European Symposium on Computer Aided Process Engineering – 15
L. Puigjaner and A. Espuña (Editors)

The Numerical Solution of Moving Boundary Problems Using the Moving Finite Element Method

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Abstract

A moving finite element method (MFEM) is developed for the numerical solutions of time-dependent partial differential equations involving solid-fluid reactions. Our MFEM generates an adaptive mesh for each dependent variable so, through spatial domain decomposition, it can be modified in order to be an efficient solver for a class of problems showing a moving internal boundary. The algorithm was tested in the numerical simulation of a non catalytic solid-fluid reaction modelled by the (a) isothermal, (b) non-isothermal shrinking core model with non-linear kinetics. This work establishes the effectiveness and applicability of the MFEM in solving moving boundary problems.

Keywords: Moving Finite Elements; Moving Boundary Problems; Adaptive Grids; Time-Dependent Partial Differential Equations; Shrinking Core Model

1. Introduction

A large number of problems in science and engineering are formulated in terms of time-dependent partial differential equations involving a moving interface. The analytic solutions of mathematical models of dynamic systems are rarely known. This has motivated many authors and different techniques have been proposed in recent years. Crank (1987) presents a wide-ranging description on mathematical and numerical methods for free and moving boundary problems. In this paper we consider the development of a MFEM to compute numerical solution of one-dimensional problems involving two phase with a moving interface. The MFEM (Sereno et. al., 1992, Coimbra et. al., 2001, 2004) generates an adaptive mesh so it can be modified in order to be an efficient solver for a class of problems showing a moving internal boundary. To modify the moving finite element equations we perform the decomposition of the spatial domain by the introduction of a moving node describing the position of the internal interface. This formulation (Robalo et. al., 2004) is expanded in this work to a

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larger class of problems by assuming the existence of non linear boundary conditions at the moving boundary. The paper is organized as follows. In section 2 we present the problem to be solved. The detailed description of the method is presented in section 3. Finally, in section 4, we apply the computer code resulting from the numerical algorithm implementation to the simulation of a non catalytic solid-fluid reaction (Carabin et.al. 1992) modelled by the (a) isothermal, (b) non-isothermal shrinking core model with non-linear kinetics.

2. The Problem

Let us define the moving boundary problem that we consider in this work. The general mathematical model of two-phase system in one-dimensional fixed space domain, with an internal moving interface, is defined by a system of *n* parabolic partial differential equations (PDE) whose *m*-th equation fill the form

$$\frac{\partial y_m}{\partial t} = f_m\left(x,t,\vec{\mathbf{y}},\frac{\partial \vec{\mathbf{y}}}{\partial x}\right)\frac{\partial^2 y_m}{\partial x^2} + g_m\left(x,t,\vec{\mathbf{y}},\frac{\partial \vec{\mathbf{y}}}{\partial x}\right) \tag{1}$$

on $a \le x \le b$, $t > 0$. We consider that the space variable satisfy $a \le x \le X_s(t)$ if $m \le n_{\mathrm{I}}$ and $X_s(t) \le x \le b$ if $n_{\mathrm{I}} < m \le n$. $n_{\mathrm{I}}, n_{\mathrm{II}}$ are the number of dependent variables in each phase, $X_s(t)$ is the position of the moving boundary at instant t and $\vec{\mathbf{y}} = \left[\vec{\mathbf{y}}^{\,\mathrm{I}}, \vec{\mathbf{y}}^{\,\mathrm{II}}\right]^T = \left[y_1,...,y_n\right]^T$, where $\vec{\mathbf{y}}^{\,\mathrm{I}\,T} = \left[y_1^{\mathrm{I}},...,y_{n_{\mathrm{I}}}^{\mathrm{I}}\right]^T$ and $\vec{\mathbf{y}}^{\,\mathrm{II}\,T} = \left[y_1^{\mathrm{II}},...,y_{n_{\mathrm{II}}}^{\mathrm{II}}\right]^T$. Let us assume some initial conditions and that equation (1) is subject to Dirichlet or Robin boundary conditions at the end points of space domain. At the interface we suppose that the boundary conditions can be expressed by general implicit conditions,

$$h_m\left(X_s,t,\vec{\mathbf{y}}\big|_{X_s},\frac{\partial \vec{\mathbf{y}}}{\partial x}\bigg|_{X_s},\frac{\partial \vec{\mathbf{y}}^{\,\mathrm{I}}}{\partial x}\bigg|_{X_s^-},\frac{\partial \vec{\mathbf{y}}^{\,\mathrm{II}}}{\partial x}\bigg|_{X_s^+}\right) = 0\,. \tag{2}$$

