Applied Thermal Engineering 100 (2016) 1292–1298

Contents lists available at ScienceDirect

Applied Thermal Engineering

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

Research Paper

Soot loading estimation model and passive regeneration characteristics of DPF system for heavy-duty engine

Shuzhan Bai [a,*], Jiao Tang [b], Guihua Wang [a], Guoxiang Li [a]

[a] School of Energy and Power Engineering, Shandong University, Jinan 250061, China
[b] Center of Research and Department, WEICHAI Power Co. Ltd., Weifang 261205, China

HIGHLIGHTS

- A new soot model was established to calculate the soot accumulation in DPF.
- The temperature field in the DPF was measured in DPF.
- The new soot model includes transient soot emission and chemical reaction module.
- Temperature and NO_2 concentration are key points for regeneration time interval.

ARTICLE INFO

Article history:
Received 23 December 2015
Accepted 20 February 2016
Available online 4 March 2016

Keywords:
Diesel particulate filter
Soot oxidation
Soot loading model
WHTC test cycle
Passive regeneration

ABSTRACT

Although the pressure differential sensor across the DPF could estimate the amount of soot in the DPF, the accuracy of the soot estimation deteriorates seriously at lower exhaust volumetric flow. In order to compensate for this defect, a new soot loading model was established to calculate the soot accumulation in the DPF for improving the accuracy of active regeneration trigger time, and passive regeneration is researched based on this model. Testing validations were taken based on WHTC test cycle. The results show that the average error between calculated and measured soot loading is about 3.4% during the soot loading process. With the increasing tailpipe temperature and NO_2 concentration, passive regeneration is accelerated and active regeneration interval is prolonged. When temperature after turbo reaches 283 °C with 289 ppm NO_2 concentration, soot loading maintains around 1.27 g/L. At this balance point, pure passive regeneration can be fulfilled.

1. Introduction

Diesel Particulate Filters (DPFs) have been widely used to remove harmful particulate matter (PM) and have become an indispensable feature of the modern diesel engines due to strict regulations on PM and particulate number (PN) emissions [1–3]. The PM, however, clogs the DPF after long-term use and affects the operation of the engine. As too much PM accumulates in the DPF, the back pressure increases resulting in low fuel economy or other problems. This has necessitated a technology for removing the PM to ensure the efficient long term operation of the engine. The trapped PM can be removed by regeneration either periodically or continuously. DPF regeneration is divided into active regeneration and passive regeneration. Typically, active regeneration depends on oxidation of the soot by O_2 at higher exhaust temperature, which operates by injecting fuel into exhaust pipe and using Diesel Oxidation Catalysts (DOC) to oxidize it to raise the temperature to approximately 600 °C [4], and passive regeneration depends on continuous oxidation of the soot by NO_2 in the temperature range 200–500 °C, which operates by DOC to oxidize NO from exhaust to NO_2 and engine exhaust NOx/PM ratio. Numerous studies have been conducted which discuss both active and passive regeneration characteristics [5–10]. The combination of both passive and active regeneration of vehicle strategies can balance PM control as well as cost.

One key (control) parameter is the accurate estimation of the actual soot loading in the DPF at any time. This is due to two main reasons: "Overloading" with soot could lead to DPF damage whereas "under-loading" results in unnecessary DPF regenerations and therefore CO_2 penalties [11–13].

Therefore, it is important to understand the key parameters affecting DPF passive regeneration, identifying the range where passive regeneration can assist in prolonging the active regeneration interval, or how to realize pure passive regeneration [14–16].

In this study, several typical steady operating points are chosen to build up soot loading model of DPF. Worldwide Harmonized Transient Cycle (WHTC) of EURO VI emission standard is adopted to validate model's transient performance. Meanwhile, impacts of

* Corresponding author. Tel.: +(86) 531 88395623; fax: +(86) 531 88392229.
E-mail address: baishuzhan@sdu.edu.cn (S. Bai).

http://dx.doi.org/10.1016/j.applthermaleng.2016.02.055
1359-4311/

Table 1
Test engine specifications.

Project	Specification
Engine type	6 cylinder in-line/inter-cooling
Bore × stroke/mm × mm	108 × 130
Swept volume/L	7.14
Compression ratio	18
Rated power/kW	200
Rated speed/r/min	2100
Max torque/N·m	1100
EGR type	Electronic control EGR

temperature and NO_2 concentration for the passive regeneration are discussed based on this model.

2. Experimental setup

The engine used in these experiments is equipped with common rail system of BOSCH. Table 1 and Fig. 1 show relating specification and detailed information about test bench, respectively. The experiments were carried out by using Electric dynamometer, Opacimeter, Exhaust gas analyzer, and Precision balance to focus on torque and speed, soot emission, concentration of NOx and O_2, and soot weight in DPF, respectively. The details of these equipments were shown in Table 2.

