LB simulation on soot combustion in porous media

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Abstract

Although diesel engines have an advantage of low fuel consumption in comparison with gasoline engines, several problems must be solved. One of the major concerns is that diesel exhaust gas has more particle matters (PM) including soot, which are suspected to be linked to human carcinogen. As one of the key technologies, a diesel particulate filter (DPF) has been developed to reduce PM in the after-treatment of exhaust gas. In this study, we conduct lattice Boltzmann (LB) simulation on combustion in porous media. Results show that the combustion reaction is well simulated to observe the decrease of soot attached to the porous wall. This information is indispensable for the better design of DPF, and LB method can be a good tool for combustion simulation in porous media.

Key words: Lattice Boltzmann Method, Combustion, Soot, Porous Media, Diesel Particulate Filter
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1 Introduction

Since diesel engines have an advantage of low fuel consumption compared with gasoline engines, the total number of cars produced in the world is gradually increased. However, several problems must be solved. One of the major concerns is that diesel exhaust gas has more particle matters (PM) including soot, which are suspected to be linked to human carcinogen. For this reason,

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more strict exhaust emissions standards such as Euro V in 2008 will be set in many countries. In Japan, the Tokyo municipal government has begun to regulate diesel-powered commercial vehicles that fail to meet the new emission standards.

As one of the key technologies, a diesel particulate filter (DPF) has been developed to reduce PM in the after-treatment of exhaust gas, which can be applied to satisfy more strict regulations for diesel emissions, coupled with improvements of combustion conditions. Some products have been already introduced at the Frankfurt Motor Show in 2003. In simple explanation of DPF, it traps the particles when exhaust gas passes its porous structure. Since the filter wall would readily be plugged with particles in a short time, the accumulated particles must be removed. Usually, the filter is heated to burn the particles in combustion. It is called filter regeneration process. However, it is expected that the outer heating with the particle burning may destroy the porous structure. Then, the thermal durable filter is plausible to maintain the low level of emissions in the long term [1]. So far, the filter has been developed mainly by experiments, and there may not be enough information to observe and understand the phenomena in DPF. For better design of DPF with efficiency and durability, it is necessary to conduct simulation with combustion in porous media. In conventional computational code, it is very challenging to deal with this process, because we need to consider the complex geometry with chemical reaction.

In the lattice Boltzmann (LB) simulation, the treatment of boundary conditions is simple and easy, and it is appropriate to calculate porous media flow [2-7]. Recently, we have simulated the flow in three-dimensional porous structure by the lattice Boltzmann method (LBM) [8]. A three-dimensional computer tomography technique (3D CT [9,10]) has been applied to obtain inner structure of a Ni-Cr metal. The flow with combustion reaction has been well simulated to discuss the local heat and mass transfer for the regeneration process of DPF.

Although the porous inner structure of DPF is not uniform, it is impossible to simulate the flow in all filters. Here, we construct the porous media structure numerically. Based on the simulation of self-aggregated fluids, the complex geometry like porous media structure is produced. In Matsukuma's group, a similar approach has been already tested by Lattice Gas Automata (LGA) [11,12]. Since we freely change the porosity and tortuosity of porous media, we can investigate the flow in any porous structure to obtain the information for better design of DPF.

2 Numerical Method

2.1 Porous Structure by Two-Phase Flow

Here, we explain the strategy to produce the porous structure. First, we simulate the self-aggregated fluids. It is like the mixture of water and oil. Initially, these are mixed randomly. At each time step, we could observe the different self-assembled structure. Then, we determine the porous geometry based on the interfaces of these fluids. As for the LB simulation, Gunstensen et al. have proposed the simple model to describe the self-aggregated fluids [13], which is based on the two-component LGA model by Rothman and Keller [14]. Here, the red and blue phases are considered. These particle distribution functions expressed in LB equation are

$$f_\alpha^k(\mathbf{x}+\mathbf{e}_\alpha, t+1) = f_\alpha^k(\mathbf{x}, t) + \Omega_\alpha^k(\mathbf{x}, t) \tag{1}$$

where k denotes either the red or blue fluid, and α is the number of local particle velocity. The collision operator is

$$\Omega_\alpha^k = \left(\Omega_\alpha^k\right)^1 + \left(\Omega_\alpha^k\right)^2 \tag{2}$$

