SPH Simulation of Pollutant Transport in Rivers

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Abstract. Two Lagrangian models are developed for the accurate simulation of advection-diffusion transport in unsteady open channel flows. The first one is based on a second-order partial differential equation (PDE) for pollutant concentration (model I), and the second one is a first-order system with diffusive flux as another primary variable (model II). To solve the two models, the meshless smoothed particle hydrodynamics (SPH) method is employed. To enforce the inlet and outlet boundary conditions, an extrapolation scheme based on cubic spline is used. Numerical results are presented for tracer distributions with boundary layer in a uniform flow and are compared with analytical solutions. It is demonstrated that both the two models can accurately solve the advection-diffusion transport problems, for which numerical diffusion and disperse oscillation are often observed in most Eulerian schemes. Therefore, the Lagrangian particle models are efficient and accurate tools to predict advection dominated transport for water quality in river systems and for transport with a boundary layer.

Introduction

Pollutant transport in open channels is one of the fundamental problems in environmental hydraulics. This problem is generally modeled by the well-known advection-diffusion equation, which also describes many other physical phenomena such as the heat conduction in the flow. These problems have the same mechanism that involves two processes of mass transport and molecular diffusion [1].

Apart from calibrating the diffusion coefficients in the equation via experimental data, another important topic is to solve the equation with robust numerical methods. To solve this kind of problems, many numerical methods have been proposed including FDMs [2], FVMs [3] and FEMs [2,3]. They are all Eulerian approaches based on meshes fixed in space, which gives rise to a number of difficulties when the transport is advection dominated. To minimize the numerical diffusion and instabilities in the sharp frontal regions, semi-Lagrangian methods are developed for weather prediction [4], in which operator splitting is often used, *i.e.* advection and diffusion are solved separately. *Gross et al.* [5] found that non-conservative semi-Lagrangian methods can decrease numerical diffusion and oscillations, but it still has problems in the vicinity of steep fronts. A full Lagrangian model with moving grid points of *Devkota and Imberger* [6] can remove the deficiencies occurred in both Eulerian and semi-Lagrangian approaches. However, its extension to high-dimensional problems is very difficult if it is not impossible, as it is still based on finite difference technique. In this paper, we aim at solving the pollutant transport problems using meshless smoothed particle hydrodynamics (SPH) method [7,8], of which the extension to high dimensions is straightforward. In addition, to avoid using standard SPH to approximate the second-order derivatives, a new Lagrangian pollutant transport model with diffusive flux is proposed. To enforce inlet and outlet boundary conditions, an extrapolation scheme based on cubic spline is developed.

The rest of the paper is organized as follows. The governing equations, the SPH method and numerical boundary conditions are firstly described. To verify the proposed models, a benchmark problem for advection-diffusion with different Peclet numbers is then solved and compared with analytical solutions. Some discussion and concluding remarks are drawn at the end.

Lagrangian Particle Models

Governing equations. The unsteady advection-diffusion equation governing the mass transport phenomenon in multi-dimensions reads

$$\frac{\partial c}{\partial t} + \boldsymbol{u} \cdot \nabla c = \nabla \cdot (\varepsilon \nabla c) \tag{1}$$

where c is pollutant concentration, $\boldsymbol{u}$ is fluid velocity, t is time and ε is diffusion coefficient, which may depend on the location or even the concentration itself. For simplicity, we assume it is a constant as often taken in practice. With the definition of material derivative $\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + \boldsymbol{u} \cdot \nabla$, Eq. (1) can be transformed into the Lagrangian form as

$$\frac{\mathrm{d}c}{\mathrm{d}t} = \varepsilon \nabla^2 c \tag{2}$$

with the moving coordinate system

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{u} \tag{3}$$

If we introduce the diffusive flux $\boldsymbol{q} = -\varepsilon \nabla c$, the second-order equation (2) can be transformed into a first-order system as

$$\begin{cases} \frac{\mathrm{d}c}{\mathrm{d}t} = -\ \nabla \cdot \boldsymbol{q} \\ \boldsymbol{q} = -\varepsilon \nabla c \end{cases} \tag{4}$$

It is clear that all three equations (1), (2) and (4) are equivalent. In addition, after Lagrangian transformation, the original advection-diffusion equation (1) becomes a pure diffusion equation (2) or (4) on the moving coordinate (3). To avoid the aforementioned various numerical difficulties in solving the advection part, we aim at solving the advection-diffusion equation in Lagrangian form, *i.e.* either Eq. (2) or Eq. (4) together with (3), but not the original one Eq. (1) in Eulerian form.

