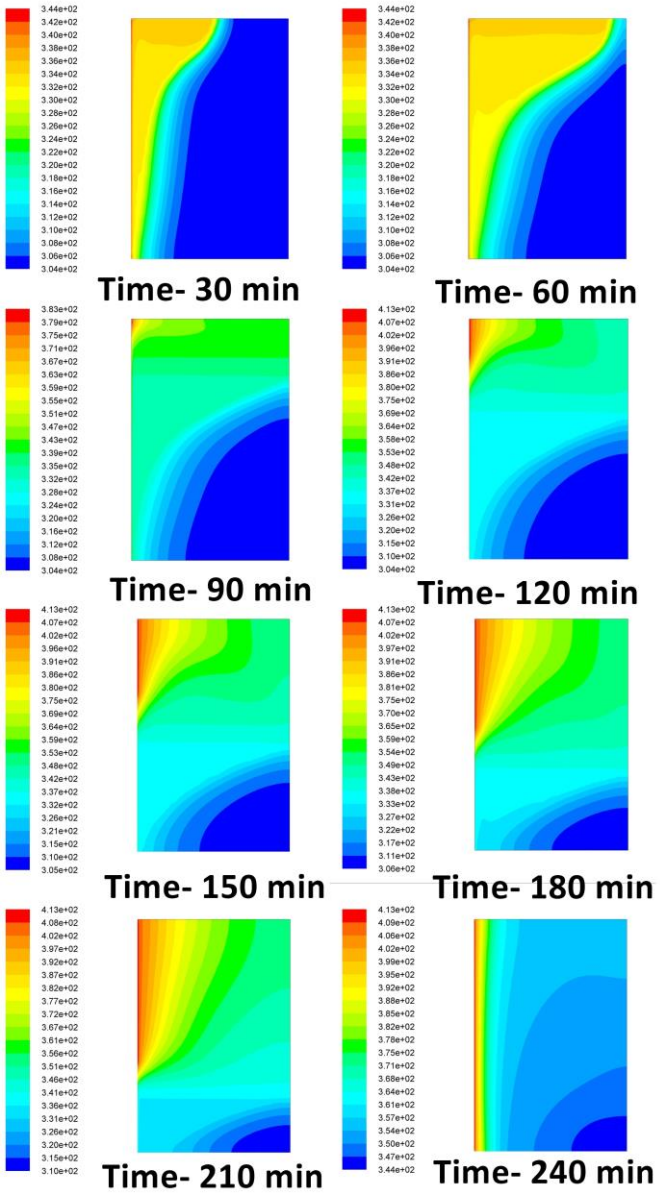

Fig -6 Contours of Temperature

3.3 Contours of Density

Fig -7 represents the contours of density and the variation in density after regular interval of 30 minutes each. The density of the PCM changes with increase in temperature. So as the temperature increases the density of the PCM decreases and it rises up, gets accumulated at the top and form a zone of low density PCM at the top; which is shown by blue color in the Fig -7. At the end of the melting process the density of the PCM domain is constant and the value of the density at time 240min is 780 kg/m^3.

