Computational analysis of encapsulated phase change materials latent heat thermal energy storage system

Mayank Srivastava*, M.K. Sinha

Department of Mechanical Engineering
National Institute of Technology Jamshedpur, India

mayank.nitjamshedpur@gmail.com

ABSTRACT. *This article proposes a computational and mathematical study to analyse interface position, rate of interface and temperature variation of encapsulated phase change thermal energy storage system (TESS) with constant heat flux for outward melting process. Conduction is the main phenomenon that governs the melting process. Spherical and cylindrical geometry is used to encapsulate the phase change material to avoid direct contact between heat transfer fluid (HTF) and phase change materials, which is under constant temperature boundary condition, applied only on one wall. Other walls are thermally insulated. The computational results are obtained for melting of solid which is initially at its fusion temperature by using computational fluid dynamics software and a matlab code has been written to develop a mathematical model for this study.*

RÉSUMÉ. *Cet article propose une étude informatique et mathématique pour analyser la position d'interface, le taux d'interface et la variation de température du système de stockage de l'énergie thermique à changement de phase encapsulé (TESS) avec flux de chaleur constant pour la fusion.La conduction est le principal phénomène qui régit le processus de fusion.La géométrie sphérique et cylindrique est utilisée pour encapsuler le matériau à changement de phase afin d'éviter le contact direct entre le fluide caloporteur (HTF) et les matériaux à changement de phase, soumis aux conditions limites de température constante, appliqués uniquement sur un mur.Les résultats informatiques sont obtenus pour la fusion d'un solide qui est initialement à sa température de fusion en utilisant un logiciel informatique de dynamique des fluides et un code matlab a été écrit pour développer un modèle mathématique pour cette étude.*

KEYWORDS: *conduction, HTF, interface position, melting, phase change materials, TEES.*

MOTS-CLÉS: *conduction, HTF, position de l'interface, fusion, matériaux à changement de phase, TEES.*

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1. Introduction

Phase change thermal energy storage has been main area of research in the last two decades and more. Regular Consumption of non-renewable energy resources led to raise the serious issues on their future scope and create a huge gap between supply and demand of energy. This problem can be overcome by either reusing the waste energy or by using the renewable energy like solar, wind, tidal etc. Solar energy is the most promising, clean and safe source of energy. The main problem associated with the use of such energy is its oscillating nature e.g. its availability is only at daytime and to utilize waste heat, we need a device to store waste energy and release when needed. Storage process of waste heat must have been at a faster rate as compared to its discharge. The consumption of energy at peak hours is higher than its generation and at the night energy generation is higher than its consumption. This difference of energy between generation and consumption can be stored in an appropriate energy storage system and may use in many industrial as well as domestic purpose. Both the problems mentioned above can be solved by the use of phase change thermal energy storage system. Likewise all other conventional energy storage system (mechanical energy storage – flywheel, electrical energy storage – battery) phase change thermal energy storage system is using sensible heat, latent heat, and thermo-chemical heat or combination of these to store energy. In sensible thermal energy storage system, energy is stored by changing the storage medium temperature whereas in latent heat thermal energy storage system, the storage medium temperature is constant during phase change. The process of solidification and melting are connected with many practical applications. They occur in wide range of industrial processes, like metal processing, casting, and thermal energy storage system in space station etc.

The material which is used to store the latent heat is called phase change material which gives an appropriate way to charge and discharge of thermal energy because of its high heat storage capacity at the constant temperature. Such type of materials is classified into mainly 3 categories: Organic, inorganic and eutectic (Zalba *et al.*, 2003). Selection of phase change materials which is going to be used in thermal energy storage system is basically based on their applications and melting temperature. For cooling purpose the melting temperature of PCM should be below 15°C and for absorption refrigeration purpose, its melting temperature should be above 90 °C. All other materials that melt in between these two temperature limit are used in heating purpose (Mohammed *et al.*, 2004). Encapsulation of thermal energy storage system is the technique which is used to separate the phase change materials and the heat transfer fluid to avoid any direct contact between them. Two geometries which are commonly used as PCM containers are the rectangular and cylindrical containers (Agyenim *et al.*, 2010).

