Chapter

The Diesel Soot Particles Fractal Growth Model and Its Agglomeration Control

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Abstract

Based on the fractal growth physical model of soot particles from large diesel agriculture machinery, this chapter simulates the morphological structure of collision for the single particles and single particles, single particle and clusters, clusters and clusters, firstly. Moreover, combining with the collision frequency, the fractal growth is controlled to agglomeration using the main environmental factors interference for diesel engine soot particles, in order to make them condensed into regular geometry or larger density particles, reduce the viscous drag for capturing by the capturer or settlement and to realize the control of the pollution of the environment. The results of numerical simulation show that the proposed method is feasible and effective, which will help to understand and analyze the physical mechanism and kinetics of non-equilibrium condensation growth behavior of the actual carbon smoke particles and provide the solution to further reduce emissions of the inhalable particulate matter from diesel engines.

Keywords: soot particles, agglomeration, fractal growth, control, diesel engine

1. Introduction

Large diesel agriculture machinery plays an important role in economic development, but it also brings sharp problems in environmental protection. Diesel emissions are one of the most important sources of air pollution. There are many kinds of harmful substances, such as HC, CO, NOX, and soot particles, but the emission of harmful gases from diesel engines, such as HC and CO, is quite low; NOX emissions are also in the same order of magnitude as gasoline engines. The soot particles emitted are respirable particles, causing the most serious air pollution [1, 2].

Particles emitted by diesel engines are usually composed of soot, organic soluble components, and sulfides [3]. The main components of particles discharged from a typical heavy-duty diesel engine under transient conditions are shown in **Figure 1**. Usually, soot accounts for 50–80% of total particulate matter. It is one of the most important harmful emissions [3]. Therefore, it is of great significance to control the emission of soot particles from diesel engine emissions.

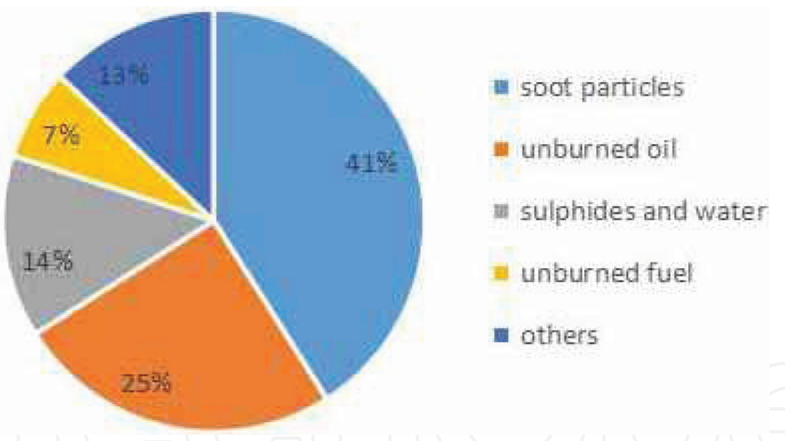

Figure 1.
The composition of particulate emissions from the heavy-duty diesel [3].

Soot is a very fine particle formed by a complex reaction mechanism in the flame of the fuel-rich region when burning hydrocarbons in the absence of air, mainly composed of a mixture of amorphous carbon and organic matter [4]. Since the concentration and particle size of soot particles emitted by the gasoline engine is lower than that of the diesel engine [5], this chapter mainly analyzes the soot particles of the diesel engine.

At present, the study of soot particles in diesel engines has focused on optical properties, chemical composition, particle size distribution, source analysis, and human health assessment [6, 7], but research on particle morphology (morphology and surface structure) is almost blank, especially the morphological structure of the particles. Most soot particles have complex fractal morphology [8, 9], affecting the nature of the particles. By studying its fractal structure, the deposition of particles, the viscous resistance of the particles and the adsorption of toxic molecules can be deduced. Therefore, it is necessary to control the fractal condensation and growth morphology of diesel soot particles.

Based on the fractal growth physical model of soot particles from large diesel agriculture machinery, this chapter simulates the morphological structure of collision for the single-single particles, single-clusters, clusters-clusters, firstly. Moreover, combining with the collision frequency, the fractal growth is controlled to agglomeration using the main environmental factors interference for diesel engine soot particles, in order to make them condensed into regular geometry or larger density particles, reduce the viscous drag for capturing by the capturer or settlement and to realize the control of the pollution of the environment.

