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Lagrangian modeling of particle concentration distribution in indoor environment with different kernel functions and particle search algorithms

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ABSTRACT

This study aims at investigating the simulation error and computational efficiency of indoor particulate matter (PM) concentration estimation for various kernel functions and particle search algorithms of the kernel method. Firstly, five kernel functions (the Gaussian, quadratic, cubic, quartic and quintic kernels) together with five released particle number are applied to establish twenty-five scenarios of indoor concentration estimation. Measured PM concentration profiles in indoor chambers are used to identify the most appropriate kernel function among the above scenarios. The simulated results show that the cubic and quartic kernel functions both give the minimum simulation error and they only need about 40% CPU time of the Gaussian kernel function. Next, two particle search algorithms (the all-pair and linked-list algorithms) with the cubic kernel function are tested for various numbers of the released particles and concentration observation points. The present study demonstrates that the linked-list algorithm provides the same accuracy as the all-pair algorithm for indoor PM concentration estimation. However, for the computational efficiency, the linked-list algorithm is proved to be much better than the widely used all-pair algorithm. The required CPU time of the all-pair algorithm can be 28 times as large as the linked-list algorithm when the number of the concentration observation points is more than $O(10^4)$.

1. Introduction

In the past decades, Lagrangian particle modeling has been extensively developed to model the dispersion of particulate matter (PM) in atmospheric environment [1,2] and indoor environment [3–6]. Lagrangian particle modeling treats PM as a discrete phase and tracks particle trajectories by solving the particle dynamic equations [7,8] or random walk models [9]. Many academic works have demonstrated the advantages of Lagrangian particle modeling compared to other Eulerian modeling [10,11]. Although Lagrangian particle modeling can accurately provide detailed temporal and spatial information of PM trajectories and dispersion history, it cannot directly give PM concentrations, which should be indirectly obtained through the statistics of a large amount of particle trajectories [10]. Basically, two methods are widely used to calculate PM concentrations. The first method is so called the sampling volume method (or called the box counting method) [2]. The computational space is divided into several imaginary rectangular sampling volumes, and PM concentration in each sampling volume is hence estimated by counting particle residence time (particle-source-in-cell) [10] or particle number (particles-in-the-box) [12] within each volume. This method is extensively adopted in atmospheric environment such as natural boundary layers [2] and urban street canopies [12], and indoor environment like single-room [4,5,10,11], two-room [3,6,13] and multi-room [14,15].

On the contrary, the second method is referred to as the kernel method [16], which treats each particle as a finite source mass. The kernel method does not need imaginary sampling volumes, so that all of the released particles in the computational domain are useful in PM concentration computation, resulting in improved accuracy and computational efficiency compared to the first method [17,18]. Chang et al. [18] have attempted to compare the numerical performance of indoor PM concentration calculation between the sampling volume method and the kernel method. Some advantages of the kernel method have been indicated, including (1) providing smooth concentration profiles, (2) requiring less computing resources, and (3) containing improved accuracy at recirculation zones of the computational domain.

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While the kernel method is used, PM concentration at a given time and location is determined as the sum of contributions from all of the particles in the computational domain through a kernel function and a particle search procedure. The kernel method can be regarded as an interpolation approach at non-ordered points. Therefore, the simulation error and computational efficiency of the kernel method critically depend on the appropriate selection of the kernel function and the particle search algorithm. In terms of kernel functions, several kernels (like the Gaussian and polynomial kernels) have been used in atmospheric PM concentration calculation [17,19–21], but little work has been done so far in indoor PM concentration estimation. On the other hand, two algorithms have been used in non-ordered particle search [22]. One is referred to as the all-pair particle search algorithm, and another is called the linked-list particle search algorithm [22]. The all-pair algorithm is the most intuitive and simplest approach, and is successfully adopted by Chang et al. [18] for indoor PM concentration estimation. The linked-list algorithm has been proved to be an efficient method for fluid dynamics [22]. However, this algorithm has not been tested in indoor PM concentration estimation. As a result, there is still a lack of research that has focused on the appropriate selection of the kernel function and the particle search algorithm of the kernel method in indoor PM concentration estimation.

To fill this gap, the aim of the study is to investigate the simulation error and computational efficiency of indoor PM concentration estimation for various kernel functions and particle search algorithms of the kernel method. Firstly, five kernel functions (the Gaussian, quadratic, cubic, quartic and quintic kernels) together with five released particle number (4, 40, 80, 400 and 800 No./s particle injection rates) are integrated into twenty-five scenarios of indoor concentration estimation to identify the most appropriate kernel function. A relative comparison of the merits and shortcomings of the scenarios is given. Next, two particle search algorithms (the all-pair and the linked-list) are combined with the previously obtained appropriate kernel function to give a series of numerical tests. The most appropriate particle search algorithm is finally emphasized.

