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NEW APPROACH OF BEM METHODS TO SOLVE SOLUTE DIFFUSION PROBLEMS WITH MOVING BOUNDARIES

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ABSTRACT

In the present paper, the boundary element method with numerical front tracking algorithm is developed to solve solute and diffusion problems with moving boundaries. The method starts by solving the problem over the entire domain with fixed boundaries and treat the moving interface as an interior point to find the temperature at that point. Then solve the problem again but as two phase problem with moving interface as a common point to find the the temperature gradient at the moving boundary. At this stage the energy balance are checked within a prescribed tolerance and upgrade the location if the accuracy is not satisfied. The same procedure is repeated for the concentration at each time step up to the end of the process.

Keywords: Stefan problem, Moving boundary problems, Boundary element method.

Nomenclature

Ω	Overall domain of the problem
Ω_1	Domain of the first phase
Ω_2	Domain of the second phase
Ω'	Initial domain
$x_1^2 = x_2^1 = s(t)$	Moving interface in case of two phase problem
$x_1^1 = 0, x_2^2 = a$	Fixed boundaries
$c_i, i = 1, 2$	Heat capacity/ unit volume

$K_i, i = 1, 2$	Thermal conductivity
$T_i, i = 1, 2$	Temperature
$C_i, i = 1, 2$	Concentration
$D_i, i = 1, 2$	Chemical diffusivity
$h_i, i = 1, 2$	Two known functions
λ	Latent heat
$A_i, i = 1, 4$	Real constants
$F_i^T(t), F_i^C(t) i = 1, 2$	Known functions
ξ	Source point
x	Field point
$\beta(\xi)$	Constant appear in the BIE-equation
r	Euclidian distance between ξ and x

INTRODUCTION

Moving boundary problems are of practical and industrial importance and widely, encountered in the metal, glass, plastic and oil industries etc. These problems are modelled through a set of partial differential equations with associated boundary and initial conditions. The solution of moving boundary problems are usually over a domain whose one or more of its boundaries are moving as a consequence of dynamics of the internal processes.

From the mathematical point of view, the inherent non-linearity of such problems poses significant theoretical difficulties [1-2], while their practical applications generally requires a numerical method of solution [3]. Direct numerical methods for solving moving boundary problems have taken two basic directions; the fixed domain methods and the front tracking method. Practical engineering problems are efficiently solved nowadays only by numerical methods [4-6]. Finite difference, finite element or more popularity boundary element method used to determine both steady-state as well as transient fields [7-8]. One of the most interesting methods of solution of phase change problems with moving interfaces is the source and sink method (SSM) [9], this method is an extension of the Lightfoot

method [10] which was originally developed for the solution of a solidification problem imposed with a constant temperature condition.

The source and sink method was then extended to solve two dimensional Stefan problems by Rathjien and Jiji [11] and Budhia and Kreith [12]. Over recent decades, the boundary element method has received much attention from researchers and has become an important technique in the computational solution of a number of physical problems. The basis of the method is to transform the original partial differential equation into an equivalent integral equation by means of the corresponding Green's representation formula or in terms of continuous distribution of singular solutions of the partial differential equation over the boundaries of the problem. The boundary element method is somewhat similar to the source and sink method and the difference appears in the Green's representation used.

In the present paper, the boundary element method with numerical front tracking algorithm is developed to solve solute and diffusion problems with moving boundaries. The method starts by solving the problem over the entire domain with fixed boundaries and treat the moving interface as an interior point to find the temperature at that point. Then solve the problem again but as two phase problem with moving interface as a common point to find the the temperature gradient at the moving boundary [13-14]. At this stage the energy balance are checked within a prescribed tolerance and upgrade the location if the accuracy is not satisfied. The same procedure is repeated for the concentration at each time step up to the end of the process.

MATHEMATICAL FORMULATION

Consider two substances diffuse simultaneously into a domain $\Omega = \Omega_1 \cup \Omega_2$, where Ω_1 and Ω_2 are two homogeneous adjacent domains separated by a moving interface $s(t)$, as shown in figure (1). This problem can be found in many fields of science and engineering, for instance in precipitant protein systems, where the crystal protein is grown with a precipitating agent such as salt [10]. The problem consists of solving two diffusion partial differential equations in each region and insuring mass and energy balance across the interface.