The simplest phase change thermal energy storage problem, which is 1-dimensional phase problem, has been analytically solved by Carslaw (1959). In 1-dimensional phase problems, only one phase is being active and other phases being at its melting point. The result obtained from the analysis shows that the rate of melting or solidification in a semi-infinite slab is governed by s non-dimensionless number, called Stefan number (S_t). Nacer *et al.*, (2006) have developed a refined integral heat balance method for time dependent 1-dimensional Stefan problem. The method is applied to phase change in the half plane and ordinary differential equation is obtained for the solid/liquid interface. The results so obtained from this method demonstrated high accuracy when compared to heat balance integral, perturbation and numerical methods including large Stefan number.

Ren (2007) analysed the one-region and two region inverse Stefan problems in Cartesian and spherical coordinates by heat balance integral method. The present method is simple and accurate for previse the temperature and heat flux variation at the fixed boundary when the movement of the phase change interface is prescribed. Kumar *et al*., (1987) have numerically solved outward radial melting process of a phase change material contained in spherical shell latent heat thermal energy storage system under constant temperature heat injection by using the three approximate analytical methods i.e. Biot variational, heat balance integral method and quasi-steady methods to evaluate phase change depth, total energy storage and heat transfer rate. These methods provide closed form solutions in the Stefan number, an independent parameter. The results obtained by these methods were almost the same. Hristov (2010) has thoroughly analysed the heat balance integral method of Goodman in the case of a parabolic profile with unspecified exponent, depending on the boundary conditions imposed to enhance the heat balance integral method and form a robust algorithm defining the parabola exponent. The results obtained from analysis were compared with the results provided by the Veinik's method. The method has also been applied to solve one dimensional heat conduction problem in cartesian coordinates including a spherical problem and over the specified boundary condition at the face of the thermal layer.

Sugawara *et al*., (2011) studied 3-D melting of ice around the tube carrying hot liquid placed inside a rectangular cavity using PHOENICS Code. The walls of the rectangular cavity were considered adiabatic. Effects of convection on the rate of melting were studied and reported. Effects of inlet temperature, tube length and cavity height were also reported in the paper. Effects of convection on melting were clearly shown through the contour plots showing the solid-liquid interface for different time periods. M. Azad *et al.* (2016) studied the effect of temperature on the melting of PCM and the factors influencing the onset of convection in the melt layer. Experimental setup was designed consisting of PCM inside a cylindrical enclosure with liquid carrying tube passing through the center. Digital camera was used to monitor the melting phenomena. COMSOL Multiphysics was used for the numerical analysis of the same. Results of the numerical model were validated using the melt profiles obtained through experiments. Temperature variation with time for different locations was plotted. An experimental setup along with a simulation model was developed for melting of paraffin wax by Tan *et al*., (2009). The study focused on the buoyancy driven melting phenomena inside a spherical capsule. Finite volume approach was used for the numerical simulation model. In the experimental setup, thermocouples were placed at different locations along the central vertical axis inside the spherical cavity to measure the temperature. It was that, initially melting was driven by diffusion and the melt layer was almost symmetrical but later on it was observed that the liquid fraction increased in the top part because of buoyancy driven convection.

Temperatures and liquid fraction were plotted at different locations and compared with the numerical results.

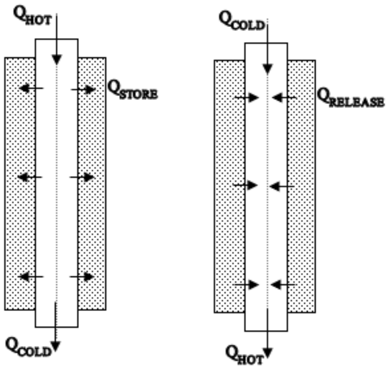

Figure 1. Thermal energy storage system

Most of the research done on PCM uses constant thermal conductivity. Amin *et al.*, (2014) tried to determine the effective thermal conductivity for the phase change process. An experimental setup and a simulation model were developed for a PCM contained in a sphere at the centre of the cylindrical shell. The heat transfer fluid was flown through this cylinder at constant flow rate. Thermal properties were assumed to be constant as they were found to have minimal effect on melting rate. Simulations were carried out for different thermal conductivities to thermal determine the effective thermal conductivity. It was observed that the simulation results agreed with the experimental results when the mass flow rate was higher. It was also concluded that the effective thermal conductivity cannot be assumed constant when the fluid temperature is varying around the sphere. Darzi *et al.*, (2012) made a comparative study of melting in horizontal concentric and eccentric annular cavity using FLUENT. Laminar and 2-D flow conditions were assumed. N-eicosane was selected as the PCM with constant thermal properties. Simulation was run to observe the movement of the interface and the time taken for melting. It was observed that time taken in eccentric case was lesser compared to the concentric one as melting occurred at faster rate in upper part due to natural convection. Flow of the fluid due to natural convection was also observed.

