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## An Integral Method for Solving Oxygen Diffusion on Unbounded Domain with Moving Boundary

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**Abstract:** In the present study, planar oxidation problem is solved using a new developed integral technique. The technique starts by assuming a profile for oxygen concentration for oxidized and metallic layers, respectively. The two profiles contain three unknowns such that one of them is common between the two layers, which is the moving (oxidation) front. Apply the first order integral moment in each layer, separately, yields the main unknown in the assumed profiles, meanwhile, the moving front remains unknown. By achieving the energy balance at the moving boundary yields a non-linear equation, its solution iteratively, yields the location of the moving boundary at each time step. The results of the present method were compared with the analytical solution and gave a good agreement between the two solutions.

**Key words:** Oxygen diffusion, moving boundary, integral moment technique

### INTRODUCTION

In advanced turbine engines and hypersonic aircraft it is required in their structure to withstand severe mechanical loading and temperature variations<sup>[1,2]</sup>. Metal matrix composites have the properties of withstanding different mechanical loads due to their high strength and relatively high temperatures. Mechanical failure in these applications is induced by a number of interacting damage modes, such as fiber cracking and slip banding.

Another type of failure can be occurred to these applications due to environmental effect 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<sup>[3,4]</sup>.

The oxidation process in metallic alloys can be modeled as phase change problem with moving interface suggested by Lagouds<sup>[5]</sup>. According to this model, the moving interface is characterized by an oxygen jump at the interface between the oxidized and metallic parts. 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<sup>[6,7]</sup>. 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 to groups, variable and fixed grid methods<sup>[8]</sup>. 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, while the fixed grid methods are often used for solving such problems<sup>[9]</sup>.

The main objective of the present study was to introduce a simple and efficient algorithm for solving one-dimensional two phase heat transfer problem. The present algorithm starts by assuming a profile for oxygen concentration for oxidized and metallic layers, in which three unknowns appear such that one of them is common between the two layers, which is the moving front.

Apply the first order integral moment in each layer, separately, yields the main unknown in the assumed profiles, meanwhile, the moving front remains unknown. By achieving the energy balance at the moving boundary yields a non-linear equation, its solution iteratively, gives the location of the moving boundary at each time step. The results of the present method were compared with the analytical solution and gave a good agreement between the two solutions.

### PROBLEM DESCRIPTION AND FORMULATION

Suppose that a semi-infinite solid, be the physical domain. Assume that the free surface of the solid  $x = 0$ , is exposed to a constant oxygen concentration  $C_0$  and initial oxygen concentration is zero.

Assume that oxygen concentration in oxidized and metallic layers is denoted by  $C_1$  and  $C_2$ , respectively.

According to Lagouds mathematical model<sup>[5]</sup>, the problem can be formulated as a one dimensional moving boundary problem. State equations describing this process can be stated as follows<sup>[10,11]</sup>:

$$\frac{\partial C_1(x,t)}{\partial t} = D_1 \frac{\partial^2 C_1(x,t)}{\partial x^2} \quad 0 \leq x \leq X(t) \quad (1)$$

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

Initial conditions:

$$X(0) = 0 \quad (3)$$

$$C_2(x,0) = 0 \quad 0 < x < \infty \quad (4)$$

Boundary conditions:

$$C_1(0,t) = C_o \quad t > 0 \quad (5)$$

$$C_1(X(t),t) = C_{cr} \quad t > 0 \quad (6)$$

$$C_2(X(t),t) = (C_{cr} - [C]) \quad t > 0 \quad (7)$$

$$D_2 \frac{\partial C_2(X(t),t)}{\partial x} - D_1 \frac{\partial C_1(X(t),t)}{\partial x} = [C] \frac{dX(t)}{dt} \quad (8)$$

Where:

$D_1$  Oxygen diffusivity for oxidized layer

$D_2$  Oxygen diffusivity for metallic layer

$C_{cr}$  Critical oxygen concentration for the oxide formation

$[C]$  Jump of oxygen concentration across the interface.

