Modeling of Solidification of PCM inside Spherical Capsules Using Moving Grid Technique

Musa M. Radwan

Abstract**—**This paper presents numerical solution of moving boundary problem manifested by freezing of phase-change material encapsulated in spherical container. The temperature distribution and solid-liquid interface position during the solidification process has been investigated. The model is based on the one-dimensional transient heat conduction with the associated boundary and interface conditions and the initial condition of the liquid face. The governing equations, boundary and interface conditions are discretized using finite difference implicit scheme. The main features of this work is adopting the moving mesh technique for spherical geometry for tracing the interface position that separates the liquid and solid phases as function of time. The results of this work are presented in terms of transient behavior of surface temperature, solidification front position, surface heat flux, and spatial temperature distribution in the solid face assuming the liquid face is maintained at the phase change temperature. Preliminary results have demonstrated a considerable effect of Stefan and Biot numbers on the solidification process as well as on the time necessary for complete solidification. Large values of Biot number leads to reducing the total time necessary for complete solidification, owing to the fact of large heat removal from the capsules.

Keywords**—**Energy Storage, Heat Transfer, Moving Boundary, Phase Change.

I. INTRODUCTION

The Phenomena of melting and solidification occurs very frequently in industrial applications and processes, such as solidification of castings, environmental engineering, metal processing, and latent heat thermal energy storage systems. In these processes, the system interacts with the surrounding resulting in a phase change. Consequently, a control surface or a boundary separating the system from the surrounding develops and moves in the matter during the phase change process. During these processes, transport properties vary considerably between phases even for a system of one component. This leads to different states of mass, momentum and energy transport from one phase to another. In phase change problems, the liquid-solid interface position is not known in advance, but has to be part of the solution procedure. The term, moving boundary problems, is associated with variation of interface position as function of time and space. Moving boundary problems are referred to as Stefan problems, were investigated as early as 1831 by Lame and Clapeyron [1]. However, the sequence of articles [2,3] written by Stefan has given his name to the moving boundary problems.

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Physical processes involving Stefan problems were solved analytically in the early stages of the nineteenth century, at that time analytical methods were the only means available to investigate physical processes involving phase change problems and hence to trace the front position as function of time. Although analytical methods are simple to implement and give an exact solution, due to their limitations, analytical solutions are mainly for one dimensional problems with simple initial or boundary conditions and constant thermo-physical properties [4]. It is well known that practical problems involving change of phase are rarely one dimensional, initial and boundary conditions may contain non-linear terms, in addition thermo-physical properties can vary with phases, temperature, concentration, and transport mechanisms (energy transfer modes) may take place simultaneously. All these constraints make the analytical methods difficult if not impossible to implement. With the availability of high speed digital computers, mathematical modeling and numerical simulations often becomes the most economical and fastest approaches to obtain an approximate solution to complicated moving boundary problems that often coincide with exact solutions if exists. Nowadays in many of engineering applications, attention has been directed toward numerical methods such as finite difference, finite volume, finite element and boundary element method which can handle complex moving boundary problems. Finite element and boundary element methods often used to handle complex geometries, but are acknowledged to be more time consuming in terms of computing and programming, finite difference or finite volume techniques are still the most popular at the present due to their simplicity and less programming efforts. The numerical methods of solving phase change problems are categorized as follows: (i) *fixed grid method*, in which the space- time domain is subdivided into a finite number of equal grids for all times. Then the position of solid-liquid interface lies between two grid points at specified time and an interpolation formula is used to locate the interface position, Crank [5] and Ehrlich [6]. (ii) *variable grid method*, in which the space-time domain is subdivided into equal intervals in one direction only and the corresponding grid side in the other direction is determined so that the moving interface always stay at the grid point. Murray and Landis [7] chose equal intervals in the time domain and allow the space interval to change keeping the same number of grid points, in other words the grid spacing is allowed to stretch, with the same number of grids, N, but changing the size of Δx. in this manner the interface position stays exactly at the grid point. (iii) *front-fixing method*, this is essentially a coordinate transformation scheme which immobilize the moving boundary hence alleviating the need to locate the interface position [8]. (iv) *enthalpy method*, this method has been suggested and implemented by several investigators for cases in which the system does not have distinct solid-liquid interface, but separated by mushy region, extended temperature range. In this approach, the total heat content of the substance is used as a dependent variable [9, 10].