Svetislav Savovic *et al.,* (2009) have reported the results of computational analysis of 1-dimensional Stefan problem with time-dependent boundary conditions describing the solidification/melting process. The variable space grid method based on finite difference method has been used to evaluate the temperature distribution, the position of the moving boundary and its velocity. The results obtained from analysis were compared with the exact solution and found more accurate from existing results. A numerical model for melting and solidification of paraffin wax was developed by Trp (2005) in FORTRAN to study PCM in shell and tube type of heat exchanger. It was decided that studying a concentric area around a single tube will serve the purpose. Accordingly an experimental setup was designed to simulate melting/solidification around a single vertical tube. Constant water mass flow rate maintained throughout the experiment. It was observed that the numerical results were in close agreement with the experimental results. It was also observed that natural convection was insignificant for solidification process. Radial dimensionless temperature distribution was plotted for different times. Experiments suggested that melting occurs non-isothermally whereas solidification occurs isothermally. Lin *et al.*, (2012) have computationally investigated the phenomena of heat energy storage and release in phase change materials, used in building retaining structure. In real life melting and solidification of PCM, the phase change material transfer model has been analysed, which only consider liquid-phase natural convection. The results obtained from analysis shows that the influence of natural convection has mainly something about circumfluence generated by liquid phase, the direction of circumfluence is opposite when heat and cool, the circumference intensity enhances as the height of face interface increases.

Aytunc Erek *et al.*, (2009) have studied the heat transfer behaviour of the encapsulated ice thermal energy storage system during charging and discharging process. The temperature of heat transfer fluid (HTF) and the heat transfer coefficient varies considerably around each capsule. A new heat transfer Coefficient correlation has been developed by simulating a series of experiments for different capsule diameter, mass flow rates and temperature of heat transfer fluid. Temperature based fixed grid solution with control volume approach has been applied for studying the heat transfer behaviour of an encapsulated ice thermal energy storage system. The results obtained from the analysis validated with some experimental data obtained from the literature. The results indicate that the heat transfer coefficient varies greatly during downstream and affects the heat transfer taking place during the process and also the solidification process is mainly governed by the Stefan number, capsule diameter and capsule row number. Gauche *et al.*, (2000) have performed a computational analysis for an electronic system that uses phase change materials to provide transient thermal control. A case study has been performed in which a system level computational fluid dynamics model of an electronic enclosure is modelled with and without phase change material retro fitted in three configurations. The results obtained from analysis shows that the proposed method simplifies the analysis without compromising the thermal integrity of the model. Unexpected results have been indicated that the system level model provides important information often lacking in an idealized (non-system) analysis.

2. Mathematical modelling

A schematic drawing of a spherical and cylindrical encapsulation containing solid PCM used in the present study is shown in figure 2. For simplicity, we consider a single phase, 1-dimensional melting problem of PCM kept inside a spherical and cylindrical capsule, whereas practical melting problem is rarely one dimensional, initial and boundary conditions are always complex. Initially, PCM is at its melting temperature T_m. The temperature at the encapsulation boundary T_s is higher than the PCM melting temperature T_m.

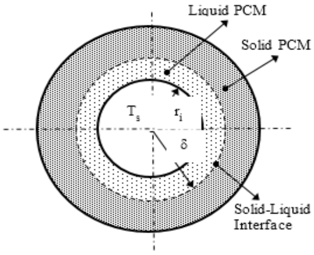

Figure 2. Schematic drawing of encapsulated PCM undergoing outward melting

The term 'moving boundary problems' is associated with time-dependent boundary problems and also referred as Stefan problems, where the position of the moving boundary must be determined as a function of time and space. As the time passes solid PCM will melt due to the boundary temperature applied at vessel and the governing equations for this process may be described by:

$$\frac{1}{r^k}\frac{\partial}{\partial r}\left[r^k\frac{\partial T}{\partial r}\right] = \frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{1}$$

where k = 1 for cylindrical vessel
k=2 for spherical vessel

Boundary Conditions:

$$r = r_i\,,\ t > 0,\ T = T_s \tag{2}$$

$$r = \delta\,,\ t > 0,\ T = T_m \tag{3}$$

$$r \geq r_i\,,\ t = 0,\ T = T_m \tag{4}$$

Energy balance at the solid-liquid interface:

$$\left[K\frac{\partial T}{\partial r}\right] = -\rho L\frac{\partial \delta}{\partial t} \tag{5}$$

