

# A Combined Collocation and Grid Methods to Solve Phase Change Problems with Moving Boundaries

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**Abstract:** Moving boundary problems require special care of treatment due to its complex nature and high non-linearity represented by so many factors, one of these factors the nature of the boundary conditions at the moving boundary. Since long time ago, numerical methods became more suitable for solution. In the present paper, a hybrid numerical method is developed to solve these types of problems. A hybrid collocation and grid method based radial basis function is derived herein with simultaneous numerical iterative algorithm to solve moving boundary problems. Two test practical problems are solved, the first is the dissolution in binary alloys and the second is the solidification in a two dimensions prism. For the first test problem, the computed results are compared with available numerical solution, while the second one, no analytical solution available, but the computed results are compared with available numerical results. The present method promises well as a new trend of numerical methods of solution for moving boundary problems.

**Keywords:** Moving boundary problem, phase change problems, binary alloys, collocation method, grid method, Precipitates dissolution.

## I. INTRODUCTION

Moving boundary problems are old field of research and still new up to more upcoming years due to its wide applications in science, technology and engineering applications. If one wants to describe or give brief definition to moving boundary problems, easiest way of definition is a set of partial differential equations with associated boundary and initial conditions, one or more of its boundaries are varying with time and should be determined as a major part of the required solution. The moving boundary problems are highly non-linear due to existence of heat balance, mass balance or both at the moving interfaces. Heat transfer is one type of moving boundary problems. Heat treatment of metals is often necessary to optimize their mechanical properties both for further processing and final use during the heat treatment the metallurgical state of the alloy changes [1-2]. This change can either involve the phases being present or the morphology of the various phases [3]. Aluminum alloys usually contain precipitates and in-homogeneities, these in-homogeneities can be removed with a thermal treatment, during which the precipitates dissolve. Although precipitate dissolution is not

the only metallurgical process-taking place during homogenization, it is often the most critical of the processes occurring. Precipitates dissolution can be modeled as one, two or three moving boundary problem. Till now, there are neither general models for micro structural changes nor general models for the kinetics of these changes [4-5]. Models describing the process as a moving boundary problem is also, referred to as Stefan problems [6]. In recent years, the simpler models covering binary and ternary alloys have been extended to cover multi-component particles [7]. Due to the complex nature of the moving boundary problems very few analytical solutions are available and limited to infinite or semi-infinite domain problems. Existence and uniqueness of analytical solutions had been proved by Evan and Douglas, respectively in [8-9]. For long time researchers recognized problems such as, labor intensive, time-consuming and error-prone task when using a mesh-based method such as finite element method [10]. One way for their efforts to overcome these problems was the automatic mesh generation the second way to overcome such problems was developing the mesh-less methods. Mesh-less methods for solving boundary value problems have been extensively popularized owing to their flexibility in engineering applications, especially for problems with discontinuities and because of high accuracy of the computed results [11]. Mesh-free methods do not require a mesh to discretize the domain of the problem under consideration, and the approximate solution is constructed entirely based on a set of scattered nodes. For long time the researchers recognized problems when using a mesh-based method such as finite element method [12-13]. One way for their efforts to overcome these problems was the automatic mesh generation. Automatic mesh generation is difficult to be fully generated in a wide range of engineering applications. The second way to overcome such problems was developing the mesh-less methods [14]. The initial idea of mesh-less methods dates back to the smooth particle hydrodynamics method for modeling astro-physical phenomena [15]. Several domain type mesh-free methods such as element free Galerkin method [16], reproducing kernel particle method [17], the point interpolation method [18] and the mesh-less Petrov-Galerkin method [19] have been proposed and achieved remarkable progress in solving a wide range of static and

dynamic problems for solid and structures. Advection-diffusion equation is one of the most important partial differential equations and observed in a wide range of engineering and industrial applications [20]. It has been used to describe heat transfer in a draining film [21], water transfer in soil [22], dispersion of tracers in porous media [23], contaminant dispersion in shallow lakes [24], the spread of solute in a liquid flowing through a tube, long-range transport of pollutants in the atmosphere [25] and dispersion of dissolved salts in groundwater [26]. Accurate numerical solution of the advection-diffusion equation is usually characterized by a dimensionless parameter, called Peclet number. These results become increasingly difficult as the Peclet number increases due to onset of spurious oscillations or excessive numerical damping if finite difference [27] or finite element formulations are used [28]. In the present paper, a hybrid numerical method is developed to solve these types of problems. A hybrid collocation and grid method based radial basis function is derived herein with simultaneous numerical iterative algorithm to solve moving boundary problems. Two test practical problems are solved, the first is the dissolution in binary alloys and the second is the solidification in a two dimensions prism. For the first test problem, the computed results are compared with available analytical solution, while the second one, no analytical solution available, but the computed results are compared with available numerical results. The present method promises well as a new trend of numerical methods of solution for moving boundary problems.

