MICROSTRUCTURE CHARACTERIZATION OF WOOD FIBER PIT ADSORBINGULTRAFINE PARTICLES EMITTED BY DIESEL ENGINE AND SIMULATION OF ITS INFLUENCE FACTORS

Xiurong Guo, Danfeng Du, Zhanfeng Qi, Peng Wang Northeast Forestry University Harbin, China

Hoseok Song University of Houston, Department of Chemical & Biomolecular Engineering Texas Center for Clean Engines, Emissions & Fuels Houston, Tx USA

(Received July 2015)

ABSTRACT

Wood fiber is a porous biomass material, which has a strong adsorption ability for the PM (particulate matter) emitted by diesel engines. Through the SEM experiments, the fact that the pits of micron wood fiber after heat-treated can adsorb lots of ultrafine particles (aerodynamic diameter is less than 1 μ m) is shown clearly. In simulation, the particle concentration equations and fibrous filtration theory are applied. The collection media around pits is assumed as a cylinder. The simulation results show that the pits have relatively lower collection efficiency for the particles within the diameter from 0.4 to 0.6 μ m. Out of the range of 0.4 to 0.6 μ m, the collection efficiency increases rapidly, which implies that the pits have higher collection efficiency to filter the particles with the diameter out of 0.4 to 0.6 μ m. Among all the affecting factors on collection efficiency, the reduction of permeate flow rate and the addition of tracheid wall thickness improve the collection efficiency. However, exhaust temperature has negligible influence on the collection efficiency.

KEYWORDS: Micron wood fiber, microstructure characterization, ultrafine particles, pits, adsorption.

INTRODUCTION

PM2.5 is defined as the particles with the aerodynamic diameter less than or equal to 2.5 μ m. Since the continuous increasing content of PM2.5 in the atmosphere, most of our cities have been shrouded in haze weather (Yang and Bai 2013). In China, nearly 30 % of the PM2.5 in the atmosphere directly comes from the vehicle exhaust (Wu 2011). According to Chinese emission standard at stage III (equivalent to EUR III), diesel vehicles emit 60 times PM than that from gasoline vehicles. Even if the light-duty diesel vehicles met the stage IV, they would emit more than 30 times PM than that from gasoline vehicles that meet the stage III (Baxter and Sacks 2014). Thus, the diesel vehicles need more improvement compared to their counterparts.

According to different sizes of particles, PM can be divided into three modes: the nuclei mode (aerodynamic diameter is $5\sim50$ nm), the accumulation mode (aerodynamic diameter is less than 1 µm), and the coarse mode (aerodynamic diameter is more than 1µm). The first two modes take up to about 90 % of all the particles. The diesel particle filter (DPF) can efficiently reduce the particle emissions. Up to date, USA, Japan and European countries have resulted in reducing PM emissions by using DPF (Baxter and Sacks 2014). However, China still needs more improvements to reduce PM emissions overcoming the high price of DPF and the requirement of high diesel quality. In addition, DPF has lower collection efficiency on ultrafine particles (aerodynamic diameter is less than 1µm), which can be easily inhaled into human respiratory system and threat human health (Mckenzie et al. 2012, Zheng et al. 2014).

In this study, micron wood fiber has been applied to filter PM to solve the issues discussed above. The advantages of wood fiber filter are low price, less requirement for diesel quality and large adsorption capacity for PM. In these respects, wood fiber filter is promising in developing countries where the sulphur contents are high in diesel fuel (Guo et al. 2011). In this paper, it is found that, after heat treatment, most pits in wood fiber are opened by the water vaporization, which increases the permeability and decreases the exhaust back pressure dramatically. The SEM experiments show that the pits of micron wood fiber can absorb ultimate particles efficiently. In simulation, the particle concentration equations and fibrous filtration theory are applied and the collection media around pits are assumed as a cylinder. Furthermore, this paper also shows the steady-state collection efficiency of pits mathematically.

