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A SPH based Lagrangian particle model for transient convection–diffusion-reaction problems

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Abstract

For numerical simulations of convection-dominated reacting flow problems governed by the convection-diffusion-reaction equations, the grid-based Eulerian methods may induce varying degrees of numerical dissipation or spurious oscillations. In this paper, the smooth particle hydrodynamics (SPH) method is applied to the autocatalytic reaction model with multicomponent reactants. For better comparison, three typical Eulerian methods are also introduced, including the high-resolution technique and the Superbee flux limiter, which is considered to be one of the most suitable methods for solving the convection-diffusion-reaction equations. Numerical results show that the Lagrangian particle algorithm has better numerical accuracy than traditional first- and second-order high-resolution methods. It can also correctly track the moving steep fronts without any numerical dispersion and spurious oscillations.

Keywords: reacting flow, smoothed particle hydrodynamics, QUICK, MTVDLF, convection dominated reacting problem.

1 Introduction

The reaction flow model with autocatalytic multiple reactants has been widely used in practical engineering, involving physics, chemistry and biology [1, 2]. The convection-diffusion-reaction system with multiple reactants is often used to describe the reacting flow model and it is composed of a set of partial differential equations

(PDEs) with nonlinear reaction terms. As this kind of problem is generally convection dominated, there are many difficulties in solving them, especially when there exists large gradient interface [1,3,4]. Since it is easy to produce numerical dissipation, phase deviation, spurious oscillation and other problems [5], sophisticated and specially designed mathematical tools are highly needed.

Smoothed particle hydrodynamics (SPH) is a meshless Lagrangian method with firm foundation in computational fluid mechanics [6]. The method was originally proposed by Gingold and Monaghan [7] and Lucy [8] for the study of astrophysical problems. In SPH, the basic idea is to approximate the governing equation by integral form and then discretize it by a group of scattered interacting particles, each of which carries the same variables, such as mass, velocity, density, concentration, etc. It mainly includes two steps namely kernel approximation and particle approximation [6]. With the Lagrangian property, SPH does not have numerical dissipation in the simulation of advection terms, so it is more suitable for modelling convection dominated transport problems than the traditional grid-based methods [9]. In addition, SPH can easily deal with large deformation and irregular boundaries, which is one of its advantages over the traditional grid-based methods. Therefore, SPH is mainly used for interface capture and real-time interface tracking in fluid dynamics [10-12].

A Lagrangian particle model based on SPH has been successfully applied to simulate convection-reaction problem in autocatalytic flow with multicomponent reactants [13]. In this paper, we extend it to convection-diffusion-reaction problems. The traditional Eulerian high-resolution mesh-based methods including Modified Total Variation Diminishing Lax-Friedrichs with Superbee limiter (MTVDLF-Superbee) [13], Upstream Difference Scheme (UDS) and the Quadratic Upstream Interpolation for Convective Kinematics (QUICK) scheme are used for comparison to elaborate its advantages.

2 Methods

For the multi-reactant reacting problems, we consider the completely stirred tank reactor (CSTR), which is an open system that provides a platform for many experiments and theories [14]. The most commonly used model in isothermal CSTR consists of three reactants which are denoted by A, B and C. The complicated chemical reactions between the three reactants generally involve the following steps [15]:

Replication of B: $A + 2B \xrightarrow{k_1} 3B$

Death of B: $B \xrightarrow{k_2} P_1$

Mutation of B into C: $A + 2B \xrightarrow{\alpha k_1} 2C + B$

Replication of C: $A + 2C \xrightarrow{\beta k_1} 3C$

Death of C: $C \xrightarrow{k_2/\beta} P_2$

where k_1 and k_2 denote the constant reaction rate during chemical reactions, α represent the constant mutation rate of reactant B and β represent the mutation efficiency of reactant C.