## II. MATHEMATICAL FORMULATION

Consider a domain  $\Omega = [0, \ell]$  that is composed by a particle whose domain is denoted by  $\Omega_{part} = [0, s(t))$  and diffusive phase  $\Omega_{diff\ ph} = [s(t), \ell]$ . We consider the concentration  $c(x, t)$  of certain material within  $\Omega = \Omega_{part} \cup \Omega_{diff\ ph}$ . Assume the concentration of the particle is constant and denoted by  $c_{part}$ . The configuration of the problem is shown in figure (1).

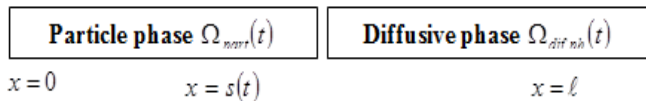


Figure (1): Problem configuration

The state equations with the associated boundary and initial conditions are as follow:

$$\frac{\partial c(x, t)}{\partial t} = \frac{\partial}{\partial x} \left( D \frac{\partial c(x, t)}{\partial x} \right) \quad x \in \Omega_{diff\ ph} = [s(t), \ell], \quad t > 0 \quad (1)$$

$$c(x, t) = c_{part} \quad x \in \Omega_{part}, \quad t \geq 0 \quad (2)$$

$$c(x, t) = c^{sol} \quad x \in \Gamma(t), \quad t \geq 0 \quad (3)$$

Condition represents the mass balance of atoms transferred to the diffusive phase:

$$v_n(x, t)(c_{part} - c^{sol}) = D \frac{\partial c(x, t)}{\partial n} \quad x = s(t), \quad t > 0 \quad (4)$$

It is assumed in the model that there is no concentration transport, i.e.,

$$\frac{\partial c(x, t)}{\partial x} = 0 \quad x \in \partial\Omega, \quad \partial\Omega = 0 \quad \text{or} \quad \ell, \quad t > 0 \quad (5)$$

Assume also a piecewise initial concentration of the form:

$$c(x, t) = \begin{cases} c_{part} & 0 \leq x < s_0 \\ c_{sol} & x = s_0 \\ c_0 & s_0 < x \leq \ell \end{cases} \quad (6)$$

## III. ANALYTICAL DERIVATION OF THE METHOD

Starting the derivation by dealing with equation (1) and let us approximate the concentration as follows:

$$c(x, t) \cong \sum_{j=1}^{N_b+N_i} a_j \phi_{ij} + \sum_{j=1}^{N_b} b_j \phi_{ij}, \quad i = 1, 2, \dots, N_b + N_a \quad (7)$$

Apply equation (7) into equation (1), the latter will be:

$$\frac{\partial c(x, t)}{\partial t} = D \left( \sum_{j=1}^{N_b+N_i} a_j \nabla^2 \phi_{ij} + \sum_{j=1}^{N_b} b_j \nabla^2 \phi_{ij} \right) \quad (8)$$

By making use of forward approximation to the time differentiation in equation (8), this will leads to:

$$\frac{c^{k+1} - c^k}{\Delta t} = D \left( \sum_{j=1}^{N_b+N_i} a_j \nabla^2 \phi_{ij} + \sum_{j=1}^{N_b} b_j \nabla^2 \phi_{ij} \right) \quad (9)$$

where  $c^{k+1}$  and  $c^k$  are the concentration at times  $(k+1)$  and  $(k)$ ,  $\Delta t$  is the time step,  $N_b, N_i$  are boundary and internal

nodes, respectively and finally,  $a_j, b_j$  are unknown constants to be determined as a major part of the proposed method. Equation (9), can now be re-written as:

$$\left( \sum_{j=1}^{N_b+N_i} a_j \nabla^2 \phi_{ij} + \sum_{j=1}^{N_b} b_j \nabla^2 \phi_{ij} \right)^{k+1} = \left( D\Delta t \sum_{j=1}^{N_b+N_i} a_j \nabla^2 \phi_{ij} + D\Delta t \sum_{j=1}^{N_b} b_j \nabla^2 \phi_{ij} + \sum_{j=1}^{N_b+N_i} a_j \phi_{ij} + D\Delta t \sum_{j=1}^{N_b} b_j \phi_{ij} \right)^k \quad (10)$$

By summing up the corresponding terms in the left hand side of equation (10), leads to:

$$\left( \sum_{j=1}^{N_b+N_i} a_j \nabla^2 \phi_{ij} + \sum_{j=1}^{N_b} b_j \nabla^2 \phi_{ij} \right)^{k+1} = \left( \sum_{j=1}^{N_b+N_i} (a_j) (\phi_{ij} + D\Delta t \nabla^2 \phi_{ij}) + \sum_{j=1}^{N_b} (b_j) (\phi_{ij} + D\Delta t \nabla^2 \phi_{ij}) \right)^k \quad (11)$$