Exhaust after-treatment system consists of DOC and DPF and Table 3 shows the detailed specification. DPF is equipped with 9 thermocouples, whose diameter is 0.5 mm, to detect the temperature field in the DPF, and Fig. 2 shows the distribution.

3. Model

3.1. Theoretical model

PM in the diesel exhaust is a complex chemical species comprising soot, soluble organic fractions (SOF) and sulfates. The SOF are generally controlled by DOC, whereas the sulfate particles are

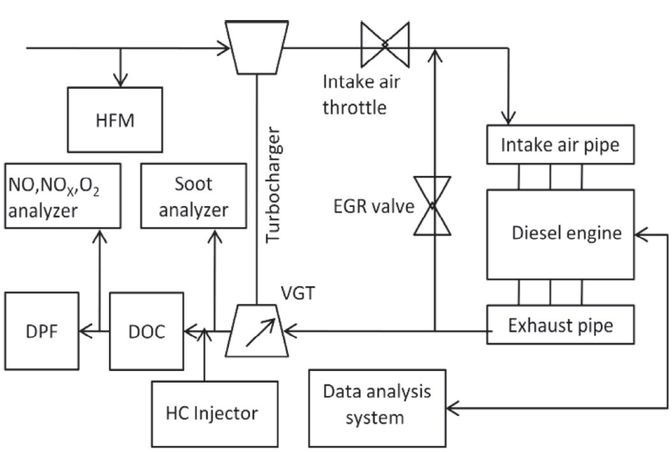

Fig. 1. Schematic of experimental setup.

Table 2
Experimental setup.

Equipment	Model	Manufacturer
Electric dynamometer	INDYS66JD	AVL
Opacimeter	483	AVL
Exhaust gas analyzer	MEXA-7100D	HORIBA
Precision balance	KA32s	METTLER TOLEDO

Table 3
DOC and DPF specification.

Parameter/Unit	DOC	DPF
PGM/g/L	1.06	0.18
Material	Cordierite	Cordierite
Pore/(cell/cm^2)	62	31
Wall thick/mm	0.10	0.32
Diameter/mm	267	267
Length/mm	102	305
Volume/L	5.7	17.0

regulated by the use of Ultra Low Sulfur Diesel (ULSD). Therefore, the main ingredient to be filtered by DPF is soot.

DPF soot loading model contains two sub-modules. Firstly, transient soot emission model is established to calculate actual soot emission which is distinguished from the stable state emission [17]. Then, chemical reaction model of soot and NO_2 is built up, which can calculate the mass of soot oxidation.

3.1.1. Transient soot emission model

Experiment result indicates that soot emission at transient state is different from stable state especially at medium and high load conditions. During the accelerating course in the actual driving, air intake system responds slowly compared with fuel injection system, and excess air coefficient will be reduced resulting in worse combustion and higher soot emission. Decelerating course is against accelerating course.

Excess air coefficient varying at transient state makes soot emission different from stable state at the same operating state. Therefore, transient soot emission can be defined as:

$$M_T = f(M_S, \lambda_S, \lambda_T) \tag{1}$$

where λ_S is the excess air coefficient at stable state; λ_T is the excess air coefficient at transient state; M_S is the soot emission at stable state, mg/s; and M_T is the soot emission at transient state, mg/s.

When the value of λ_S is small, changing its value will make great impact on soot emission. However, when the value of λ_S is relatively big, changing its value will make little effect. In order to identify the λ_S range that soot emission is greatly affected by it, four full-power points and one middle-power point are selected to test, as shown in Fig. 3. By adjusting the EGR valve and throttle valve reasonably, the engine can be considered as running in transient state and M_T under different λ_T can be obtained at the same load point. To ensure enough torque with depressed excess air coefficient, the fuel quantity should be adjusted accordingly.

Fig. 4 shows the relationship between soot emission and excess air coefficient. When $\lambda_S = 1.3$, M_T/M_S is about 25, and M_T/M_S is only about 5 with $\lambda_S = 2$. With this trend, if λ_S continues increasing, the difference between transient and steady soot emission is becoming smaller, so it is reasonable for us to choose the above five points to calculate transient emission including the low load operating range.

Through curve fitting, the above Equation (1) can be rewritten as follows:

$$\frac{M_T}{M_S} = c_0 \cdot e^{\frac{1}{c_1}\frac{\lambda_S}{\lambda_T}} + c_2 \tag{2}$$

where c_0, c_1, c_2 are the relating correction factors.