To complete the model let us assume that the interface movement is governed by

$$\frac{dX_s}{dt} = \mathrm{w}\left(X_s,t,\vec{\mathbf{y}}\big|_{X_s},\frac{\partial \vec{\mathbf{y}}}{\partial x}\bigg|_{X_s},\frac{\partial \vec{\mathbf{y}}^{\,\mathrm{I}}}{\partial x}\bigg|_{X_s^-},\frac{\partial \vec{\mathbf{y}}^{\,\mathrm{II}}}{\partial x}\bigg|_{X_s^+}\right) \tag{3}$$

This class of problems is an extension of those considered in (Sereno et. al., 1992, Coimbra et. al., 2001) where all differential equations have the same fixed one-dimensional spatial domain but each dependent variable has its own moving mesh. The main idea to solve this problem is to combine the domain decomposition and these different moving finite element meshes.

3. Method Development

The MFEM is a discretization process in two stages: first spatial discretization using finite elements and allowing the movement of the space nodes, in which we focus our attention, and secondly the time integration of the resulting ordinary differential

equations (ODE) system. To solve this implicit time-dependent ODE system we use the package LSODI , (Hindmarsh, 1980).

3.1 Spatial Discretization

The grid connected to the *m*-th dependent variable, y_m , is obtained by partitioning the spatial domain in N_m finite elements by $N_m - 1$ interior separation nodes,

$$P_m : \quad X_{m,1}(t) < X_{m,2}(t) < \ldots < X_{m,N_m}(t) < X_{m,N_m+1}(t), \quad t \geq 0 \tag{4}$$

One of the nodes $X_{m,1}$ or X_{m,N_m+1} is fixed and the other is defined by the interface position along time. In each of the finite element of grid P_m we define the approximate solution by a polynomial obtained by Lagrange interpolation. The relative positions of the interpolation points are optimized as in the orthogonal collocation method (Sereno, 1991). The degree of the polynomial approximation may be chosen by the user. This local approximation guides to a global approximation Y_m to y_m in the spatial domain. It is a continuous piecewise polynomial function that depends, at each instant, on the value of the the *m*-th dependent on the i-th collocation node of the *j*-th finite element, $Y^i_{m,j}$, and on the nodal position, $X_{m,j+1}$ (Sereno et. al., 1992, Coimbra et. al., 2001).

3.2 Residual Minimization, Penalty functions and Integrals Calculation

Following the ideas and implementation of the MFEM expressed in (Sereno et. al., 1992, Coimbra et. al., 2001, 2004), to establish the semi-discrete variables $Y^i_{m,j}$ and $X_{m,j+1}$ we must integrate, in time, the system of ODE´s generated by minimization of the following objective function

$$F = \sum_{m=1}^{n} \left[\left\| \frac{\partial Y_m}{\partial t} - f_m\left(x, t, \vec{\mathbf{Y}}, \frac{\partial \vec{\mathbf{Y}}}{\partial x}\right) \frac{\partial^2 Y_m}{\partial x^2} - g_m\left(x, t, \vec{\mathbf{Y}}, \frac{\partial \vec{\mathbf{Y}}}{\partial x}\right) \right\|^2_{L_2} + P_{enalty} \right] \tag{5}$$

with respect to time derivatives of nodal amplitudes and nodes positions, where P_{enalty} is a penalty term depending on the internodal viscosity and spring penalty functions of the *j*-th finite element of the *m*-th grid, $\varepsilon_{m,j}$ and $S_{m,j}$, respectively (Sereno, 1991). Here we introduce Miller's penalty functions (Miller, 1981) into the minimization process to avoid the singularities associated with the method, due to parallelism and element folding. The penalty functions depend on small positive constants supplied by the user for each element of each grid. To get the explicit form of general equations of method is necessary, first, define the partial derivatives of Y_m in order to time variable and also in order to $Y^i_{m,j}$ and $X_{m,j+1}$ and, secondly, calculate the integrals that results from minimization of F . To define the approximations of spatial derivatives of Y_m we use a smoothing process based on cubic Hermite polynomials in a neighbourhood of the separation nodes. By this process (Sereno et. al., 1991, 1992, Coimbra et. al., 2001) show that all the integrals are well defined as a limit when the amplitude of the neighbourhood tends to zero.

