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The QMOM Method to Solve The PBE Equations of the Urban Haze

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Abstract. Mega and medium-sized cities in China are facing the increasingly serious aerosol pollution, among them Xi'an is one of the typical cities. During the early stage of ash haze, aerosol concentration is rising so fast that the simulation of the process is difficult. This article uses the population balance equation (PBE) describing the distribution of fine particles, and solves the changing process of particle size distribution by the moment method. Population balance equation**,** a non-linear hyperbolic equation about number density function**,** is employed to describe micro-behaviors **(**aggregation**,** breakage**,** growth**)** of disperse phase and resulting variation of particle size distribution. By expressing PBEs for both batch and continuous operations in a general form, and using weighted residual method to derive the moment equations, different moments can be tracked directly. Three examples of simulation results show that compared with the analytical solution, relative error of this method is within 10^{-5} and has the characteristics of high precision and low computation amount. In early 2016, the early stage of $PM_{2.5}$ pollution in Xi'an is simulated and the simulation results and experimental results are highly consistent.

1. Introduction

Atmospheric aerosol is a solid and liquid polyphase microparticle system suspended in the atmosphere with a diameter of 0.001~100 m. Due to its important influence on atmospheric environment, human health and earth radiation, it has become one of the hot issues in the field of earth science. In recent years, with the acceleration of urbanization and rapid economic growth, the aerosol pollution in China's large cities has become more and more serious, which has attracted wide attention from the academic, political and public sectors. In the early stage of haze development, the quality concentration of $PM_{2.5}$ increased rapidly, and the explosive growth of more than 100ug•m-3 was frequently seen in the hours. It is difficult to complete process simulation with emission source and migration model due to sudden growth rate and atmospheric stability in urban center area. Population balance equation can describe the discrete phase system (such as bubbling bed, fluidized bed reaction process) of the distribution of the scale of the discrete phase entities (particle size distribution, etc.) and alternate with microscopic behavior (aggregation and breakage, etc.), so as to become and traditional double fluid equation of coupling an effective tool to describe the discrete phase system[1,2].

2. Solution methods for population balance equations

The first paragraph after a heading is not indented (Bodytext style). In the discrete phase system, the numerical density function $f(\varepsilon;x,t)$ can be used to describe the distribution of the entity number in the attribute space ε, the position space x and the time space t. If you consider only the volume coordinates of a single property, the property vector will become a scalar V. The model can be expressed as[4,5]:

$$\frac{\partial f(V;x,t)}{\partial t}+\frac{\partial}{\partial x_i}\left(<u_i>_V f(V;x,t)\right)=S(V)$$

$$\frac{\partial f(V;t)}{\partial t}+\frac{f(V;t)\text{-}f(V)_{in}}{\tau}=S(V)$$

In the formula, $f(V;x,t)$ is a numerical density function with volume V as the internal coordinate; $<u_i>_V$ is the velocity of the velocity u of V in the x_I direction; $S(V)$ is the source term of entity property change caused by the aggregation, fragmentation or growth of the entity.

In the group equilibrium equation, there are often differential, single weight integral and multiple integrals, and the form is extremely complex, so it is not possible to analyze the general meaning at present, and the numerical solution becomes the main method. Mcgraw[3] uses the gaussian integral of the entity distribution to assume that the equation is closed, and the moment integral method (QMOM) is proposed, which has been widely used.

QMOM directly tracks the product component of the entity distribution - the moment of particle distribution.

$$m_k(t)=\int_0^\infty V^k f(V;t)dV$$

The ratio of the total volume to the total area is represented by the Sauter particle size d_{32}.

$$d_{32}=\frac{\int_0^\infty Vf(V;t)dV}{\int_0^\infty V^{\frac{2}{3}}f(V;t)dV}$$

We use the PBE moment integral method to calculate the process, the breakage process and the growing process, and fully simulate the variation of the particle distribution. The accuracy of the model is verified by CFD analytical solution.

The microscopic description of the polymerization process:

$$\mathrm{S}(V)=\frac{1}{2}\int_0^{\mathrm{v}}\beta(V\text{-}v,v)f(V\text{-}v;t)f(v;t)dv\text{-}f(V;t)\int_0^\infty\beta(V,v)f(v;t)dv$$

In the equation, $\beta(V,v)$ is the aggregation rate of the volume V entities and volume v entity, depends on the entity's collision rate and efficiency of merger, but the quantity is determined by the environment fluid characteristics and its entity itself attribute, so we need to use two-way coupling method to solve the S(V) equation, the equation of fluid motion and the equation of chemical reaction.