MATERIAL AND METHODS

Material

The *Cunninghamia lanceolata* was manufactured into a new type of wood fiber by longitudinal cutting, which was dozens of microns thick, hundreds of microns wide, thousands of microns length. By a pressing machine, micron wood fiber was made into a filter. In order to open the pit membrane and improve it to adsorb more ultrafine particles, we put the filters in a drying oven and rise temperature at a rate of 5°C per minute, then keep warm for 2 hours when temperature reaches 200°C. After the fabrication process, the filter can be installed in a detachable DPF case where the temperature inside can be controlled below 220°C (Guo and Liu 2014). Fig. 1 shows the manufacturing process of heat-treated micron wood fiber DPF.



d) Heat-treated micron wood fiber filter e) Sealed shell of detachable DPF $% \mathcal{A}(\mathcal{A})$

Fig. 1: Manufacturing Process of heat-treated micron wood fiber DPF.

The SEM was used to observe the microscopic structure of micron wood fiber. As shown in Fig. 2a, the external force deforms the tracheids and also reduces the specific surface area of micron wood fiber. Fig. 2b shows that most pits are in a closed state leading to a lower permeability.



b) The pits in a closed state (3000×)

Fig. 2: SEM picture of micron wood fiber.

a) The deformed tracheids by external force (100×)

As shown in Fig. 3, the deformed tracheids restore the fluffy natural state because of the heat treatment and its specific surface-area increases greatly. Furthermore, Fig. 3b shows that many pits are opened by the water vaporization, which means that heat treatment method can improve the permeability of micron wood fiber.



a) The natural, unsqueezed state tracheids (100×)



b) The opened pits (3000×)

Fig. 3: SEM picture of heat-treated micron wood fiber.

A heat-treated micron wood fiber filter was used to filter PM emitted by an Isuzu diesel engine.

WOOD RESEARCH

Fig. 4a and b show that the PM is adsorbed onto the surface of heat-treated micron wood. As the magnification increased in Fig. 4c and d, it can be observed that a lot of PM are collected by tracheids and wood rays. When the magnification is increased to 10000 as Fig. 4e, we can easily see that the opened pits capture the ultrafine PM whose aerodynamic diameter is less than 1 μ m. Since the pits have better collection efficiency on ultrafine particles, this paper is focused on ultrafine particles to understand the collection mechanism of the pits. The mathematical approach is introduced in the following section.



a) The adsorbed PM onto the surface (100×,





b) The adsorbed PM is onto the surface 300×)



c) Collected PM with small size by tracheids d) Collected PM with small size by wood rays (1000×) (3000×)



e) The collected PM with smaller size by pits (10000×)

Fig. 4: SEM of heat-treated micron wood fiber after filtering.

Model descriptions

Microscopic model of heat-treated micron wood fiber

As shown in Fig. 5, the tracheid structure of coniferous wood is regular and contains many pits with various sizes. In order to describe it by mathematical method, the cross section could be simplified into 2 dimensional hexagonal structure (Yang et al. 2013, Li and Zhao 2003). Assuming that all the pits have the same size, regular shape (circle) and uniformly distribute in the tracheid, according to the characteristics of heat-treated tracheid structure, 3D simulation

software and geometric transformation are used to get a 3 dimensional simulation of heat-treated micron wood fiber cell structure (Fig. 5c).



c) 3D model of micron wood fiber cell structure

Fig. 5: Micron wood fiber microstructure.

Control equation of exhaust particle concentration in pits

This paper mainly discusses the steady-state collection efficiency of pits. In the study, the collection process of clean filter to capture particles is defined as steady-state collection process. Before building a mathematic model of steady-state collection efficiency, some assumptions need to be made:

- 1) Micron wood fiber is perpendicular to the direction of exhaust;
- 2) The changes of the exhaust velocity through the pits are not obvious. Thus, it can be considered as a constant (Bissett 1984);
- 3) The particles will not rebound or fall off after being collected.

As shown in Fig. 6, the hexahedron is considered as a particle concentration control body in the pits.



Fig. 6: Particle concentration control body.