In a simple compact matrix form, equation (11) can now take the form:

$$(A_{ij} a_j + B_{ij} b_j)^{k+1} = (C_{ij} b_j + C_{ij}^* b_j)^k \quad (12)$$

where

$$A_{ij} = \begin{bmatrix} \phi_{11} & \phi_{12} & \dots & \phi_{1N_b+N_i} \\ \phi_{21} & \phi_{22} & \dots & \phi_{2N_b+N_i} \\ \dots & \dots & \dots & \dots \\ \phi_{N_b+N_i1} & \phi_{N_b+N_i2} & \dots & \phi_{N_b+N_iN_b+N_i} \end{bmatrix}$$

$$B_{ij} = \begin{bmatrix} \phi_{11} & \phi_{12} & \dots & \phi_{1N_b} \\ \phi_{21} & \phi_{22} & \dots & \phi_{2N_b} \\ \dots & \dots & \dots & \dots \\ \phi_{N_b+N_i1} & \phi_{N_b+N_i2} & \dots & \phi_{N_b+N_iN_b} \end{bmatrix}$$

$$C_i = \begin{bmatrix} \phi_{11} + D\Delta t \nabla^2 \phi_{11} & \phi_{12} + D\Delta t \nabla^2 \phi_{12} & \dots & \phi_{1N_b+N_i} + D\Delta t \nabla^2 \phi_{1N_b+N_i} \\ \phi_{21} + D\Delta t \nabla^2 \phi_{21} & \phi_{22} + D\Delta t \nabla^2 \phi_{22} & \dots & \phi_{2N_b+N_i} + D\Delta t \nabla^2 \phi_{2N_b+N_i} \\ \dots & \dots & \dots & \dots \\ \phi_{N_b+N_i1} + D\Delta t \nabla^2 \phi_{N_b+N_i1} & \phi_{N_b+N_i2} + D\Delta t \nabla^2 \phi_{N_b+N_i2} & \dots & \phi_{N_b+N_iN_b+N_i} + D\Delta t \nabla^2 \phi_{N_b+N_iN_b+N_i} \end{bmatrix}$$

$$C_j^* = \begin{bmatrix} \phi_{11} + D\Delta t \nabla^2 \phi_{11} & \phi_{12} + D\Delta t \nabla^2 \phi_{12} & \dots & \phi_{1N_b+N_i} + D\Delta t \nabla^2 \phi_{1N_b+N_i} \\ \phi_{21} + D\Delta t \nabla^2 \phi_{21} & \phi_{22} + D\Delta t \nabla^2 \phi_{22} & \dots & \phi_{2N_b+N_i} + D\Delta t \nabla^2 \phi_{2N_b+N_i} \\ \dots & \dots & \dots & \dots \\ \phi_{N_b+N_i1} + D\Delta t \nabla^2 \phi_{N_b+N_i1} & \phi_{N_b+N_i2} + D\Delta t \nabla^2 \phi_{N_b+N_i2} & \dots & \phi_{N_b+N_iN_b+N_i} + D\Delta t \nabla^2 \phi_{N_b+N_iN_b+N_i} \end{bmatrix}$$

The next step is to deal with the boundary conditions at the moving boundary, and let us start with the boundary condition given by equation (3):

$$\sum_{j=1}^{N_b+N_i} a_j \phi_{ij} + \sum_{j=1}^{N_b} b_j \phi_{ij} = c^{\text{sol}} \mathbf{I} \quad (13)$$

where  $\mathbf{I}$  is a unit vector of dimension  $(N_b + N_i \times 1)$ . This equation in a simplified matrix form takes the following form:

$$D_{ij} b_j + F_{ij} (a_j) = u^{\text{sol}} \quad (14)$$

where

$$D_{ij} = \begin{bmatrix} \phi_{11} & \phi_{12} & \phi_{13} & \dots & \phi_{1N_b+N_i} \\ \phi_{21} & \phi_{22} & \phi_{23} & \dots & \phi_{2N_b+N_i} \\ \dots & \dots & \dots & \dots & \dots \\ \phi_{N_b+N_i1} & \phi_{N_b+N_i2} & \phi_{N_b+N_i3} & \dots & \phi_{N_b+N_iN_b+N_i} \end{bmatrix}$$

And

$$F_{ij} = \begin{bmatrix} \phi_{11} & \phi_{12} & \phi_{13} & \dots & \phi_{1N_b} \\ \phi_{21} & \phi_{22} & \phi_{23} & \dots & \phi_{2N_b} \\ \dots & \dots & \dots & \dots & \dots \\ \phi_{N_b+N_i1} & \phi_{N_b+N_i2} & \phi_{N_b+N_i3} & \dots & \phi_{N_b+N_iN_b} \end{bmatrix}$$