The moment transformation and gaussian distribution hypothesis for the equation:

$$\overline{S}_k(t)=\frac{1}{2}\sum_{i=1}^{N}\omega_i\sum_{j=1}^{N}\beta_{i,j}\left(V_i+V_j\right)^k\text{-}\sum_{i=1}^{N}V_i^k\omega_i\sum_{j=1}^{N}\beta_{i,j}\omega_j$$

In the equation, $\beta_{i,j}=\beta(V_i,V_j)$.

In general, the expression of aggregation is very complicated, so that the equation cannot be analyzed. When $\beta(V,v)$ is C_0, the change of entity number is analyzed.

$$N(t)=2N_0/(C_0N_0t+2)$$

When C_0=1, the calculation results of particle changes are shown as Fig1 and Fig2, which is exactly the same as the analytical solution.

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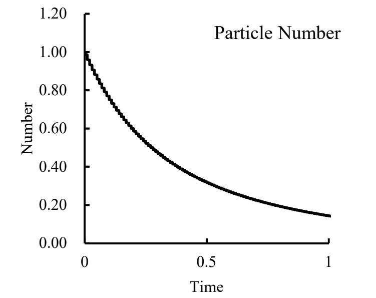

Figure 1. The variation of particle number in the process of aggregation.

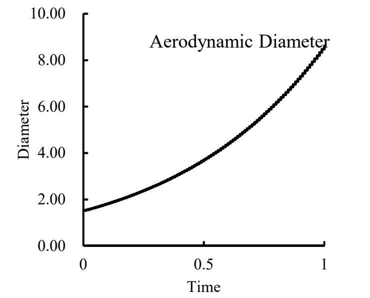

Figure 2. The variation of aerodynamic diameter in the process of aggregation.

The microscopic description of the breakage process:

$$S(V)=\int_{V}^{\infty} a(v)b(V|v)f(v;t)dv\text{-}a(V)f(V;t)$$

In the equation, a(v) is the breakage rate, and the bubbles and droplets are mainly determined by the vortex motion of the environment fluid. For the particles, a(v) is determined by the thermal stress of the environment and the physical properties of the particles. b(V|v) is the probability that the volume V is generated by volume v, depending on the strength of the vortex or the intensity of the thermal stress.

The moment transformation and gaussian distribution hypothesis for the equation:

$$\overline{S}_k(t)=\sum_{i=1}^{N} a_i\overline{b}_i\omega_i\text{-}\sum_{t=1}^{N} a_t\overline{b}_t\omega_t$$

When the breakage rate is C_0; There are analytic solutions to the uniform distribution of the fragments.

$$m_k=m_k(0)exp(\frac{1\text{-}k}{1+k}C_0t)$$

When C_0=1, the particle changes are as Fig 3 and Fig 4, which is exactly the same as the analytical solution.

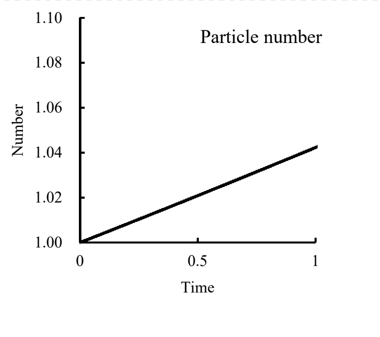

Figure 3. The variation of particle number in the process of breakage.

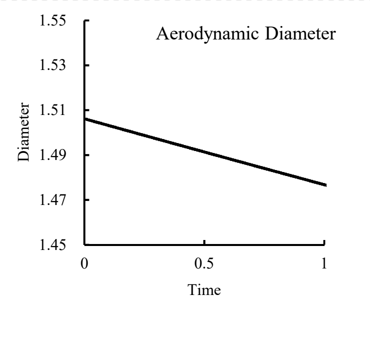

Figure4. The variation of aerodynamic diameter in the process of breakage.

The microscopic description of the growth process:

$$S(V)=\text{-}\frac{\partial}{\partial V}[G(V)f(V;t)]$$

In the equation, *G(V)* is the growth rate for entities, depending on the specific physical or chemical process, and is determined by the environment fluid and its discrete phase entity itself characteristics, which are obtained from fluid equations and reaction equations.

The moment transformation and gaussian distribution hypothesis for the equation:

$$\overline{S_k}(t) = k\sum_{i=1}^{N}\omega_i G(V_i)V_i^{k-1}$$

Assuming that the number of particles in the growing process remains unchanged, the equation has an analytic solution.

$$m_{Qk}(t) = \sum_{i=0}^{k} C_k^i (G_0 t)^i m_{Q(k\text{-}i)}\ (t=0)$$

When C_0=1, the particle changes are as Fig 5 and Fig 6, which is exactly the same as the analytical solution.