2.1. Non-dimensional analysis

To reduce dependent variables we introduce the non-dimensional variables,

$$\xi = \frac{r}{r_i} \qquad \eta = \frac{\delta}{\mathrm{r_i}} \qquad \tau = \frac{\alpha\, t}{{r_i}^2}$$

$$\theta = \frac{T - T_f}{T_s - T_f} \qquad S_t = \frac{C\,(T_s - T_f)}{L}$$

Put these non-dimensional variables to above equations, to get non-dimensional governing equations

Equation (1) becomes,

$$\frac{1}{\xi^k}\frac{\partial}{\partial \xi}\left[\xi^k\ \frac{\partial \theta}{\partial \xi}\right] = \ \frac{\partial \theta}{\partial \tau} \tag{6}$$

And all boundary conditions becomes,

$$\xi = 1, \tau > 0, \theta = 1 \tag{7}$$

$$\xi = \eta\ , \tau > 0, \theta = 0 \tag{8}$$

$$\xi \geq 1, \tau = 0, \theta = 0 \tag{9}$$

Now non-dimensional energy balance equation at the solid-liquid interface is,

$$\left[\frac{\partial \theta}{\partial \xi}\right] = \ -\frac{1}{S_t}\frac{\partial \eta}{\partial \tau} \tag{10}$$

2.2. Heat balance integral method

The heat balance integral method (HBIM) is simple approximate technique developed for solving transport problems like phase change problems. Goodman [21] introduced HBIM, which converts the governing partial differential equations to ordinary differential equations by integrate the heat conduction equation with respect to the space variable over a suitable interval to create a heat balance integral equation and solve the integral equation to obtain the interface location and temperature distribution.

Now, integrate the energy equation (10) with respect to space variable,

$$\int_1^\eta \frac{\partial}{\partial \xi}\left[\xi^k\frac{\partial \theta}{\partial \xi}\right] d\xi\ =\ \int_1^\eta \left[\xi^k\frac{\partial \theta}{\partial \tau}\right] d\xi \tag{11}$$

$$\frac{\partial}{\partial \tau}\left[\int_1^\eta (\xi^k\theta) d\xi\right] -\ (\xi^k\theta)_{\xi=\eta}\dot{\eta}\ =\ \left[\xi^k\frac{\partial \theta}{\partial \xi}\right]_{\xi=\eta} -\ \left[\xi^k\frac{\partial \theta}{\partial \xi}\right]_{\xi=1} \tag{12}$$

Now assume a suitable linear temperature profile with negligible temperature drop within the solid layer, which satisfies the boundary conditions:

$$\theta = 1 - \left[\frac{1-\frac{1}{\xi}}{1-\frac{1}{\eta}}\right] \tag{13}$$

Substituting eq. (13) into eq. (12) leads to

2.3. Interface location

For spherical geometry (k=2),

$$\tau = \frac{\eta^3}{3} - \frac{\eta^2}{2} - \frac{1}{6} + [\eta^2 - \log(\eta) - \eta]\left(\frac{S_t}{6}\right) \tag{14}$$

For cylindrical geometry (k=1),

$$\tau = \frac{\eta^2}{3} - \eta + \frac{1}{2} + [\eta - \log(\eta) - 1]\left(\frac{S_t}{2}\right) \tag{15}$$

2.4. Heat transfer analysis

$$\mathrm{Q} = \int_1^{\eta} (\text{Latent heat} + \text{Sensible heat})\, d\xi \tag{16}$$

For sphere:

$$Q_\tau = \left[\frac{\eta^3 - 1}{S_t} + 3\int_1^{\eta} \xi^2 \theta \, d\xi\right] \tag{17}$$

$$Q_\tau = \left[\frac{\eta^3 - 1}{S_t} + (\eta^3 - 1) - 3\left(\frac{\eta}{\eta - 1}\right)\left(\frac{\eta^3 - 1}{3} - \frac{\eta^2 - 1}{2}\right)\right] \tag{18}$$

