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A new method for simulating aerosols Brownian coagulation based on finite active samples assumption

Yu Li, Weiguo Gu *, Jinpeng He, Dezhong Wang *

School of Nuclear Science and Engineering, School of Mechanical Engineering, Shanghai Jiao Tong University, Shanghai 200240, China

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ABSTRACT

Aerosol dynamics are of great importance in the concept of Leak Before Break (LBB) in the Nuclear Power Plant (NPP). Coagulation is of common interest due to its influence on the particle size distribution and number concentration during the diffusion process. In this paper, a new method for simulating aerosols Brownian collision and coagulation based on Monte Carlo algorithm and Finite Active Samples Assumption (MC-FASA) is proposed, and the corresponding software is developed. This MC-FASA method can directly simulate the collision process and obtain the coagulation coefficient as well as the time evolution of particle size distribution and number concentration. The method can reduce the computation amount without the loss of accuracy. The results are validated by the analytical solutions both for the monodisperse and polydisperse aerosol particles. The method provides the confidence to cover more aerosol dynamic processes in the coolant leakage from the reactor coolant pressure boundary (RCPB).

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1. Introduction

Safety is the primary consideration in nuclear power development. The leakage of the reactor coolant will destroy the integrity of the reactor coolant pressure boundary (RCPB) and threaten the safe operation of a nuclear power plant (NPP). Since an accident usually begins with a discharge of coolant into the containment system, it is of great importance to detect the leak and quantify its flow rate (Zheng et al., 2016) as soon as possible. The U.S. Nuclear Regulatory Commission Guide 1.45 (USNRC Regulatory Guide, 1973) recommends the use of at least three different detection methods in reactors to detect a leakage rate of 1 Gal/min with a response time of no greater than 1 h. There are many monitoring methods for NPP RCPB leakage measurement, one of which is monitoring the activity concentration of radionuclides (e.g., ^{18}F) that leak from the RCPB to the containment. The radionuclides will be released mainly in the form of sub-micron and micron sized aerosols (Sun, 2017). Hence, mastering the mechanism of aerosol movement is essential for ensuring the accuracy of the evaluation of the leak rate.

The aerosol dynamic characteristics, such as diffusion, gravitational settling, thermophoresis, coagulation, and deposition, are all related to the physical properties of particles, especially the particle size. The relative motion between two particles may lead to the contact and collision of them and adhere to form a larger particle, which is called coagulation. Coagulation can cause a change in particle size distribution, and then change the particle motion, and in turn affect the coagulation. For sub-micron and micron particles, an important aerosol behavior mechanism affecting the size distribution is Brownian coagulation (Lee et al., 1984). In many basic and applied fields, the time-dependent size distribution due to coagulation is therefore of fundamental importance and interest (Yu et al., 2016).

The population balance equation (PBE), proposed by Smoluchowski (1927), can be used to describe the time-dependent size distribution of particles. The collision kernel in PBE is related to particle size. But, the particle size changes all the time due to coagulation. So, it is difficult to solve the PBE accurately. The analytical solution to PBE is only possible in the case of simple collision kernels. In the case of complex coagulation kernels, the problem has to be solved by numerical means (Kruis et al., 2000). Many researchers have done a lot of research in solving the PBE. There are basically three methods (Morgan, 2006), the moment method (Yu et al., 2008), the sectional method (Gelbard et al., 1980) and stochastic particle method (Xu et al., 2014, 2015), to study the coagulation of particles by solving the PBE.

The moment method uses a series of equations describing the evolution of particle moments to calculate the particle dynamic evolution. The method is of high efficiency and is relatively easy to implement. However, the moment method cannot obtain the

* Corresponding authors.
E-mail addresses: guweiguo@sjtu.edu.cn (W. Gu), dzwang_sjtu@sina.com (D. Wang).

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complete particle size distribution. The sectional method is a kind of finite element method. The particle size distribution can be divided into several sections. The sectional method can obtain the particle size distribution. However, when more complicated systems have to be dealt with, the sectional method results in very complex algorithms (Maisels et al., 1999). Moreover, the moment method and the sectional method cannot obtain the information about the history of each particle.

The stochastic particle method, or Monte Carlo method is known as an effective method. The Monte Carlo method can obtain the history change of particle size and the internal structure of particles. It is convenient to deal with multicomponent and polydisperse aerosol particles. The Monte Carlo method can be divided into two groups. One is based on the random trajectories of particles. When a sufficient number of particles is taken, collisions will result from the random Brownian motions and a change in the particle size distribution can be recorded. This trajectory random method is computationally expensive and time-consuming, hence, the number of particles simulated are limited to 500–1000. The other is based on a known collision rate, and then choose collision particle pairs randomly (Palaniswaamy and Loyalka, 2006). To meet the demand of statistical analysis, numerous particles should be involved in the simulation. It is assumed that the number concentration and the particle size remain constant or change slowly to obtain the collision rate. The assumption is valid when the concentration is low and the time for coagulation is short. However, the situation becomes complicated when polydisperse aerosol particles are considered. The size distribution and the proportion of particles of a particular size are changing with time. So, the mathematics become much more complicated and no explicit solution exists (William, 1982).