2. The condensation growth process of the soot and its simulation method

2.1 The generation process of soot

The soot particles generation process undergoes complex chemical reactions and physical processes. Firstly, it undergoes gas phase reactions, phase transitions from gaseous to solid state. Then the formation of soot particles in diesel cylinders undergoes the evolution of kinetic events such as nucleation, condensation, collision fragmentation, growth, and surface oxidation [10–14]. The specific formation process described by the soot particle model is shown in **Figure 2**.

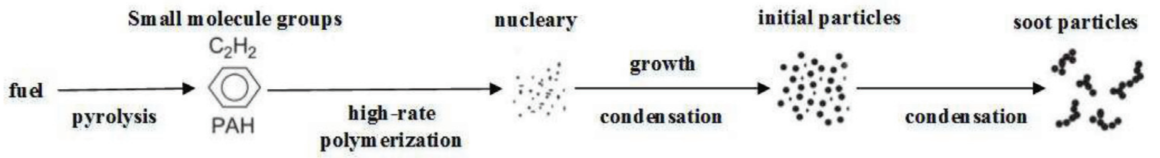

Figure 2.
The soot generation process.

2.2 The simulation method of soot structure

According to the characteristics of the soot growth process, the dynamic Monte Carlo method [15] is used to establish the soot fractal growth model. As shown in **Figure 3**, in a two-dimensional Euclidean space with many particles, one initial particle is set as the target particle, and the other particles are candidate particles. One of the candidate particles is selected to collide with the target particle according to a randomly generated locus, and adheres according to the adhesion probability. One other candidate particle repeats the above process, and the analogy eventually forms an agglomerate. If the motion reaches the boundary of the space, the particle is absorbed by the target particle and disappears. After the particles are released, they do Brownian motion, and they are required to move to the neighboring left, right, upper, and lower surrounding squares with a probability of 1/4. The process will continue until the particles leave the boundary or reach the agglomerate. There are two kinds of collision for particles: the collision of the particle with particle (**Figure 4**), the collision of the cluster with cluster (**Figure 5**).

Taking the collision of the single particle as an example to illustrate the collision of the particles, the trajectory vectors of two collision particles is firstly determined

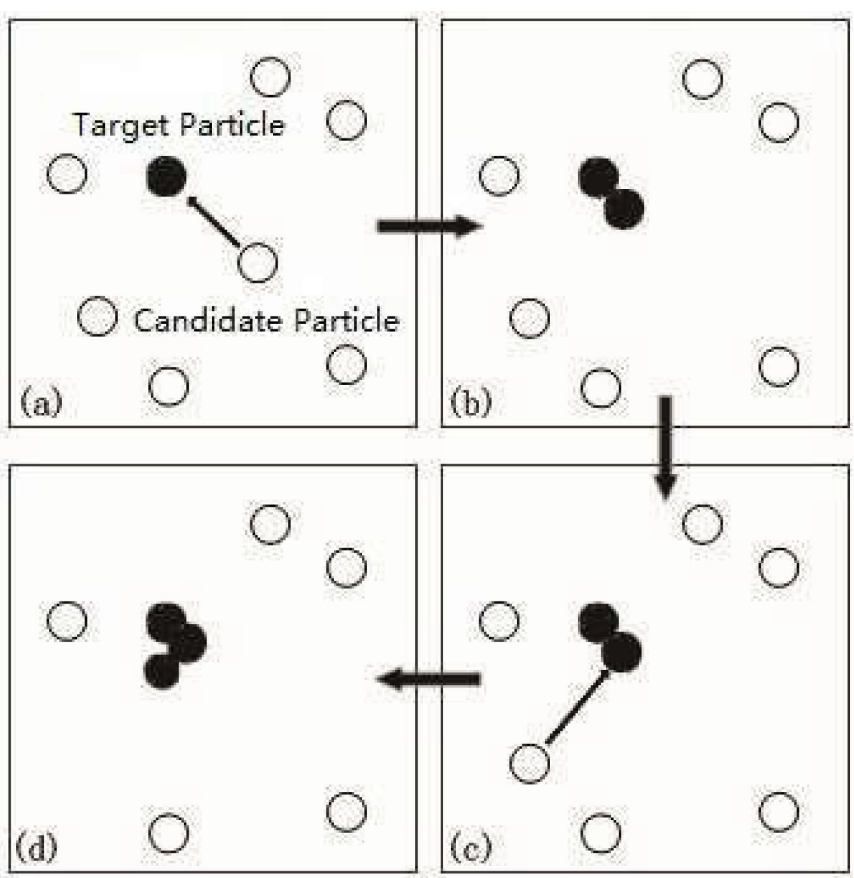

Figure 3.
The diagram of growth process. ((a) set target particle; (b) collide with target particle; (c) analogy of collide with target particle; (d) form an agglomerate).

