A VARIATIONAL PRINCIPLE FOR THE PHOTOCATALYTIC NO_x ABATEMENT

by

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Numerical study of NO_x abatement in a photocatalytic reactor has been caught much attention recently. There are two ways for the numerical simulation, one is the CFD model, the other is the variational-based approach. The latter leads to a conservation algorithm with less requirement for the trial functions in the numerical study. In this paper we establish a variational principle for the problem, giving an alternative numerical method for NO_x abatement.

Key words: *CFD model, semi-inverse method, free surface, variational principle, photocatalytic NO_x abatement, fractal Fick's law, fractal derivative, fractal variational principle*

Introduction

Recently Lira *et al.* [1] suggested a 2-D CFD model for the numerical simulation of NO_x abatement in a photocatalytic reactor, and good results were obtained. The numerical simulation has two general approaches, one is to use the governing equations to construct algorithms like that in the CFD simulation [1], the other is to establish a variational principle for the discussed problem, which is an energy form and can suggest suitable boundary conditions and trial functions [2]. The variational-based finite element method (FEM) [2] has many advantages over its traditional FEM partner, and we should not ignore the convenience and effectiveness of the variational-based simulation for NO_x abatement in a photocatalytic reactor.

Mathematical model

We introduce a potential function Φ defined as:

$$\frac{\partial \Phi}{\partial x} = u \tag{1}$$

$$\frac{\partial \Phi}{\partial y} = v \tag{2}$$

to replace the Navier-Stokes equations, where u and v are velocity components in x- and y-directions, respectively. Equations (1) and (2) imply that:

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$$\frac{\partial u}{\partial y}-\frac{\partial v}{\partial x}=0 \tag{3}$$

The mass conservation requires that:

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0, \quad \text{or} \quad \frac{\partial^2 \Phi}{\partial x^2}+\frac{\partial^2 \Phi}{\partial y^2}=0 \tag{4}$$

The conservation of NO, NO_2, and H_2O requires that [1]:

$$\frac{\partial}{\partial x}(\rho u\omega_i)+\frac{\partial}{\partial y}(\rho v\omega_i)+\frac{\partial}{\partial x}(J_{i,x})+\frac{\partial}{\partial y}(J_{i,y})=0 \tag{5}$$

where ω_i is the species mass fraction and $J_{i,x}$ and $J_{i,y}$ – the diffusive flux of the species i in the x- and y-co-ordinates, given by Fick's law [1]:

$$J_{i,x}=-\rho D_{i,\mathrm{m}}\frac{\partial \omega_i}{\partial x} \tag{6}$$

$$J_{i,y}=-\rho D_{i,\mathrm{m}}\frac{\partial \omega_i}{\partial y} \tag{7}$$

where $D_{i,\mathrm{m}}$ is the species diffusivity in the mixture. Equation (5) becomes:

$$\frac{\partial}{\partial x}(\rho u\omega_i)+\frac{\partial}{\partial y}(\rho v\omega_i)-\frac{\partial}{\partial x}\left(\rho D_{i,\mathrm{m}}\frac{\partial \omega_i}{\partial x}\right)-\frac{\partial}{\partial y}\left(\rho D_{i,\mathrm{m}}\frac{\partial \omega_i}{\partial y}\right)=0 \tag{8}$$

Variational principle for the photocatalytic NO_x abatement

Using the semi-inverse method [3-18], we can obtain the following variational principle:

$$J(\Phi,u,v)=\iint L\mathrm{d}x\mathrm{d}y \tag{9}$$

where the Lagrange function, L, is given by:

$$L=a\rho\omega_i\left(\frac{\partial \Phi}{\partial x}-u\right)^2+a\rho\omega_i\left(\frac{\partial \Phi}{\partial y}-v\right)^2+\rho\omega_i u\frac{\partial \Phi}{\partial x}+\rho\omega_i v\frac{\partial \Phi}{\partial y}-$$

$$-\rho D_{i,m}\frac{\partial \omega_i}{\partial x}\frac{\partial \Phi}{\partial x}-\rho D_{i,m}\frac{\partial \omega_i}{\partial y}\frac{\partial \Phi}{\partial y}-\frac{1}{2}\rho\omega_i(u^2+v^2) \tag{10}$$

where a is a free parameter satisfying:

$$2a+1\neq 0 \tag{11}$$

The stationary condition (Euler-Lagrange equation) for eq. (9) with respect to some an independent function, Ψ, can be written:

$$\frac{\partial L}{\partial \Psi}-\frac{\partial}{\partial x}\frac{\partial L}{\partial \Psi_x}-\frac{\partial}{\partial y}\frac{\partial L}{\partial \Psi_y}=0 \tag{12}$$

where Ψ is an independent function of u, or v, or Φ, the subscribe means the partial derivation.

The Euler-Lagrange equations with respect to u, v, and Φ, respectively, are given:

$$2a\rho\omega_i\left(\frac{\partial\Phi}{\partial x}-u\right)+\rho\omega_i\frac{\partial\Phi}{\partial x}-\rho\omega_i u=0 \tag{13}$$

$$2a\rho\omega_i\left(\frac{\partial\Phi}{\partial y}-v\right)+\rho\omega_i\frac{\partial\Phi}{\partial y}-\rho\omega_i v=0 \tag{14}$$

$$-2a\frac{\partial}{\partial x}\left\{\rho\omega_i\left(\frac{\partial\Phi}{\partial x}-u\right)\right\}-2a\frac{\partial}{\partial y}\left\{\rho\omega_i\left(\frac{\partial\Phi}{\partial y}-v\right)\right\}-\frac{\partial}{\partial x}(\rho\omega_i u)-\frac{\partial}{\partial y}(\rho\omega_i v)+$$

$$+\frac{\partial}{\partial x}\left(\rho D_{i,m}\frac{\partial\omega_i}{\partial x}\right)+\frac{\partial}{\partial y}\left(\rho D_{i,m}\frac{\partial\omega_i}{\partial y}\right)=0 \tag{15}$$

It is obvious that eqs. (13) and (14) are equivalent to, respectively, eqs. (1) and (2) when $2a + 1 \neq 0$. In view of eqs. (1) and (2), we can obtain eq. (8) from eq. (15).

Discussion and conclusion

As we can see from eq. (10), the highest order is the first order, while that in eqs. (4) and (8) are second order. During the numerical simulation, the trial functions for ω_i and Φ must be at least two-order differential in the CFD model, while the variational principle requires only first-order differential trial functions, making the simulation process much simpler. Additionally, the variational model can effectively deal with free or moving boundaries for multiple phase problems, which cannot be done effectively by the CFD model, a detailed discussion on the free boundary problem by the variational principle was given in [2].

Fick's law can also be further improved using fractal calculus [19-26]:

$$J_{i,x}=-\rho D_{i,\mathrm{m}}\frac{\partial\omega_i}{\partial x^\alpha} \tag{16}$$

$$J_{i,y}=-\rho D_{i,\mathrm{m}}\frac{\partial\omega_i}{\partial y^\beta} \tag{17}$$

where $\partial/\partial x^\alpha$ and $\partial/\partial y^\beta$ are fractal derivatives with respect to x and y, respectively. The α and β are fractal dimensions in x- and y-directions, respectively. Detailed discussion of the fractal calculus and its applications are available in [19-26]. The semi-inverse method was successfully applied to establishment of a variational principle in a fractal space [27, 28].

To be concluded, for the first time ever, a variational principle is established in this paper to deal with NO_x abatement in a photocatalytic reactor.

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