Catalysis Today 242 (2015) 357–362

Contents lists available at ScienceDirect

Catalysis Today

journal homepage: www.elsevier.com/locate/cattod

Simulation of continuously regenerating trap with catalyzed DPF

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ARTICLE INFO

Article history:
Received 25 March 2014
Received in revised form 8 July 2014
Accepted 10 July 2014
Available online 8 August 2014

Keywords:
Catalyst
DPF
Continuously regenerating trap
Diesel exhaust
Computed Tomography

ABSTRACT

For reduction of particulate matter (PM) including soot in diesel exhaust gas, a diesel particulate filter (DPF) has been developed. However, it would be plugged with PM to cause an increase of filter backpressure. If the backpressure is too high, the fuel consumption rate unexpectedly increases and the engine output may decrease. Then, the filter must be regenerated by oxidizing PM. The system where PM is trapped and oxidized simultaneously is called a continuously regenerating DPF. A catalyst such as platinum is used for the reduction of PM oxidation temperature. Since platinum is a precious and rare metal, the amount of catalyst must be suppressed. In this study, we simulated the continuously regenerating trap system with catalyzed DPF by a lattice Boltzmann method (LBM). For the soot oxidation rate with catalysts, reaction parameters such as activation energy were evaluated by an engine test bench. In the simulation, five cases with different catalyst-coating were considered. Based on the filter backpressure, the coating area for the reduction of catalysts was discussed.

1. Introduction

The reduction of carbon dioxide (CO_2) emissions is essential for inhibiting global warming. The use of fuel-efficient diesel vehicles is one strategy for reducing CO_2 emissions [1], and the number of diesel vehicles has been increasing, particularly in Europe. However, diesel vehicles emit nitrogen oxides (NO_x) and particulate matter (PM) in the form of soot, which cause air pollution. Measures to reduce nanoparticulate soot emission are particularly important, because nanoparticles pose particular health risks for diseases such as cancers [2–4]. Therefore, regulations for the control of automobile exhaust gas emissions are being strengthened year after year [5]. Meeting these regulations requires not only increasing fuel efficiency but also improving the exhaust gas after-treatment system. Diesel particulate filters (DPFs), which collect PM, are widely used for exhaust gas treatment [4,6,7].

Fig. 1 shows a schematic of DPF. Upper figure shows PM trap inside porous filter wall. A typical DPF is made of porous ceramics with a honeycomb structure, and has the alternate closure of the inlets and outlets of its many channel holes. The mechanism for PM trap is simple: when the exhaust gas passes through the cell walls (the filter's sidewalls), which separate cells at inlet and outlet sides of the filter, PM contained in the gas phase is deposited within the filter wall. However, as PM is continuously collected, the filter eventually clogs, and the exhaust pressure (filter backpressure) increases [8,9]. Consequently, the fuel consumption rate unexpectedly increases and the engine output may decrease. These disadvantages can be avoided by using a continuously regenerating DPF [4,5], which collects PM and simultaneously oxidizes it. To oxidize the PM at low temperature, DPFs with precious metal catalysts such as platinum are in practical use [10,11].

However, since catalysts made of precious and rare metals are very expensive, the amount of catalysts must be reduced to make these filters cost-effective. This requires an understanding of the phenomena occurring within the thin sidewalls of DPFs. Therefore, processes that would allow visualization of these phenomena and examination of the effects of catalysts would be valuable, but these are very difficult in experiments [12]. Our research group has been investigating the phenomena occurring within DPFs by conducting numerical simulations using a lattice Boltzmann method (LBM) [13–16], which is effective for analyzing a porous media flow [17]. The present study numerically simulated a continuously regenerating DPF for the reduction of the catalyst amount required to support its operation.

2. Numerical analysis

2.1. Lattice Boltzmann method

Firstly, the numerical approach for exhaust gas flow with soot oxidation is explained, followed by the soot deposition model described at the next section. The lattice Boltzmann method (LBM)

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http://dx.doi.org/10.1016/j.cattod.2014.07.022
0920-5861/

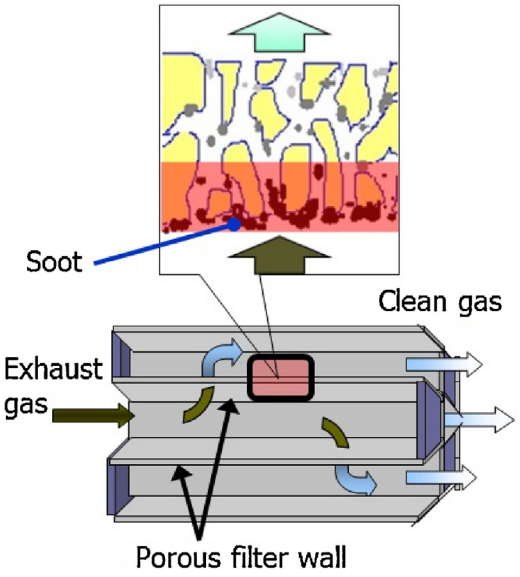

Fig. 1. A schematic of diesel particulate filter is shown. Upper figure shows PM trap inside porous filter wall.

was used in the simulation, which is a simplification of Boltzmann equation [17]. The LBM analyses the flow based on the movement and collision processes of artificial particles moving at lattice nodes. So far, many fluid simulations by LBM have been conducted, including the flow in DPF [12–16]. The model of D3Q15 using cubic lattices is applied for 3D calculation [18].