In the present paper, solidification of phase-change material (pcm) inside spherical capsule is considered. This work originates from the need of assessing the quantity of heat removal for thermal storage unit that contains spherical capsules filled with pcm and staggered in fluidized bed system; hence these capsules serve as distributed heat sources in the fluidized bed, so knowledge of heat transfer parameters such as Stefan number, Biot number, temperature distribution, and solid mass fraction as well as total solidification time during the process are valuable information to model the latent heat thermal storage unit.

II. Mathematical model

The present work, considers solidification of a liquid initially at the phase-change temperature T_m, confined to the region $0 \le r \le R$. For times > 0, the boundary surface at r = R is subjected to convective cooling into an ambient at constant temperature T_∞ less than the freezing temperature of the phase change material inside the sphere with a heat transfer coefficient h, while the boundary at the center of the sphere at r = 0 is considered to be well insulated or satisfy the symmetry boundary condition, nil temperature gradient. The solidification of PCM starts at the boundary surface r = R and the solid liquid interface moves in the r direction toward the center of the sphere. The temperature T(r,t) varies only in the solid phase, since the liquid region is assumed to be maintained at the phase change temperature, T_m. The main objective is to determine the temperature distribution T(r,t) in the solid phase and the location of interface position as function of time $r_f(t)$. The mathematical formulation of the solidification process is described by the heat conduction equation with the associated boundary and initial conditions.
For the solid region the governing equations are,

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c}\left(\frac{2}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial r^2}\right);\ r_f < r < R \qquad (1)$$

$$\frac{\partial r}{\partial t} = \frac{k}{\rho L}\frac{\partial T}{\partial r} \qquad r = r_f \qquad (2)$$

$$-\frac{\partial T}{\partial r} = \frac{h}{k}(T - T_\infty) \qquad r = R \qquad (3)$$

$$T = T_m \ \ , t = 0\ ;\ 0 < r < R \qquad (4)$$

$$T = T_m \ \ , t = 0\ ;\ 0 < r < r_f \qquad (5)$$

In the above equations r_f is the position of the solidification front, L is the latent heat of fusion of the PCM, T_m is the phase change temperature and k, ρ, c are respectively the thermal conductivity, density, and specific heat of the PCM.

III. Numerical Solution

To obtain the solution in a dimensionless form, the following dimensionless variables are defined,

$$x = 1 - \frac{r}{R} \quad ; \qquad \epsilon = \frac{r_f}{R}$$

$$\tau = \frac{\alpha t}{R^2} \quad ; \quad \theta = \frac{T - T_\infty}{T_m - T_\infty}$$

$$Ste = \frac{c(T_m - T_\infty)}{L} \quad ; \qquad Bi = \frac{hR}{k}$$

When equations (1-5) are rewritten using the dimensionless variables defined above, the result is

$$\frac{\partial \theta}{\partial \tau} = \frac{2}{x-1}\frac{\partial \theta}{\partial x} + \frac{\partial^2 \theta}{\partial x^2} \ \ ;\ 0 < x \qquad (6)$$

$$Ste\,\frac{\partial \theta}{\partial x} = \frac{dx}{d\tau}\,; \qquad x = \epsilon \qquad (7)$$

$$\frac{\partial \theta}{\partial x} = Bi\theta \ \ ; \qquad x = 0 \qquad (8)$$

$$\theta = 1 \ \ , \tau = 0\ ;\ 0 < x < 1 \qquad (9)$$

$$\theta = 1 \ \ ;\ \tau > 0\ ;\ \epsilon < x < 1 \qquad (10)$$

At this point, it is noted that if the sensible heat of the solid is much less than the latent heat of fusion of the PCM, in other words Ste<< 1, then equation 6 is transformed to steady-state equation which can be solved using equation 10.

