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Modeling the dynamics of molecular concentration during the diffusion procedure

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Abstract: *In this paper, a numerical method is proposed to solving a reaction-diffusion system. The systems describe the solid state reaction mechanism of all the reaction components at the preparatory stage of yttrium aluminum garnet (YAG) in one dimension. Kansa's method and forward Euler method are employed to discrete the spatial variable and time respectively.*

Keywords*: Kansa's method, reaction-diffusion system, molecular concentration*

I. INTRODUCTION

In this paper, we employ the Kansa's method to solve the nonlinear partial differential equation system defined on the space $x \in I \subset R^1$ as following.

$$\frac{\partial c_1}{\partial t} = D_1 \frac{\partial^2 c_1}{\partial x^2} - 3\kappa c_1 c_2 \quad (1)$$

$$\frac{\partial c_2}{\partial t} = D_2 \frac{\partial^2 c_2}{\partial x^2} - 5\kappa c_1 c_2 \quad (2)$$

$$\frac{\partial c_3}{\partial t} = D_3 \frac{\partial^2 c_3}{\partial x^2} + 2\kappa c_1 c_2 \quad (3)$$

with initial conditions $c_i(x,0) = c_i^0(x)$, $x \in I = (a,b)$ and with zero Neumann boundary conditions on the boundary $x = a$ and $x = b$, that is, $\frac{\partial c_i}{\partial x}\Big|_{x=a \cup x=b} = 0, i = 1,2,3,$when $t > 0$.

The mathematical model above is a reaction-diffusion system, which describes the solid state reaction mechanism of all the reaction components at the preparatory stage of yttrium aluminium garnet (YAG). Where $c_i = c_i(x,t)$ (i=1,2,3) are the concentrations of the i-th reactant respectively, i.e., Al_2O_3, Y_2O_3 and $Y_3Al_5O_{12}$ in the reaction

$3Al_2O_3+5Y_2O_3 \rightarrow 2Y_3Al_5O_{12}$,

of the synthesis at a point $x \in (a,b)$ at time t. D are the diffusion coefficients, that is, we consider all the diffusion coefficients coincide. This assumption is general when this sizes of molecules are nearly the same. For details, we refer the references [1–7].

It is well known that the system (1)-(3) in common three-dimensional case is complicated and so it is difficult to implement the numerical modeling. In [2], the authors carried out the solution of the system (1)-(3) numerically by using finite difference techniques in one-dimensional case and in two-dimensional case. Sysmmetric implicit scheme and alternating direction scheme are employed in the former case and in the latter case respectively. Both schemes were solved using stream sweeping method [8]. However, to guarantee the convergence of the method of finite difference, it is necessary that the Courant-Friedrichs-Lewy (CFL) condition, which says that the time step should be less than a certain time in many explicit time-marching computer simulations, must be satisfied[9].

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In this paper, a meshless method is employed to compute the concentrations of the reactant of Al_2O_3, Y_2O_3 and $Y_3Al_5O_{12}$ in the reaction

$3Al_2O_3+5Y_2O_3 \rightarrow 2Y_3Al_5O_{12}$.

Generally, numerical methods, such as the finite element method (FEM), finite differences (FD) and finite volumes (FV), transform a partial differential equation over continuum into a finite set of algebra equations. In order to accomplish this tast, it is needed to discretize the domain into a grid, mesh or set of points with a fixed connection among them. However, the generation of a well-behaved mesh is not a trivial question except in very regular geometries. To compensate the difficulties in traditional mesh-based numerical methods, meshless methods are emerged. Moreover, meshless methods are very fit for solving the problems in three dimension space or when the domain is complicated, because there are no fixed connectivities among the nodes.