From equation (14), one can get:

$$a_j = u^{\text{sol}} F_{ij}^{-1} - F_{ij}^{-1} D_{ij} b_j \quad (15)$$

Next, let us dealing with the other boundary condition as follows:

$$v_n(x, t) (c_{\text{part}} - c^{\text{sol}}) = D \sum_{j=1}^{N_b+N_i} a_j \frac{\partial}{\partial n} \phi_{ij} + \sum_{j=1}^{N_b} b_j \frac{\partial}{\partial n} \phi_{ij}, i = 1, 2, \dots, N_b + N_a \quad (16)$$

In a compact matrix form, equation (16) can be re-written as:

$$\Phi_{ij} a_j + \Psi_{ij} b_j = \left( \frac{\mathbf{u}^{\text{part}} - \mathbf{u}^{\text{sol}}}{\mathbf{D}} \right) \mathbf{v}_j \quad (17)$$

From equation (17), one can get the unknown  $a_j$  as follows:

$$a_j = \left( \frac{\mathbf{u}^{\text{part}} - \mathbf{u}^{\text{sol}}}{\mathbf{D}} \right) \Phi_{ij}^{-1} \mathbf{v}_j - \Phi_{ij}^{-1} \Psi_{ij} b_j \quad (18)$$

Equating equations (15) and (18), leads to:

$$\left( \frac{\mathbf{u}^{\text{part}} - \mathbf{u}^{\text{sol}}}{\mathbf{D}} \right) \Phi_{ij}^{-1} \mathbf{v}_j - \Phi_{ij}^{-1} \Psi_{ij} b_j = \mathbf{u}^{\text{sol}} F_{ij}^{-1} - F_{ij}^{-1} D_{ij} b_j \quad (19)$$

Simplifying equation (19), leads to:

$$b_j = \frac{\left( \frac{\mathbf{u}^{\text{part}} - \mathbf{u}^{\text{sol}}}{\mathbf{D}} \right) \Phi_{ij}^{-1} \mathbf{v}_j - \mathbf{u}^{\text{sol}} F_{ij}^{-1}}{(\Phi_{ij}^{-1} \Psi_{ij} - F_{ij}^{-1} D_{ij})} \quad (20)$$

Finally, let us deal with the boundary condition given by equation (5), leads to:

$$\frac{\partial}{\partial x} \sum_{j=1}^{N_b+N_i} a_j \phi_{ij} + \sum_{j=1}^{N_b} b_j \phi_{ij} = 0, i = 1, 2, \dots, N_b + N_a \quad (21)$$

In a compact matrix form, equation (21) can be re-written as follows:

$$\mathbf{L}_{ij} a_j = \mathbf{K}_{ij} b_j \quad (22)$$

where

$$\mathbf{L}_{ij} = \begin{bmatrix} \frac{\partial \phi_{11}}{\partial n} & \frac{\partial \phi_{12}}{\partial n} & \frac{\partial \phi_{13}}{\partial n} & \dots & \frac{\partial \phi_{1N_b+N_i}}{\partial n} \\ \frac{\partial \phi_{21}}{\partial n} & \frac{\partial \phi_{22}}{\partial n} & \frac{\partial \phi_{23}}{\partial n} & \dots & \frac{\partial \phi_{2N_b+N_i}}{\partial n} \\ \dots & \dots & \dots & \dots & \dots \\ \frac{\partial \phi_{N_b+N_i+1}}{\partial n} & \frac{\partial \phi_{N_b+N_i+2}}{\partial n} & \frac{\partial \phi_{N_b+N_i+3}}{\partial n} & \dots & \frac{\partial \phi_{N_b+N_i+N_b+N_i}}{\partial n} \end{bmatrix} \quad (23)$$

$$\mathbf{K}_{ij} = (-) \begin{bmatrix} \frac{\partial \phi_{11}}{\partial n} & \frac{\partial \phi_{12}}{\partial n} & \frac{\partial \phi_{13}}{\partial n} & \dots & \frac{\partial \phi_{1N_b}}{\partial n} \\ \frac{\partial \phi_{21}}{\partial n} & \frac{\partial \phi_{22}}{\partial n} & \frac{\partial \phi_{23}}{\partial n} & \dots & \frac{\partial \phi_{2N_b}}{\partial n} \\ \dots & \dots & \dots & \dots & \dots \\ \frac{\partial \phi_{N_b+N_i+1}}{\partial n} & \frac{\partial \phi_{N_b+N_i+2}}{\partial n} & \frac{\partial \phi_{N_b+N_i+3}}{\partial n} & \dots & \frac{\partial \phi_{N_b+N_i+N_b}}{\partial n} \end{bmatrix} \quad (24)$$

Equation (22) is a direct relation between the unknown constants  $a_j$  &  $b_j$ , from which one can get the following form:

$$a_j = \mathbf{L}_{ij}^{-1} \mathbf{K}_{ij} b_j \quad (25)$$

Now then, we have two direct system of relations for the unknown  $a_j$  and two systems for  $b_j$  one of them is direct and the other is indirect. These relations will be used in two different ways, the first is a computation purpose and the other is a check in the iterative procedure, as will be seen in the next section.