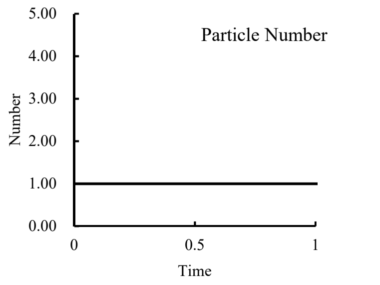

Figure 5. The variation of particle number in the process of growth.

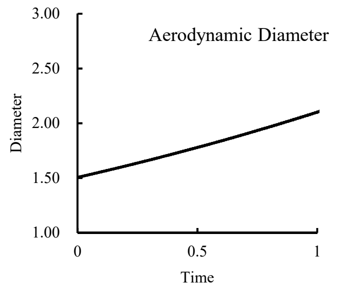

Figure 6. The variation of aerodynamic diameter in the process of growth.

The source term of PBE is the linear superposition of the source term of the aggregation, growing and breakage processes. The discrete moment calculation was carried out by using the particle size distribution of particle size observed by FMPS. Assuming that the particle logarithm distribution is a gaussian distribution, the initial moment distribution M[0]~M[6] is obtained, and the changes of each moment in the tracking calculation can be obtained with the change of particle size distribution over time. At the same time, by adjusting the moment integral, the effects of growth, aggregation and breakage process can be classified separately.

3. The simulation of the formation of a severe haze episode in Xi'an, China

During the haze aggravation process in the big city, the rapid growth of mass concentration of particulate matter is frequent. In view of this phenomenon, that real-time monitor and analysis of high time resolution is carried out by use FMPS to real-time monitor and analyze the particle spectrum distribution in the process of heavy grey haze, so as the weight of haze is increased, the total volume (mass) of particulate matter rises rapidly, the median particle diameter is increased, the concentration of ultrafine particle is obviously reduced, the concentration of fine particles is accelerated, and the fine particles are accelerated. The monitoring results of particle size distribution of a typical $PM_{2.5}$ rapid growth process in Xi'an on December 21, 2015 are shown in Figure 7.

In the process, the $PM_{2.5}$ concentrations increased by more than 100 μg m^{-3} in 6 hours, reaching more than 250 μg m^{-3}, forming serious ash haze pollution. In view of this process, the PBE described in the paper is adopted to construct the model, and the distribution is resolved into 6 different moments by the moment method. Figure 8 shows that the simulation results are highly consistent with the experimental results. This method can simultaneously output the effects of aggregation, growth and breakage process, and we focus on the aggregation and growth process.

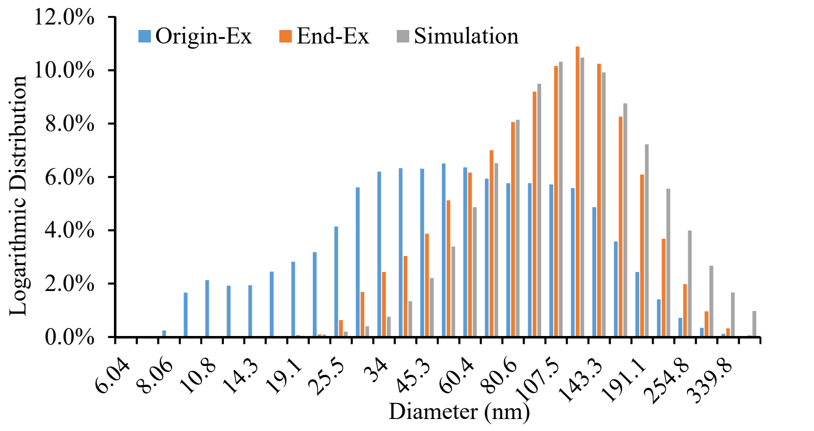

Figure 7. The simulation result of the haze incident.

In the early stage of haze, the concentration of $PM_{2.5}$ increased rapidly, and the average particle size gradually increased and the distribution range became more concentrated. Among them, the increase of the average particle size is mainly due to the strengthening of the role of growth, from the point of the simulation results, the contribution of growth process on the average grain size growth above 80%, and this is also the main reason for the rapid growth of $PM_{2.5}$ mass concentration. The reduction of particle size distribution is mainly affected by the polymerization. The simulation results show that aggregation and breakage process have positive and negative effects on the concentration of particle size.

4. Conclusion

For the characteristics of rapid increase of $PM_{2.5}$ concentration in the early stage of haze, this paper describes the polyphase state of particles with PBE, and puts forward a method of point moment which can track arbitrary number of moments. Through the direct tracking of the moment, the high-precision solution of each order moment is realized, and the process of aggregation, growth and breakage is tracked, and the dynamic monitoring and development process simulation is realized. A high precision simulation of the haze development in Xi'an on December 21, 2015 has been carried out with good simulation results. The important contribution of aggregation and growth function to the mass concentration of $PM_{2.5}$ and the change of particle size distribution were analyzed by the method of moments.

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