Meshless methods have gained much attention in recent years, not only in the mathematics but also in the engineering community. Much of the work concerning meshless approximation methods is the interdisciplinary between mathematics and engineering. Many traditional numerical methods can either not handle such problems at all, or are limited to very special situations. Meshless method is often better suited to cope with the changes in the geometry of the domain of interest than classical discretization techniques such as finite difference, finite elements or finite volumes. Another obvious advantage of meshless discretizations is their independence from a mesh. Mesh generation is still the most time consuming part of any mesh-based numerical simulation. Since meshless discretization techniques are based only on a set of independent points, these costs of mesh generation are eliminated. Meshless approximation methods can be seen to provide a new generation of numerical tools.

There are many kind of meshless method, here we make a brief introduction of Kansa's method, for more details, we refer to the references [10].

A function $\Phi: R^s \to R$ is called radial provided there exists an univariate function $\phi: [0, +\infty) \to R$ such that

$\Phi(x) = \varphi(r), \text{where } r = \|x\|.$

$\|.\|$usually is the Euclidean norm on R^s. It is obvious that for a radial function Φ, $\Phi(x_1) = \Phi(x_2)$ holds for all $\|x_1\| = \|x_2\|$ $(x_1, x_2 \in R^s)$. In standard Gaussian radial basis function (RBFs) approximant, the approximate form of function c is written as

$c(x) \approx \sum_{i=1}^{N} \alpha_i \phi(\|x - x_i\|), x \in V.$ (4)

where $\{\alpha_i (i = 1,2, \dots, N)\} \in R$ are the unknown coefficients to be determined.

$\sum_{i=1}^{N} \alpha_i \phi(\|x - x_i\|) = c(x_k), k = 1,2, \dots, N.$ (5)

It is to be noted that there is a large class of RBF Φ available and one have to choose appropriate one according to his need. The most studied RBF including the multiquadric (MQ) $\phi(r) = \sqrt{r^2 + c^2}$, inverse MQ $\phi(r) = (r^2 + c^2)^{-s}$, thin plate splines $\phi(r) = r^2 \log(r)$and Gaussian $\exp[-\left(\frac{r}{c}\right)^2]$. For more details about RBF, we refer the famous review of 29 interpolation method over scattered data [11].

In early 1990s, Kansa made the first attempt to extent RBF interpolation with multiquadrics to the solution of PDEs in the strong form collocation formulation [12, 13]. The method, named the Kansa's method, is a domain type numerical technique in the sense that the problem is discretized not only on the boundary to satisfy boundary conditions but also inside domain to satisfy the governing equation.

II. NUMERICAL METHOD FOR SOLVING THE PROBLEM

To solve the systems (1)-(3) with the given initial and boundary conditions when $I \subset R^1$,we make assumption that all particles are of the same shape of cube shape and its volume is small enough. These are the same as in the papers [2, 3] and readers can find more details in them.

In light of Kansa's method, we write the concentrations $c_l, (l = 1,2,3)$ as

$c_l(x, t) = \sum_{i=1}^{N} \alpha_i^l(t) \phi(x - x_i).$ (6)

Here, the set $\{x_i, i = 1,2,3, \dots, N\}$ is consisted by Halton points [14] in I and is chosen as the central set. $x \in I \cup (a, b)$ are known as the test points.

For simplicity, we introduce some other notations

$\phi_i = \phi(\|x - x_i\|)$,

$\phi_{i_k} = \phi(\|x - x_i\|)|_{x=x_k}$,

$\phi_i^{(1)} = \frac{\partial \phi(\|x - x_i\|)}{\partial x}$,

$\phi_{ik}^{(1)} = \frac{\partial \phi(\|x - x_i\|)}{\partial x}\Big|_{x=x_k}$,

$\phi_i^{(2)} = \frac{\partial^2 \phi(\|x - x_i\|)}{\partial x^2}$,

$\phi_{ik}^{(2)} = \frac{\partial^2 \phi(\|x - x_i\|)}{\partial x^2}\Big|_{x=x_k}$,