The first term represents the process of relaxation to the local equilibrium in the lattice BGK model.

$$\left(\Omega_\alpha^k\right)^1 = -\frac{1}{\tau_k}\left(f_\alpha^k - f_\alpha^{k(eq)}\right) \tag{3}$$

Here, τ_k is the characteristic relaxation time determined by the viscosity for species k, and the distribution function with the superscript of eq expresses the local equilibrium distribution depending on the local macroscopic variables such as density and velocity. The densities of red and blue phases and the total momentum are given by

$$\rho_r = \sum_\alpha f_\alpha^r \qquad \rho_b = \sum_\alpha f_\alpha^b \tag{4}$$

$$\rho\mathbf{u} = (\rho_r + \rho_b)\,\mathbf{u} = \sum_{\alpha,k} f_\alpha^k \mathbf{e}_\alpha \tag{5}$$

The second collision operator contributes to the dynamics in the interfaces to generate a surface tension.

$$\left(\Omega_\alpha^k\right)^2 = \frac{A_k}{2}\left|\mathbf{F}\right|\left(\frac{\left(\mathbf{e}_\alpha\cdot\mathbf{F}\right)}{\left|\mathbf{F}\right|^2}-\frac{1}{2}\right) \tag{6}$$

$$\mathbf{F} = \sum_\alpha \mathbf{e}_\alpha\left(\rho_r(\mathbf{x}+\mathbf{e}_\alpha)-\rho_b(\mathbf{x}+\mathbf{e}_\alpha)\right) \tag{7}$$

where $\mathbf{F}$ is the local color gradient. The parameter A_k is used to determine the surface tension. In Eq. (6), for d2q9 model, we replace 1/2 with 2/3 in the parentheses to satisfy the local momentum conservation, because 1/2 is for the 7-bit model with hexagonal lattice. In addition, the following local color momentum, $\mathbf{j}$, is used to separate the different phases.

$$\mathbf{j} = \sum_\alpha (f_\alpha^r - f_\alpha^b)\mathbf{e}_\alpha \tag{8}$$

The distribution function for each phase is given to maximize $\mathbf{-j}\cdot\mathbf{F}$, which forces colored fluids to move towards fluids with the same colors.

2.2 Combustion Simulation by LBM

As for the combustion simulation, we have already proposed a numerical scheme by the LBM [15]. For example, the LB equation for temperature is,

$$F_{T,\alpha}(\mathbf{x}+\mathbf{e}_\alpha, t+1) - F_{T,\alpha}(\mathbf{x},t) = -\frac{1}{\tau_T}[F_{T,\alpha}(\mathbf{x},t) - F_{T,\alpha}^{eq}(\mathbf{x},t)] + w_\alpha Q_T \tag{9}$$

where F_T is the distribution function for temperature, τ_T is the relaxation time determined by thermal diffusivity, and w_0=4/9, w_α=1/9 (α=1:4), w_α=1/36 (α=5:8) for 9-bit lattice BGK model in two-dimensional square lattice space. The source term, Q_T, is heat release by chemical reaction. In this study, we consider the soot combustion [12]. In our simulation, the soot is uniformly attached to the porous wall surface, which is similar situation in the regeneration process of DPF. The porous structure is determined by self-aggregated fluid simulation. The over-all reaction by Lee et al. is adopted for soot oxidation [16]. More information on the soot oxidation is found in the review article by Stanmore et al. [17]. For simplicity, any catalytic effect is not considered.