Fig. 5 shows the soot emission of WHTC cycle. As is observed in the figure, the results show a good correlation of soot emission between the model and test during WHTC cycle. Different λ_S should have different correction factors; for this study we take the average correction factor resulting in smaller simulated value compared to measured value when λ_S is lower than the average value and bigger

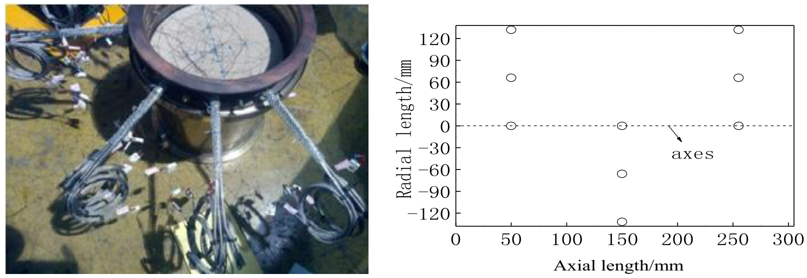

Fig. 2. Thermocouples distribution in DPF.

ones when λ_S is higher than the average value. The average soot emission of measured and calculated is 0.62 mg/s and 0.64 mg/s separately, with only 3.2% error.

3.1.2. Chemical reaction model of soot and NO_2

Fig. 6 shows the NO conversion efficiency of DOC under the space velocity of 50,000 h^{-1}. As can be observed in the figure, at low temperature, NO conversion efficiency is lower, and at high temperature, chemical balance limits the production of NO_2. Hence, the optimal efficiency can be obtained at temperature about 300 °C.

Continuous chemical reaction happens between NO_2 and soot with equations as followed:

$$C + 2NO_2 \rightarrow CO_2 + 2NO \quad (3)$$

$$C + NO_2 \rightarrow CO + NO \quad (4)$$

Some studies [18] indicate that calculation accuracy can be improved by ignoring the reaction (4). Because NO_2 is a strong oxidizer, reaction(4) can only happen with 15% probability. Therefore, the rate of soot oxidation by NO_2 is expressed by chemical reaction kinetics:

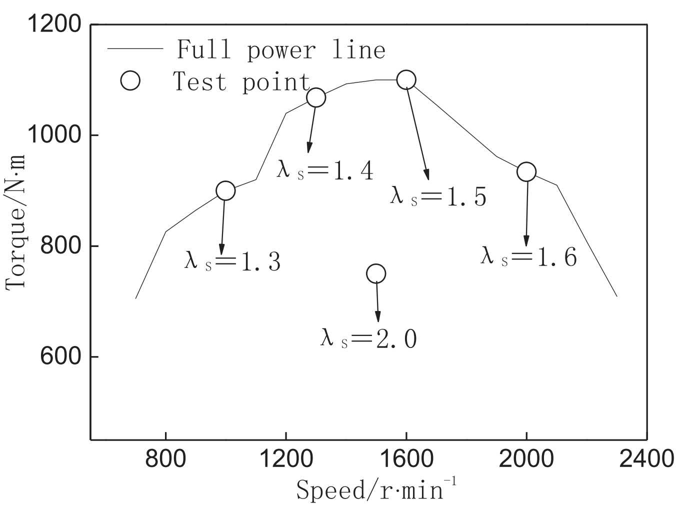

Fig. 3. The test points.

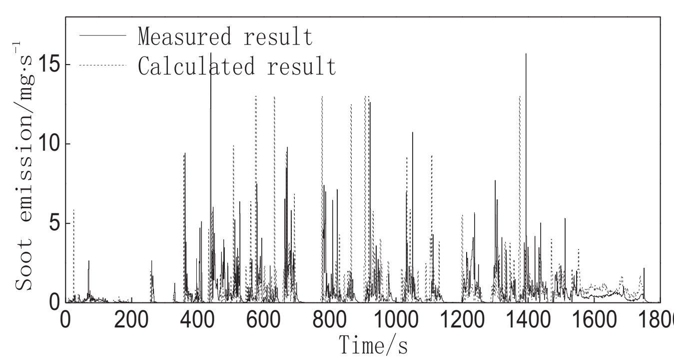

Fig. 5. Soot emission of WHTC cycle.

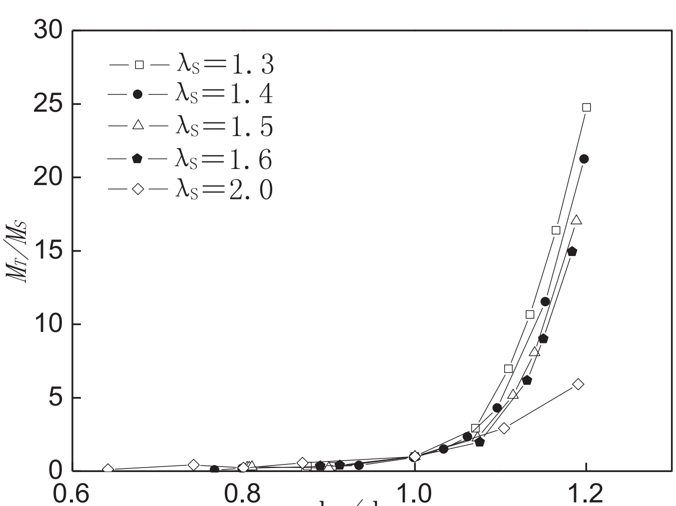

Fig. 4. Soot emission vs. Excess air coefficient.