#### IV. NUMERICAL ITERATIVE ALGORITHM

In the present paper, a new suggested iterative numerical algorithm is developed as follows:

1. Guess an initial position for the moving boundary and subsequently its velocity, assuming linear variation between them.
2. Solve system given by equation (15) at the time step  $t = k$  to get  $\{a_j\}_{\text{Eq.15}}$
3. Solve system given by equation (25) at the time step  $t = k$  to get  $\{a_j\}_{\text{Eq.25}}$
4. Compute the error  $E = \left| \{a_j\}_{\text{Eq.25}} - \{a_j\}_{\text{Eq.15}} \right|$
5. Solve system given by equation (20) at the time step  $t = k$  to get  $b_j$
6. Check step, if  $E \leq \varepsilon_{\text{Prescribed}}$ , go to the next time step, if not update both moving interface position and its velocity and repeat steps 2-6

#### V. NUMERICAL RESULTS

##### Example -I-

This example is a direct application of the proposed new method to the problem given by the system of the governing equation and the associated boundary and initial condition given by equations (1-6) with the numerical data given in table (1).

Table 1: Numerical data

$C_{Part}$	$C_o$	$\ell$	$s_0$	$D$
0.53	0.1	1.0	0.2	1

Starting the computations based on the proposed new method and the proposed iterative algorithm, the movement of the moving boundary is shown in figure (2).

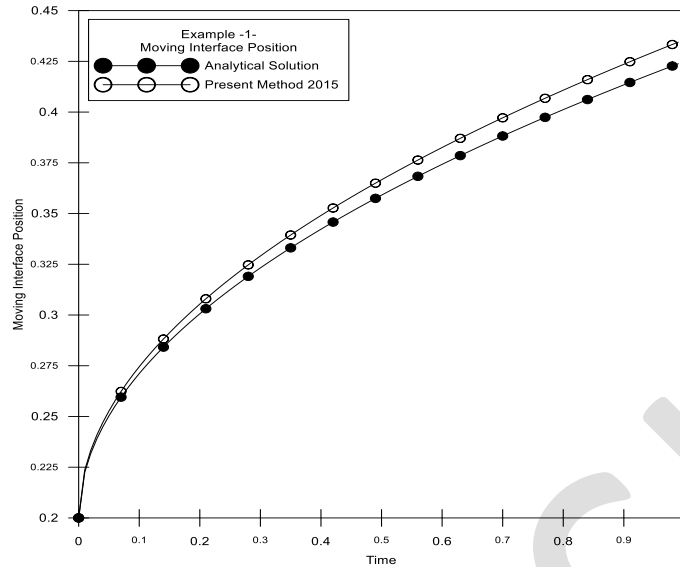


Figure (2): Movement of the moving boundary for example -1-

As it is appear the present solution is close to the analytical similarity solution. In the beginning of the time and up to time nearly equal 0.3 an agreement between the two solutions with some errors. Follow up the computations based the proposed new method, the concentration in both phases via space variable at different times 0.01, 0.05, 0.1, 1.0 are plotted as shown in figures (3-6), respectively.

