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Abstract

A variational formulation is used to solve a moving boundary problem in a sphere. The fix-domain and the finite element methods are employed to obtain the motion of the reaction front and concentration profiles. The times to complete reaction are given for various values of the density of nondiffusing reactant in the particle and compared with previous results.

1 INTRODUCTION

In this paper we consider a numerical approach for solving a moving boundary problem related to the study of a chemical reaction within spherical particles.

This problem is a classical one and it has been studied by many authors (see [2, 3, 5, 6]). Interest in such problems have been growing because of their applications in chemical engineering and many industrial processes. Several techniques, such as Bergman-Type series expansion method (see [1, 7, 8]), have been used by several authors (see [2, 5]) to find an approximate solution

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to this problem. Here the fix-domain method is presented and a numerical approximation by means of finite elements is used to obtain an approximate solution in one space dimension.

The outline ot the paper is the following:

In section 2 the model problem is presented. Section 3 is devoted to the variational formulation of the problem. In section 4 a finite element method is described and the discretized problem is derived. Finally, in section 5 and 6 a numerical scheme is described and numerical results are obtained.

2 THE MODEL PROBLEM

We consider the following moving-boudary-value problem which corresponds to the shrinking-core model describing a chemical reaction within a spherical particle of radius a, namely

Problem (P1):

$$r^* \frac{\partial c^*}{\partial \tau} = D \frac{\partial}{\partial r^*} \left(r^{*2} \frac{\partial c^*}{\partial r^*} \right), \quad R^*(\tau^*) < r^* < a \tag{1}$$

$$c^*(r^*, \tau^*) = 0, \quad \text{at } r^* = R^*(\tau^*) \tag{2}$$

$$c^*(r^*, \tau^*) = c_0, \quad \text{at } r^* = a \tag{3}$$

$$D \frac{\partial c^*}{\partial r^*}(R^*(\tau^*), \tau^*) = -\alpha^* \frac{d}{d\tau} R^*(\tau^*), \quad R^*(0) = a \tag{4}$$

where $c^*(r^*, \tau^*)$ is the concentration of the diffusing reactant, $R^*(\tau^*)$ is the position of the moving boundary at time τ^*, D is the diffusion coefficient and

α^* is a measure of the density of nondiffusing reactant in the particle.

Following [5], non-dimensionlal variables

$$\tau = \frac{D\tau^*}{a^2}, \quad c = \frac{c^*}{c_0}, \quad r = \frac{r^*}{a}, \quad R = \frac{R^*}{a}. \tag{5}$$

are introduced to obtain:

Problem (P2): Given T_0 and α find the pair $\{U(r,\tau), R(\tau)\}$ such that

$$\frac{\partial U}{\partial \tau} = \frac{\partial^2 U}{\partial r^2}, \tag{6}$$

$$\text{in} \quad \Omega = \{(r,\tau) | R(\tau) < r < 1,\ 0 < \tau \leq T_0\}$$

$$U(R(\tau),\tau) = 0, \tag{7}$$

$$U(1,\tau) = 1, \qquad \text{for} \quad 0 < \tau < T_0 \tag{8}$$

$$\frac{\partial}{\partial r} U(R(\tau),\tau) = -\alpha R(\tau) \frac{dR(\tau)}{d\tau}, \quad R(0) = 1, \tag{9}$$

where

$$c(r,\tau) = \frac{U(r,\tau)}{r} \qquad \text{and} \qquad \alpha = \alpha^*/c_0 \tag{10}$$

3 VARIATIONAL FORMULATION

To avoid the difficulties arising from having an unknown domain for the differential equation (6), we will now use the well known Landau transformation to transform problem (P2) to a one with fixed boundaries. To do that we introduce the new space variable

$$x = \frac{r-1}{R(\tau)-1} \tag{11}$$

while the new time variable $t = t(\tau)$ will be defined as the unique solution to the ordinary differential equation

$$\frac{dt}{d\tau} = \frac{1}{R^2(\tau)} \qquad \text{with} \qquad t(0) = 0 \tag{12}$$

and we set

$$\begin{cases} u(x,t) = U(r,\tau) \\ s(t) = R(\tau) \end{cases} \tag{13}$$

Then in the new variables the transformed problem (P2) becomes

Problem (P3): Given T and α find the pair $\{u(x,t), s(t)\}$ such that

$$s(t)b(t)u_{xx} - u_t = \frac{b(t)}{\alpha} u_x(1,t) x u_x(x,t) \tag{14}$$

$$\text{in} \quad Q = \{(x,t) |\ 0 < x < 1, 0 < t \leq T\}$$

$$u(1,t) = 0 \tag{15}$$

$$u(0,t) = 1 \tag{16}$$

$$\frac{ds(t)}{dt} = \frac{s}{\alpha(1-s)} u_x(1,t), \qquad s(0) = 1 \tag{17}$$

where

$$b(t) = \frac{s}{(1-s)^2} \tag{18}$$

and $t = T$ is the corresponding value of $\tau = T_0$.