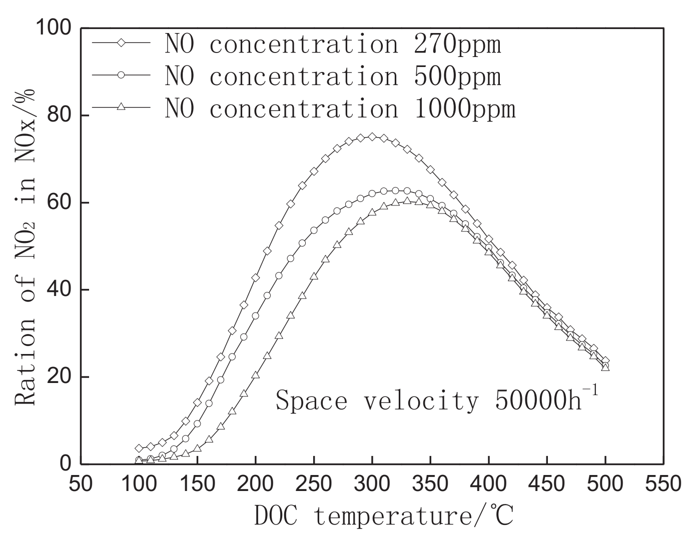

Fig. 6. The conversion efficiency of NO by DOC oxidation.

Table 4
Value of reaction Equation (3) parameter.

Parameter/Unit	Value	Chemical equation
α	1.13	(3)
γ	1	(3)
E_a/(J/mol)	45,500	(3)
A / (1/s)	4200	(3)

$$\frac{1}{m^{\gamma}}\frac{dm}{dt}=kC_{NO_2}^{\alpha} \tag{5}$$

where dm/dt is the rate of soot oxidation by NO_2, mg/s; m is the soot loading, mg; α and γ are the reaction progression; C_{NO_2} is the NO_2 concentration upstream DPF, ppm; and k is the rate constant of reaction(3), 1/s.

NO_2 concentration upstream DPF can be calculated:

$$C_{NO_2}=C_{NO_X}\times\eta \tag{6}$$

where C_{NO_X} is the NO concentration upstream DOC, ppm; η is the NO conversion efficiency by DOC.

Rate constant k is expressed by Arrhenius function:

$$k=Ae^{-E_a/RT} \tag{7}$$

where A and E_a are the pre-exponential factor and the apparent activation energy, respectively. R is the molar gas constant, 8.314 J/(mol·K). T is the temperature in DPF, K.

In the previous study [19], the result shows that O_2 and H_2O can be catalyst for the reaction of NO_2 and soot. While in the actual driving, the O_2 in the exhaust is a little high. In order to get the actual soot reaction rate, the mass of soot oxidation by NO_2 under different temperature is obtained. Then according to Equations (5) and (7), the value of A can be obtained. Considering the common engine operating state and NO_2 distribution in Fig. 6, the value should ensure the veracity of reaction rate when the temperature is between 250 °C and 350 °C. The values are listed in Table 4.

Four steady state points A, B, C and D are selected to verify Equation (5). To minimize the effect of O_2, temperature of selected points is limited up to 400 °C and EGR valve is closed to increase NOx concentration. Before the test of every point, initial soot loading is weighed and recorded. Because the rate of soot oxidation is very slow at low temperature, longer time is needed to monitor the reaction process, which can minimize the error between calculated results and measured results. During the experiment, average temperature of DPF, NO_2 concentration, soot emission and soot loading are recorded in Table 5.

Fig. 7 shows the mass of soot oxidation by NO_2. Errors of four measured points are 10.3%, 4.4%, 4.1%, and 5.4%, respectively. Obviously, the preexponential factor A by the test-bench experiment can correct the reaction rate; the average error is only about 6.1%. During the heating up process of DPF, temperature adopted by calculation is higher than the actual temperature, resulting in higher calculated results.

3.1.3. Chemical reaction model of soot and O_2

The oxidation reaction of soot by O_2 will happen in the appropriate temperature range, with the equation as follows:

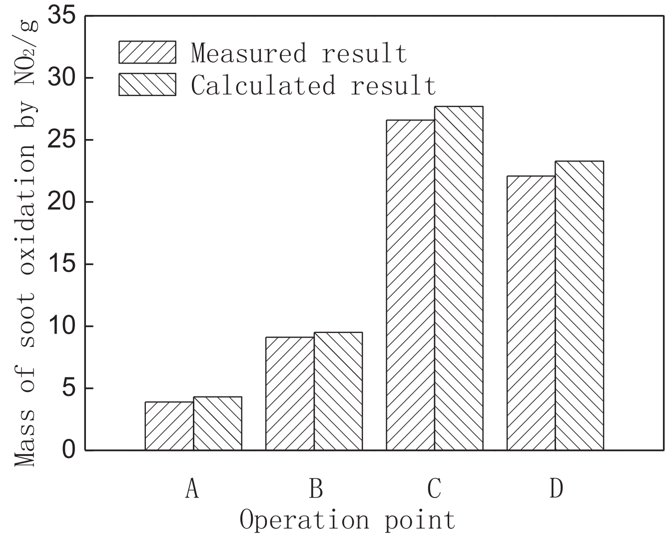

Fig. 7. Comparison of calculated and measured soot oxidation mass by NO_2.