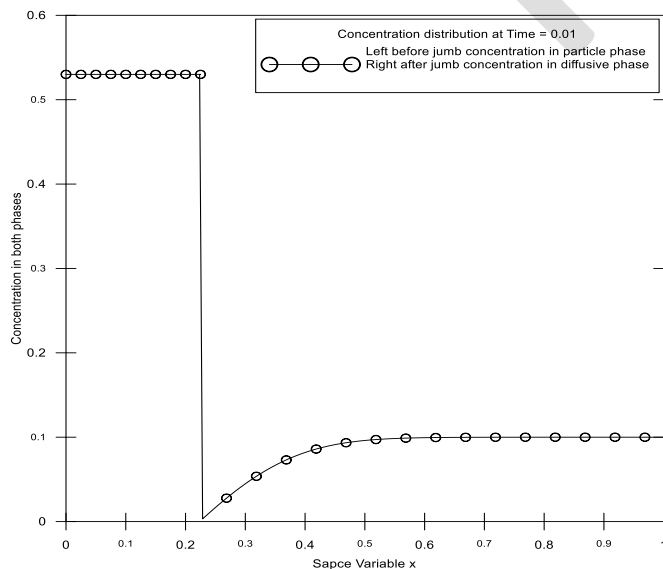


Figure (3): Concentration in both phases at time = 0.01

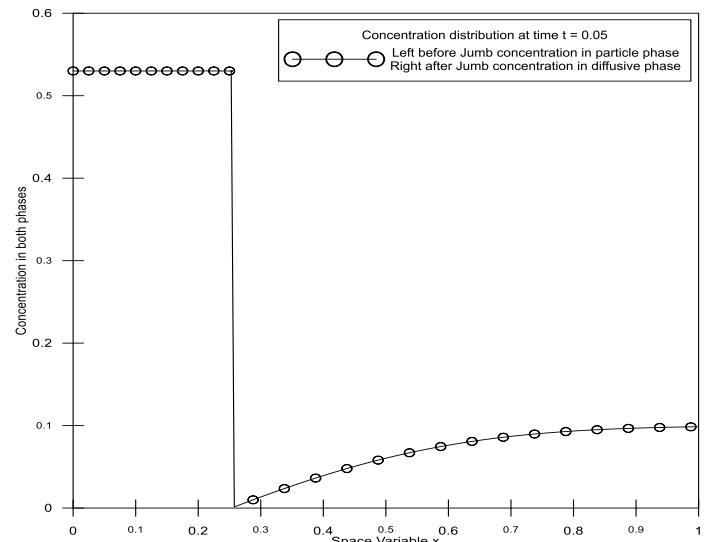


Figure (4): Concentration in both phases at time = 0.05

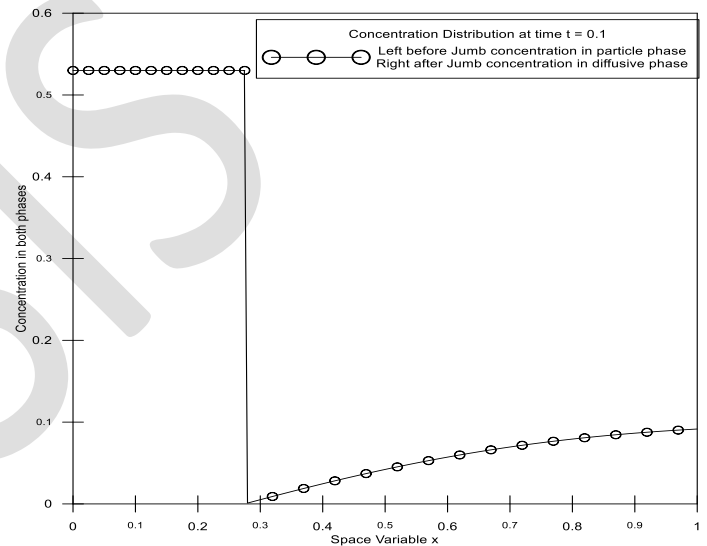


Figure (5): Concentration in both phases at time = 0.10

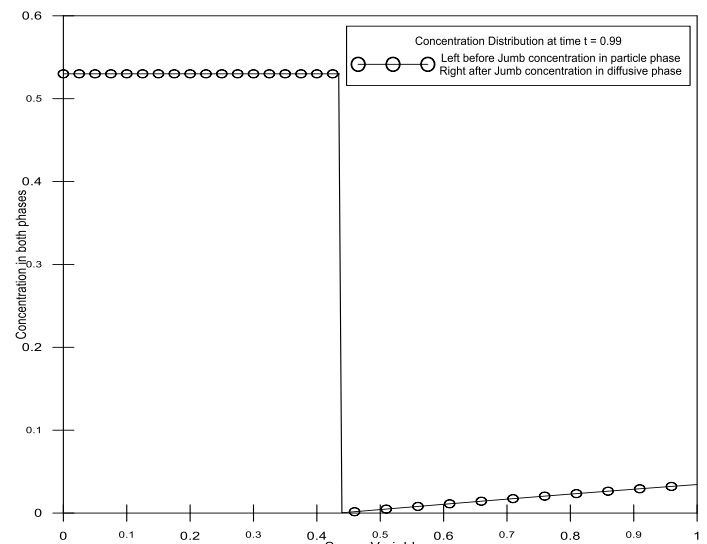


Figure (6): Concentration in both phases at time = 1.0

As it is clear the concentration in the particle domain is always constant and equals to the boundary condition 0.53. On the other side the concentration in the diffusive phase starts at the point very close to the moving boundary at the time of computations. Therefore, the starting point of these curves is different from case to another due to the position of the moving boundary at these times. The behavior of the concentration at these times is the same and agrees with physical behavior of the problem. The variation of the concentration with time at three different points is also computed using the present method and the results are shown in figures (7-9) respectively.