IV. The Moving Grid

As was mentioned earlier, the disadvantage of the fixed grid method is that the solidification front stays between two grid points and an interpolation scheme has to be used to locate the interface position. To overcome this drawback, Murray and Landis [7] proposed and developed a system of moving mesh for cylindrical geometry. In the present work, the same model is adopted for spherical geometry, where the first grid point is located on the external surface of the sphere and the last grid point is located at the proper solid - liquid interface toward the center of the sphere. In this manner as the sphere is cooled, solid layer builds up and the solidification front is dislocated with time traveling toward the center, with the number of grid points being fixed the mesh is stretched, increasing the size of space increment and at each time level the grid spacing grows but stays uniform. Figure1. Illustrates the model of moving grids at two time levels $\tau and \tau + \Delta\tau$for N = 5.

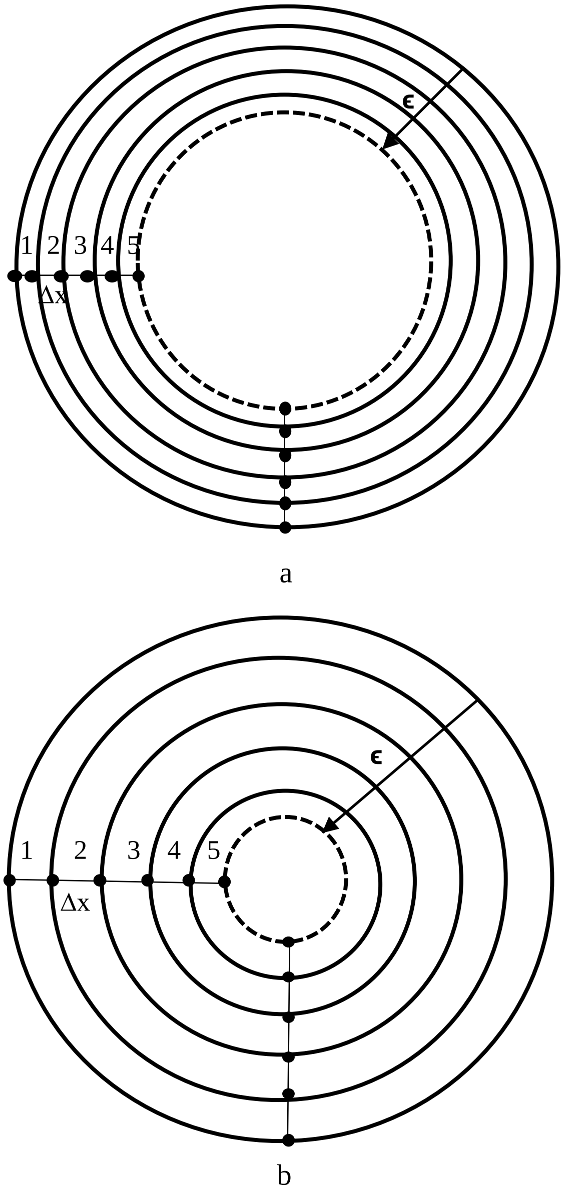

Fig. 1 The model of Moving Mesh Exemplified for N = 5, (a) at τ ; (b) at $\tau + \Delta\tau$

In Order to obtain the solution of the moving boundary problem, the dimensionless form of the conservation equations (6-10) are transformed to an implicit finite difference form following the central differencing scheme for approximating the second derivative and the two-point formulas for the first derivative. The discretization process results in a number of discrete equations which can be solved iteratively to yield the temperature distribution and interface location at each time level. Due to the ease and simplicity, the Gauss-Seidel method has been used to solve the system of algebraic equations where the most recently determined values are used in each round of iteration.