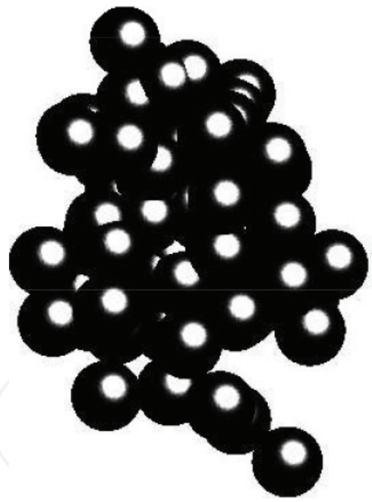

Figure 4.
The collision of single particles and single particle.

Figure 5.
The collision of clusters and clusters.

in **Figure 6**. Two small balls are defined as B_1 (target particles) and B_m (random particles) to represent two separate particles, with radius R_1 and R_m, respectively. The coordinates of B_1 are given, the coordinates of B_m are random, and the radius of the concentric sphere B_s of the small ball B_1 is defined as $R_s(R_s = R_1 + R_m)$. Then let B_m move according to a random trajectory. When B_m meets the fixed ball B_1, Eq.(1) is satisfied, where x_s^0 is the center of the ball B_1.

$$|x_s - x_s^0| = R_s. \tag{1}$$

When the random particle B_m adsorbs and condenses on the target particle B_1, its random motion trajectory vector v exactly intersects with or intersects the ball B_1, and can be defined as Eq.(2),

$$x_m = x_m^0 + c_n v, \qquad c_n \in [0, \infty). \tag{2}$$

where x_m is the sphere center coordinate after the collision of the ball B_m, and x_m^0 is the initial sphere center coordinate of the ball B_m.

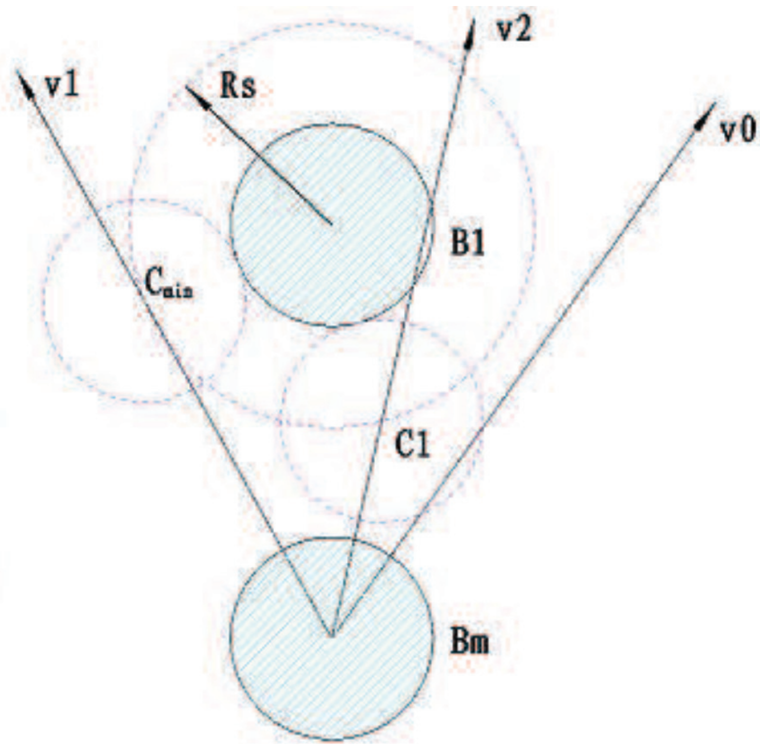

Figure 6.
The diagram of single particle collisions.