Note that we now have a problem with fixed boundaries but at the cost of having a nonlinear governing equation. Also, one should note that the governing equation (14) and Eq. (17) are coupled while in (P2) there are uncoupled.

In order to reach a weak formulation of (P3) we make another change of

variable

$$v(x,t) = u_x(x,t) \tag{19}$$

then we introduce, for t fixed, the usual soboleve space $H^1(0,1)$. The reader interested in Sobolve Spaces used in this paper can refer to [4].

Note that from (19),(16) and (15), we obtain the relation

$$u(x,t) = \frac{1}{2}\int_0^x v(z,t)dz - \frac{1}{2}\int_x^1 v(z,t)dz + \frac{1}{2} \tag{20}$$

We now multiply (14) by $w_x \in H^1$ and integrate it with respect to x to get

Problem (P4): Find the pair $\{v(x,t), s(t)\}$ with

$$v(x,t) : (0,T] \to H^1$$

such that

$$sb(v',w') + (\dot{v},w) = \frac{b}{\alpha}v(1)(xv,w') \text{ for all } w \in H^1 \tag{21}$$

$$\dot{s} = \frac{s}{\alpha(1-s)}v(1), \qquad s(0) = 1. \tag{22}$$

where here and in the following v' and $\dot{v}$ denote, respectively, differentiation with respect to x and t. The dependence on t is usually suppressed and $v(1)$ means $v(1,t)$. The L_2-product is denoted by (.,.).

4 A FINITE ELEMENT METHOD

Given a subdivision of the interval $(0,1)$ into $N = 1/h$ equal parts, we introduce a finite element space S_h of continuous functions which are piecewise polynomials of degree less than an integer r.

The discretized problem now reads as follows.

Problem (P5): Find $\{v_h(x,t)$ and $s_h(t)\}$ with

$$v_h(.,t) : (0,T] \to S_h$$

such that

$$s_h b_h(v_h', w') + (\dot{v}_h, w) = \frac{b_h}{\alpha} v_h(1)(x v_h, w') \tag{23}$$

for all $w \in S_h$.

$$\dot{s}_h = \frac{s_h}{\alpha(1-s_h)} v_h(1), \qquad s_h(0) = 1. \tag{24}$$

5 NUMERICAL SCHEME

Let S_h be the space of continuous functions which are piecewise polynomial of degree three. For any positive integer M, divide the interval $(0,T]$ into M subintervals of equal length $k = 1/M$ and let

$$t_n = nk, \qquad n = 1, 2, ..., M.$$

We discretize the time derivative $\dot{v}_h$ at time $t = t_{n+1}$ using the backward difference

$$\dot{v}(x,t) = \frac{v_h^{n+1}(x) - v_h^n(x)}{k} \tag{25}$$

where

$$v_h^n(x) = v_h(x, nk).$$

We now linearize Eq. (23) by evaluating the nonlinear term at the previous time step, in order to get known terms. Hence,

$$\frac{1}{k}\left[(v_h^{n+1},w)-(v_h^n,w)\right]+s_h^n b_h^n(v_{h,x}^{n+1},w_x)=\frac{b_h^n}{\alpha}v_h^n(1)(xv_h^n,w_x) \qquad (26)$$

for all $w \in S_h$ where

$$s_h^n = s_h(nk), \quad v_{h,x}^{n+1}=\frac{\partial}{\partial x}v_h^{n+1}(x) \quad \text{and} \quad w_x=\frac{\partial}{\partial x}w(x).$$

Next, we solve the ordinary differential equations (12) and (24) by means of Heun's method to get

$$s_h^{n+1} = s_h^n\left\{1+\frac{k}{2\alpha}\left[\frac{v_h^n(1)}{(1-s_h^n)}+v_h^{n+1}(1)\frac{\alpha(1-s_h^n)+kv_h^n(1)}{\alpha(1-s_h^n)^2-ks_h^n v_h^n(1)}\right]\right\} \qquad (27)$$

$$\tau_h^{n+1} = \tau_h^n+\frac{k}{2}\left[(s_h^n)^2+(s_h^{n+1})^2\right] \qquad (28)$$

We now set

$$v_h^{n+1}(x)=\sum_{j=0}^{N}\beta_j^{n+1}\psi_j(x), \qquad (29)$$

where $\psi_j(x)$ are basis functions of S_h defined by the cubic splines at equally spaced knots $x = jh,\ j = 0,1,\ldots,N$.