V. Results And Discussions

In this work the solidification process of phase change material has been investigated and the results of temperature distribution, tracking of interface position, surface temperature and heat flux are presented in dimensionless form. The solution of the conduction equation, with associated boundary and interface conditions, was conducted through the development of computer code written in FORTRAN, with the implementation of moving grid and variable time step. The time step size was monitored in a manner that the Van Newman criterion is satisfied to insure solution stability. A mesh dependency test has been performed to insure that the solution is converged, this is conducted through mesh refining, hence N = 20 have met the mesh sensitivity test. The final results are demonstrated through figures 2 to 5. Figure 2 shows the time dependence of the solid-liquid interface, as can be seen this curve actually separates two phases, the liquid phase at the phase change temperature and the solid phase which experience temperature gradient over its domain. As expected the variation of surface temperature of the sphere is shown in Figure 3, as can be seen the surface temperature drops drastically at the beginning of the process then approximately smoothed out to the exponential behavior. This can be attributed to the temperature difference between the cooling fluid and the surface of the sphere and also to the high convection coefficient. The heat removal from the sphere (PCM) is demonstrated in figure 4, as can be seen at early times the heat flux is large as expected, and drops significantly as the total solidification time is reached. Finally, the temperature distribution through the solid phase is shown in figure 5. This temperature profile is reached at the end of the solidification process. It is clear that the maximum temperature occurs at the center of the sphere, the point where the dimensionless variable, x = 1 and the minimum temperature occurs at the surface of the sphere where the variable, x equal to zero.

VI. Conclusions

This work has presented the numerical solution of moving boundary problem using numerical method that is well suited to phase change problems. The main features of this work is that moving grid has been adopted to spherical geometry and can be used to track the solid liquid interface without the need to interpolate between grid points to locate the front position. As mentioned earlier, knowledge of the heat pumped by the PCM to the surrounding fluid which is depicted by the present work is very significant when dealing with modeling of phase change suspension.