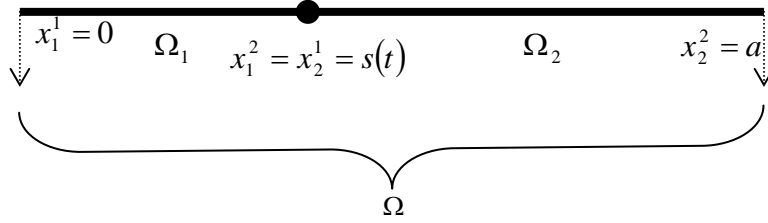


Figure 1: Domain of the problem

The problem is governed with the associated boundary and initial conditions by:

$$c_j \frac{\partial T_j}{\partial t} = K_j \frac{\partial^2 T_j}{\partial x^2} \quad \forall (x, t) \in \Omega_j(t), j = 1, 2 \quad (1)$$

$$\frac{\partial C_j}{\partial t} = D_j \frac{\partial^2 C_j}{\partial x^2} \quad \forall (x, t) \in \Omega_j(t), j = 1, 2 \quad (2)$$

Conditions at the moving boundary

$$T_1(x, t) = T_2(x, t) = h_1(C_1(x, t)) = h_2(C_2(x, t)) \quad x = s(t) \quad (3)$$

$$\lambda \frac{ds(t)}{dt} = K_1 \frac{\partial T_1(x, t)}{\partial x} - K_2 \frac{\partial T_2(x, t)}{\partial x} \quad x = s(t) \quad (4)$$

$$D_2 \frac{\partial C_2(x, t)}{\partial x} - D_1 \frac{\partial C_1(x, t)}{\partial x} = \frac{ds(t)}{dt} (C_1(x, t) - C_2(x, t)) \quad x = s(t) \quad (5)$$

Boundary Conditions

$$\left. \begin{array}{l} A_1 T_1 = F_1^T(t) \\ A_2 C_1 = F_1^C(t) \end{array} \right\} \quad x = 0 \quad (6)$$

$$\left. \begin{aligned} A_3 T_2 &= F_2^T(t) \\ A_4 C_2 &= F_2^C(t) \end{aligned} \right\} \quad x = a \quad (7)$$

Initial Conditions

$$\begin{aligned} T_2(x, t_o) &= T_o \\ C_2(x, t_o) &= C_o \end{aligned} \quad (8)$$

BOUNDARY ELEMENT FORMULATION

For simplicity, equations (1) and (2) can be written as one equation:

$$\frac{\partial u(x, t)}{\partial t} = \gamma \nabla^2 u(x, t) \quad (9)$$

Equation (9) is equivalent to equation (1) if:

$$\begin{aligned} u(x, t) &= T(x, t) \\ \gamma &= \frac{K}{c} \end{aligned} \quad (10)$$

and is equivalent to equation (2) if:

$$\begin{aligned} u(x, t) &= C(x, t) \\ \gamma &= D \end{aligned} \quad (11)$$

An integral equation corresponding to equation (9) over the entire space-time domain can be obtained from the following weighted residual statement:

$$\int_{t_o}^{\tau} dt \int_{\Omega(t)} u^* \left(\gamma \nabla^2 u - \frac{\partial u}{\partial t} \right) d\Omega = 0 \quad (12)$$

where u^* is the free-space Green's formula or the fundamental solution given by:

$$u_j^*(\xi, x, t_n, t) = \frac{1}{(4\pi\gamma(t_n - t))^{m/2}} \exp\left(-\frac{\|\xi - x\|^2}{4\alpha_j(t_n - t)}\right) \quad (13)$$

which is a solution of:

$$\frac{\partial u^*}{\partial t} + \gamma \nabla^2 u^* = -\delta(\xi - x)\delta(\tau - t) \quad (14)$$

where δ denotes the Dirac delta function, m is the dimension of the problem, and $r = \|\xi - x\|$ is the Euclidian distance between the field point x and the source point ξ . Using the Green's second identity and making use of Reynolds transport theorem, the integral representation of equation (9) is obtained in the form [11-12]:

$$\beta(\xi)u(\xi, \tau) = \gamma \int_{t_o}^{\tau} dt \int_{\Gamma(t)} \left[u^* \frac{\partial u}{\partial n} - u \frac{\partial u^*}{\partial n} + \frac{1}{\gamma} uu^* \vec{v} \cdot \vec{n} \right] d\Gamma + \int_{\Omega(t_o)} [uu^*] d\Omega \quad (15)$$

where $\beta(\xi)$ is a constant which depends on the position of the source point ξ , smoothness and the shape of the boundary.

