A combined domain and integral techniques to solve planar oxidation problem

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Abstract

In this paper, a semi-analytical method is developed to solve planar oxidation problems in a semi-infinite domain. The proposed method is based mainly on a combined procedure for both domain transformation and boundary layer integral techniques in the oxide layer. A numerical algorithm is then developed to find the unknowns in the assumed profiles for oxygen concentration in both layers. The results of the proposed method were compared with previous available approximate solutions and gave a good agreement.

1 Introduction

In some applications of engineering industries, especially where elevated high temperature is a factor, it is recommended special types of metal matrix composites be used. Metal matrix composites have been proposed for this purpose due to their high strength and ability to retain their mechanical integrity at relatively high temperature.

Applications anticipated for structural components in advanced turbine engines and hypersonic aircraft require the structural composite to withstand severe mechanical loading and temperature variations [1-2]. In these applications, mechanical failure is induced by a number of interacting damage modes, such as fibre cracking and slip banding.

Other types of failure can occur in these applications due to environmental effects such as oxidation. The oxidation process in metallic alloys is a complicated chemical process based on a two-way ionic diffusion and flow of molecular oxygen through the porosity of the oxide scale [3-5]. The oxidation process in metallic alloys can be considered and modeled as a phase change problem with moving interface.
Diffusion problems with moving interfaces, especially, solidification problems have been investigated by numerous authors [6-7]. Due to the unknown moving interface involved such problems are essentially nonlinear boundary value problems. As pointed in [8], there are very few cases where exact analytical solutions are available except for those problems where the moving interfaces vary with the square root of time. Therefore, many efforts have been emphasized on developing numerical techniques. Numerical methods for solving boundary value problems with moving interfaces can be generally divided into groups, variable and fixed grid methods [9].

The major advantage of numerical methods in the first group is capturing the unknown moving interface explicitly, where the exact location of the moving interface is evaluated on a grid at every time level. However, the usage of variable grid methods to solve multi-dimensional boundary value problems with moving interface is algorithmically complicated [10], while the fixed grid methods are often used for solving such problems.

In the present paper, an oxygen diffusion model with moving oxidation front suggested by Lagoudas [1] is used. The method developed herein is mainly based on a combined procedure for both domain transformation and boundary layer integral techniques. Then, a numerical procedure is developed to find the unknowns in oxygen profiles for both oxide and non-oxide layers. The results achieved by the present method gave a good agreement with previous numerical solution.

2 Problem description and formulation

Let $\Omega = \mathbb{R}^2_+$ a semi-infinite solid, be the physical domain. Assume that the free surface of the solid, $\partial \Omega = \{(0, x_2), x_2 \in \mathbb{R}\}$, is exposed to a constant oxygen concentration $C_o$, and initial oxygen concentration is zero.

From figure (1), the oxide layer can be written as:
Oxygen concentration in oxide and non-oxide layers is denoted by $C_1$ and $C_2$ respectively. The oxygen concentration depends mainly on $x$, $-$ coordinate and the time $t$. The state equations describing this process can be stated as follows:

$$\frac{\partial C_1(x,t)}{\partial t} = D_1 \frac{\partial^2 C_1(x,t)}{\partial x^2} \quad 0 \leq x \leq X(t)$$

$$\frac{\partial C_2(x,t)}{\partial t} = D_2 \frac{\partial^2 C_2(x,t)}{\partial x^2} \quad X(t) < x < \infty$$

Where $D_1$ and $D_2$ are oxygen diffusivities in both layers, respectively. With the following initial and boundary conditions:

$$X(0) = 0 \& C_2(x,0) = 0, 0 < x < \infty$$

$$C_1(0,t) = C_o, C_1(X(t),t) = C_{cr}, t > 0$$

$$C_2(X(t),t) = (C_{cr} - [C]), \lim_{t \to \infty} C_2(x,t) = 0, t > 0$$

$$\frac{D_2}{\partial x} \frac{\partial C_2(X(t),t)}{\partial x} - D_1 \frac{\partial C_1(X(t),t)}{\partial x} = [C] \frac{dX(t)}{dt}$$

In these equations, $C_{cr}$ and $[C]$ are the critical oxygen concentration for the oxide formation and jump of oxygen concentration across the interface respectively.

3 Development of the proposed method

- For the oxide layer

Let us start applying the domain transformation technique suggested by Ding et. al. [11], defined as:

$$\rho = \frac{x}{X(t)}, \quad \tau = X(t) \Rightarrow C_1(x,t) = C_1(\rho, \tau)$$

Then, the diffusion equation in the oxide layer becomes [11]:

$$\left(-\rho \frac{\partial C_1(\rho, \tau)}{\partial \rho} + \frac{\partial C_1(\rho, \tau)}{\partial \tau} \tau \right) \frac{\partial X(t)}{\partial t} = D_1 \frac{1}{X^2(t)} \frac{\partial^2 C_1(\rho, \tau)}{\partial \rho^2}$$

In the proposed method, we try to choose a profile for the oxygen concentrations in both layers that appear throughout the process, such that these profiles...
satisfies the boundary conditions for both layers. Assume oxygen concentration profile for oxide layer as follows:

\[
C_1(x, t) = C_{cr} \left( \frac{x}{X(t)} \right) + C_o e^{-\frac{x}{X(t)}} + a(t) \left( \frac{x}{X(t)} \right)^2 + b(t) \left( \frac{x}{X(t)} \right)^2
\]  

(9)