For cylinder:

$$Q_\tau = \left[\frac{\eta^2 - 1}{S_t} + 2\int_1^{\eta} \xi \, \theta \, d\xi\right] \tag{19}$$

$$Q_\tau = \left[\frac{\eta^3 - 1}{S_t} + (\eta^3 - 1) - 3\left(\frac{\eta}{\eta - 1}\right)\left(\frac{\eta^3 - 1}{3} - \frac{\eta^2 - 1}{2}\right)\right] \tag{20}$$

3. Computational modelling

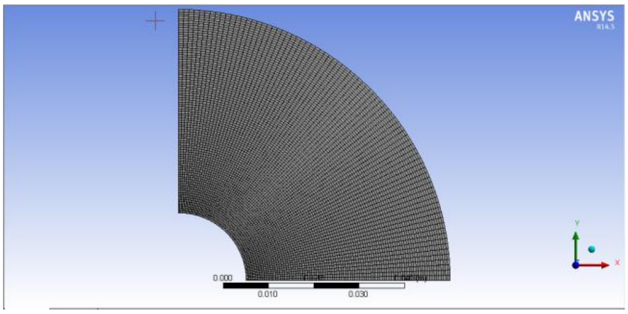

Figure 3. Schematic drawing of computational domain

4. Results and discussion

The temperature of the lower part of the capsule is higher than that of the outer part and the isotherms are clearly radially symmetric. The maximum temperature reached at the inner wall of the capsule which is at fixed temperature. The temperature of inner wall is higher than the melting temperature of the phase change material. Hence melting in the phase change material has started near the inner wall of the capsule. As shown in the figure, the interface separating the liquid PCM from the solid PCM propagates radially outward as the melting process progresses. The temperature is much higher at inner wall of the capsule. The dark blue region represents the solid phase and red region represents the liquid phase whereas in between blue & red region, both the phases present. Figure shows the location of the propagating liquid/solid interface at various times. Results are presented during the charging process of PCM.

4.1. Contours at different times

For cylinder

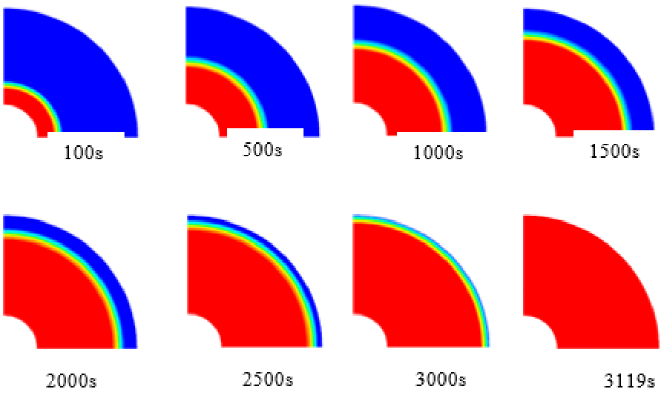

Figure 4. Contours at different times (For cylindrical geometry)

For sphere

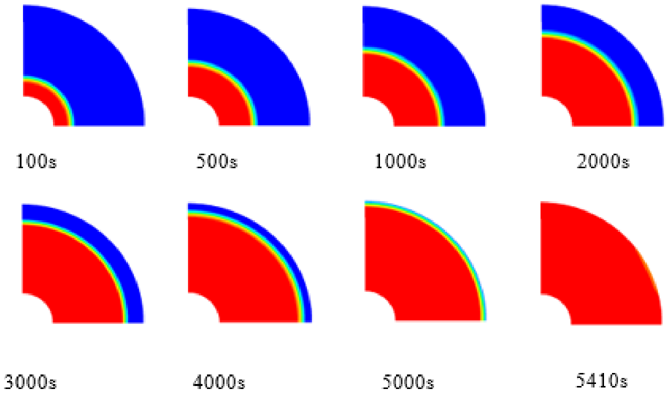

Figure 5. Contours at different times (For cylindrical geometry)

