공학석사학위논문

접근성 높은 변수 기반의 디젤 차량 실도로 주행 질소산화물 제어를 위한 희박 질소산화물 트랩의 효율 예측

Prediction of Lean NOx Trap Efficiency by Using Accessible Parameters for Controlling Real Driving NOx Emissions in Diesel Vehicles

2020 년 2 월

서울대학교 대학원

기계항공공학부

현 재 우

Abstract

Prediction of Lean NOx Trap Efficiency by Using Accessible Parameters for Controlling Real Driving NOx Emissions in Diesel Vehicles

Jaewoo Hyun

Department of Mechanical & Aerospace Engineering

College of Engineering

Seoul National University

In Korea, Euro 6D-TEMP has been applied since September 2019, which includes the Real Driving Emission(RDE) tests. Unlike conventional emissions-measurement conducted in chassis dynamometer, the actual road measurement can be very high depending on outside temperature, drivers' tendency, and road conditions. Therefore, in terms of after-treatment system that reduces vehicle emissions, not only the specifications of the after-treatment device itself such as the purification efficiency according to temperature, but also the engine operating

condition control method for the after-treatment device to work well are very important. In case of diesel vehicles, Lean NOx Trap(LNT) and Selective Catalytic Reduction(SCR) are used as after-treatment devices to deoxidize nitrogen oxides(NOx), but because real road driving considers driver's tendency and traffic conditions, the operating temperature of after-treatment devices can't always be satisfied. In particular, the SCR does not operate in the beginning or the long stop section, so only LNT reduces NOx, and the RDE data showed that the NOx emissions in this section accounted for 40% of the total NOx emission. That is, in real road driving, the change in the efficiency of LNT has a big influence on the NOx emission. Therefore, in this paper, LNT efficiency is predicted with as few and accessible variables as possible such as Onboard Diagnostics(OBD), so that it can be used in emission control methods applicable to real driving. The effect of concentration and flow rate of NOx and oxygen at LNT inlet is first considered to model LNT efficiency. Then the temperature at LNT inlet as a parameter is included which can affect LNT by two separate ways. Finally, in that degradation cause the change of temperature difference through LNT, change of NOx in mole fraction can be expressed by the total change of temperature and heat convection, substituted in the form of LNT efficiency. Therefore, the entire model is developed, and then the undefined coefficients were fitted by least squares method. The result indicated that the correlation of the

measured data and the model is 0.80898, and the tendency of the prediction model matched well shown in the last figure.

Keywords: Euro 6D, RDE, NOx, after-treatment, Diesel vehicles, LNT, OBD

Student Number: 2018-26825

List of Tables

List of Figures

Nomenclature

A	pre-exponential factor
c	ratio of NO_2 in NOx by mass
c'	ratio of NO in NOx by mole
c_h	specific heat
C_h	heat capacity
EFF	effect
E_a	activation energy
f	Maxwell-Boltzmann distribution
F	cumulative Maxwell-Boltzmann distribution
$\triangle h$	enthalpy difference
k	Boltzmann constant
k_r	reaction rate constant
R	universal gas constant
m	mass of a molecule
m_1	exponent of NO
m_2	exponent of O_2
$\dot{m}$	mass flow rate (g/s)
M	molecular weight
n	number of moles
r	reaction rate (M/s)
T	gas temperature (K)
$\mathrm{v}_{\lim}$	maximum speed of molecule possible to adsorb
x	mole fraction

Greek symbols

α	1st fitting coefficient
β	2nd fitting coefficient
γ	3rd fitting coefficient
δ	4th fitting coefficient
ϵ	5th fitting coefficient
ζ	6th fitting coefficient
η	7th fitting coefficient
θ	8th fitting coefficient
κ	non-dimensional reaction rate coefficient
λ	9th fitting coefficient
μ	10th fitting coefficient

Subscripts

avg	average
CF	concentration and flow rate considered
D	degradation considered
exh	exhaust gas
i	LNT inlet
o	LNT outlet
reac	reaction
red	reduced
R_2	reaction 2.2
s	surface
tran	heat transfer
T	temperature considered

Notation

[X]	molar concentration of the X species (mol/cm^3)
$\triangle X$	(X at LNT outlet) - (X at LNT inlet)