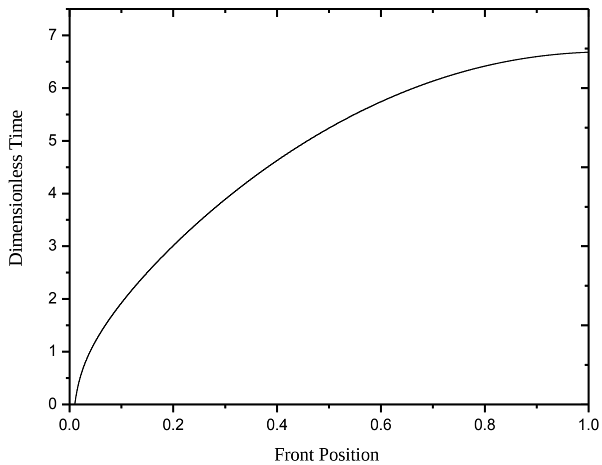

Fig.2. Dimensionless Front Position vs Dimensionless Time

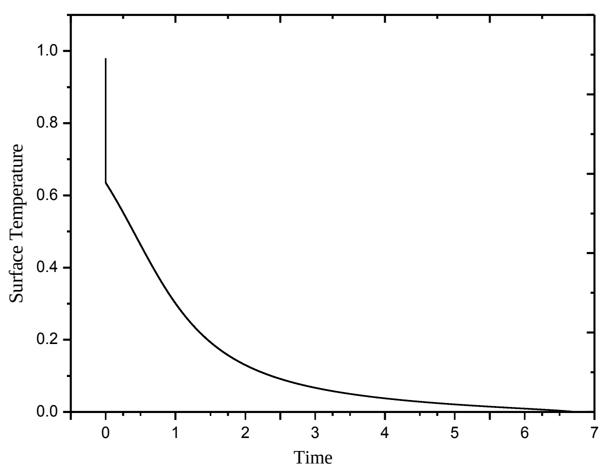

Fig. 3 Dimensionless Surface Temperature vs Dimensionless Time

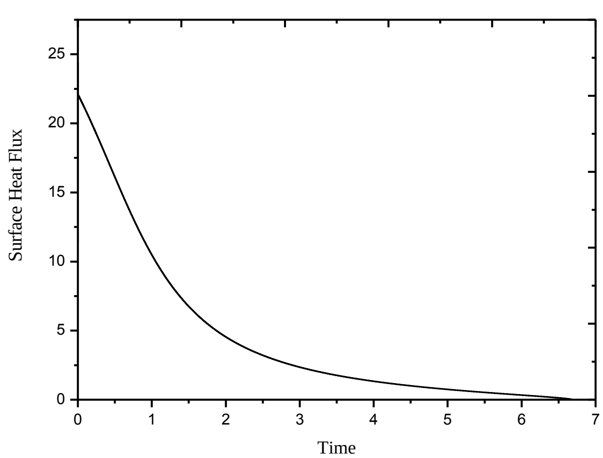

Fig. 4 Surface Heat Flux (dimensionless) vs Dimensionless Time

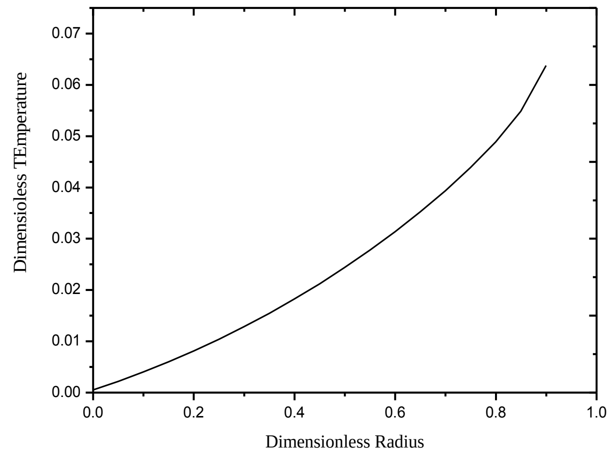

Fig 5. Tmperature distribution vs Dimensionless Coordinate, x

References

[1] Lame G & Clapeyron B.P.E 1831 Memoire sur la solidification par refroidissment d'un globe solid *Ann. Chem. Phys*. **47** 250-60.
[2] Stefan J 1889 *S B Wein Akad. Mat. Natur*. **98** 473-84, 965-83
[3] Stefan J 1891 Uber die theorie der eisbildung, inbesondere uber die eisbildung im polameer *Ann Chem. Phys*. **42** 269-86
[4] Crank J 1984 *free and moving boundary problems* (Oxford: Clarendon).
[5] J. Crank, *J. Mech. Appl. Math*. **10**, 220-231, 1957.
[6] L. W. Ehrlick, *J. Assn. Comp. Math*. **5**, 161-176, 1958.
[7] W. D. Murry & F. Landis, *Trans. Am. Soc. Mech. Eng.* **81,** 106, 1959.
[8] R. M. Furzeland, *J. Inst. Math. Appl*. **26,** 411-429, 1980.
[9] N. Shamsunder & E. M. Sparrow, *J. Heat Tranaser***97c**, 333-340, 1975.
[10] K. H. Tacke, *Int. J. Num. Meth. Eng*. **21**, 147-150, 1985.
[11] Vasilios Alexiades, Alan D. Solomon, Mathematical modeling of melting and freezing processes, Hemisphere Publishing Corporation, 1993.
[12] M. Necati OZISik, Heat Conduction, second edition (Chapter 11). *Phase Change Problems John Wiley&Sons, Inc*, 1993.