CSTR can be described by a one-dimensional model, in which the flow velocity can be regarded as a constant. The governing equation for the reactant A, B and C can be written in the following format

$$\frac{\partial U_1}{\partial T}+V\frac{\partial U_1}{\partial X}=D_1\frac{\partial^2 U_1}{\partial X^2}+(1-U_1)\left[(1+\alpha)U_2^2+\beta U_3^2\right] \tag{1}$$

$$\frac{\partial U_2}{\partial T}+V\frac{\partial U_2}{\partial X}=D_2\frac{\partial^2 U_2}{\partial X^2}+(1-\alpha)(1-U_1)U_2^2-\gamma U_2 \tag{2}$$

$$\frac{\partial U_3}{\partial T}+V\frac{\partial U_3}{\partial X}=D_3\frac{\partial^2 U_3}{\partial X^2}+(1-U_1)(\beta U_3^2+2\alpha U_2^2)-\frac{\gamma}{\beta}U_3 \tag{3}$$

with the following initial and Dirichlet boundary conditions

$$\begin{aligned} &U_1(X,0)=1,\ U_2(X,0)=0,\ U_3(X,0)=0\\ &U_1(0,T)=0,\ U_2(0,T)=1,\ \ U_3(0,T)=0\\ &U_1(1,T)=1,\ U_2(1,T)=0,\ \ U_3(1,T)=0 \end{aligned} \tag{4}$$

All the dimensionless parameters in Eqs. (1)-(3) are given by

$$U_1=\frac{u_f-u_1}{u_f},\ U_2=\frac{u_2}{u_f},\ U_3=\frac{u_3}{u_f},\ X=\frac{x}{L},\ T=k_1u_f^2t,\ V=\frac{a}{k_1u_f^2L},\ \gamma=\frac{k_2}{k_1u_f^2} \tag{5}$$

where $U_i(i=1,2,3)$ and $D_i(i=1,2,3)$ are the dimensionless concentration and diffusion parameters of reactant A, B and C, respectively, V is the dimensionless convection velocity and T is the dimensionless time, X is the dimensionless coordinate, u_f represent the substrate concentration, L is the length of tubular reactor, x and t represent coordinate and time, respectively.

The smoothed particle hydrodynamics (SPH) method is a fully meshless method in Lagrangian system. And it was proposed to overcome the difficulties and limitations of the grid-based methods in dealing with the interaction between stars in astrophysics. There are two basic ideas in SPH namely kernel function approximation and particle approximation.

The kernel approximation rewrites any function in the following integral form

$$f(x)=\int_\Omega f(x')\delta(x-x')dx' \tag{6}$$

where Ω is the problem domain, $\delta(x-x')$ is the Dirac function defined as

$$\delta(x-x')=\begin{cases}1 & x=x'\\ 0 & x\neq x'\end{cases} \tag{7}$$

Considering the ideal properties of the Dirac function, in SPH the kernel function $W(x-x',h)$ is used to approximately replace the Dirac function, and Eq. (6) can be converted into

$$\langle f(x)\rangle=\int_\Omega f(x')W(x-x',h)dx' \tag{8}$$

where $\langle f(x)\rangle$ represents kernel approximation of the function $f(x)$, h is the smoothing length of the kernel function W.

The SPH method discretizes the problem domain into a set of particles and replaces the integral function with discrete summation. The function at the central particle i

is then further approximated by its neighbor particle j

$$\langle f(x_i)\rangle = \sum_{j=1}^{n} \frac{m_j}{\rho_j} f(x_j) W(x_i - x_j, h) \tag{9}$$

The derivative of Eq. (9) can be obtained as

$$\langle \nabla f(x_i)\rangle = - \sum_{j=1}^{n} \frac{m_j}{\rho_j} f(x_j) \nabla_i W(x_i - x_j, h) \tag{10}$$

where m_j and ρ_j are mass and density of the particle, ∇W is the gradient of the kernel function. Since the derivative of the kernel function has the property of anti-symmetry

$$\sum_{j=1}^{n} \frac{m_j}{\rho_j} \nabla_i W(x_i - x_j, h) = 0 \tag{11}$$

The most widely used spatial derivative can be obtained

$$\langle \nabla f_i\rangle = \sum_{j=1}^{n} \frac{m_j}{\rho_j} (f_j - f_i) \nabla_i W_{ij} \tag{12}$$

where $f_i = f(x_i)$ and $\nabla_i W_{ij} = \partial W(|x_i - x_j|, h_i)/\partial x_i$. Similarly, the second spatial derivative of the function at particle i can be written as [9]

$$\langle \nabla^2 f_i\rangle = \sum_{j=1}^{n} \frac{2m_j}{\rho_j} (f_j - f_i) \frac{x_j - x_i}{|x_j - x_i|^2} \nabla_i W_{ij} \tag{13}$$