1. Introduction

1.1. Research background

Emission measurement methods for vehicles are becoming more complex.[1] The indoor measurement method has now shifted from the New European Driving Cycle(NEDC) to the Worldwide Harmonized Light-duty Vehicles Test Cycle(WLTC), which consists of relatively more acceleration and more realistic than the old one as can be seen in Fig. 1.1. In the case of diesel cars, the generation of NOx is high due to the characteristics of compression ignition(CI), and it is essential to reduce NOx emissions.[2] As the emission measurement changed to RDE, the role of the after-treatment in diesel vehicles became more important.[3] However, since RDE includes a wide operating range, there are some sections in which the efficiency of the after-treatment mainly using catalytic reaction is low or the device does not work at all.[4] Therefore, it can be said that it is effective to increase the efficiency of the after-treatment device in such sections in order to satisfy the NOx emission regulations.

Widely used after-treatment units for reducing NOx in diesel vehicles are LNT and SCR. LNT serves to reduce NOx by adsorption and SCR deoxidize NOx by urea. For LNT, regeneration is necessary when NOx is adsorbed so much that available sites of LNT are insufficient, because the efficiency of the LNT could be lowered. In the period of regeneration, the engine conducts rich combustion, which produces reducing agents such as Carbon Oxide or Unburned Hydrocarbon. LNT generally operates over a wide temperature range, but overall purification efficiency is lower than SCR. In SCR, the injected urea water is decomposed into ammonia to reduce nitrogen oxides. However, since the minimum temperature for this reaction is around 160 degrees Celsius, urea is not discharged below this temperature that could cause worse emission characteristics due to not reacting ammonia. Despite these shortcomings, the SCR shows high purification efficiency once it is operated. In particular, in the case of high-speed driving, the amount of emitted NOx is very small even though a large amount of NOx is generated from the engine.

Diesel vehicles with LNT and SCR tend to have lower NOx emissions, but vary significantly with emission measurement cycles. Since both devices are based on catalytic reactions, the efficiency is lower than that in the optimum temperature conditions, and the temperature of the catalyst section and the amount of NOx produced in the engine also vary depending on the operating conditions. Therefore, the NOx control method used to satisfy emission regulations before when RDE is applied is not well suited to RDE.

In terms of RDE, the most effective method of controlling NOx is to create conditions for improving the purification efficiency of LNT or SCR.

Using existing LNT and SCR, and controlling them to meet the conditions under which LNT and SCR work well, can have a good effect on the cost and final emissions of the after-treatment unit. However, because LNT and SCR have different operating ranges, consideration of final NOx emission is needed.[5] What's important is that SCR is very efficient above a certain temperature and has the ability to meet Euro 6D-TEMP criteria, but in the section where SCR does not operate and only LNT operates, in some cases, NOx emission exceeds Euro 6D-TEMP criterion significantly. Therefore, controlling LNT is a key solution in reducing final NOx emissions.