Based on the above assumptions and the law of conservation of mass, it is concluded that the sum of the volume flow rate of particles that flow and diffuse in the control body and the volume change rate of particles caused by the source term is zero (Liu 2009), namely:

$$\begin{bmatrix} U_{wx} \left(C - \frac{\partial C}{\partial x} \cdot \frac{dx}{2} \right) dy dz - U_{wx} \left(C + \frac{\partial C}{\partial x} \cdot \frac{dx}{x} \right) dy dz \end{bmatrix}$$

$$\cdot \left[-D_p \frac{\partial}{\partial x} \left(C - \frac{\partial C}{\partial x} \cdot \frac{dx}{2} \right) dy dz + D_p \frac{\partial}{\partial x} \left(C + \frac{\partial C}{\partial x} \cdot \frac{dx}{2} \right) dy dz \end{bmatrix} + S_e = 0$$
(1)

where: C - the particle volume concentration,

 U_{wx} - the permeate flow rate of micron wood fiber,

$$\begin{split} D_p &= \frac{k_b T}{3\pi \mu d_p} & \text{the particle diffusion coefficient,} \\ k_b &= 1.38 \times 10^{-23} \text{J/K the Boltzmann constant,} \\ \mu &= \frac{832 \times 10^{-15} \times T^3 - 296 \times 10^{-11} \times T^2 + 624 \times 10^{-6} \times T + 231 \times 10^{-6}}{100} & \text{the exhaust-gas viscosity (Ober 1971),} \end{split}$$

T - the exhaust temperature, $S_t = -E \cdot C \cdot U_0 \cdot S_M - \text{the particle change rate caused by source term in the control body (Kong 1999),$ $U_0 = U_{wx} / \varepsilon - \text{the velocity in the pits,}$ $\varepsilon - \text{the interstitial porosity of the tracheid,}$ $S_M - \text{the filter area, which is perpendicular to the exhaust velocity,}$ E - the comprehensive collection coefficient of the capture unit.

 ${\cal E}$ means the sum of composite collection coefficient from all kinds of filtration mechanism to particles.

If the particle is captured by one of the collection methods, it will not be captured by others. In this case, E is defined as (Ning et al. 2005)

$$E = E_R + E_D + E_I - E_R \cdot E_D - E_R \cdot E_I - E_D \cdot E_I$$
⁽²⁾

where:

 E_R - the direct interception coefficient, E_D - the brown diffusion coefficient, E_I - the inertial collision coefficient.

Steady-state collection model based on fibrous filtration theory

The collection unit is assumed as a cylinder in the fibrous filtration theory as shown in Fig. 7. The diameter of cylindrical collection media can be obtained from the porous medium theory (Kong 1999).

$$d_{c} = \frac{3}{2} \cdot \frac{1 - \varepsilon}{\varepsilon} d_{pore}$$
(3)

where: d_{pare} - the diameter of pits.



Fig. 7: Cylindrical collection unit.

According to the research by Rumpf and Gupte (Masoudi et al. 2001), the Brownian diffusion coefficient can be defined as

$$E_{D} = 2.86 \left[1 + 0.388 Kn \left(\frac{Pe}{H + 1.996 Kn(H + 0.5)} \right)^{\frac{1}{3}} \right] (H + 1.996 Kn(H + 0.5))^{-\frac{1}{3}} \cdot Pe^{-\frac{2}{3}}$$
(4)

where:

$$Kn = \frac{2\lambda}{d_c} \text{ is the Knudsen Number,}$$
$$\lambda = \frac{\mu}{0.499P} \cdot \sqrt{\frac{\pi TR_s}{8}} \text{ the mean free path,}$$

180

P - the exhaust pressure, $R_b - \text{the gas constant,}$ $H = \frac{3}{4} - \frac{1}{2} \ln(1-\varepsilon) \text{ the constant,}$ $Pe = \frac{U_0 d_c}{D_p} \text{ the Peclet number.}$