Using the above theories and formulas, the multicomponent reacting model (1)-(3) can be written in Lagrangian form as

$$\frac{d\boldsymbol{U}}{dt} = \boldsymbol{D} \cdot \nabla^2 \boldsymbol{U} + \boldsymbol{G}(\boldsymbol{U}) \tag{14}$$

$$\frac{dx}{dt} = v \tag{15}$$

Discretizing Eqs. (14) and (15) with SPH approximations give

$$\begin{aligned} \frac{d\boldsymbol{U}_i}{dt} = & \sum_{j=1}^{n} \frac{2m_j}{\rho_j} \boldsymbol{D}(\boldsymbol{U}_j - \boldsymbol{U}_i) \frac{x_j - x_i}{|x_j - x_i|^2} \nabla_i W_{ij} \\ & + \sum_{j=1}^{n} \frac{m_j}{\rho_j} \boldsymbol{G}(\boldsymbol{U}_i) W(x_i - x_j, h) \end{aligned} \tag{16}$$

$$\frac{dx_i}{dt} = v_j \tag{17}$$

3 Results

In the section, the numerical results are presented and the following parameters are taken into consideration: $\alpha = 0.065$, $\beta = 2.0$, $\gamma = 0.025$, $V = 1.0$. The diffusion coefficient of A, B and C are taken the same as $D = 0.05$. The time step is $\Delta t = 0.00002$ and the simulation time is 1. As no analytical solution is available for the problem studied herein, it is indispensable to obtain a reference solution. As a grid-based Eulerian method, the upstream difference scheme (UDS) has been confirmed with convergence to theoretical solution in convection diffusion problems [16].

With different grid number, the time history of the dimensionless concentration at

$X = 0.5$ and the concentration profile for reactant A gained by UDS are shown in Fig. 1(a) and 1(b), respectively. Numerical convergence is clearly observed. The UDS solution with N = 500 is then taken as the reference.

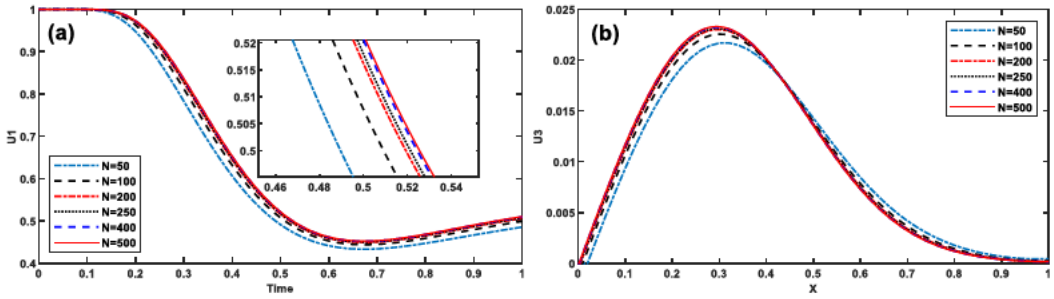

Figure 1: Concentration of reactant A obtained by UDS at X = 0.5 changing with time and grid numbers.

To get more accurate results under the same conditions, spatial step of $\Delta x = 0.002$ is adopted for SPH, MTVDLF-Superbee and QUICK in the following simulations with Courant number $Cr = \dfrac{V\Delta t}{\Delta x} = 0.02$. The concentration comparison of reactant (U_1), substrate (U_2), and mutant (U_3) obtained by different scheme are presented in Fig. 2.