The collision of two small balls can be defined Eq.(3).

$$|x_m - x_m^0| = |(x_m^0 - x_s^0) + c_n v| = R_s. \tag{3}$$

Solve both sides of squared Eq.(3) simultaneously to obtain a quadratic equation with unknown c_n. c_n is the judgment factor, if c_n has no solution, two balls cannot collide; if c_n has a solution, the two balls collide with two cases. One is that when there is a unique solution, the two balls just collide with each other; when there are two solutions, the smallest solution is c_{min} according to the physical conditions. Then the coordinates of randomly moving ball B_m are also determined as Eq.(4). This process describes a simple collision process between particles and particles. Based on this, it can be used to simulate the collision and clustering process between clusters and clusters. The collision process is still established by using Monte Carlo method.

$$x_m = \begin{cases} x_m^0 + c_{min} v, & \text{intersect,} \\ x_m^0 + c_{min} v, & \text{tangent.} \end{cases} \tag{4}$$

The shape of aggregates formed by fractal growth of soot is closely related to the radius of gyration, soot radius, and fractal dimension, which is shown in **Figure 7**. The R_g characterizes the compactness of soot condensation growth, R_e characterizes the size of the soot agglomerates formed by fractal growth. The fractal dimension of the surface roughness of soot agglomerates is closely related to the adsorption of particles. The calculation of fractal dimension D_f of soot agglomerates is based on the box calculation method [16] and shown in Eq.(5), where $N_n(A)$ is the minimum number of boxes needed to contain A, $1/T_n$ is the boundary of the small box. When T_n is large enough, the box dimension is approximate as Eq.(6), and the fractal dimension calculation method for soot agglomerates is shown in **Figure 7**.

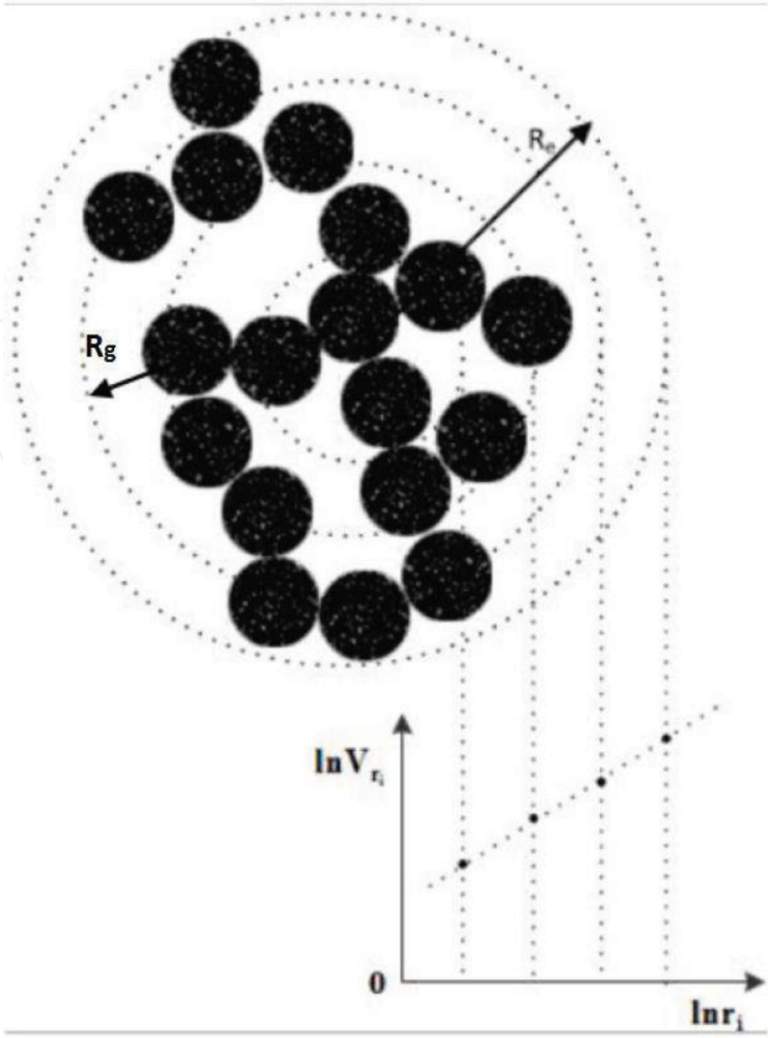

Figure 7.
The sandbox method for the fractal dimension of soot condensed matter.