Equation (15) in any region Ω_j bounded by two moving boundaries $x_j^1(t)$ and $x_j^2(t)$ is as follow according to [14-15]:

$$\begin{aligned} \beta(\xi)u_j(\xi, t_n) = & \alpha_j \int_{t_0}^{t_n} \left[u_j^*(\xi, x, t_n, t) \frac{\partial u_j(x, t)}{\partial x} - u_j(x, t) \frac{\partial u_j^*(\xi, x, t_n, t)}{\partial x} \right]_{x_j^1(t)}^{x_j^2(t)} dt \\ & + \int_{t_0}^{t_n} \left[u_j(x, t) u_j^*(\xi, x, t_n, t) \left(\frac{ds(t)}{dt} \right) \right]_{x_j^1(t)}^{x_j^2(t)} dt + D_j^n(\xi, t_n) \end{aligned} \quad (18)$$

In which $D_j^n(\xi, t_n)$ is a domain integral corresponds the initial condition.

Re-write equation (18) for the two phases appear in the appear problem under-hand.

- **For the phase, Ω_j , $j=1$**

$$\begin{aligned} \frac{1}{2}u_1(\xi, t_n) = & \alpha_1 \int_{t_0}^{t_n} \left[u_1^*(\xi, x, t_n, t) \frac{\partial u_1(x, t)}{\partial x} - u_1(x, t) \frac{\partial u_1^*(\xi, x, t_n, t)}{\partial x} \right]_0^{s(t)} dt \\ & + \int_{t_0}^{t_n} \left[u_1(x, t) u_1^*(\xi, x, t_n, t) \left(\frac{ds(t)}{dt} \right) \right]_0^{s(t)} dt + D_1^n(\xi, t_n) \end{aligned} \quad (19)$$

With

$$D_1^n(\xi, t_n) = 0 \quad (20)$$

- **For the phase, Ω_j , $j=2$**

$$\begin{aligned} \frac{1}{2}u_2(\xi, t_n) = & \alpha_2 \int_{t_0}^{t_n} \left[u_2^*(\xi, x, t_n, t) \frac{\partial u_2(x, t)}{\partial x} - u_2(x, t) \frac{\partial u_2^*(\xi, x, t_n, t)}{\partial x} \right]_{s(t)}^a dt \\ & + \int_{t_0}^{t_n} \left[u_2(x, t) u_2^*(\xi, x, t_n, t) \left(\frac{ds(t)}{dt} \right) \right]_{s(t)}^a dt + D_2^n(\xi, t_n) \end{aligned} \quad (21)$$

With

$$D_2^n(\xi, t_n) = \int_0^a u_2(x, 0) u_2^*(\xi, x, t_n, 0) dx \quad (22)$$

Discretisation

Assume a step-wise variation for u and its derivative a linear variation within the time for the moving interface. The discretised form of equation (19) will be:

$$\begin{aligned}
\frac{1}{2}u_\xi^n &= \alpha_1 \sum_{i=0}^n \int_{t_{i-1}}^{t_i} [u_1^*(\xi, s, t_n, t_i) dt] \frac{\partial u_1(s, t)}{\partial x} - \alpha_1 \sum_{i=0}^n \int_{t_{i-1}}^{t_i} \left[\frac{\partial u_1^*(\xi, s, t_n, t_i)}{\partial x} dt \right] u_1(s, t) \\
&+ \sum_{i=0}^n \int_{t_0}^{t_n} [u_1^*(\xi, s, t_n, t_i) dt] u_1(s, t) \left(\frac{ds(t)}{dt} \right)_{t_n} - \alpha_1 \sum_{i=0}^n \int_{t_{i-1}}^{t_i} [u_1^*(\xi, 0, t_n, t_i) dt] \frac{\partial u_1(0, t)}{\partial x} \\
&+ \alpha_1 \sum_{i=0}^n \int_{t_{i-1}}^{t_i} \left[\frac{\partial u_1^*(\xi, 0, t_n, t_i)}{\partial x} dt \right] u_1(0, t)
\end{aligned} \tag{23}$$