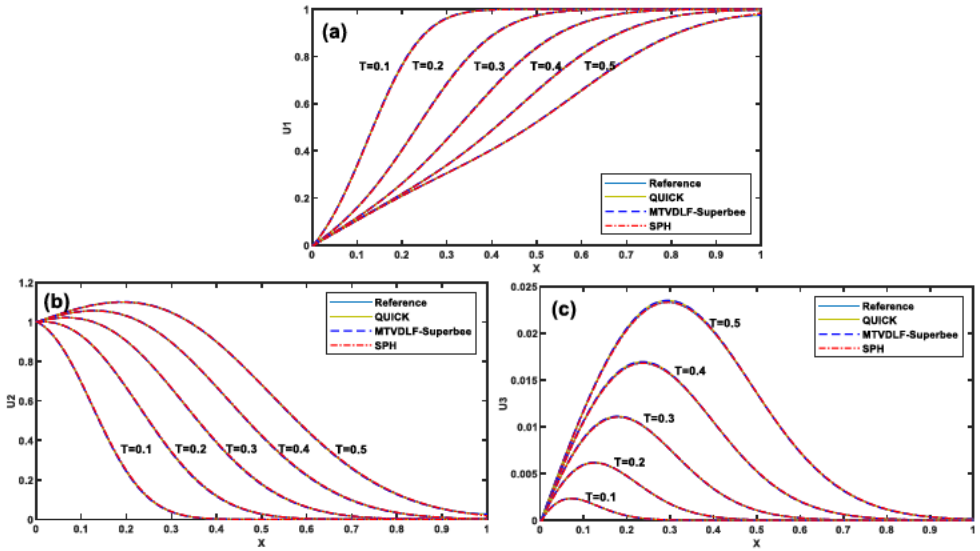

Figure 2: Concentration profiles of numerical reactants A (a), B (b) and C (c) at five time levels for Pe = 200.

The above results illustrate that for the case of Peclet number Pe = 200, under the same conditions of sufficient refinement, the SPH results have excellent agreement with the reference solutions. So are the high-resolution grid-based methods. However, with the increase of the Peclet number, the advantage of SPH in dealing with convection dominant reacting problems with multiple reactants becomes obvious as shown in Fig. 3.

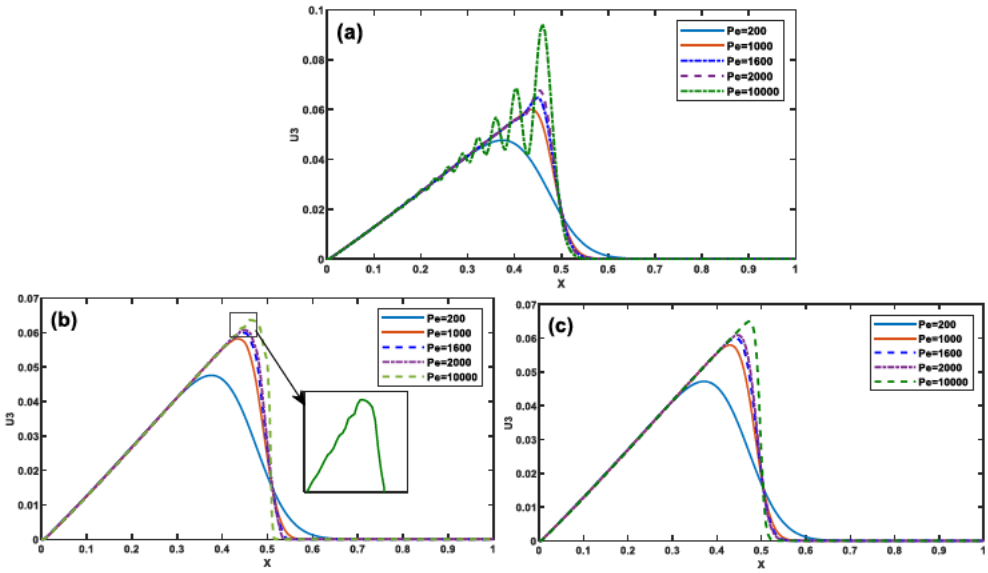

Figure 3: Concentration profile of reactant C obtained by (a) QUICK, (b) MTVDLF and (c) SPH under different Peclet number.

4 Conclusions and Contributions

The aim of the paper is to develop a numerical method for convection-dominated reacting flow problems without suffering from numerical dissipation and unphysical oscillations that existed in traditional grid-based Eulerian methods. The meshless smoothed particle hydrodynamics (SPH) method has been applied for solving the autocatalytic reaction model with multicomponent reactants. For a better illustration of the scheme, typical Eulerian methods were also studied, including the high-resolution QUICK and the MTVDLF with Superbee limiter.

Numerical results indicated that the MTVDLF-Superbee scheme is capable of yielding more accurate solutions. This is consistent with Alhumaizi's conclusion that the MTVDLF-Superbee scheme is the most appropriate method for simulating the autocatalytic reaction model [15]. However, MTVDLF-Superbee still suffers from spurious oscillations near the shock region for a certain component reactant. This will greatly reduce the accuracy of the solution. While the SPH algorithm can solve the autocatalytic reaction model without any numerical diffusion and spurious oscillations, even for convection dominant problems with high Peclet numbers. It is therefore considered to be an effective numerical method for completing the convection-reaction model with multicomponent reactants.

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