$$C+O_2\rightarrow CO_2 \tag{8}$$

$$2C+O_2\rightarrow 2CO \tag{9}$$

Research shows that the reaction Equation (9) and the effect of O_2 concentration on reaction rate could be ignored because of the higher O_2 concentration in diesel engine exhaust. So the oxidized soot quality during operation of diesel engine could be calculated by the following equation based on the law of mass action:

$$\frac{1}{m^{\gamma}}\frac{dm}{dt}=k \tag{10}$$

in which dm/dt is the derivative of oxidized soot mass to time; γ is the reaction order of Equation (8); k is reaction rate constant of Equation (8).

Reaction order and reaction activation energy were derived from References [14] and [15], the reaction rate constant k is expressed by Arrhenius function, and the pre-exponential factor is obtained by the engine test bench. The values are listed in Table 6.

Four steady state points E, F, G and H are selected to verify Equation (10), the exhaust temperatures of G and H are raised to 550 °C and 600 °C by fuel injection in exhaust and DOC. The soot loading of DPF is 4.0 g/L before experiment, and certain amount of soot should be remained in DPF after the experiment in order to guarantee the rationality of the oxidation test. EGR valve is opened to reduce NOx concentration during the experiment. The results are recorded in Table 7.

The oxidized soot by O_2 of experiment and calculated are showed in Fig. 8 . Errors of four steady state points are 8.3%, 6.3%, 6.5%, and 7.6%, respectively. Obviously, the pre-exponential factor A by the test-bench experiment can correct the reaction rate; the average error is only 7.2%, which is bigger than NO_2 reaction model; the main reason is the difference of temperature value in DPF; temperature

Table 5
Value of main test parameter.

Test point	Speed [r/min]	Torque [N·m]	DPF temp. [°C]	NO_2 concentration [ppm]	Soot emission [mg/s]	Test time [h]	Initial soot [g]	Soot left [g]
A	900	468	250	223	0.2	2.0	69.5	67.1
B	1000	662	300	258	0.2	1.5	71.4	63.4
C	1100	713	350	551	0.2	1.0	72.7	46.8
D	1200	878	400	487	0.3	0.5	70.5	48.9

Table 6
Value of reaction Equation (8) parameter.

Parameter/Unit	Value	Chemical equation
γ	1	(8)
E_a/(J/mol)	408,000	(8)
A / (1/s)	16,000	(8)

adopted by calculation is the average temperature; temperature distribution is uniform in NO_2 reaction experiments, but it is non-uniform at these experiments, in which center is higher at the radial direction, while back-end is higher at the axial direction.

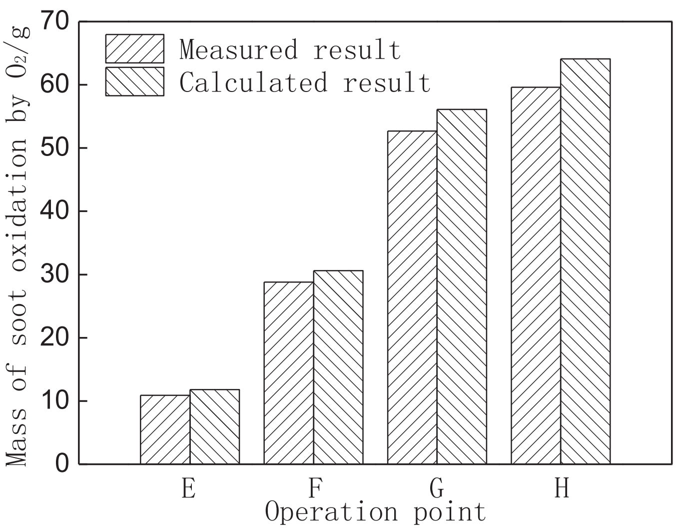

Fig. 8. Comparison of calculated and measured soot oxidation mass by O_2.

3.2. Simulation model

3.2.1. Model established

DPF soot loading model including both transient soot emission and chemical reaction module is established with Simulink. The sampling period is 100 ms, which is the test interval of the test-bench. Fig. 9 shows the main structure of the model and it is used to calculate the soot loading in DPF.

3.2.2. Calculated and measured results

The soot balance of the DPF is defined by the soot entry described by the engine emission model and the soot oxidation depending on the soot loading in the DPF, the gas composition and the exhaust temperature. Fig. 10 shows the soot loading at balance point based on temperature and NO_2 concentration. At low temperature, soot emission does an obvious impact on the balance point, while with temperature increasing up to 250 °C, temperature and NO_2 concentration are becoming more important. Therefore, appropriate temperature and NO_2 concentration are the key points to prolong the active regeneration interval and to realize continuous regeneration.