$$D_f = \lim_{n\to\infty} \frac{N_n(A)}{-lnT_n}, \quad (5)$$

$$D_f = slope\{\ln(N_n(A)), \ln(T_n)\}. \quad (6)$$

3. The analysis and condensation control of soot particles fractal growth

3.1 The theory of control

The formation of soot particles in diesel engines is affected by factors such as temperature, pressure, soot particle concentration, and oxidation rate [17]. According to the characteristics of free particles moving in a continuous medium state, it can be considered that the soot growth of a soot particle (condensation collision) has a distribution parameter equation of motion with boundary conditions as Eq.(7).

$$\frac{\partial\eta(x,y,t)}{\partial t} = \delta\left(\frac{\partial\eta^2(x,y,t)}{\partial x^2} + \frac{\partial\eta^2(x,y,t)}{\partial y^2}\right), \quad (7)$$

The condensation growth frequency of soot particles satisfies the distribution parameter system Eq.(8).

$$\nabla^2\eta(x,y) = F\left(\eta(x,y), \frac{\partial\eta}{\partial t}, u(x,y)\right), \tag{8}$$

$\eta(x,y)$ is the condensation temperature. F represents the environmental disturbance term, called the forcing term, which is a non-linear function term. $u(x,y)$ is the initial value of the digitization, called the source term. The solution to the system Eq.(8) is very tedious. To facilitate the analysis of the solution, a discrete power system of Eq.(8) is introduced as Eq.(9).

$$\eta_{m+1,n} + \eta_{m-1,n} + \eta_{m,n+1} + \eta_{m,n-1} - 4\eta_{m,n} = F\big[\eta_{m,n}, \left(\eta_{m+1,n} - \eta_{m,n}\right)\left(m_{t+1} - m_t\right) + \left(\eta_{m,n+1} - \eta_{m,n}\right)\left(n_{t+1} - n_t\right), u_{m,n}\big], \tag{9}$$

Considering the boundedness and variability of soot particle agglomeration, the nonlinear function F is set as Eq.(10).

$$F = \alpha\, sin\left(\eta_{m,n}\right) + u_{m,n}, \tag{10}$$

For more generalized processing problems, the system Eq.(11) is hereby introduced.

$$\Omega(r) = \alpha\, sin(\Omega(r-1)) + \Omega(r-1) + u_{m,n}, \tag{11}$$

where

$$\Omega(r) = \eta_{m+r,n} + \eta_{m-r,n} + \eta_{m,n+r} + \eta_{m,n-r}, r = 1, 2, \cdots. \tag{12}$$

Obviously, when $r = 1$, Eq.(12) becomes system Eq.(9). By iterating simplification of Eq.(9), a simple control system can be obtained as Eq.(13).

$$\Omega(r) = ru + \alpha\, sin(\Omega(r-1)) + \alpha\, sin(\Omega(r-2)) + \cdots + \alpha\, sin(\Omega(0)) + \Omega(0), r = 1, 2, \cdots \tag{13}$$

3.2 The control of fractal growth for diesel engines' soot particles from source item and nonlinear term

According to the control method of [18], this chapter analyzes the effect of this control method on the fractal growth of soot particles. Assuming that $\mathcal{H}$ is a condensed region, $\overline{\mathcal{H}}$ is a condensed boundary, and $\mathcal{M}$ is the scope of control of the source item $u(x,y)$, and satisfies $Mathcal\,M \in \mathcal{H}$. In addition, for any $(x,y) \in \mathcal{H}$, there is $0 \le \eta(x,y) \le 1$ established. Since the analytical function $u(x,y)$ satisfies the maximum principle in $\mathcal{H}$, for any $(x,y) \in \mathcal{H} - \overline{\mathcal{H}}$, condition $0 \le \eta(xy) < 1$ must be true, so α and u in Eq.(11) must be as small as possible, represented by an inequality:

$$0 \le \eta_{m+r,n} + \eta_{m-r,n} + \eta_{m,n+r} + \eta_{m,n-r} < 1,$$

$0 \le \Omega(r) < 1$, where $r = 1, 2, \cdots$. Since $0 \le \sin(\Omega(t)) < \Omega(r) < 1$ holds, the system (10) satisfies the relationship Eq.(14).