Similarly, equation (21) can be discretised, yield:

$$\begin{aligned}
\frac{1}{2}u_\xi^n &= \alpha_2 \sum_{i=0}^n \int_{t_0}^{t_n} [u_2^*(\xi, a, t_n, t_i) dt] \frac{\partial u_2(a, t)}{\partial x} - \alpha_2 \sum_{i=0}^n \int_{t_0}^{t_n} \left[\frac{\partial u_2^*(\xi, a, t_n, t_i)}{\partial x} dt \right] u_2(a, t) \\
&- \alpha_2 \sum_{i=0}^n \int_{t_0}^{t_n} [u_2^*(\xi, s, t_n, t_i) dt] \frac{\partial u_2(s, t)}{\partial x} + \alpha_2 \sum_{i=0}^n \int_{t_0}^{t_n} \left[\frac{\partial u_2^*(\xi, s, t_n, t_i)}{\partial x} dt \right] u_2(s, t) \\
&+ \sum_{i=0}^n \int_{t_0}^{t_n} [u_2^*(\xi, s, t_n, t_i) dt] u_2(s, t) \left(\frac{ds(t)}{dt} \right)_{t_n} + \int_0^a u_2(x, 0) u_2^*(\xi, x, t_n, 0) dx
\end{aligned} \tag{24}$$

Define:

$$g_j(\xi, x, \tau, t) = \int_{t_0}^{t_n} u_2^*(\xi, x, \tau, t) dt, \quad h_j(\xi, x, \tau, t) = \int_{t_0}^{t_n} \frac{\partial u_2^*(\xi, x, \tau, t)}{\partial x} dt \tag{25}$$

Therefore, equations (23) and (24) can take the following discretising form, respectively:

$$\begin{aligned}
\frac{1}{2}u_\xi^n &= \alpha_1 \sum_{i=0}^n \left[g_1(\xi, s, t_n, t_i) \frac{\partial u_1(s, t)}{\partial x} - h_1(\xi, s, t_n, t_i) u_1(s, t) \right] \\
&- \alpha_1 \sum_{i=0}^n \left[g_1(\xi, 0, t_n, t_i) \frac{\partial u_1(0, t)}{\partial x} - h_1(\xi, 0, t_n, t_i) u_1(0, t) \right] \\
&+ \sum_{i=0}^n g_1(\xi, s, t_n, t_i) u_1(s, t_i) \left(\frac{ds(t)}{dt} \right)_{t_n} \\
\frac{1}{2}u_\xi^n &= \alpha_2 \sum_{i=0}^n \left[g_2(\xi, a, t_n, t_i) \frac{\partial u_2(a, t_i)}{\partial x} - h_2(\xi, a, t_n, t_i) u_2(a, t_i) \right] \\
&- \alpha_2 \sum_{i=0}^n \left[g_2(\xi, s, t_n, t_i) \frac{\partial u_2(s, t_i)}{\partial x} - h_2(\xi, s, t_n, t_i) u_2(s, t_i) \right] \\
&- \alpha_2 \sum_{i=0}^n \left[g_2(\xi, s, t_n, t_i) u_2(s, t_i) \left(\frac{dx}{dt} \right)_{t_n} \right] + \int_0^a u_2(x, 0) u_2^*(\xi, x, t_n, 0) dx
\end{aligned} \tag{26}$$

$$\tag{27}$$

Four different integrals that appear in equations (26) and (27) can be evaluated analytically. These integrals are of the Green's formula and its derivative with respect to space when the field point is fixed.

$$I_1 = \int_{t_1}^{t_2} u_j^*(\xi, x, t_n, t) dt = \frac{-r}{2\alpha_j \sqrt{\pi}} \left[\frac{1}{a} \exp(-a^2) + \sqrt{\pi} \operatorname{erf}(a) \right]_{a_1}^{a_2} \tag{28}$$

$$I_2 = \int_{t_1}^{t_2} \frac{\partial u_j^*(\xi, x, t_n, t)}{\partial x} dt = \frac{\text{sign}(\xi - x)}{2\alpha_j} [\text{erf}(a_1) - \text{erf}(a_2)] \quad (29)$$

$$I_3 = \int_{t_1}^{t_2} u_j^*(\xi, s(t), t_n, t) dt =$$

$$= \frac{-1}{2v} \left\{ \exp\left(-\frac{bv}{\alpha_j}\right) \left[\text{erf}\left(-\frac{v(t_n - t) - b}{\sqrt{4\alpha_j(t_n - t)}}\right) \right]_{t_1}^{t_2} + \left[\text{erf}\left(-\frac{v(t_n - t) + b}{\sqrt{4\alpha_j(t_n - t)}}\right) \right]_{t_1}^{t_2} \right\} \quad (30)$$