4. Numerical Examples

We are interested in solving numerically a fluid-solid non-catalytic heterogeneous reactions problem described by the Shrinking Core Model (Carabin et. al.) to illustrate the working and performance of our MFEM. All the numerical results presented are obtained on a Pentium 4 computer at 1.6 GHz. Some parameters of the method are kept constant. It is the case of the penalty constants and the ODE solver tolerances. We use Lobatto's quadrature with 11 interior quadrature points to compute the integrals appearing in each one of the equations of the ODE systems.

4.1 The Shrinking Core Model, Isothermal Case

Here we take up the simplest model for the reaction of fluid species A with spherical particles of unchanging size of solid S. Considering the stoichiometric coefficients, ϑ_i, the reaction of the shrinking coke takes the form:

$$\vartheta_A A_{(f)} + \vartheta_S S_{(s)} \rightarrow \vartheta_B B_{(f)} + \vartheta_P P_{(s)} \tag{6}$$

The mathematical problem is to determine the values of the dimensionless concentration of reactant A, $C(x,t)$, $X_s(t) \le x \le 1$, $t \ge 0$, normalized by the bulk molar concentration of A, C_{Ab}. $X_S(t)$ is the position of the interface of the solid unreacted core. The equation for diffusion of reactant A is, in dimensionless form:

$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial x^2} + \frac{2}{x}\frac{\partial C}{\partial x}, \quad X_s(t) \le x \le 1, \quad t > 0 \tag{7}$$

subject to the boundary conditions

$$\frac{\partial C}{\partial x} = DaC^n, \quad x = X_s(t), \quad t \ge 0, \tag{8}$$

$$\frac{\partial C}{\partial x} = Bi_m(1 - C), \quad x = 1, \quad t \ge 0, \tag{9}$$

$$\frac{dX_s}{dt} = -\gamma \ DaC^n, \quad x = X_s(t), \quad t \ge 0 \tag{10}$$

and initial conditions $C(x,0) = 1$, $X_s(0) \le x \le 1$, $X_s(0) = 1$. Here n is the reaction order, Bi_m is the Biot number for mass transfer and $\gamma = \upsilon_S M_S C_{Ab} / \upsilon_S \rho_S$ is a dimensionless number, M_S is the molecular weight of S, ρ_S is the density of S. $Da = Ae^{-\beta} R_S C_{Ab}^{n-1} / D$ is the Damköhler number. Here A is the pre-exponential factor, $\beta = E/(RT_b)$ is the Arrhenius number at bulk temperature, T_b, D is the effective diffusivity of A and R_S the radius in sphere. Figure 1(a) shows the conversion of the solid reactant, $1 - (X_S)^3$ as a function of dimensionless time t/t_f (t_f is the finite time for complete solid conversion) for different Da numbers and fixed γ. We consider $Bi_m = 10^3$ and first order reaction, $n = 1$. For these runs CPU time take values from 0.42 to 0.78 seconds, using cubic approximations and 4 finite elements. Figure 1(b)

shows the time evolution of the moving boundary position, for higher values of Da and γ using approximations of degree 6. The CPU is 3.3 seconds.

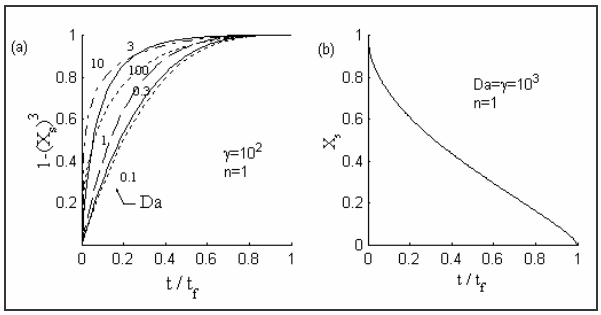

Figure 1. Conversion (a) and evolution of the interface (b) as functions of scaled time