In which, \(a(t)\) and \(b(t)\) are unknown functions to be determined as a part of the solution. By substituting from equation (7) into equation (9), leads to:

\[
C_1(\rho, \tau) = C_{cr}(\rho) + C_o e^{-\rho} + a(\rho) + b(\rho)^2
\]  

(10)

The next step in the proposed method is to apply the boundary layer integral technique by integrating both sides of the transformed diffusion equation given by equation (8) as follows:

\[
\int_0^1 \left( -\rho \frac{\partial C_1(\rho, \tau)}{\partial \rho} + \frac{\partial C_1(\rho, \tau)}{\partial \tau} \right) \frac{\partial X(t)}{\partial t} d\rho = \int_0^1 D_1 \frac{1}{X^2(t)} \frac{\partial^2 C_1(\rho, \tau)}{\partial \rho^2} d\rho
\]  

(11)

By evaluating the integrals in both sides of the above equation, taking into consideration the equation (10), leads to:

\[
a(t) \left( \frac{dX(t)}{dt} \right) + b(t) \left( 2 \frac{dX(t)}{dt} + \frac{2D_1}{X^2(t)} \right) = \frac{D_1}{X^2(t)} \left( C_o \left( e^{-1} - 1 \right) \right)
\]  

(12)

\[
+ \left\{ \frac{D_1}{X^2(t)} \frac{dX(t)}{dt} \right\} \left( C_o - 2C_o e^{-1} - C_o e^{-1} X(t) - e^{-1} + \frac{1}{2} C_{cr} \right)
\]

- For non-oxide layer

Let us start the solution in this layer, also by assuming a profile for oxygen concentration as follows:

\[
C_2(x, t) = \left\{ C_{cr} - [C] \right\} \left( \frac{X(t)}{x} \right) + a(t) \left( 1 - \frac{X(t)}{x} \right) + b(t) \left( 1 - \frac{X(t)}{x} \right)^2
\]  

(13)

By making use of equation (9) into equation (6), and after some mathematical manipulation, we get the following equation:

\[
a(t) \left( \frac{D_2 - D_1}{X(t)} \right) + b(t) \left( \frac{-2D_1}{X(t)} \right) = D_1 \left\{ \frac{C_{cr} - C_o e^{-1}}{X(t)} \right\}
\]  

\[
- D_2 \left\{ \frac{[C] - C_{cr}}{X(t)} \right\} + [C] \frac{dX(t)}{dt}
\]  

(14)
- Solution procedure

The following flow chart describing the solution procedure for the present method is shown below in figure (2).

Start

Guess an initial position for the oxide front and assume linear variation between position and its speed

Solve equation (12) and (14) to get first approximation for the unknown functions $a_j(t), b_j(t)$

Use the first approximation for both $a_j(t), b_j(t)$ to check the oxygen concentration jump at the oxide front, then compute the absolute error, say $E$

Guess another speed and position

Go to next time step

Check $E < \varepsilon$

Stop

If $t = t_F$

Figure 2
4 Numerical results and discussion

In the present paper, we take the following quantity [11],

\[
\begin{align*}
D_1 &= 0.274 \mu m^2 / sec \\
D_2 &= 0.166 \mu m^2 / sec \\
C_o &= 1 \\
[C] &= 0.25 \\
C_{cr} &= 0.65
\end{align*}
\]

Table 1

Since the exact analytical solution to the planar oxidation problem is available, a comparison between the present solution, exact solution [6] and recently numerical solution developed by Ding et. al.[11] is made. Table (2) summarize the results of the oxide front based on the three methods.

<table>
<thead>
<tr>
<th>Time (h)</th>
<th>Oxide Front (X(t)) in &quot;Micron&quot;</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Time Step</td>
</tr>
<tr>
<td></td>
<td>0.1</td>
</tr>
<tr>
<td>0.5</td>
<td>17.873</td>
</tr>
<tr>
<td>1</td>
<td>25.276</td>
</tr>
<tr>
<td>2</td>
<td>35.745</td>
</tr>
<tr>
<td>5</td>
<td>56.519</td>
</tr>
<tr>
<td>10</td>
<td>79.930</td>
</tr>
</tbody>
</table>

Table 2

Another comparison between the present solution and the numerical solution is made and shown in figure (3). From table (2) and figure (3) that there is a good agreement the present method and the other available solutions. Since the exact solution is available for tracking the oxide front, a comparison for the oxygen concentration in the oxide layer is made between the present solution and the numerical solution developed by Ding et. al. as shown in figure (4).
Figure 3: Location of the oxide front

Figure 4: Oxygen concentration comparison
After 1-hour
After 3-hour
After 5-hour
After 7-hour
After 9-hour

Distance from the surface (Micron)

Figure 5

Oxygen Concentration in the Non-oxidized layer

Distance from the surface (Micron)

Figure 6
It is clear from figure (4) that, the solution describes the physical behavior of the problem. Also, it is clear that at the same time step, the error between the two solutions decreases by going away from the surface. The oxygen concentration in the oxide and the non-oxide layers based on the present method are shown in figure (5) and (6), respectively.

5 Conclusion

Domain transformation technique was first suggested by Landau [12] but it was applied to space variables only which result in complexity in numerical algorithms. The domain transformation applied, herein, that suggested and developed by Ding et al., which transformed the oxidation problem to non-linear boundary-value problem on a fixed domain. To overcome this non-linearity, a boundary layer integral technique is applied. The combination of the two-technique result in a system of linear equations in the unknown functions in the oxygen concentration profiles assumed. The proposed method has the advantage that it is simple in mathematical handling and simple algorithm for computation.

References