Directly study on the particle trajectory, motion and collision can reveal the evolution law of the coagulation coefficient, the particle size distribution, and the number concentration dynamically. The trajectories of particles are fully determined by the particles initial locations, initial velocities and the forces acting on the particles. The collisions can be treated as a geometric interception of particle trajectories. One of the biggest challenges for direct simulating the particle coagulation is numerous particles are required to guarantee the statistical analysis, and the collision judgment of every two particles is really computational expensive.

Aiming at the above problems, this paper proposes a new method based on Monte Carlo algorithm and Finite Active Samples Assumption (MC-FASA), to directly simulate the collision and coagulation. With the MC-FASA method, this paper performs the simulation on the particle motion, collision and coagulation directly, both for monodisperse and polydisperse aerosol particles. Substantial computation savings can result from avoiding every two particles in the calculation domain from the judgment for collision.

2. Methodology

The method proposed in this paper divides the particles in the calculation domain into two parts, the sample particles and the environmental particles, as shown in Fig. 1 (left). The coagulation process of aerosol particles is simulated based on the real-time collision judgment between the sample particles and the environmental particles. The sample particles are tracked and analyzed to obtain the collision times and the coagulation coefficient, and then get the change of particle number concentration and particle size distribution as a function of time.

The particle motion is subject to the initial status and the forces acting on it. The Lagrangian method is applied to simulate the motion and collision of particles. The sample particles are generated randomly based on the corresponding model by Monte Carlo method. The Mersenne Twister (MT19937) method is selected to generate the random number. It is by far the most widely used general-purpose pseudorandom number generator with a very long period of 2^{19937}-1.

It is assumed that the particles are spherical and the number (N) of sample particles is finite. The sample particles are released randomly in the calculation domain. The sizes of the particles are selected randomly and the probability of the occurrence of a size should obey the size distribution function.

The right of Fig. 1 shows the collision computational domain of one sample particle. The collisions only take place between the environmental particles and the sample particle. The collision surface (William, 1982) is an imaginary surface with a radius of $R = r_p + r_p'$ around the sample particle, where r_p and r_p' are the radius of the sample particle and the environmental particle respectively. The red sphere in the center of the collision calculation domain represents the sample particle. The blue spheres represent the environmental particles.

The boundary of the collision domain should be large enough to contain an adequate amount of environmental particles and encircle the range of their movements. The initial value of the radius (R_S) of the collision domain is determined by $R_S = \max(10 \times \bar{L}_p, 10 \times r_p)$, where $\bar{L}_p$ and r_p are the particle's average displacement within one time step and the radius of sample particles respectively. Then R_S is adjusted in order to guarantee the number (N_{Sp}) of particles existing in the domain being in the range from 10 to 100. The environmental particles are distributed uniformly along the circumferential direction. In the radial direction, the concentration distribution of environmental particles satisfies Eq. (1).

$$\frac{C}{C_\infty} = 1 - \exp\left(\frac{R - r}{r_p}\right) \tag{1}$$

where C is the number concentration of the environmental particles, C_∞ is the average particle concentration of the whole calcula-

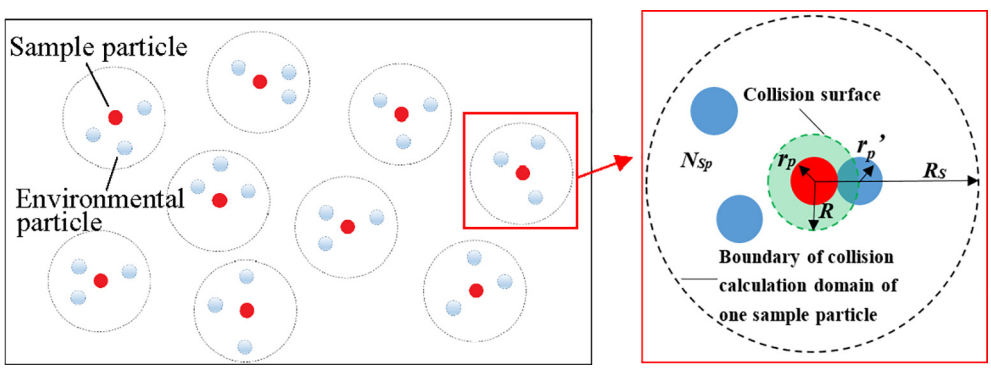

Fig. 1. The calculation domain (left) and the collision computational domain (right) of one sample particle.

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