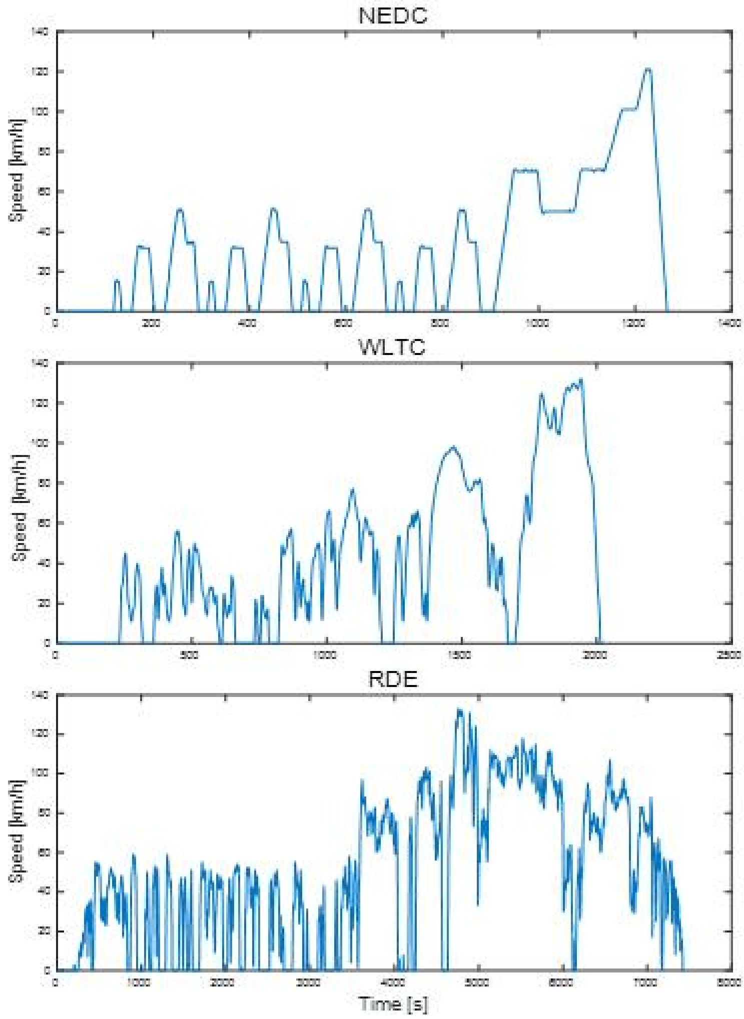

Fig. 1.1. Comparison of NEDC, WLTC, and RDE by speed variation

1.2. Previous researches

Wang et al. simplified the chemical reactions in LNT and predicted the amount of subsequent NOx by distinguishing between lean and rich conditions.[6] However, the flow rate of CO is required to calculate the amount of outlet NOx in this report. In reality, not only CO, but also reducing agents such as HC or hydrogen could affect the reaction of NOx. In addition, to know the flow rate of CO, predictions about combustion products in the engine must be accomplished or sensors must be attached to the front of the LNT. However, predicting CO in an RDE with a wide variety of operating points can be inaccurate, and the CO sensor is typically not used as an OBD, which adds a new kind of sensor.

Ratts et al. conducted chemical reaction modeling that was slightly more detailed than Wang et al.[7] As a result, they have verified the distinction between nitrogen monoxide and nitrogen dioxide and the temperature change depending on the location within the LNT, but there is no discussion of the emission of NOx when RDE conditions are applied. In addition, there is a disadvantage that it is difficult to be applied at real-time emission control, because most variables used in the result are not the values of OBD sensors equipped in vehicles.

In Yang et al., a study on the adsorption of NOx in LNT by nonlinear autoregressive exogenous(NARX) is presented.[8] The NARX technique derives the result from a lot of data, so the accuracy is high, but it requires a lot of input data and requires excessive learning time. In addition, since the physical meaning of each input cannot be interpreted, it may be limited to be applied to various vehicles.

1.3. Research subjects

In this paper, easy-to-get data is used as input for modeling LNT. The OBD sensor values, which are widely used, are selected mainly, and additional sensor installations are minimized, but descriptions are included if necessary. And when applied to NOx control in real driving, the calculation time could be short enough to reduce NOx emissions in real time.

2. After-treatment system

Fig. 2.1 shows the typical after-treatment system of diesel vehicles. The exhaust gas first pass LNT, then DPF, and finally SCR with NOx and PM being reduced.[9]

2.1. LNT

As can be seen in Fig. 2.1, LNT plays an crucial role in terms of absolute value of NOx reduction because it directly accepts NOx generated from the engine. Additionally, efficiency of LNT itself equals the efficiency of the whole NOx after-treatment system in the period that SCR operating condition is not satisfied.

2.1.1. LNT reactions

Catalytic chemical reaction that occur in LNT can be divided into 2 steps as seen in Fig. 2.2. The first step is that nitrogen monoxide is oxidized to nitrogen dioxide and the second step is that nitrogen dioxide is stored in adsorber. Reaction. 2.1 and 2.2 correspond to the first and the second step each.[10]

$$2NO + O_2 \rightarrow 2NO_2 \qquad (2.1)$$

$$2NO_2 + BaCO_3 + \frac{1}{2}O_2 \rightarrow Ba(NO_3)_2 + CO_2 \qquad (2.2)$$

The activation energy of Reaction. 2.1 and 2.2 is around 82 kJ/mol and 5 kJ/mol each, which means that Reaction. 2.1 is the weight limiting factor of LNT kinetics.