According to the analyses and deduction of a large number of the test results by Davies (Pratim and Flagan 1988), the inertial collision coefficient can be defined as

$$E_I = 0.16 \left[N_R + (0.5 + 0.8N_R)St - 0.103St^2 \right]$$
(5)

where:

1

$$N_{R} = \frac{a_{p}}{d_{c}} - \text{ the intercept coefficient,}$$

$$s_{t} = \frac{(\rho_{p} - \rho_{s})d_{p}^{2}U_{s}}{18\mu d_{c}} \quad \text{the stokes number,}$$

$$\rho_{p} \text{ and } \rho_{g} - \text{ the intake and exhaust density of particles respectively.}$$

Based on the experimental study and theoretical analysis, the direct interception coefficient can be defined as

$$E_{R} = \frac{N_{R} \left(N_{R} + 1.996 Kn \right)}{H_{a} + 1.996 Kn \left(H_{a} + 0.5 \right)} \tag{6}$$

where: $H_a = 2 - \ln \operatorname{Re}$ is the constant,

 $\operatorname{Re} = \frac{\rho_g U_0 d_c}{\mu}$ the Reynolds number.

According to the characteristics of cylindrical collection unit, SM can be expressed as

$$S_{M} = \frac{4(1-\varepsilon)}{\pi \cdot d_{c}} \cdot dx dy dz \tag{7}$$

Substituting Eq. (7) in (3), Eq. (8) becomes

$$S_{c} = -\frac{4E(1-\varepsilon)}{\pi\cdot\varepsilon\cdot d_{\varepsilon}} \cdot C \cdot U_{wx} dx dy dz$$
(8)

Substituting the results of Eq. (8) in Eq. (1), Eq. (9) becomes

$$D_{P} \frac{\partial^{2} C}{\partial^{2} x} - U_{wx} \frac{\partial C}{\partial x} - U_{wx} \frac{4E(1-\varepsilon)}{\pi \varepsilon d_{c}} C = 0$$
⁽⁹⁾

with the boundary conditions:

$$\begin{cases} x = 0, C = C_0 \\ x \to \infty, C = 0 \end{cases}$$
(10)

where: C_0 - the particle volume concentration from the entrance of cylindrical collection unit.

According to Eq.(10), Eq.(11) has the solution:

$$C = C_0 \cdot \exp\left(\frac{U_{wx} - \sqrt{U_{wx}^2 + 6E(1-\varepsilon)D_p U_{wx}/(\varepsilon d_\varepsilon)}}{2D_p} \cdot x\right)$$
(11)

Set the tracheid wall thickness as h and the particle volume concentration that passed through the unit as C_{2h} , which can be expressed as

$$C_{2h} = C_0 \cdot \exp\left(\frac{U_{uu} - \sqrt{U_{uu}^2 + 6E(1-\varepsilon)D_p U_{uu}/(\varepsilon d_\varepsilon)}}{2D_p} \cdot 2h\right)$$
(12)

According to the fibrous filtration theory, the solution of the steady-state collection efficiency equation is

$$\eta = \frac{C_0 - C_{2h}}{C_0} = 1 - \exp\left(\frac{2hU_{wx}}{2D_p} - 2h\sqrt{\frac{U_{wx}^2}{4D_p^2} + \frac{3E(1-\varepsilon)U_{wx}}{2D_p\varepsilon d_c}}\right)$$
(13)

RESULTS AND DISCUSSION

According to the method mentioned above, the influence factors on steady-state collection efficiency of pits is researched. The average tangential diameter of early coniferous wood is about 40 and the late is about 36 μ m. The diameter of its pit is 17 to 24 μ m given in (Zhou 2001). The tracheid wall thickness is 1.2 to 10 µm given in (Yang et al. 2012). The average void volume fraction of tracheid is 92 % given in (Fang and Wu 2007). Based on the above data, the steadystate collection efficiency of pits was calculated by Eq. (13).