Smoothed Particle Hydrodynamics (SPH). In SPH method, continuous media are discretized into a finite number of N particles. Each particle $a \in [1, N]$ carries a mass m_a, density ρ_a, velocity $\boldsymbol{u}_a$, concentration c_a and other properties depending on the specific problem. The particle mass $m_a = \rho_a^0 V_a^0$ depends on the discretized medium's initial density distribution ρ_a^0 and the chosen volume partitioning V_a^0 of the physical domain Ω. In general, particles are initially distributed at Cartesian grid points with an equal distance $\Delta \boldsymbol{x}$. The volume of a particle can then be written as $V_a = \Delta x^d$, where d denotes the spatial dimension number. During motion, a particle is allowed to change its density and volume, but its mass keeps constant. In this paper Eqs. (2) and (4) are solved using SPH. For details of standard SPH, the readers are referred to recent reviews by Monaghan [7,8] and the text book of Violeau [9].

Model I. The semi-discretization of Eq. (2), in standard SPH particle form, is

$$\frac{\mathrm{d}c_a}{\mathrm{d}t} = \varepsilon \sum_b \frac{m_b}{\rho_b} (c_b - c_a) \nabla_a^2 W_{ab} \tag{5}$$

where $W_{ab} = W(\boldsymbol{x}_a - \boldsymbol{x}_b, h_a)$ is the kernel function, $\nabla_a^2 W_{ab}$ denotes the Laplacian of the kernel taken with respect to the coordinates of particle a, and h_a is the smoothing length for particle a.

Model II. The semi-discretization of Eq. (4) reads

$$\begin{cases} \frac{\mathrm{d}c_a}{\mathrm{d}t} = \sum_b \frac{m_b}{\rho_b} (\boldsymbol{q}_b - \boldsymbol{q}_a) \cdot \nabla_a W_{ab} \\ \boldsymbol{q}_a = \varepsilon \sum_b \frac{m_b}{\rho_b} (c_b - c_a) \nabla_a W_{ab} \end{cases} \tag{6}$$

where $\nabla_a W_{ab}$ is the kernel gradient. The cubic spline function [9] widely used in SPH is employed herein as the kernel.

Particles are moved according to

$$\frac{\mathrm{d}\boldsymbol{x}_a}{\mathrm{d}t} = \boldsymbol{u}_a \tag{7}$$

Boundary Condition. Although SPH has been successful in a broad range of applications, several stumbling problems need to be overcome, among which boundary condition implementation is a subtle but difficult issue. The logical difficulty is that SPH was invented to deal with astrophysical problems, for which an important task is to find the system boundary. However, in many practical applications, the influence of boundaries has to be taken into account. It is noted that there is no

reason to assume correct boundary conditions will be automatically implemented in SPH, as the physical boundary of a system domain does not coincide with the SPH interaction boundary. In this paper, the dummy particle method proposed by Takeda et al. [10] is used, in which some particles are located outside the system boundary but are included in the SPH interaction range. To specify accurate values for dummy particles, the cubic spline is used to extrapolate the boundary information.

Numerical Results

Together with (7), the semi-discrete SPH equations (5) and (6) are marched in time by the second-order predictor-corrector method. A sufficiently small time step is used to satisfy the CFL condition. For validation, the two models developed in Section 2 are used for solving the non-dimensionalized pollutant transport problem in one dimension

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = \varepsilon\frac{\partial^2 c}{\partial x^2}, \quad x \in [0,1] \tag{8}$$

with boundary conditions

$$c(0,t) = 1 \text{ and } c(1,t) = 0 \tag{9}$$

At steady state, it has the exact solution

$$c(x) = 1 - \frac{\exp(Pe\, x) - 1}{\exp(Pe) - 1} \tag{10}$$

where $Pe = u/\varepsilon$ is the dimensionless Peclet number. The exact solution is used to evaluate the numerical behavior of the proposed models.

The simulation results together with exact solutions for two Peclet numbers with the two models are shown in Fig. 1 and Fig. 2, respectively. It is seen that although both of them give results comparable to exact solutions, Model II has better performance than Model I.

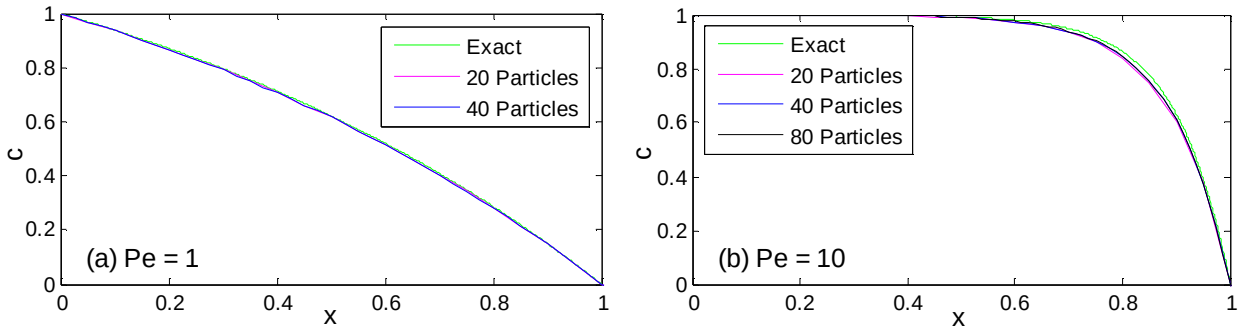

Fig. 1 Model I solutions for pollutant transport with different Peclet number. (a) Pe = 1 and (b) Pe = 10.