By substituting (29) into (26) and setting $w = \psi_i(x),\ i = 0,1,\ldots,N$, we get a linear system in $(N+1)$ equations and $(N+1)$ unknows $\beta_0^{n+1},\beta_1^{n+1},\ldots,\beta_N^{n+1}$ of the form

$$\mathbf{A}\beta = b \qquad (30)$$

where $\mathbf{A}$ is a $(N+1)\times(N+1)$ matrix

$$a_{ij}=\sum_{j=0}^{N}\beta_j^{n+1}\left[\int_0^1(\psi_i\psi_j+ks_h^n b_h^n\psi_i'\psi_j')dx\right], \quad i=0,1,\ldots,N \qquad (31)$$

and b is the known coefficient vector

$$b_i = \int_0^1 \left[\frac{k}{\alpha} b_h^n (\frac{1}{4}\beta_{N-1}^n + \beta_N^n) x v_h^n \psi_i' + v_h^n \psi_i \right] dx, \quad i = 0, 1, \ldots, N \qquad (32)$$

By solving the system (30) we get the values of v_h^{n+1} at each point $(ih, (n+1)k)$ and at the same time we calculate s_h^{n+1} and τ_h^{n+1} using Eqs. (27) and (28). Next, relation (20) is used to obtain $u_h(x,t)$ which is the solution of problem (P3); then the values of $U_h(r_h, \tau_h)$ are obtained at the point r_h, τ_h with

$$r_h = ih[s_h(nk) - 1] + 1 \quad \text{and} \quad \tau_h = \tau(nk)$$

using relation (13). Finally, the values of the solution $c_h(r_h, \tau_h)$ of our original problem are obtained by using transformation (10).

6 NUMERICAL RESULTS

For the numerical results the analytical approximation for U and R obtained by Rogers & Mc.Innis [5] is used as the starting point for the numerical scheme. It is

$$\begin{aligned} U(r,\tau) &= a_0 \text{erfc}[\frac{1-r}{2\eta}] + b_0 \text{erfc}[-\frac{1-r}{2\eta}] \\ R(\tau) &= 1 - 2s_0\eta, \qquad \text{with} \quad \eta = \sqrt{\tau} \end{aligned}$$

where a_0, b_0 and s_0 are given by the solution of the system

$$\begin{aligned} a_0 + b_0 &= 1 \\ (b_0 - a_0)e^{-s_0^2} &= -\alpha\sqrt{\pi} s_0 \\ a_0 \text{erfc}(s_0) + b_0 \text{erfc}(-s_0) &= 0 \end{aligned}$$

here

$$\text{erfc}(\xi) = 1 - \text{erf}(\xi) = 1 - \frac{2}{\sqrt{\pi}} \int_0^{\xi} e^{-y^2} dy$$

Table 1: Times for the moving front to reach the center of the sphere for different values of α.

α	Davis Hill	Present work
0.015	0.10	0.107
0.025	0.131	0.134
1.0	0.291	0.292

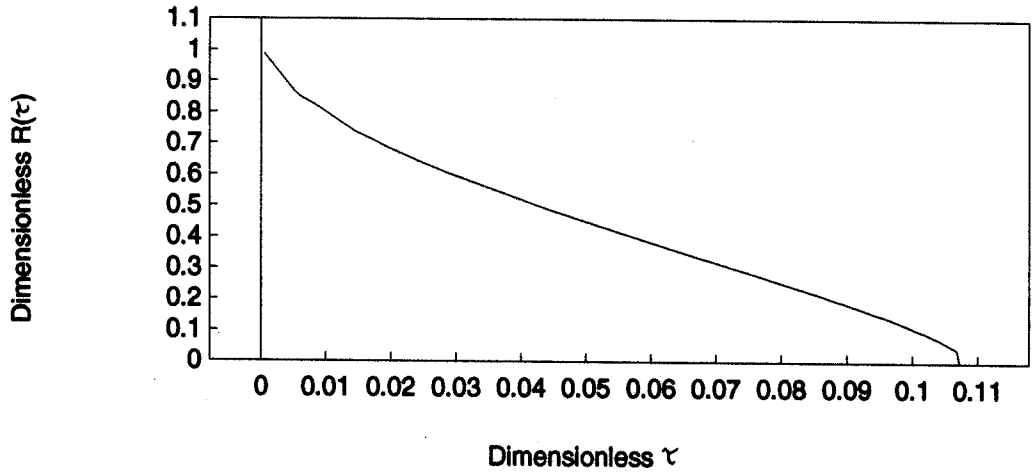
The time for the moving front to reach the center of the sphere or to complete reaction is an important parameter in an industrial situation. Table 1 shows the time to complete reaction with $\alpha = 0.015, 0.025$ and 1.0 and it can be observed that the results of this work are in good agreement with the ones obtained by Davis & Hill [2].