As for the combustion simulation, we followed the same numerical scheme proposed in our previous study [12,19]. The flow field was determined using the distribution function of pressure, p. The evolution equation and the equilibrium distribution function are expressed as follows:

$$F_{p,\alpha}(\vec{x}+\vec{e}_\alpha\delta_t, t+\delta_t) - F_{p,\alpha}(\vec{x}, t) = -\frac{1}{\tau_p}[F_{p,\alpha}(\vec{x}, t) - F^{\mathrm{eq}}_{p,\alpha}(\vec{x}, t)] \quad (1)$$

$$F^{(\mathrm{eq})}_{p,\alpha} = w_\alpha \left\{ p + p_0 \left[3\left(\frac{\vec{e}_\alpha\times\vec{u}}{c^2}\right) + \frac{9}{2}\left(\frac{\vec{e}_\alpha\times\vec{u}}{c^2}\right)^2 - \frac{3}{2}\left(\frac{\vec{u}}{c}\right)^2 \right] \right\} \quad (2)$$

where δ_t is the time step, τ is the relaxation time which controls the rate of approach to equilibrium, and $\vec{e}_\alpha$ (α = 1– 15) is the unit vector of D3Q15 model in lattice space. The constants in Eq. (2) are $w_{1\text{-}6} = 1/9$, $w_{7\text{-}14} = 1/72$, and $w_{15} = 2/9$. The pressure, p, and the local velocity of $\vec{u} = (u, v, w)$ are obtained using the low Mach number approximation [19] as follows:

$$p = \sum_\alpha F_{p,\alpha} \quad (3)$$

$$\vec{u} = \sum_\alpha \frac{F_{p,\alpha}}{P_{\mathrm{out}}} \times \frac{T}{T_0}\vec{e}_\alpha \quad (4)$$

where P_{out} represents atmospheric pressure. The kinematic viscosity of ν in LBM is related with the relaxation time of τ, using the following formula:

$$\nu = \frac{2\tau_p - 1}{6}\frac{\delta_x^2}{\delta_t} \quad (5)$$

Through the Chapman–Enskog procedure, the Navier–Stokes equations are derived from these equations [17]. In the calculation, all of the variables were set to be dimensionless, and the same dimensionless quantities such as the Reynolds number ($\mathrm{Re} = U_{\mathrm{in}}W/\nu$) were used [19], where U_{in} is the inlet velocity of exhaust gas, and W is the width of numerical domain in Fig. 3.

Similar to the flow field, the scalar quantities of temperature and species concentrations were also determined by their distribution functions [12–16,19]. The evolution equation and the equilibrium distribution function for the scalar quantities are expressed as follows:

$$F_{s,\alpha}(\vec{x}+\vec{e}_\alpha\delta_t, t+\delta_t) - F_{s,\alpha}(\vec{x}, t) = -\frac{s}{\tau_s}[F_{s,\alpha}(\vec{x}, t) - F^{(\mathrm{eq})}_{s,\alpha}(\vec{x}, t)] + w_\alpha Q_s \quad (6)$$

$$F^{(\mathrm{eq})}_{s,\alpha}(\vec{x}, t) = w_\alpha s \left\{ 1 + 3\left(\frac{\vec{e}_\alpha\times\vec{u}}{c^2}\right) + \frac{9}{2}\left(\frac{\vec{e}_\alpha\times\vec{u}}{c^2}\right)^2 - \frac{3}{2}\left(\frac{\vec{u}}{c}\right)^2 \right\} \quad s = T,\ Y \quad (7)$$

where s is the value of temperature and mass fraction of species i, and Q_s represents the source term due to the chemical reaction in the soot oxidation process. The procedure to evaluate the soot oxidation rate in catalyzed DPF will be explained later. An overall one-step reaction of $C + O_2 \rightarrow CO_2$ was used [12,20]. For relaxation time of τ_s, which is required for calculating the concentration and temperature fields, the same value as that of τ_p in Eq. (5) was used. The temperature and the mass fraction of species i (mass fraction) are obtained as follows:

$$T = \sum_\alpha F_{T,\alpha} \quad (8)$$

$$Y_i = \sum_\alpha F_{Y_i,\alpha} \quad (9)$$

2.2. Soot deposition model

In this section, a soot deposition model is explained. Generally, the soot has complex geometry of nanoparticles [2,21,22]. Since the size of diesel soot has a nano-scale, it is difficult to realize the deposition phenomenon of soot particles precisely. Then, the soot deposition is described by the modified particle deposition model [23]. Different from Lagrangian approach through the equation of motion, individual particles were not considered. Instead, the soot concentration was monitored. The mass fraction of deposited soot is given by

$$Y_{C,s}(\vec{x},\ t+\delta_t) = \sum_\alpha F_{C,\alpha}(\vec{x},\ t) \times P_D + Y_{C,s}(\vec{x},\ t) \quad (10)$$

where $Y_{C,s}$ is the mass fraction of deposited soot of solid phase, and P_D is the soot deposition probability, which controls the amount of soot attached to the filter substrate. If P_D is unity, soot is thoroughly deposited on the filter without reflection. Else, a part of soot is bounced back and transported downstream. As the soot deposition is continued, the soot mass fraction sometime becomes unity. When this limit is reached, the solid site is piled up, and the deposited soot region is treated as non-slip wall, which implies a change of boundary condition for fluid. In the simulation, we adopted $P_D = 0.002$, which is the value determined in experiments [15,16].

2.3. Numerical domain

Here, we describe the numerical domain in the simulation. Fig. 2 shows an image of the filter obtained by a three-dimensional X-ray CT measurement. The image area was 0.66 mm (y) × 0.66 mm (z), and the spatial resolution was 1.15 μm/pix. Fig. 3 shows the filter and the coordinate system used in the simulation. The direction