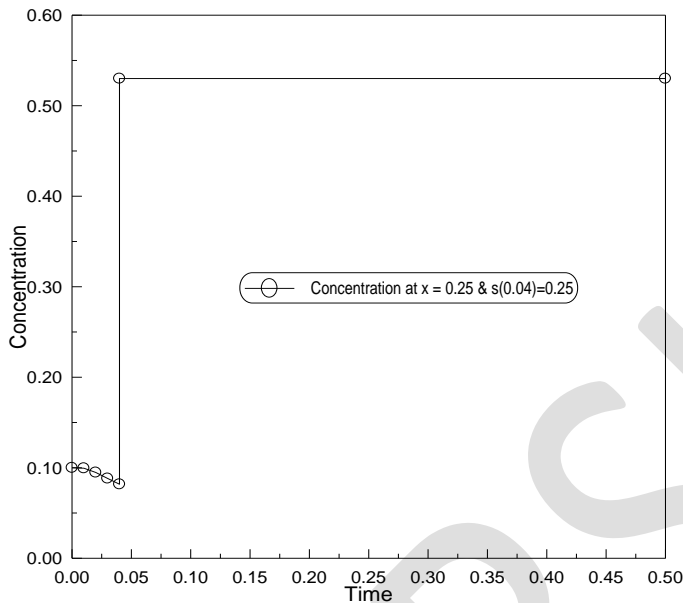


Figure (7): Concentration at  $x = 0.25$  -Example (1)

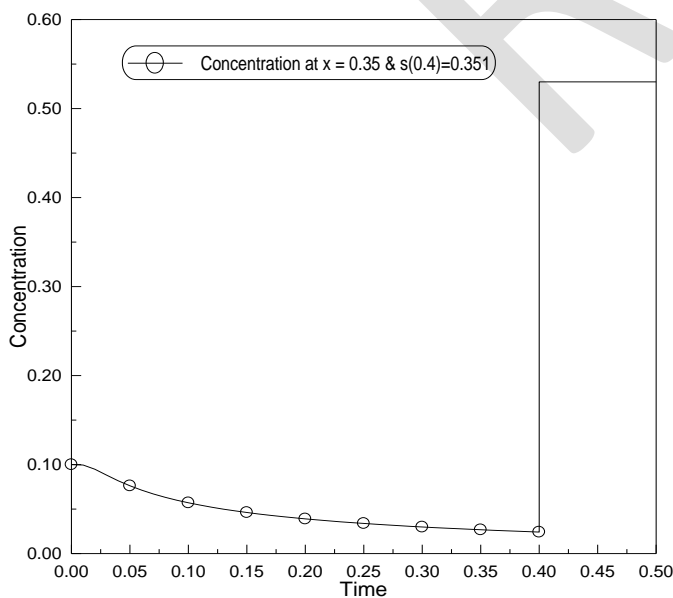


Figure (8): Concentration at  $x = 0.35$  - Example (1)

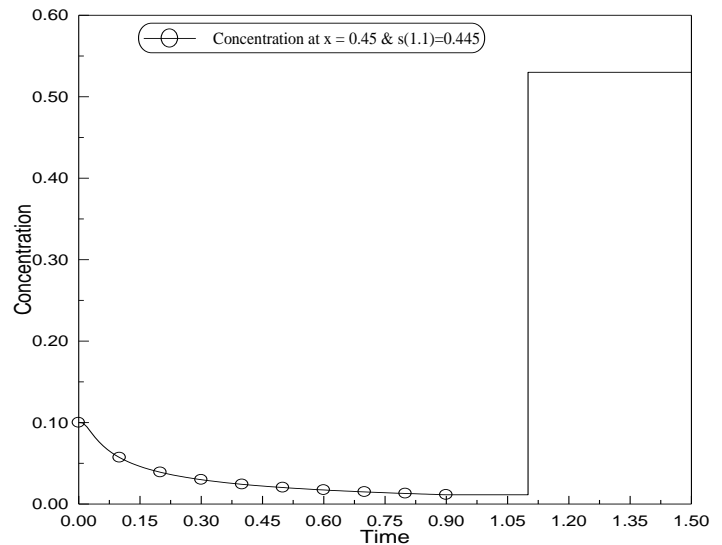


Figure (9): Concentration at  $x = 0.45$ -Example (1)

It is clear from figures (7-9) that the concentrations at time zero equal the initial condition. The behavior of the concentration after that decreases till the concentration at the moving boundary, then jump in the concentration profile occur at behave constant value at equal to the particle concentration.