Where

$$a_i = \frac{r}{\sqrt{4\alpha_j(t_n - t_i)}}, \quad i = 1, 2 \quad (31)$$

$$r = \|\xi - x\| \quad (32)$$

$$\text{sign}(\xi - x) = \frac{\|\xi - x\|}{(\xi - x)} \quad (33)$$

$$s(t) = x + v(t - t') \quad (34)$$

$$b(t) = \xi - s(t) \quad (35)$$

The other integrals can be evaluated numerically taking into consideration the singularities that appear when the source and field point coincides. After some mathematical manipulations, equations (26) and (27) lead to a system of equations, solved at each time step, for more details see [15].

PROPOSED SCHEME

The scheme at each time step can be summarized as follow:

- (1) Guess an initial position and subsequently its velocity.
- (2) Solve the problem as fixed domain problem considering the moving interface as a fixed internal point.
- (3) Solve again the problem as a two phase problem to find the temperature gradient at the moving boundary for each phase.
- (4) Check energy equation at the moving boundary within certain prescribed tolerance and update its location till the energy equation satisfied.
- (5) Repeat steps (1) to (4) up to the end of the process.

These steps are also repeated for concentration, but it should be mention that these steps are repeated at each time step simultaneously.

NUMERICAL RESULTS AND DISCUSSIONS

In the present paper, two different examples were solved in order to test the validity and the applicability of the present technique.

Example (1)

In this example [15]:

$$h_1 = \gamma_1 C + \zeta_1 \quad (36)$$

$$h_2 = \gamma_2 C + \zeta_2 \quad (37)$$

$$A_1 = A_3 = A_4 = 1.0 \quad (38)$$

$$A_2 = 0.0 \quad (39)$$

$$\left. \begin{aligned} F_1^T(t) &= T_o \\ F_1^C(t) &= 0.0 \end{aligned} \right\} \quad (40)$$

$$\left. \begin{aligned} F_2^T(t) &= T_\infty \\ F_2^C(t) &= C_\infty \end{aligned} \right\} \quad (41)$$

With

$$c_1 = 0.1, c_2 = 0.5, K_1 = K_2 = 1.0, \gamma_1 = 20, \gamma_2 = 40 \quad (42)$$

$$D_1 = D_2 = 1., \zeta_1 = \zeta_2 = 83., T_\infty = 115, C_\infty = 0.1$$

Rubnastien [1] had been introduced an analytical solution for this problem but for semi-infinite domain. The variation of the moving boundary with time is plotted as shown in figure (2). It is clear a good agreement between the analytical results and the results from the present scheme.

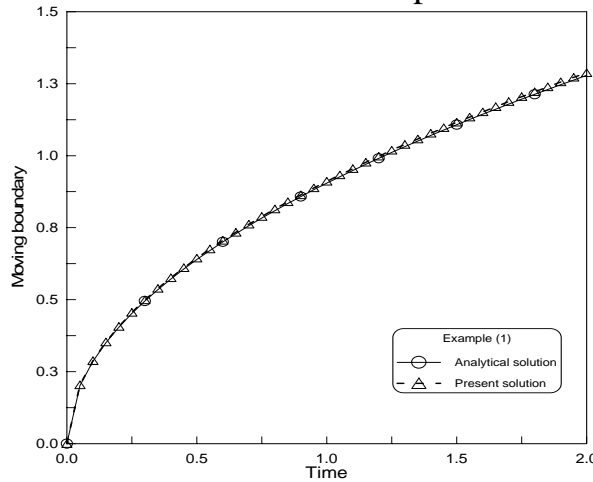


Figure 2: Moving boundary of example (1)

The temperature variation with the space x at two different times is also computed from the present scheme, as shown in figures (3) and (4) respectively. Figure (3) shows the first phase temperature variation at the times $t = 0.5$ and $t = 0.9$, while figure (4) is for the second phase temperature distribution at the same times. It can be seen that at any fixed x and by

increasing the time the temperature decreases and this coincides with the physics of the problem. Also, a comparison between the analytical, the boundary element and the present methods for computing the temperature and the concentration against x is summarized in table (1) at time $t = 0.4$. The concentration distribution for both phases according to the present scheme is plotted in figure (5). As expected the concentration in the first phase behaves constant in the first phase then sudden jump occurs at the moving boundary. The concentration variation is computed at two different times, $t = 0.5$ and $t = 1.1$.