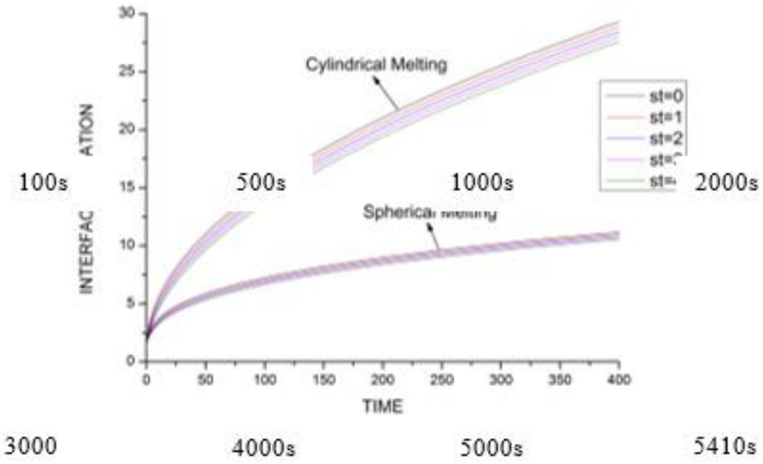

Figure 6. Behaviour of the non-dimensional interface location with non-dimensional time, Stefan's number is taken as a parameter

In figure 6, the plot shows the position of interface with time for different values of Stefan's number which is a non-dimensional parameter. At initial time, interface position increases very rapidly with time for each values of stefan's number and after some time interval it will become almost linear. This happens because during starting time heat transfer rate increases more sharply. The solution obtained for present problem by using HBIM depends upon Stefan's number. It is observed that at any time instance as St. number decreases interface depth increases.

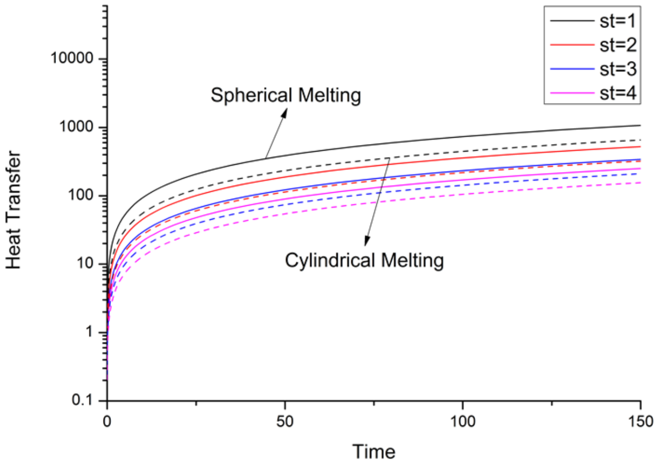

Figure 7. Non-dimensional heat transfer with non-dimensional time, Stefan's number is taken as a parameter

Figure 7 shows the heat transfer variation with time in spherical and cylindrical melting at different values of Stefan’s number. During starting time of melting, the heat transfer increases more rapidly because of large temperature difference available between two phases. But as the time passes, heat transfer becomes linear with time. This happens because temperature difference between two phases decreases. The time taken to absorb a fixed amount of heat in spherical melting process is lower than that of cylindrical melting process.

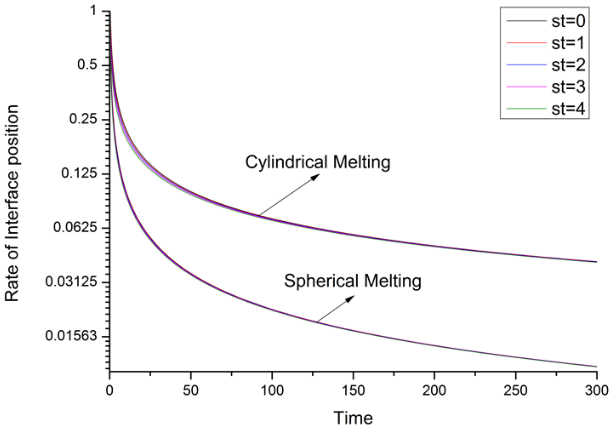

Figure 8. Behaviour of the non-dimensional rate interface position with non-dimensional time, Stefan’s number is taken as a parameter

Figure 8 shows the variation of rate of interface position with time. The interface location is a function of Stefan’s number (Eq.14, 16). The plot between rate of interface position and time is almost a single curve for all values of Stena’s number. Rate of interface position decreases with time for all values of Stefan’s number.

5. Conclusions

The melting phenomenon in Cylindrical and Spherical encapsulated thermal energy storage system with phase change materials at fixed temperature heat transfer is investigated computationally. In present work, HBIM and computational method are used for single phase change models in cylindrical and spherical melting. This method can be further applied on more complicated and realistic melting/solidification problems. Conduction is the main heat transfer phenomenon between different phases. The effect of other heat transfer mode is being neglected.

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