$\alpha_i^{l,m} = \alpha_i^l(x, t^m)$,

$\omega_\tau = \{t^m : t^m = m\tau, m = 0,1, \dots, M\}, M\tau = T.$

To solve the non-linear system (3), we propose an alternative iteration algorithm. The scheme is given as

$\frac{c_l(x, t^{m+1}) - c_l(x, t^m)}{\tau} = D \sum_{i=1}^{N} \alpha_i^{l,m+1} \phi_i^{(2)} + D_l \kappa \sum_{i=1}^{N} \alpha_i^{1,m} \phi_i \sum_{i=1}^{N} \alpha_i^{2,m} \phi_i,$

or equivalently,

$\sum_{i=1}^{N} \alpha_i^{l,m+1} \phi_i = \tau[D \sum_{i=1}^{N} \alpha_i^{l,m} \phi_i^{(2)} + D_l \kappa\left(\sum_{i=1}^{N} \alpha_i^{1,m} \phi_i\right)\left(\sum_{i=1}^{N} \alpha_i^{2,m} \phi_i\right)] + \sum_{i=1}^{N} \alpha_i^{l,m} \phi_i.$

Where D_l equals to$-3, -5, 2$ when$l = 1,2,3$, respectively. In the form of system, it can be written as follows,

$$\begin{cases} \sum_{i=1}^{N} \alpha_i^{1,m+1}\phi_i = \tau[D\sum_{i=1}^{N} \alpha_i^{1,m}\,\phi_i^{(2)} - 3\kappa\left(\sum_{i=1}^{N} \alpha_i^{1,m}\,\phi_i\right)(\sum_{i=1}^{N} \alpha_i^{2,m}\,\phi_i)] + \sum_{i=1}^{N} \alpha_i^{1,m}\phi_i \\ \sum_{i=1}^{N} \alpha_i^{2,m+1}\phi_i = \tau[D\sum_{i=1}^{N} \alpha_i^{2,m}\,\phi_i^{(2)} - 5\kappa\left(\sum_{i=1}^{N} \alpha_i^{1,m}\,\phi_i\right)(\sum_{i=1}^{N} \alpha_i^{2,m}\,\phi_i)] + \sum_{i=1}^{N} \alpha_i^{2,m}\phi_i \\ \sum_{i=1}^{N} \alpha_i^{3,m+1}\phi_i = \tau[D\sum_{i=1}^{N} \alpha_i^{m}\,\phi_i^{(2)} + 2\kappa\left(\sum_{i=1}^{N} \alpha_i^{1,m}\,\phi_i\right)(\sum_{i=1}^{N} \alpha_i^{2,m}\,\phi_i)] + \sum_{i=1}^{N} \alpha_i^{3,m}\phi_i \end{cases}$$

(7)

When considering the boundary conditions, we denote

$$\phi_i^{(1)}(a) = \frac{\partial\phi(\|a - x_i\|)}{\partial x}$$

$$\phi_i^{(1)}(b) = \frac{\partial\phi(\|b - x_i\|)}{\partial x}$$

Then we can obtain the following linear systems.

$A^l X^l = F^l$, (8)

where $A^l \in R^{(N+2)\times(N+2)}$ with its entry $A_{ki}^l = \phi_{ik}$ when $k = 1,2,\dots,N, A_{ki}^l = \phi_i^{(1)}(a)$ and $A_{ki}^l = \phi_i^{(1)}(b)$ when $k = N+1$ and $k = N+2$ respectively.

$F_k^l = \tau[D\sum_{i=1}^{N} \alpha_i^{l,m}\left(\sum_{j=1}^{3} \phi_{jk}^{(2)}\right) + D_l\kappa\left(\sum_{i=1}^{N} \alpha_i^{1,m}\,\phi_{ik}\right)(\sum_{i=1}^{N} \alpha_i^{2,m}\,\phi_{ik})] + \sum_{i=1}^{N} \alpha_i^{l,m}\phi_{ik}$

when $k = 1,2,\dots,N$ and $F^l = 0$ $k = N+1$ and $k = N+2$.

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