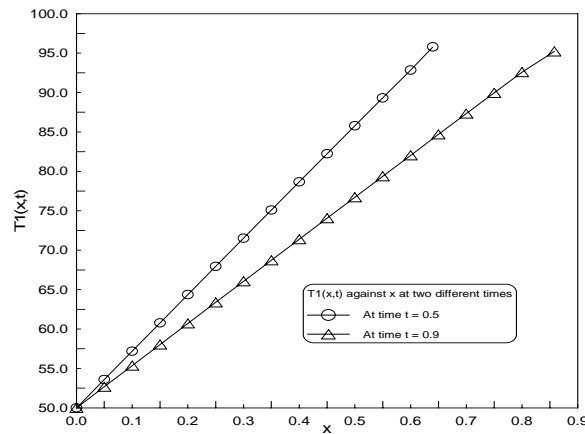


Figure 3: First phase temperature distribution

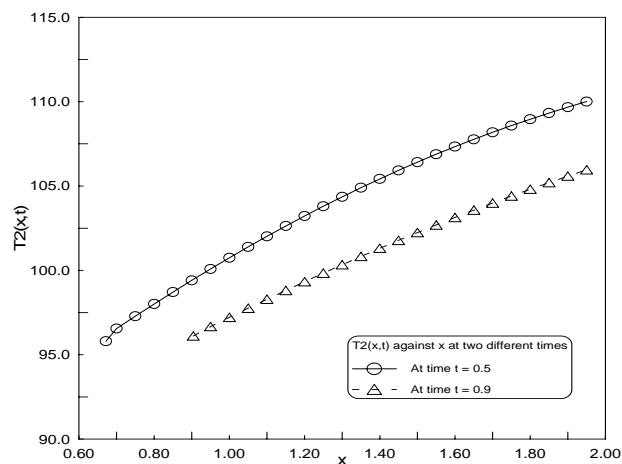


Figure 4: Second phase temperature distribution

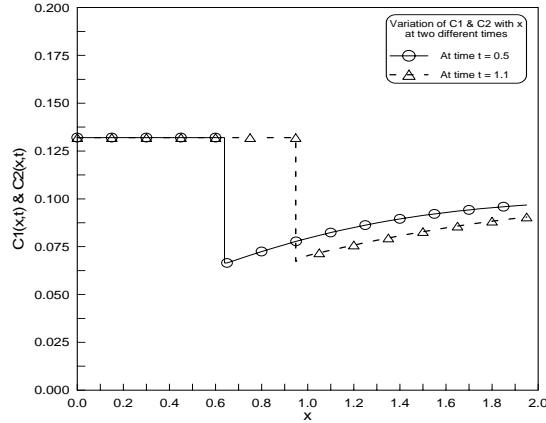


Figure 5: Concentration variation for example (1)

Table 1: Temperature and concentration for example (1), compared with previous analytical and numerical solutions.