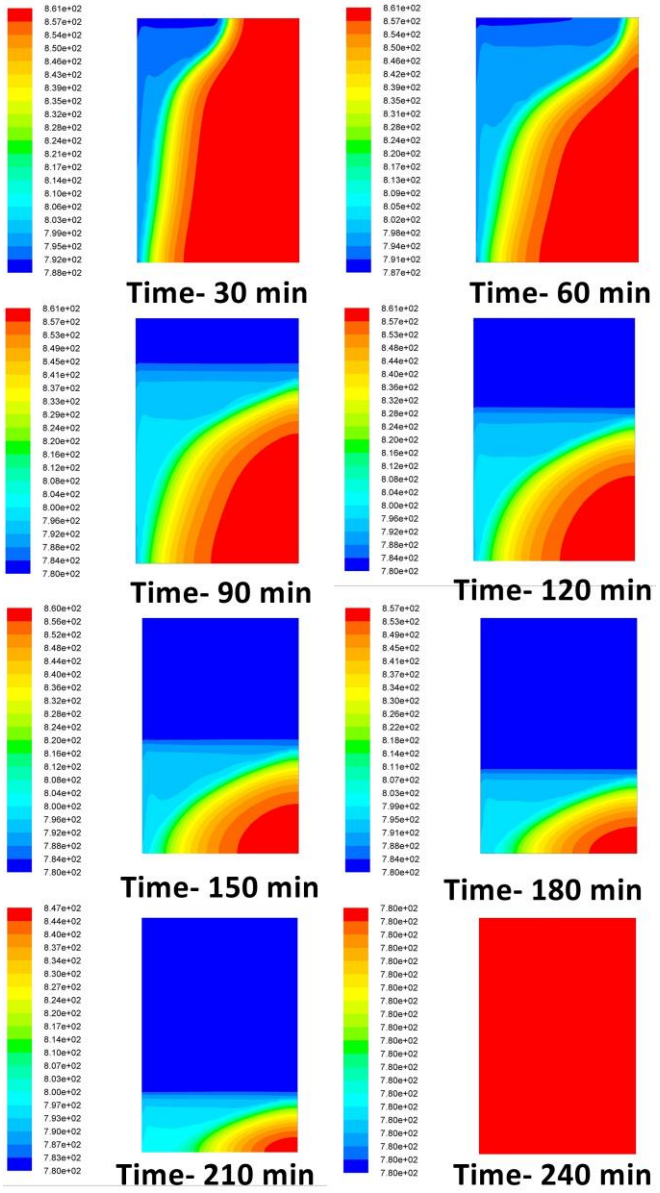

Fig -7 Contours of density

3.4 Contours of Velocity vector

Fig -8 represents the contours of velocity vector and the variation in velocity after regular interval of 30 minutes each. We can observe that there is a red zone in the liquid PCM near the left (hot) wall which has the highest magnitude of velocity. At the end of the melting process all the PCM is in liquid state and also the density of the PCM becomes constant. Thus the buoyancy effects become zero after complete melting. Hence all the molecules at the end of the melting process become at rest.

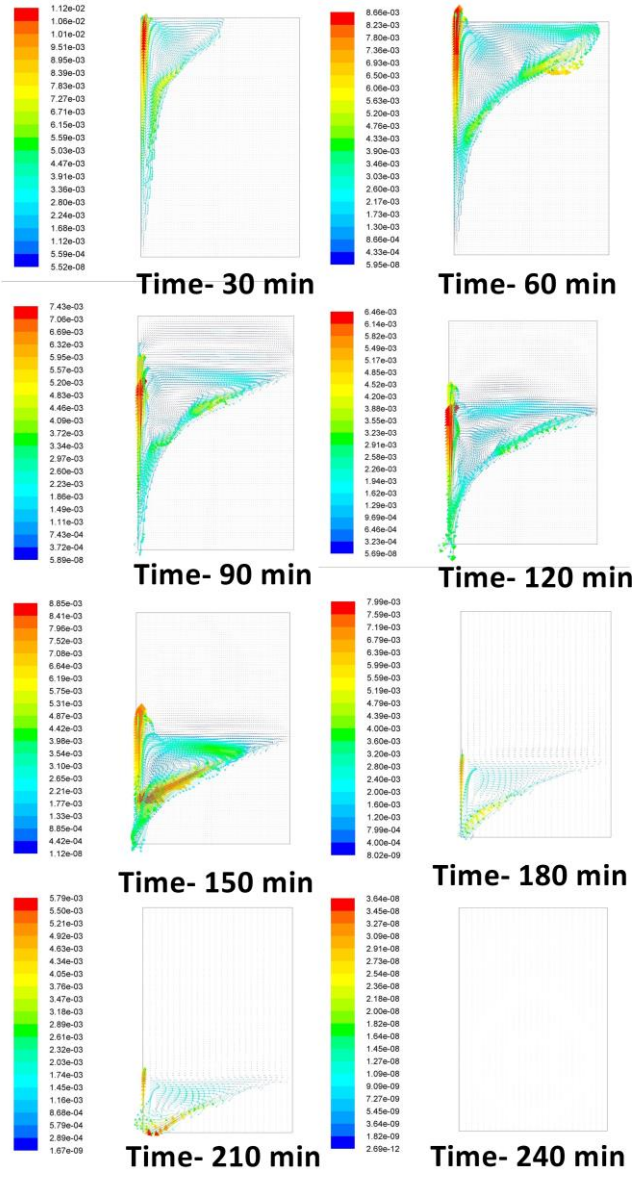

Fig -7 Contours of velocity vector

4. CONCLUSIONS

After this numerical modelling and simulation of PCM melting process with constant heat flux condition the following conclusions can be drawn:

1. For this case with vertical heating wall melting starts from the top and then proceeds in the downward direction.

2. The melting rate increases as the time proceeds. It is almost same at the initial stages and increases in the middle and the end of the melting process.

3. In the early stages (0-30 min) of melting process the heat transfer is mainly by conduction and after further heating it changes to natural convection.

4. Proper meshing and the selection of time steps should be done while simulating melting problem on ANSYS (Fluent), otherwise there will be divergence error during solution.

It is concluded that with using proper settings the simulation of melting of PCM for latent heat storage can be done with the help of ANSYS (Fluent) software.

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BIOGRAPHIES

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