$$\Omega(r) < ru + \alpha\Omega(r-1) + \alpha\Omega(r-2) + \cdots + (\alpha+1)\Omega(0). \tag{14}$$

According to Eq.(13) and combined with mathematical induction, Eq.(15) can be get.

$$\Omega(r) < \left[(\alpha+1)^{r-1} + (\alpha+1)^{r-2} + \cdots + (\alpha+1) + 1\right]u + (\alpha+1)^r\Omega(0), r = 1, 2, \cdots. \tag{15}$$

Eq.(16) is get by changing the inequality of $\Omega(r)$ to $\Psi(\alpha, u, r)$

$$\Psi(\alpha, u, r) = \left[(\alpha+1)^{r-1} + (\alpha+1)^{r-2} + \cdots + (\alpha+1) + 1\right]u + (\alpha+1)^r\Omega(0) \tag{16}$$

And because $0 < \alpha \leq 1$, $0 < u \leq 1$, it turns out to have $\frac{\partial\Psi}{\partial\alpha} > 0$ and $\frac{\partial\Psi}{\partial u} > 0$ is true, $\Omega(r)$ is monotonically increasing about α and u, respectively.

The particle condensation temperature η will increase with the increase of the nonlinear term $\alpha\, sin(\eta)$ and the source term u. For system Eq. (8), when the action region of source item u is circular (r is a radius), the values of u are constants and random numbers(rand represents a random number in the range (0,1), respectively, and the resulting simulated pictures are shown in **Figures 8–10**. Comparing with **Figure 3** and **Figure 4** without interference and other model [19] shown in **Figure 11**, this chapter simulates the morphological structure of collision for the single-single particles, single-clusters, clusters-clusters, and it is obvious that the effect of the increase of the interference term and the action region on the control of the aggregation of particles is more and more condensed than in the absence of the

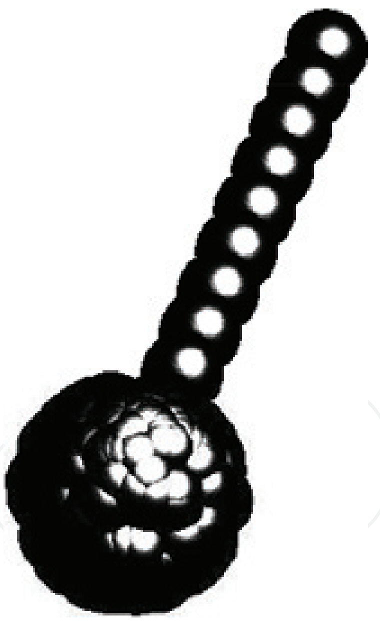

Figure 8.
The control of single direction.

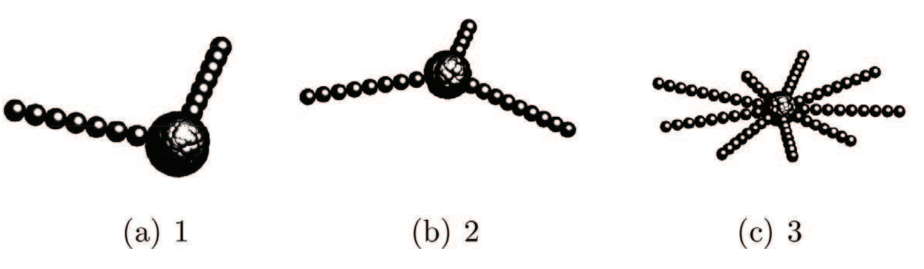

Figure 9.
The control of multiple direction.

Figure 10.
Particles' center point coagulation control.