x	Temperature			Concentration		
	Analytical	BEM	Present	Analytical	BEM	Present
0.00	50.000	50.000	50.0925	0.132	0.132	0.130
0.05	53.136	53.137	53.1500	0.132	0.132	0.130
0.10	56.272	56.271	56.2860	0.132	0.132	0.130
0.15	59.405	59.401	59.4180	0.132	0.132	0.130
0.20	62.536	62.527	62.5470	0.132	0.132	0.130
0.25	65.663	65.649	65.6720	0.132	0.132	0.130
0.30	68.785	68.766	68.7930	0.132	0.132	0.130
0.35	71.901	71.877	71.9070	0.132	0.132	0.130
0.40	75.010	74.981	75.0140	0.132	0.132	0.130
0.45	78.111	78.079	78.1150	0.132	0.132	0.130
0.50	81.204	81.169	81.2070	0.132	0.132	0.130
0.55	84.287	84.251	84.2900	0.132	0.132	0.130
0.60	86.355	86.343	86.3710	0.068	0.068	0.0683
0.65	87.614	87.596	87.6270	0.070	0.070	0.0710
0.70	88.847	88.822	88.8570	0.072	0.072	0.0726
0.75	90.054	90.022	90.0610	0.074	0.074	0.0738
0.80	91.233	91.194	91.2360	0.076	0.076	0.0763
0.85	92.382	92.338	92.3830	0.078	0.078	0.0789
0.90	93.502	93.452	93.5000	0.080	0.080	0.0821
0.95	94.590	94.535	94.5860	0.082	0.082	0.0823
1.00	95.647	95.587	95.6410	0.083	0.083	0.0836

Example (2)

In this example:

$$c_1 = 1, c_2 = 2, K_1 = 1000, K_2 = 100, \gamma_1 = 40, \gamma_2 = 20 \quad (46)$$

$$D_1 = D_2 = 0.1, \zeta_1 = \zeta_2 = 83., T_\infty = 115, C_\infty = 0.8 \quad (47)$$

This example has no analytical solution, therefore, the results of the present method were compared with previous approximate solution introduced by Wilson, et al. [16]. Figure (6) shows the moving boundary interface compared with Wilson's solution. It is clear that a good agreement between the two solutions was achieved. Table (2) shows a comparison between the present method and Wilson results for temperature variations with x at two different times.

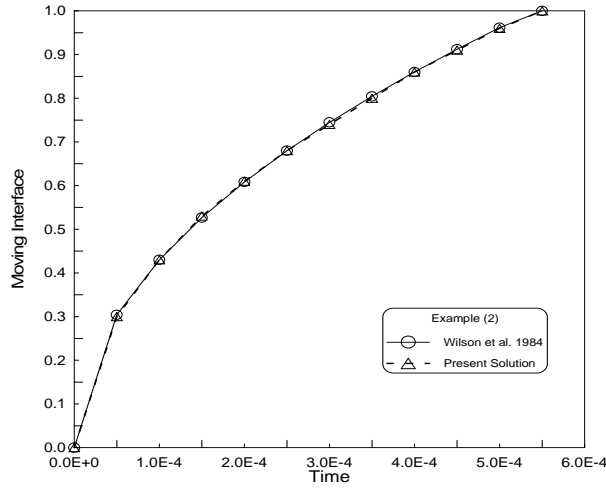


Figure 6: Moving boundary of example (2)

Table 2: Present and Wilson results for temperature at $t = 1.0 \times 10^{-4}$

Time	Temperature			
	x	Wilson 1984	x	Present
1.0×10^{-4}	0.00	50.0	0.00	50.000
	0.05	56.1	0.05	55.772
	0.10	62.1	0.10	61.539
	0.15	68.2	0.15	67.293
	0.20	74.2	0.20	73.029
	0.25	82.2	0.25	78.739
	0.30	86.2	0.30	84.419
	0.35	92.1	0.35	90.062
	0.40	98.0	0.40	95.663
	0.45	103.8	0.43	99.000

Table 3: Present and Wilson results for temperature at $t = 2.0 \times 10^{-4}$

Time	2.0×10^{-4}							
	x	0.00	0.05	0.10	0.15	0.20	0.25	0.30
T	50.000	54.082	58.162	62.238	66.307	70.367	74.417	
x	0.35	0.40	0.45	0.50	0.55	0.60	0.61	
T	78.452	82.473	86.477	90.461	94.424	98.363	99.148	

CONCLUSION

In the present paper, the boundary element method is used as a numerical tool with new algorithm of solution. The main feature of the new algorithm is to solve the problem twice at the same time. Once time as a fixed domain problem dealing with the moving interface as an internal and fixed point, and once more as a two phase moving boundary problem with the moving interface as a moving point. The updating procedure of the moving interface depends mainly on a prescribed error in the numerical scheme. It is found from the solution procedure that there is a proportional relation between the prescribed error and the number of iterations per time step. Also it is found that the maximum number of iterations not exceed thirty iterations per time step to achieve a good accuracy. The mathematics of the present algorithm is easy to handle higher dimensional problems.

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