In order to validate the model accuracy and observe soot loading at balance point, run the WHTC cycle repeatedly. Fig. 11 shows the comparison of calculated (with different boundary conditions during the calculation process) and measured DPF soot loading. Average error between measured and calculated results is about 2.4%, and soot is still accumulating after 50 WHTC cycles with no appearance of balance point. During the WHTC cycle, average exhaust temperature is 238 °C, NO_2 concentration is 213 ppm, and soot emission is 0.64 mg/s. According to Fig. 9, presumed balance point is about 5.6 g/L and the relating calculated result (with single boundary conditions) is 6.2 g/L. But soot loading increases back pressure of the actual engine, resulting in the worse combustion and higher soot emission. Appearance of balance point is delayed by the increased

Table 7
Value of main test parameter.

Test point	Speed [r/min]	Torque [N·m]	DPF temp. [°C]	NO_2 concentration [ppm]	Soot emission [mg/s]	Test time [h]	Initial soot [g]	Soot left [g]
E	1300	976	450	71	0.5	0.2	72.3	59.7
F	1600	1028	500	67	0.6	0.2	71.2	40.2
G	1700	980	550	18	0.6	0.2	70.5	17.6
H	1800	950	600	3	0.6	0.1	74.3	14.8

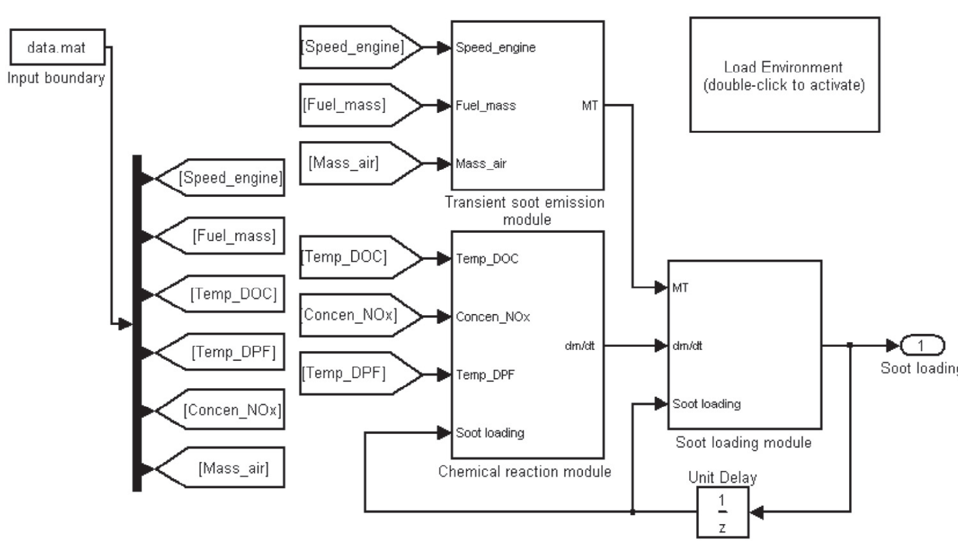

Fig. 9. Simulation model of soot loading in DPF.