### DEVELOPMENT OF THE INTEGRAL METHOD

Assume a quadratic profile for oxidized and metallic layers of the following forms:

$$c_1(x,t) = x \left\{ \frac{c_{cr}}{x(t)} + a(t) \left( \frac{x-x(t)}{x(t)} \right) \right\} + (x(t)-x) \left\{ c_{cr} \left( \frac{x}{x(t)} \right) + c_o \left( \frac{1-x}{x(t)} \right) \right\} \quad (9)$$

$$c_2(x,t) = x \left\{ \left( \frac{c_{cr} - [C]}{x} \right) + b(t) \left( \frac{x-x(t)}{x(t)} \right) \right\} \quad (10)$$

In these equations,  $a(t)$  and  $b(t)$  are three unknowns are to be determined as a major and principle part of the

required solution. Because the physical plane is a semi infinite solid  $L$  is a truncated boundary long enough for accurate solution. The next step is to take the first integral moment for oxidized layer from  $x = 0$  to  $x = x(t)$  and the metallic layer from  $x = x(t)$  to  $x = L$ , i.e.,

$$\int_{x=0}^{x=x(t)} \frac{\partial C_1(x,t)}{\partial t} dx = D_1 \int_{x=0}^{x=x(t)} \frac{\partial^2 C_1(x,t)}{\partial x^2} dx \quad (11)$$

$$\int_{x=x(t)}^{x=L} \frac{\partial C_2(x,t)}{\partial t} dx = D_2 \int_{x=x(t)}^{x=L} \frac{\partial^2 C_2(x,t)}{\partial x^2} dx \quad (12)$$

Integrate both sides of Eq. 11 and make use of the oxidized profile given by Eq. 9 and boundary conditions given by Eq. 5 and 6 leads to:

$$a(t) = c_{cr} - c_o \quad (13)$$

Similarly, integrate both sides of Eq. 12 and make use of the metallic profile given by Eq. 10 and boundary conditions given by Eq. 7 and 8 leads to:

$$b(t) = -x(t) \left\{ \frac{(c_{cr} - [C])}{(L-x(t))^2} \right\} \quad (14)$$

The three unknowns are now reduced to only one that is the location of the oxidation front. To find the oxidation front follow up the following procedure:

(1) From Eq. (9) find  $\left. \frac{\partial c_1}{\partial x} \right|_{x=x(t)}$

(2) From Eq. (10) find  $\left. \frac{\partial c_2}{\partial x} \right|_{x=x(t)}$

(3) Substitute from step (1) and (2) into Eq. 8 and simplify, leads to:

$$\frac{dx(t)}{dt} = \frac{B_1}{L-x(t)} + \frac{B_2}{x(t)} \quad (15)$$

Its exact solution is given by:

$$x^2(t) - 2 \left( L + \frac{\eta_2}{\eta_1} \right) x(t) + 2 \left( \frac{\eta_2}{\eta_1} \right) \left( L + \frac{\eta_2}{\eta_1} \right) \ln \left( \frac{\eta_1 x(t) + \eta_2}{\eta_2} \right) + 2\eta_1 t = 0 \quad (16)$$

Where:

$$\eta_1 = B_1 - B_2 \quad (17)$$

$$\eta_2 = LB_2 \tag{18}$$

$$B_1 = -D_2 \left( \frac{c_{cr} - [c]}{[c]} \right) \tag{19}$$

$$B_2 = -D_1 \left( \frac{c_{cr} - c_o}{[c]} \right) \tag{20}$$

**RESULTS AND DISCUSSION**

The following numerical data are taken from<sup>[10,11]</sup>.

$D_1 = 0.274 \mu\text{m}^2$        $D_2 = 0.166 \mu\text{m}^2$        $C_{cr} = 0.65$   
 $C_o = 1.0$                $C_{cr} = 0.65$                $[C] = 0.25$

Since the exact analytical solution to the planar oxidation problem is available, a comparison between exact solution<sup>[6]</sup> and the present method is made as shown in Fig. 1 in which it is clear that there is a good agreement between the two solutions with very small error can be neglected.