Fig. 8 describes the effect of permeate flow rate on steady-state collection efficiency of pits. It shows that particles with the diameter of 0.01 µm have the highest collection efficiency that could reach 90 % or more. The figure also illustrates that the collection efficiency decreases sharply as the ranging from 0.01 to 0.4 μ m and reaches a minimum as the diameter between 0.4 and 0.6 μ m. However, when the diameter from 0.6 to 1.0 μ m, the collection efficiency will increase slowly and for the particle with same diameter the efficiency decreases as the permeate flow rate increases. Furthermore, with the diameter approaching 1µm, the collection efficiency has no obvious changes when the permeate flow rate increases.



Fig. 8: The effect of permeate flow rate on steadystate collection efficiency of pits (T=453.15 K, steady-state collection efficiency of pits $b=6\ \mu m,\ \varepsilon=92\ \%,\ d_{pore}=20\ \mu m).$

Fig. 9: The effect of exhaust temperature on $(U_{wx}=1.0 \text{ m.s}^{-1}, .b=6 \mu m, \varepsilon = 92 \%, d_{pore}=20 \mu m).$

Fig. 9 demonstrates the effect of exhaust temperature on steady-state collection efficiency. It implies that, in the diameter ranges from 0.01 to 0.4 μ m, the collection efficiency decreases, and it decreases to a minimum within the diameter from 0.4 to 0.6 µm. At the same temperature, with the diameter from 0.6 to 1.0 μ m, there is a positive relationship between the collection efficiency and the diameter. With the same diameter, exhaust temperature has a negligible influence on collection efficiency.



Fig. 10: The effect of tracheid wall thickness on steady-state collection efficiency of pits(T=453.15 K, U_{uux} =1.0 m.s⁻¹, ε =92 %, d_{hore} =20 µm).

Fig. 10 depicts the effect of the tracheid wall thickness on steady-state collection efficiency. With the same tracheid wall thickness, the collection efficiency decreases rapidly as the diameter ranging from 0.01 to 0.4 μ m, and it reaches a minimum with the diameter between 0.4 and 0.6 μ m. This figure also implies that under the same condition of thickness, the collection efficiency is inching up with the diameter ranging from 0.6 to 1.0 μ m. However, as the tracheid wall thickness increases, the collection efficiency slowly increases.

CONCLUSIONS

After studying the microstructure of micron wood fiber, the results show that under the condition of external force the tracheids can be deformed and the pits are in a closed state. However, when the micron wood fiber was heat-treated, the deformed tracheids could return to the natural state and most pits were open. This method can efficiently increase the specific surface-area and permeability. Based on these results, micron wood fiber filter made by special process can be applied in filtering material of the DPF. It has higher permeability and lower exhaust back pressure. Moreover, it has better collection efficiency for ultrafine particles. According to the particle concentration equations and fibrous filtration theory, the collection media around pits can be assumed as a cylinder. The numerical method is applied to analyze the steady-state collection efficiency. The results show that the pits have relatively low collection efficiency for the particles within the diameter from 0.4 to 0.6 μ m, and when the influence factors change, the collection efficiency has no obvious changes. Out of the range of 0.4 to 0.6 µm, the collection efficiency increases rapidly, which implies that the pits have higher collection efficiency to filter the particles with the diameter out of 0.4 to 0.6 μ m. The explanations of this interesting phenomenon is as follows: When diameter of particles is between 0.01 and 0.4 µm, the high collection efficiency may be due to Brown diffusion effect, i.e. the smaller particles are easier to be adsorbed into pits and stuck to the tracheid wall; when diameter is between 0.6 and 1 μ m, the reason for increase of collection efficiency may be the inertial collision effect, i.e. the bigger particles are easier to be captured when they collide with pits relying on inertia; when diameter is between 0.4 and 0.6 μ m, the collection efficiency is lowest, it is probably

WOOD RESEARCH

due to the fact that the inertial collision effect and Brownian diffusion effect are all not obvious. Among all the factors that can affect the collection efficiency, the reduction of permeate flow rate and the increase of tracheid wall thickness will help improve the collection efficiency. However, the exhaust temperature has a negligible influence on collection efficiency.