#### Example -2-

A square of dimensions  $2 \times 2$  initially filled with liquid at the melting temperature. The surface is suddenly cooled at time zero to the temperature  $u_0$  and the solidification proceeds inwards. Two phases will appear, solid and liquid, respectively. This problem is a classical Stefan problem and solved using different numerical methods before. One of these methods given by Rao, and the results due to the present method are compared with the results due to Rao. The following non-dimensional (normalized) parameters are used in the computation.

$$\overline{k_s} = 1$$

$$\overline{c_s} = 1$$

$$\overline{x} = \frac{x}{R}$$

$$\overline{y} = \frac{y}{R}$$

$$\overline{k_\ell} = k_\ell / k_s$$

$$\overline{c_\ell} = c_\ell / c_s$$

$$\tau = \frac{k_s t}{R^2}$$

$$\Theta = \frac{(u - u_m)}{(u - u_0)}$$

$$\overline{L} = \frac{1}{\text{Stef number}}$$

$$\text{Stef number} = \frac{c_s (u_m - u_0)}{L}$$



The results started by a comparison between the present method and the method proposed by Rao *et. al.*. The comparison started by plotting the moving interfaces due to both methods at three different times as shown in figure (6). As it is clear there is a very good agreement between the results. Also it is clear that the behavior of the moving interface moves as a one-dimensional case at the beginning of the process and the effect of two dimension starts appearing at later times.

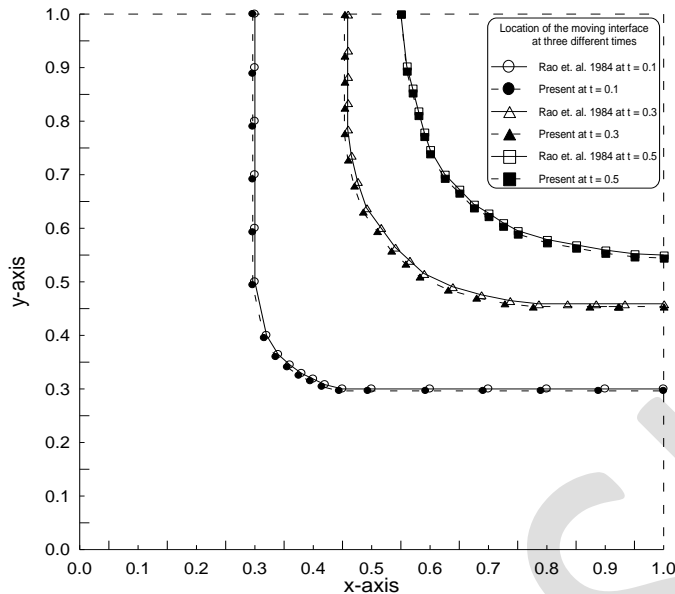


Figure (7): 2-D moving interface without mushy zone at three different times

The normalized temperature due to the present algorithm is presented in figure (7) and compared with the results due to Rao *et. al.*. The temperature verses time at two different points (1,0.2) and (1,0.4) is plotted, as seen an acceptable agreement is obtained and the error can be neglected.

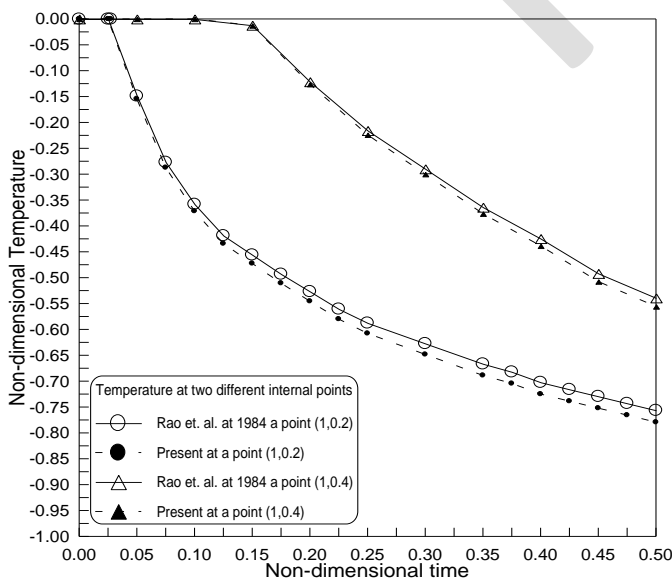


Figure (8): Non-dimensional temperature variation at two different times

## VI. CONCLUSION

Dealing with moving boundary problems in general case, needs special care due to the non-linearity inherent at the moving boundary as well as its complex nature. The proposed method herein, is a hybrid collocation and Cartesian grid numerical method. It is clear that the mathematics of the proposed method is so simple compared with other numerical methods such as finite element and boundary elements methods. The computations of the proposed method are so easily just need careful with matrices. The collocation based radial basis function itself is an easy numerical technique and it does not need to deal with the overall domain, also the Cartesian grid method is easily manipulated but requires special care. The proposed hybrid method collects the advantages of both methods and avoid the disadvantages. The results due to the present method give promises to solve wide range of moving boundary problems with acceptable error.

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