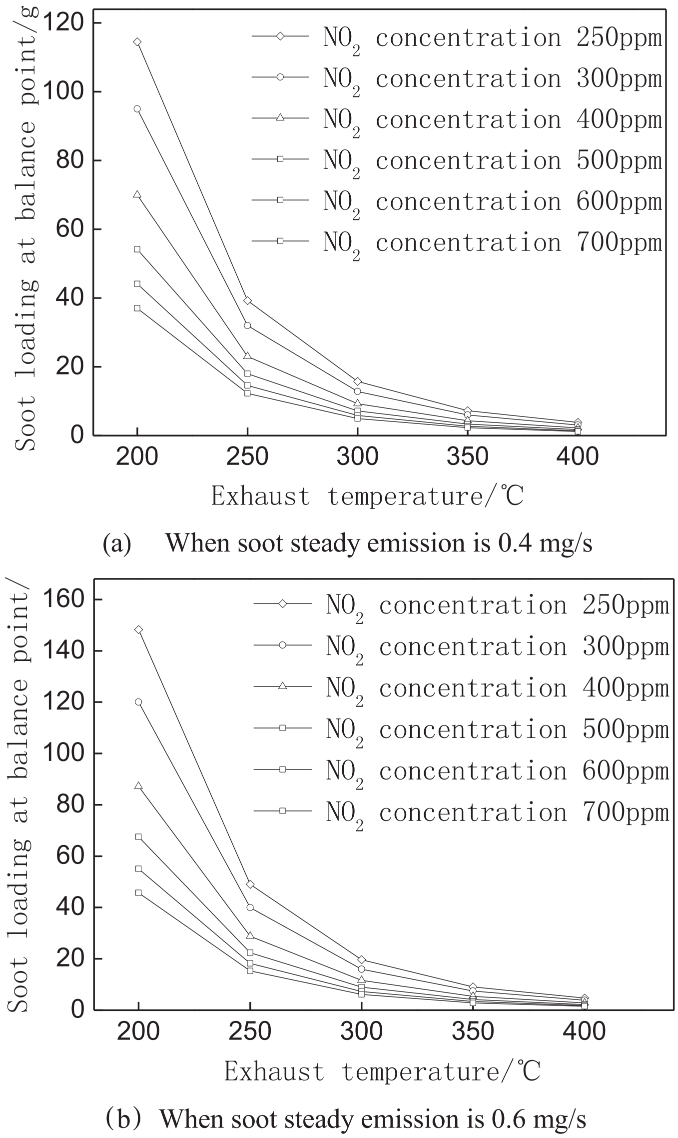

Fig. 10. Soot loading at balance point.

soot emission, and more severely, light off caused by high back pressure may induce no balance point. In conclusion, pure regeneration only occurs when back pressure is low enough, and under which conditions the soot loading can be on a balance of the soot emission and soot oxidation.

4. Engine adjusted and experiments

4.1. Raised exhaust temperature and reduced EGR rate

To insure the back pressure is low enough, the soot loading at balance point is set to about 1.0 g/L. According to Fig. 9, exhaust temperature should be about 280 °C with NO_2 concentration about 300 ppm. Intake air throttle and EGR valve can be used to improve exhaust temperature and NOx concentration. By these measures, average temperature is raised from 238 °C up to 283 °C, NO_2 concentration is increased from 213 ppm up to 289 ppm, and soot emission is decreased from 0.64 mg/s to 0.43 mg/s.

4.2. Results and discussion

Fig. 12 shows the comparison of measured and calculated results of soot loading in DPF. The soot loading increases with more WHTC cycle running. At the beginning soot is loaded fast, but with time passed, it has lowered down until to the balance point. Error between measured and calculated soot loading is small, and when it comes to 100 cycles, the soot loading becomes stable, at which point the soot loading is about 1.27 g/L.

5. Conclusion

This paper describes a new model for the soot loading estimation of DPF based on the balance of engine soot emission and soot oxidation in the DPF as well as measures to enforce the soot oxidation. Below is a summary of our study and the findings:

(1) The soot loading in the DPF can be predicted by the proposed model. During the soot loading process under WHTC cycle, the average error between calculated and measured results is about 3.4%.
(2) Proper exhaust temperature and NO_2 concentration are key points to prolong the interval of active regeneration and realize

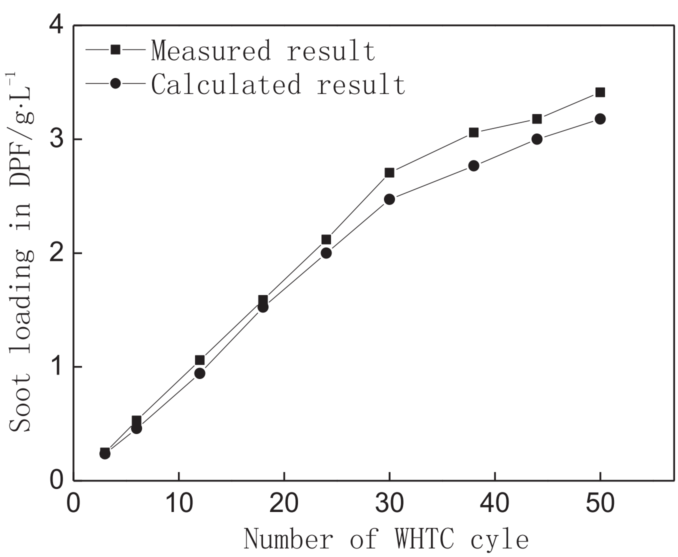

Fig. 11. Comparison of calculated and measured DPF soot loading.

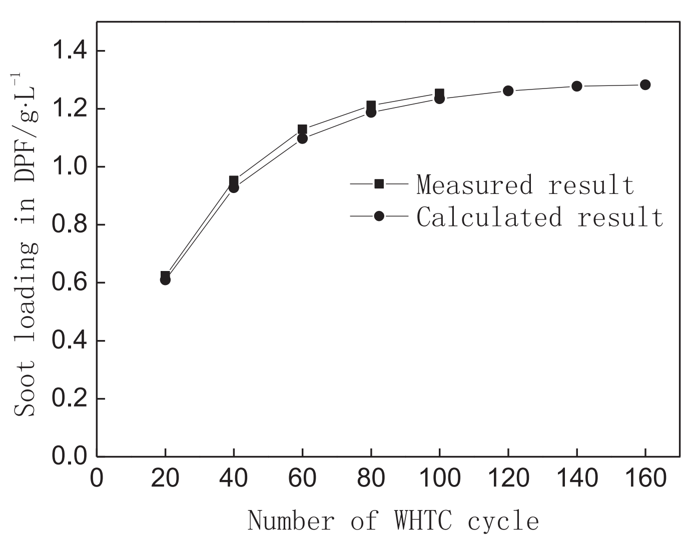

Fig. 12. Comparison of calculated and measured DPF soot loading.

purely passive regeneration. The soot loading at balance point should be controlled at reasonable range, and accordingly, reduce the fluctuation of exhaust temperature, soot emission and NOx emission caused by the soot loading.