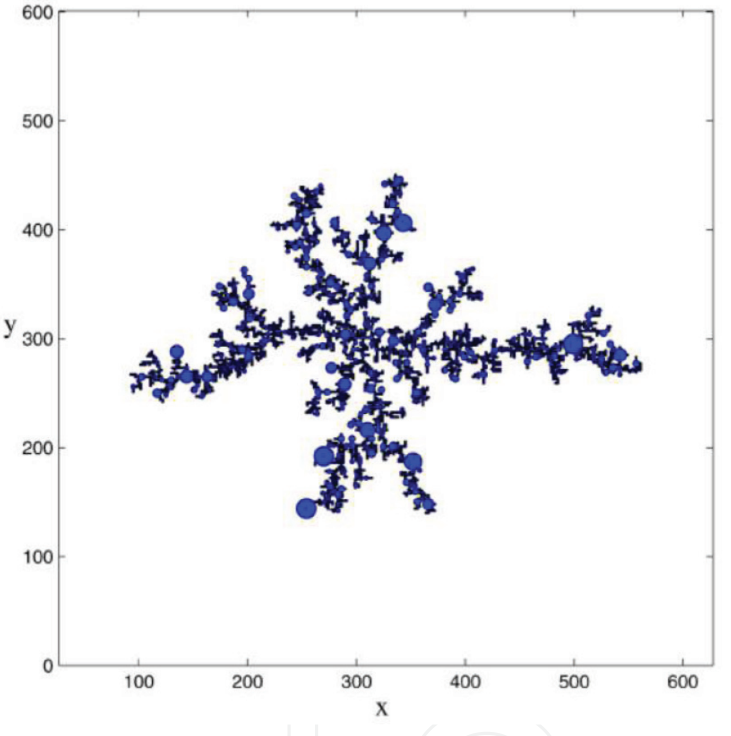

Figure 11.
Fractal diffusion of soot particles established by others [19].

interference term. The concentration of the particles after the condensation is greater for the settlement and the aggregation. Condensation can also have a fixed direction. The control method on the fractal growth reduces the complexity of the surface area of aggregated particles and reflects the effectiveness of the control method.

4. The meaning of the soot particles condensed control

The fractal structure of the particles is closely related to the binding resistance and the adsorption of the particles. The literature [20] investigated the relationship between the viscous resistance and the fractal structure of the particles during the descending process. Particles with a fractal structure will have a larger fractal dimension, the smaller the viscous resistance, and the faster the sedimentation rate than spherical particles of the same volume. The fractal dimension of the particle before control shown in **Figures 3** and **4** is 2.029 and 2.236, respectively. The fractal dimension of the particle after control in **Figure 8** is 2.3273. Obviously, the viscous resistance of the particle in **Figure 8** is small, which is conducive to the settlement of particles.

The fractal dimension of particles directly affects the surface adsorption. The relationship between the number of saturated molecules adsorbed in single layer N_m and the cross-sectional area of adsorbed molecules S_m is given by Eq. (17), where ξ is the scale factor and D_f is the fractal dimension of the particle.

$$N_m = \xi(S_m)^{\left(-\frac{D_f}{2}\right)}, \tag{17}$$

If the adsorbate molecular weight is M and the density is ρ, then the adsorption amount Q' is Eq.(18).

$$\begin{aligned} Q' &= N_m \frac{M}{\rho}, \\ Q' &= \varepsilon \frac{M}{\rho} (S_m)^{\left(-\frac{D_f}{2}\right)}. \end{aligned} \tag{18}$$

Obviously, the adsorption of toxic particulates by atmospheric particles is not only related to the composition and chemical properties of gas molecules but also related to the fractal dimension of the particle surface. The roughness of the surface of atmospheric particles also affects the adsorption of toxic gases in the atmosphere. The bigger fractal dimension particles have, the stronger adsorption of toxic particulate matter atmospheric particles have. Then, atmospheric particles will greatly affect human health.

The controlled particulate matter (**Figure 8**) can adsorb more toxic particulate matter and cause it to control the settlement and reduce the environmental pollution. In addition, if the particulate matter still cannot settle after control, it will be controlled as in **Figure 6** (fractal dimension is 2.029) and **Figure 7** (fractal dimension 2.021, 2.031 and 2.038, respectively) shape structure, in order to reduce the adsorption of particles on toxic particles and the harm to human health.

5. Conclusions

The analysis and its agglomeration control of soot particles fractal growth provides a new idea for the development of particulate matter traps and also provides a new solution for reducing environmental pollution. Based on the fractal growth physical model of soot particles from large diesel agriculture machinery, this chapter simulates the morphological structure of collision for the single particles and single particles, single particle and clusters, clusters and clusters, firstly. Moreover, combining with the collision frequency, the fractal growth is controlled to agglomeration using the main environmental factors interference for diesel engine soot particles, in order to make them condensed into regular geometry or larger density particles, reduce the viscous drag for capturing by the capturer or settlement and to realize the control of the pollution of the environment.