2. Methodology

2.1. PM transport modeling (the particle pre-process)

The Eulerian airflow model and the Lagrangian particle model in the commercial computational fluid dynamics code ANSYS FLUENT 12.0 [23] are herein adopted to simulate PM transport processes in indoor environment. In the Eulerian airflow model, the airflow velocity contains the time-averaged part and the fluctuation part. The time-averaged part is conducted through solving the renormalization group (RNG) k-ε model of the turbulent flows [23], and the fluctuation part can be gained by using the discrete random walk (DRW) model [23]. The computed airflow velocity distributions obtained from the Eulerian airflow model are next input into the Lagrangian particle model to calculate 3D PM trajectories in the airflow field. More detailed information of the Eulerian airflow model and the Lagrangian particle model can be found in [10,11,23].

2.2. PM concentration estimation with the kernel method (the particle post-process)

As indoor PM trajectories in the entire computational domain have been given, the present study introduces the kernel method to compute indoor PM concentrations. In the kernel method, indoor PM concentration at a given time and location is determined as the weighted summation of all the particles in computational environment through a kernel function and a particle search procedure. Thus, the indoor PM concentration $c(\mathbf{x}_i)$ at the position $\mathbf{x}_i$ (x_i, y_i, z_i) (or called the concentration observation point) can be expressed as

$$c(\mathbf{x}_i) = \sum_{j=1}^{n} \frac{m_j}{l_i^3} \cdot W\left(\left|\mathbf{x}_i - \mathbf{x}_j\right|, l_i\right) \tag{1}$$

where n is the total number of particles in the computational domain, $\mathbf{x}_j$ (x_j, y_j, z_j) and m_j are the position and the mass of the jth particle, respectively, l_i is the smoothing length which equals to 1.2 times the grid size in space of airflow computation, and $W_{ij} = W(|\mathbf{x}_i - \mathbf{x}_j|, l_i)$ is the kernel function.

2.2.1. Kernel function

Five different kernel functions (the Gaussian, quadratic, cubic, quartic and quintic kernels) are applied to investigate the simulation error and computational efficiency of indoor PM concentration estimation [22]. The Gaussian kernel function has been widely used in atmospheric environment applications and can be expressed as

$$W_{ij} = \frac{1}{\pi^{3/2} l_i^3} \exp\left(-q_{ij}^2\right) \tag{2}$$

where $q_{ij} = |\mathbf{x}_i - \mathbf{x}_j|/l_i$ is the relative distance between the ith concentration observation point and the jth particle.

Other polynomial kernel functions are the quadratic kernel function

$$W_{ij} = \frac{5}{4\pi l_i^3} \begin{cases} \frac{3}{4} - \frac{3}{4} q_{ij} + \frac{3}{16} q_{ij}^2 & \text{if } 0 \le q_{ij} \le 2 \\ 0 & \text{elsewhere} \end{cases} \tag{3}$$

the cubic kernel function

$$W_{ij} = \frac{3}{2\pi l_i^3} \begin{cases} \frac{2}{3} - q_{ij}^2 + \frac{1}{2} q_{ij}^3 & \text{if } 0 \le q_{ij} < 1 \\ \frac{1}{6}\left(2 - q_{ij}\right)^3 & \text{if } 1 \le q_{ij} \le 2 \\ 0 & \text{elsewhere} \end{cases} \tag{4}$$

the quartic kernel function

$$W_{ij} = \frac{315}{208\pi l_i^3} \begin{cases} \frac{2}{3} - \frac{9}{8} q_{ij}^2 + \frac{19}{24} q_{ij}^3 - \frac{5}{32} q_{ij}^4 & \text{if } 0 \le q_{ij} \le 2 \\ 0 & \text{elsewhere} \end{cases} \tag{5}$$

and the quintic kernel function

$$W_{ij} = \frac{3}{359\pi l_i^3} \begin{cases} \left(3 - q_{ij}\right)^5 - 6\left(2 - q_{ij}\right)^5 + 15\left(1 - q_{ij}\right)^5 & \text{if } 0 \le q_{ij} < 1 \\ \left(3 - q_{ij}\right)^5 - 6\left(2 - q_{ij}\right)^5 & \text{if } 1 \le q_{ij} < 2 \\ \left(3 - q_{ij}\right)^5 & \text{if } 2 \le q_{ij} \le 3 \\ 0 & \text{elsewhere} \end{cases} \tag{6}$$

In Fig. 1, these five kernel functions are plotted together for comparison. They are displayed as the function of inter-particle distance, given in units of the smoothing length. Each kernel function has a support domain, within which the function gives the weighted impact. The size of the support domain is controlled by the smoothing length. It should be noted that the support domain is infinite for the Gaussian kernel function and other polynomial kernel functions have finite compact supports [22]. In this study, the support domain shape is spherical. For the quadratic, cubic and quartic kernel functions, their support domains are all a spherical zone with a radius of $2l_i$ ($W_{ij}(q_{ij} > 2) = 0$), and for the quintic kernel