Figures 1, 2 and 3 show the position of the moving boundary $R(\tau)$ versus time for various values of α. It can be observed that it takes more time for the reaction to complete for larger α. This is due to the fact that a greater amount of the diffusing reactant is required to advance the reaction interface than is the case for a smaller α.

Figure 4 shows the concentration of the diffusing reactant within the spherical particales for $R(\tau) = 0.12$ and 0.23 with $\alpha = 0.15$.

Finally, the actual computation were carried out using $h = 0.05$ and $k = 0.0001$. To compute $u_h(x,t)$ from (20), we used an exact formula since

Figure 1: Position of moving boundary for $\alpha = 0.15$.



v_h is piecewise quadratic.

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Figure 2: Position of moving boundary for $\alpha = 0.25$.

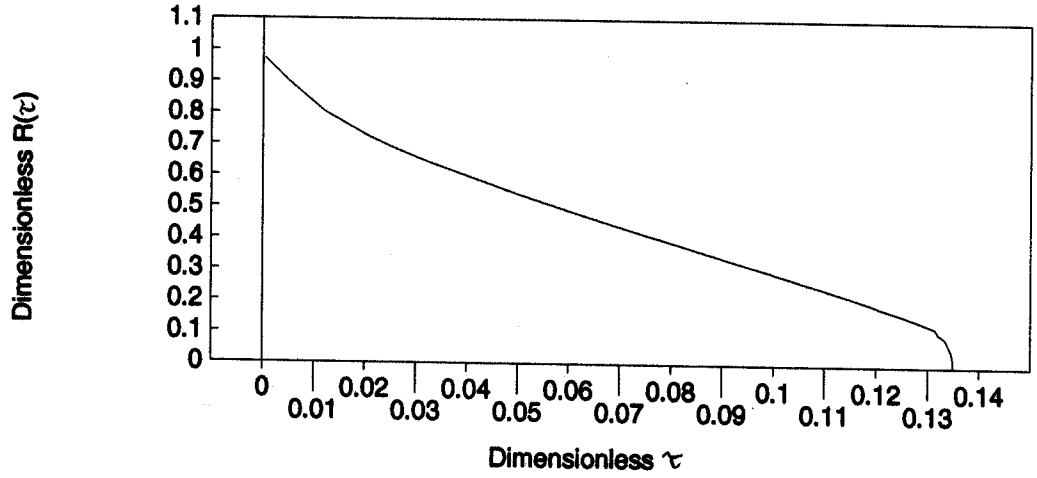

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Figure 3: Position of moving boundary for $\alpha = 1.0$.

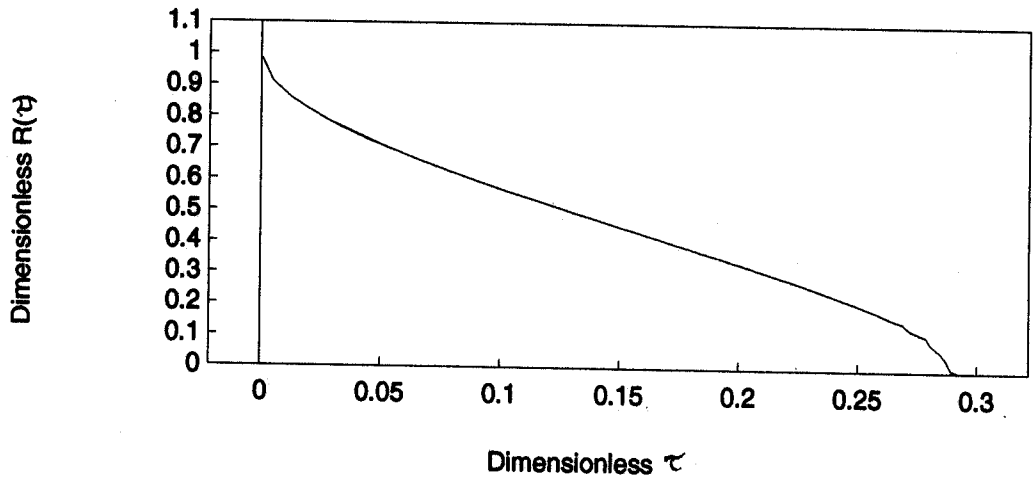

Figure 4: Concentration of diffusing reactant for $\alpha = 1.0$.