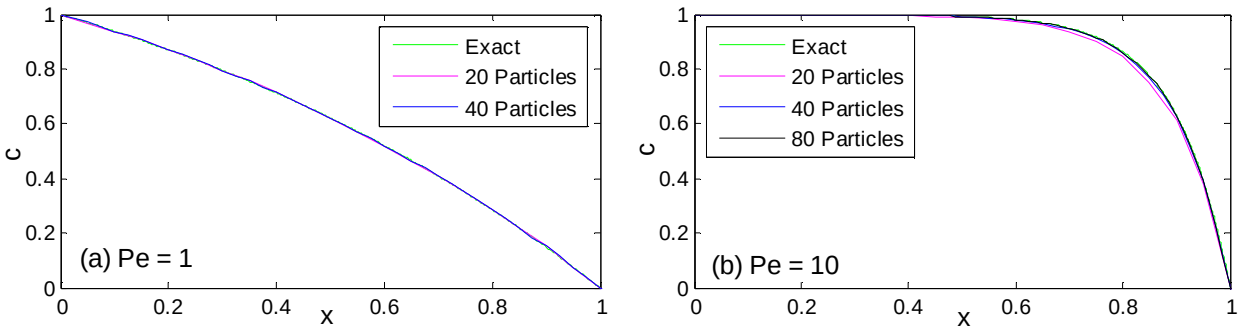

Fig. 2 Model II solutions for pollutant transport with different Peclet number. (a) Pe = 1 and (b) Pe = 10.

To show the accuracy and convergence behavior of the two models, the convergence rate with exact boundary condition is shown in Fig. 3, which is about 1.6 for Model II and only 0.6 for Model I. This is consistent with the conclusion that standard SPH approximation for second-order derivatives had better not to be used due to the low accuracy [8, 9]. As shown in Figs. 1 and 2 for Pe =10 and Fig. 4 for Pe = 100, neither of the two models shows numerical oscillations at the right-end boundary layer, which is a notorious phenomenon in mesh-based methods [2].

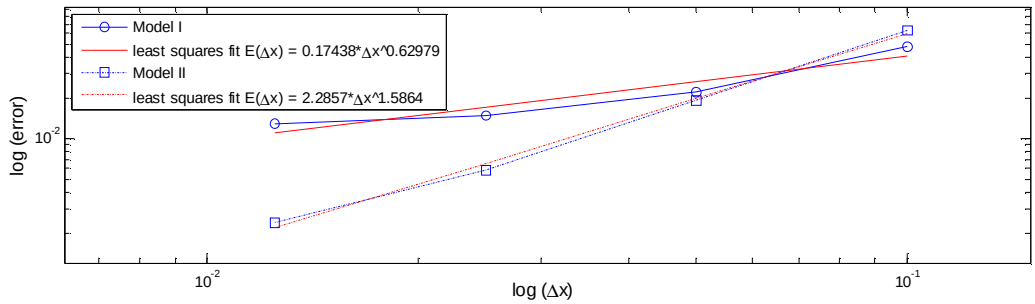

Fig. 3 Convergence rate of the Lagrangian particle models for pollutant transport.

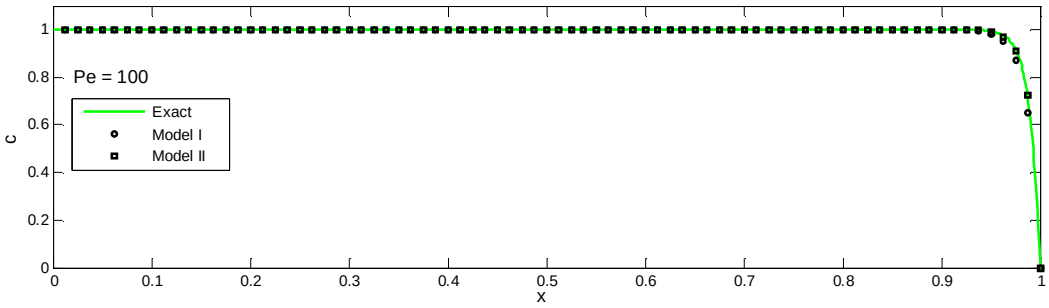

Fig. 4 SPH solutions for pollutant transport with Pe = 100.

Conclusions

This paper reports two Lagrangian particle models for the simulation of pollutant transport in open channel flows. Although both of them can give good solutions, Model II without a second-order derivative approximation has better convergence behavior. As all the developed formulations are in multi-dimensional form, the extension to high dimensions is straightforward and being worked on.

Acknowledgements

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