Figure 1 shows the coordinate and boundary conditions. The calculation domain is 5 cm × 1 cm, and the inflow velocity, U_{in}, is 10 cm/s. The total number of grids is 201×41, with grid size of 0.25 mm. The porous structure of 100 grid length (L) is placed in the center part in this figure. In the calculation, all equations are non-dimensionalized based on similarity to obtain the temperature and concentration fields. As for the boundary condition, the inflow boundary is adopted at the inlet [18]. The temperature and mass fractions are those of the air at room temperature. At the sidewall, the slip boundary conditions are adopted, considering the symmetry [19]. At the outlet, the pressure

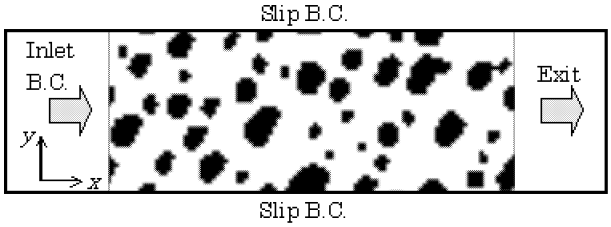

Fig. 1. Coordinate and boundary conditions in porous media flow.

is constant, and the gradient of scalar such as temperature is set to be zero. On the surface of the porous wall, the bounceback rule for non-slip boundary condition is adopted.

3 Results and Discussion

Figure 2 shows time evolution of self-aggregation. The fraction of red phase is shown. The total density ratio of blue particles to red particles is about three, corresponding to the porosity of 0.74. Time steps are 0, 10, 100, 600, 1200, and 3000, respectively. At initial condition ($t = 0$), particles for both phases are placed randomly. As seen in this figure, the phase separation is observed. At later time step, the red spot colligate each other to become larger spot. The final equilibrium state is full separation with a few large red spots. Resultantly, the surface of interface is decreased monotonically.

Here, we consider the blue phase as volume available for flow and red phase as solid media. The interface of two-phases is regarded as porous wall surface. The key parameters of porous structure are porosity and total wetted surface. The pore size distribution may be important, but the porosity and total wetted surface are only used to describe the porous structure in the theoretical formula [20]. These two parameters are shown in Fig.3 to see the time dependence. In 2D calculation, the wetted surface corresponds to the wetted perimeter. The

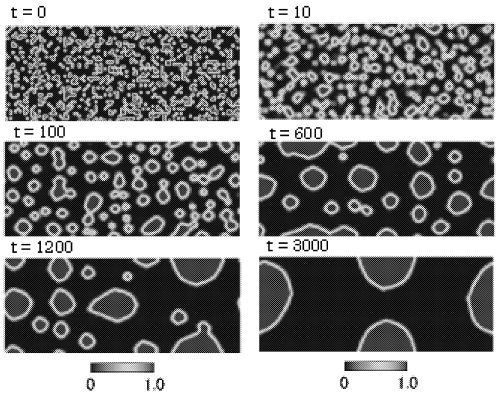

Fig. 2. Time evolution of self- aggregation at representative time steps.

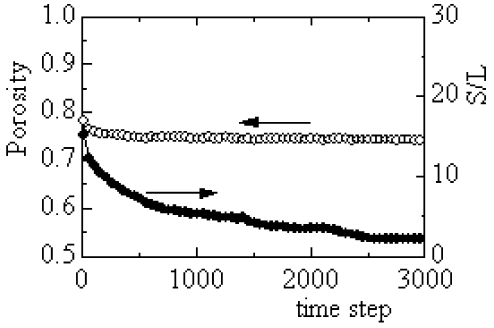

Fig. 3. Porosity and total wetted surface.

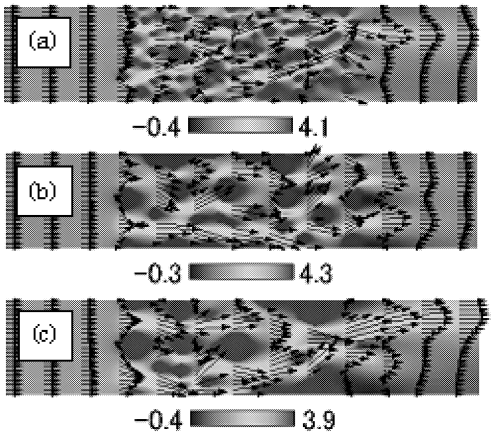

Fig. 4. Flow field in porous media of (a)case 1, (b)case 2, and (c)case 3.