It is clear from this Fig. 2 that at the same depth from the surface oxygen concentration increases by growing up the time, meanwhile, at the same time and by going inside the domain oxygen concentration decreases which describes the physics of the process very well.

On the other side, oxygen concentration in the metallic layer verses depth from the surface at the same three different times is shown in Fig. 3. Each curve in this Fig. 3. starts from the same oxygen concentration at the oxidation front due to the assumed profile for metallic layer in the beginning of the present method.

Another topic to check the ability of the present method for tracking the oxidation front and physical behavior of the process is evaluation of oxygen concentrations against time at different depths from the surface, this is clearly shown in Fig. 4. It is clear that, at the same time if the depth is closer to the surface its oxygen concentration is much higher than that of other depth away from the surface.

Oxygen concentration in the metallic layer against time at different depths from the location of the oxidized front is studied and the results are shown in Fig. 5.

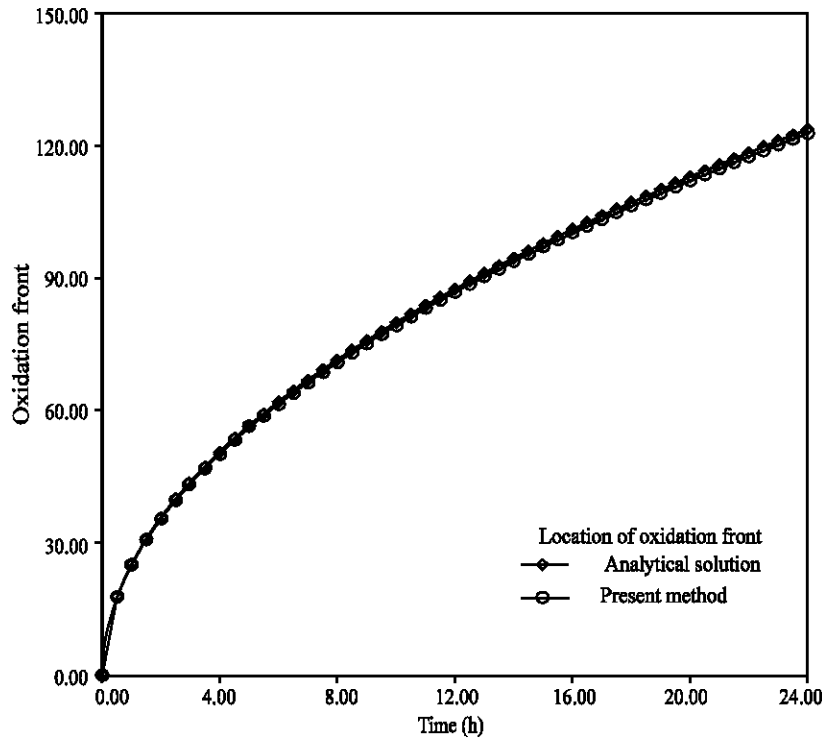


Fig. 1: Location of oxidation front

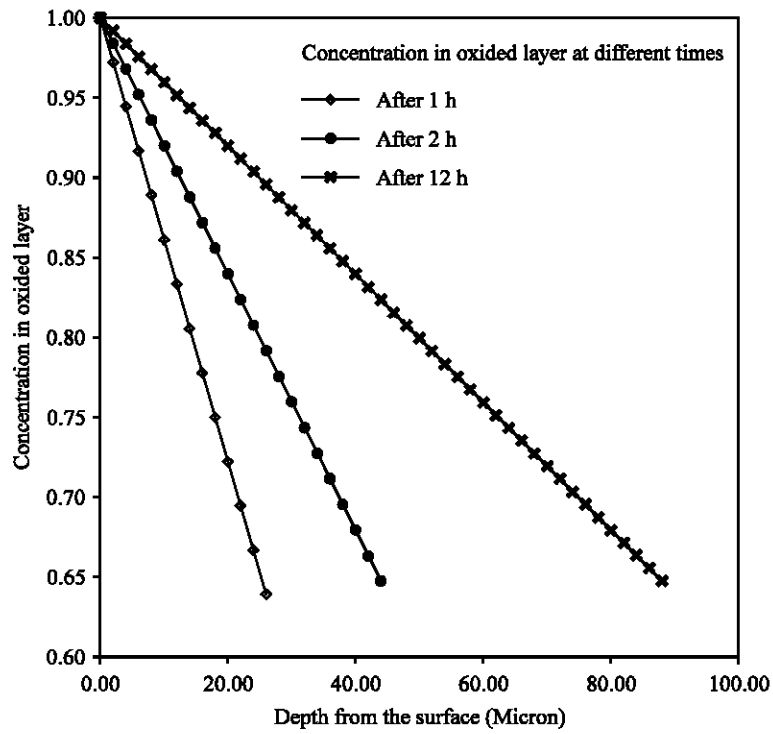


Fig. 2: Oxygen concentrations in oxidized layer at different times

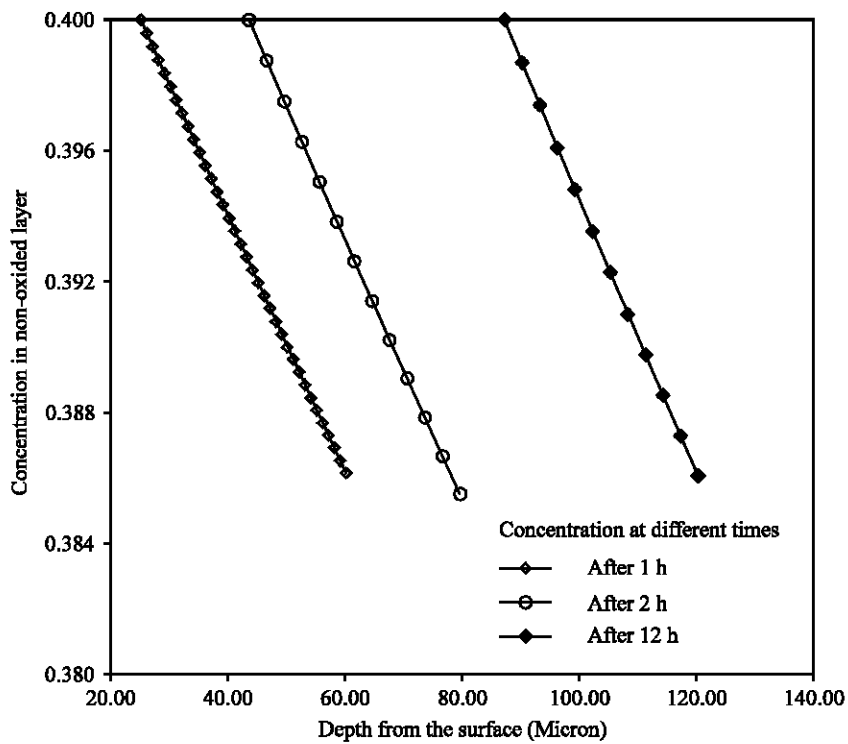


Fig. 3: Oxygen concentrations in metallic layer

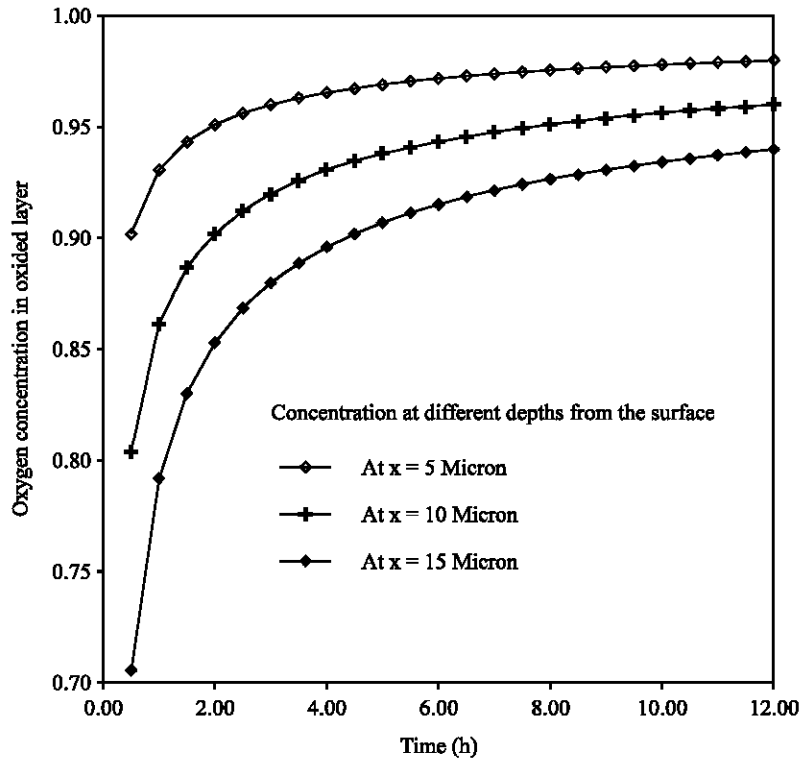


Fig. 4: Oxygen concentrations in oxidized layer at different depths

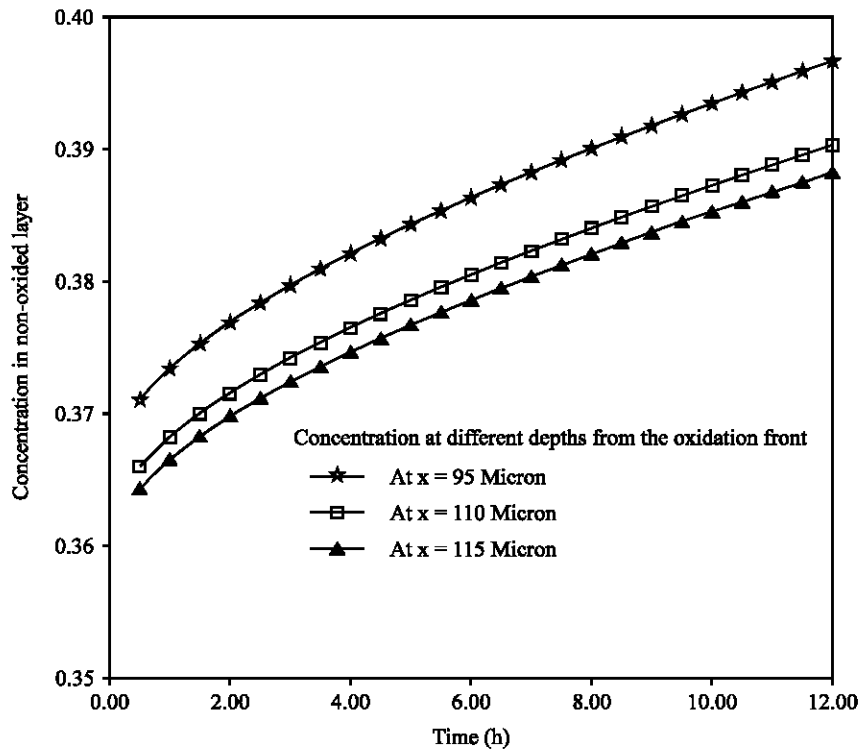


Fig. 5: Oxygen concentrations in metallic layer at different depths

## CONCLUSIONS

In the present study, the planar oxidation problem was studied due to its practical importance in engineering and industry. The problem is solved through a new computational integral method. A profile for each phase that appears is assumed in a quadratic form and three unknowns appear throughout the analysis. Once applying the first order integral moment the three unknowns reduces to only one, that the oxidation front. Achieving the energy balance thermodynamically at the oxidation front yields a non-linear equation. Its solution, iteratively leads to the position of the oxidation front at each time step. The present method has the advantage of easy mathematical manipulation, small errors occur that can be neglected and low number of iterations to achieve the required accuracy. Finally, the present method succeeded to explain the physical behavior of the problem.

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