If the particles cannot settle, they can be controlled to reduce the adsorption of inhalable particles to toxic particles and reduce the harm to human health.

This chapter simulates the control of the aggregation fractal growth trend of diesel soot particles. The results of numerical simulation show that the proposed method is feasible and effective, which will help to understand and analyze the physical mechanism and kinetics of non-equilibrium condensation growth behavior of the actual carbon smoke particles and provide the solution to further reduce emissions of the inhalable particulate matter from diesel engines.

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Nomenclature

α	the coefficient of equation.
$\eta(x,y)$	the condensation temperature.
c_n	the judgment factor.
$u(x,y)$	the initial value of the digitization.
x_s	the center of the ball B_m.

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References

[1] Poran A, Tartakovsky L. Performance and emissions of a direct injection internal combustion engine devised for joint operation with a high-pressure thermochemical recuperation system. Energy. 2017;**124**:214-226

[2] Robelia B, Mcneill K, Wammer K, et al. Investigating the impact of adding an environmental focus to a developmental chemistry course. Journal of Chemical Education. 2010; **87**(2):216-220

[3] Kittelson DB. Engines and nanoparticles: A review. Journal of Aerosol Science. 1998;**29**(5–6):575-588

[4] Tian H, Liao Z. Progress on the formation mechanism of biomass soot particles. Clean Coal Technology. 2017; **23**(3):7-15

[5] Shuai J et al. Review of formation mechanism and emission characteristics of particulate matter from automotive gasoline engines. Transactions of CSICE;**2016**(2):105-116

[6] Maozhao XIE. The Computational Combustion Theory of the Internal Combustion Engine. Dalian: Dalian Institute of Technology Press; 2005

[7] M Balthasar, M Frenklach. Monte-Carlo simulation of soot particle coagulation and aggregation: The effect of a realistic size distribution. Proceedings of the Combustion. 2005; **30**(1):1467-1475

[8] Zhang L, Liu ST. Directed control for fractal growth with environmental disturbance. Control Theory & Applications. 2011;**28**(12):1786-1790

[9] Liu P, Liu ST. Nonlinear generalized synchronization of two different spatial Julia sets. Control Theory & Applications. 2013;**30**(9):1159-1164

[10] Hu E, Hu X, Liu T, et al. The role of soot particles in the tribological behavior of engine lubricating oils. Wear. 2013;**304**(1–2):152-161

[11] Liu Y, Tao F, Foster DE, et al. Application of a multiple-step phenomenological soot model to HSDT diesel multiple injection modeling. In: 2005 SAE World Congress. Warrendale: SAE Transactions; 2005. pp. 1141-1156

[12] Pang KM, Ng HK, Gan S. Investigation of fuel injection pattern on soot formation and oxidation processes in a light-duty diesel engine using integrated CFD-reduced chemistry. Fuel. 2012;**96**(7):404-418

[13] Ming-rui W, Hui-ya Z, Liang K, Wei-dong Z. Numerical simulation for the growth of diesel particulate matter and its influential factor analysis. Advances in Natural Science. 2008; **9**(18):1028-1033

[14] Koto F, Yanagimoto T, Mori K, et al. The Clarification of Fuel-Vapor Concentration on the Process of Initial Combustion and Soot Formation in a Di Diesel Engine. 2017;**2003**.1:1-253-1-258

[15] A Witten T, Sander LM. Diffusion-limited aggregation, a kinetic critical phenomenon. Physical Review Letters. 1981;**47**(19):1400 (p 4)

[16] Jizhong Z. Fractal. Beijing: Tsinghua University Press; 2011

[17] Deng X, Dav RN. Breakage of fractal agglomerates. Chemical Engineering Science. 2017;**161**:117-126

[18] Pfeifer P, Avnir D. Chemistry in noninteger dimensions between two and three. I. Fractal theory of heterogeneous surfaces. The Journal of Chemical Physics. 1983;**79**(7):3558-3565

[19] Sun J, Qiao W, Liu S. Controlling fractal diffusion of differently-sized soot particles. International Journal of Bifurcation and Chaos. 2018

[20] Chou CK, Lee CT. On the aerodynamic behavior of fractal agglomerates. Journal of Aerosol Science. 1997;**28**(2):620-635