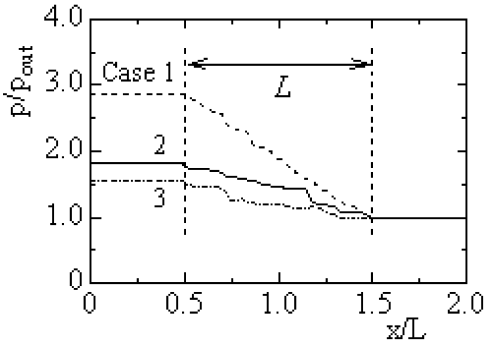

Fig. 5. Pressure distributions in porous media in cases 1 to 3.

wetted surface, S, is non-dimensionalized by the porous region length of L. It is clearly shown that only the wetted surface is decreased as the time step goes. Then, by this model, we can choose any wetted surface of porous media with porosity constant.

Next, we simulate the flow field in porous structure created in this study. We choose three structures at the time steps of 100, 600, and 1200 shown in Fig.2. These are set to be cases 1, 2, and 3, and the wetted surface of porous media is smaller from cases 1 to 3. Figure 4 shows the distribution of non-dimensional velocity in the x-direction, u_x/U_{in}. It is found that the flow is fluctuated in the porous region and the flow direction is largely changed, even when the flow is uniform at the inlet. The velocity is locally accelerated in the narrow path. The negative velocity is observed, which means that the recirculation flow exists. With different porous structure, the flow pattern is changed at the same porosity.

The pressure distribution is shown for the above three cases. Figure 5 is the averaged pressure distribution along y-direction, which is normalized by the constant pressure at the outlet. In the porous region shown by length of L, the pressure starts to decrease almost linearly, although it slightly fluctuates in cases 2 and 3. After passing this region, the pressure is almost constant. To compare three cases, it is found that the pressure at the inlet is increased as the wetted surface is larger, which could be due to the larger effect of shear forces. In future study, our numerical scheme will be extended to produce 3D porous structure to consider the real porous media.

Finally, the combustion flow is simulated. It is assumed that the soot is homogeneously attached to the wall surface with its mass fraction of 0.1. The mass fraction of oxygen in the air is 0.233. When the porous wall is heated, the soot is burned to react with oxygen. Time, t, is counted after we set the wall temperature for 1200 K. Figure 6 shows the distributions for temperature of T, mass fraction of oxygen and soot, Y_{O_2} and Y_C. The temperature is non-dimensionalized by inflow temperature. The real time corresponds to 0.12 s

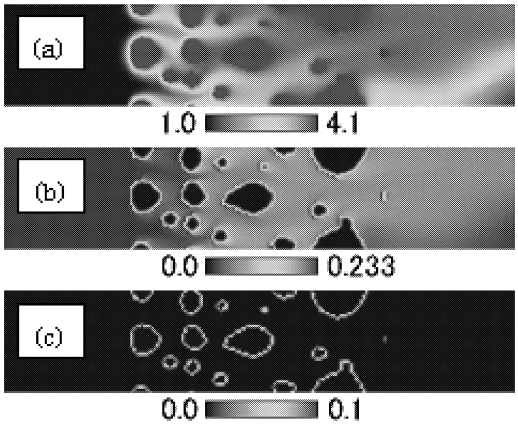

Fig. 6. Distributions of (a) temperature, (b) mass fraction of oxygen, and (c) mass fraction of soot in case 3.

after heating, and the porous structure is that of case 3 in Fig.4. It is found that the oxygen concentration around the wall surface is decreased by the reaction with soot. Then, the maximum temperature is higher than the wall temperature. It is interesting to note that the degree of soot consumption reaction is locally defferent, simply because the oxygen transport is different by the convection.

4 Conclusions

We have used the lattice Boltzmann method (LBM) to simulate the combustion flow in porous media. The distribution function for flow, temperature, and concentration fields are solved to simulate the regeneration process of diesel particulate filter (DPF). The porous stricture is formed by the self-aggregated fluids using the model proposed by Gunstensen et al. Then, the porosity and tortuosity are freely chosen to change the porous inner structure. Results show that soot combustion is well simulated, assuming that soot is uniformly attached to the wall surface. This information is indispensable for the better design of DPF. LBM can be a good tool for combustion simulation in porous media.

Acknowledgements

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