ACKNOWLEDGMENTS

This paper is supported by the Fundamental Research Funds for the Central Universities (grant number: 2572014EB04) and the National Natural Science Foundation of China (grant numbers: 51378096 and c160402).

REFERENCES

- Baxter, L.K., Sacks, J.D., 2014: Clustering cities with similar fine particulate matter exposure characteristics based on residential infiltration and in-vehicle commuting factors. Science of the Total Environment 470-471: 631-638.
- 2. Bissett, E.J., 1984: Mathematical model of the thermal regeneration of a wall-flow monolith diesel particulate filter. Chemical Engineering Science 39: 1233-1244.
- Fang, W.B., Wu, Y.Q., 2007: Tissue ratio of conifer wood. Journal of Northeast Forestry University 35(2): 12-14.
- Guo, X.R., Du, D.F., Wang, F.H., Ma, Y., 2011: Study on test instrument and filtration theory of the carbonized micron wood fiber DPF. Microporous and mesoporous materials 1422): 655-660.
- Guo, X.R., Liu, Y.X., 2014: Diesel PM filter device cooler with the long wood fiber filter (P). China: 201420116735, 2014.09.10.
- 6. Kong, X., 1999: See page mechanics. Press of University of Science and Technology of China., Pp 21-52.
- 7. Li, Y., Zhao, G., 2003: Wood resources in materials science. Beijing: China Forestry Publishing House. Pp 64-65.
- 8. Liu, Y., 2009: Mechanisms study on filtration and microwave regeneration of wall-flow diesel particulate filter. Hunan University. Pp 30-35.
- McKenzie, L., Witter, R.Z., Newman, L.S., Adgate, J.L., 2012: Human health risk assessment of air emissions from development of unconventional natural gas resources. Science of the Total Environment 424: 79-87.
- Masoudi, M., Konstandopoulos, A, Nikitidis, M.S., 2001: Validation of a model and development of a simulator for predicting the pressure drop of diesel particulate filters. SAE World Congress. Pp 911-917.
- 11. Ning, Z., Song, B., Zi, X.Y., Liu, J., 2005: Study on the trap mechanisms and effect factors of the diesel ceramic wall flow filter. Journal of Beijing Jiaotong University 29: 69-73.
- 12. Ober, E.F., 1971: Internal combustion engines and air pollution. Automotive Engineering 43: 367-375.
- 13. Pratim, B., , Flagan, R.C., 1988: The particle trap impactor. Journal of Aerosol Science 19(1): 113-121.
- 14. Wu, Q.T., 2011: PM_{2.5} and vehicle emission standards. Automobile & Parts 52(12): 18-19.

- 15. Yang, X.B., Bai, Z.P., 2013: Causes of fog and frost weather conditions to deal with the legal aspects of the operational level policy recommendations. Energy of China 35(4): 6-10.
- Yang, D.X., Ma, Y., Yang, C.M., 2013: Theoretical calculation of coniferous wood cell wall. Journal of Nanjing Forestry University: Natural Sciences Edition 37(3): 97-102.
- 17. Yang, D.X., Ma, Y., Yang, C.M., 2012: Theoretical calculation of cell wall fracture of coniferous timber. Journal of West China Forestry Science 41(3): 42-47.
- Zheng, Y., Liu, Y., Harold, M.P., Luss, D., 2014: LNT-SCR dual layer catalysts optimized for lean NOx reduction by H₂ and CO, Applied Catalysis B: Environmental 148-149: 311-321.
- 19. Zhou, J., 2001: Chinese larch wood. Beijing: China Forestry Publishing House. Pp 23-61.

Xiurong Guo, Danfeng Du^{*}, Zhanfeng Qi, Peng Wang Northeast Forestry University Harbin 150040 China Corresponding author: ddf72@163.com

Hoseok Song University of Houston Department of Chemical & Biomolecular Engineering Texas Center For Clean Engines, Emissions & Fuels Houston Tx 77204, USA WOOD RESEARCH