Acknowledgements

This work was supported by the National Natural Science Foundation of China (Grant Nos. 51306105, 51576116), the Key R & D projects in Shandong Province (Grant No. 2015GSF117013) and the Fundamental Research Funds of Shandong University (Grant No. 2014QY001). The authors would like to thank the reviews whose constructive and detailed critique contributed to the quality of this paper.

References

[1] T.V. Johnson, Diesel Emission Control in Review. SAE 2009-01-0121, 2009.
[2] T.V. Johnson, Review of Diesel Emissions and Control. SAE 2010-01-0301, 2010.
[3] L.M. Oliveira, Controlling Particulate Matter Emissions in Vehicles Using Different Strategies under the Heavy-Duty Test Cycle. SAE 2012-01-0885, 2012.
[4] A. Mayer, T. Lutz, C. Lammle, M. Wyser, F. Legerer, Engine Intake Throttling for Active Regeneration of Diesel Engine. SAE 2003-01-0381, 2003.
[5] J.R. Warner, D. Dobson, G. Cavataio, A Study of Active and Passive Regeneration Using Laboratory Generated Soot on a Variety of SiC Diesel Particulate Filter Formulations. SAE 2010-01-0533, 2010.
[6] S.-J. Lee, S.-J. Jeong, W.-S. Kim, Numerical design of the diesel particulate filter for optimum thermal performances during regeneration, Appl. Energy 86 (7) (2009) 1124–1135.
[7] A. Kotrba, L. Bai, A. Yetkin, R. Shotwell, T. Gardner, DPF Regeneration Response: Coupling Various DPFs with a Thermal Regeneration Unit to Assess System Behaviors. SAE 2011-01-2200, 2011.
[8] N. Schmidt, T. Root, E. Wirojsakunchai, E. Schroeder, C. Kolodziej, D.E. Foster, et al. Detailed Diesel Exhaust Particulate Characterization and DPF Regeneration Behavior Measurements for Two Different Regeneration Systems. SAE 2007-01-1063, 2007.
[9] T. Kuwahara, S. Nishii, T. Kuroki, M. Okubo, Complete regeneration characteristics of diesel particulate filter using ozone injection, Appl. Energy 111 (2013) 652–656.
[10] P. Chen, J. Wang, Air-fraction modeling for simultaneous Diesel engine NOX and PM emissions control during active DPF regenerations, Appl. Energy 122 (2014) 310–320.
[11] O. Naohisa, N. Tomohiko, D. Shigeki, New Concept Catalyzed DPF for Estimating Soot Loadings from Pressure Drop. SAE 2008-01-0620, 2008.
[12] R. Dominik, B. Thorsten, Different Approaches to Soot Estimation as Key Requirement for DPF Applications. SAE 2009-01-1262, 2009.
[13] S. Nishant, M. Silpa, DPF Soot Estimation Challenges and Mitigation Strategies and Assessment of Available DPF Technologies. SAE 2013-01-0838, 2003.
[14] A. Kotrba, T.P. Gardner, L. Bang, A. Yetkin, Passive Regeneration Response Characteristics of a DPF System. SAE 2013-01-0520, 2013.
[15] H. Bülte, J. Weyers, S. Jerzembeck, H. Zimmerman, A. Qriqra, Monitoring Model for the Soot Load of a CRT System, Aachen Colloquium Automobile and Engine Technology, 2011, Aachen.
[16] R. Allansson, P.G. Blakeman, B.J. Cooper, H. Hess, P.J. Silcock, A.P. Walker, Optimising the Low Temperature Performance and Regeneration Efficiency of the Continuously Regenerating Diesel Particulate Filter(CR-DPF) System. SAE 2002-01-0428, 2002.
[17] K. Boulouchos, P. Kirchen, A phenomenological mean value soot model for transient engine operation [J], MTZ 69 (7) (2008) 58–65.
[18] A. Messerer, R. Niessner, U. Poschl, Comprehensive kinetic characterization of the oxidation and gasification of model and real diesel soot by nitrogen oxides and oxygen under engine exhaust conditions: measurement, Langmuir-Hinshelwood, and Arrhenius parameters [J], Carbon 44 (2006) 307–324.
[19] F. Jacquot, V. Logie, F. Brilhac, Kinetics of the oxidation of carbon black by NO_2 Influence of the presence of water and oxygen [J], Carbon 40 (2002) 335–343.