4.2 The Shrinking Core Model, Non-Isothermal Case

In the non-isothermal case the dependent variables are the dimensionless concentration of reactant A, C and the dimensionless temperature, $\nu = (T - T_b)/T_b$. For simplicity we denote by ν_1 the temperature for $0 \le x \le X_S(t)$ and by ν_2 the temperature for $X_S(t) \le x \le 1$. The model is now defined by the mass balance equations (7)-(10), taking into account that the Damköhler number is now a function of temperature, $Da = Ae^{-\beta/(1+\nu_2)} R_S C_{Ab}^{n-1} / D$, combined with the dimensionless energy balance equations:

$$\frac{\partial \nu_i}{\partial t} = \frac{\partial^2 \nu_i}{\partial x^2} + \frac{2}{x}\frac{\partial \nu_i}{\partial x}, \quad i = 1,2, \quad 0 \le x \le 1, \quad t > 0 \tag{11}$$

with initial conditions, $\nu_1 = \nu_2 = 0$ and boundary conditions

$$\frac{\partial \nu_1}{\partial x} = 0, \quad \frac{\partial \nu_2}{\partial x} = -Bi_h C, \quad x = 1 \tag{12}$$

$$\nu_1 = \nu_2, \quad -\kappa \frac{\partial \nu_1}{\partial x} + \frac{\partial \nu_2}{\partial x} - \alpha C^n e^{-\beta/(1+\nu_2)} = 0, \quad x = X_S(t) \tag{13}$$

Bi_h is the Biot number for heat transfer, α is the dimensionless heat of reaction and $\kappa = 1.4$. Figure 2 shows the temperature (a) and concentration (b) profiles for $n = 2$.

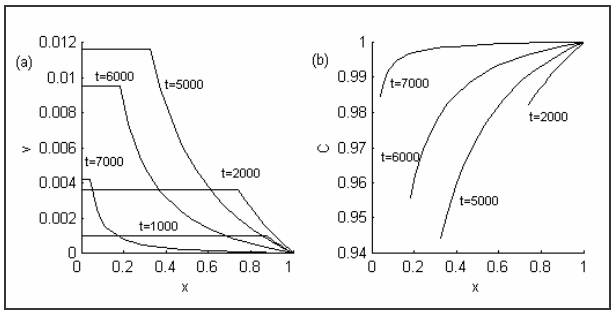

Figure 2. Temperature (a) and concentration (b) profiles at different times

This run test was performed considering $\beta = 20.9$, $\gamma = 4.1\times10^{-4}$, $Bi_m = Bi_h = 10^3$, $\alpha = -7.5\times10^7$ and $Da(t=0) = 0.31$. We use 3 finite elements in the grid associated to ν_1, and 4 in the two other grids associated to ν_2 and C. Using cubic approximations the CPU time for this run is 2.6 seconds. Figure 3(a) and 3(b) present the trajectories of nodes separation associated to temperature and concentration respectively. Initially nodes are concentrated near x=1.

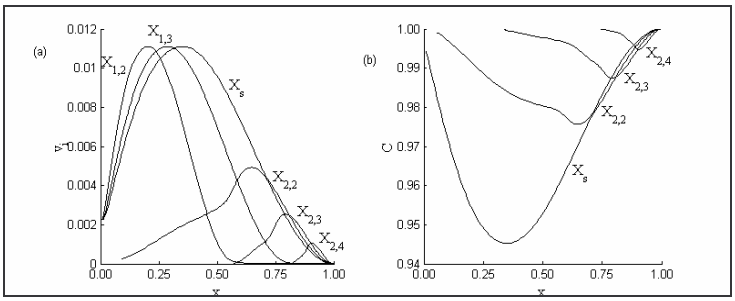

Figure 3. Temperature (a) and concentration (b) at nodes position and interface

5. Conclusions

In this paper we have presented a MFEM for moving boundary problems. The main advantages of the method are its simplicity and performance, which account for its widespread use. The complexity of the numerical examples considered requires a robust and efficient algorithm. In fact, the numerical results obtained by this formulation of MFEM exhibit very good agreement with those obtained by previous methods so, this work establishes the effectiveness and applicability of the MFEM in solving moving boundary problems.

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