2.1.2. LNT capacity

The number of available sites at the wall of LNT increases that causes less adsorption of NOx because former NOx is stored in adsorbers in LNT as can be seen in Fig. 2.3.[11] Although empty sites are created through regeneration process, capacity must be considered for modeling of LNT because degradation of LNT can occur as time passes before regeneration.

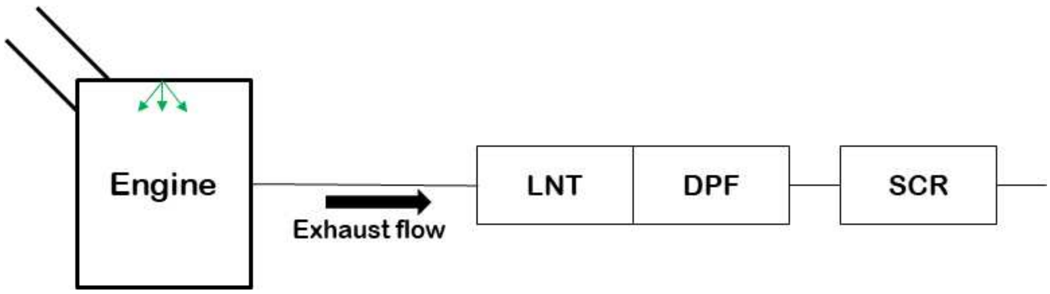

Fig. 2.1. Typical after-treatment system of diesel vehicles

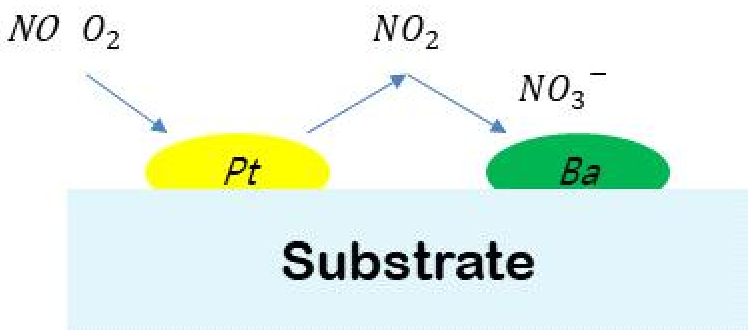

Fig. 2.2. Chemical schematic at LNT

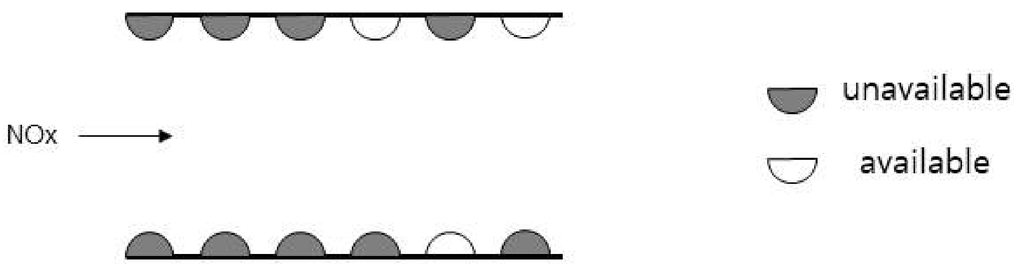

Fig. 2.3. Empty and filled LNT sites

3. Methodology

The descriptions of the target vehicle is shown in Table. 3.1. Fig. 3.1 shows simple schematic of LNT operation with parameters used in the LNT modeling. Temperature of LNT inlet and outlet(T_i and T_o), and NOx flow rate of LNT outlet($\dot{m}_{NOx,o}$) is measured by OBD sensors in frequency of 10 Hz. On the other hand, NOx flow rate and oxygen fraction of LNT inlet($\dot{m}_{NOx,i}$ and $x_{O_2,i}$) is measured by additional sensors with 10 Hz, because the target vehicle does not have these kinds of sensors. Whole sensors employed in this research in the after-treatment system is represented in Fig. 3.2. The driving cycle is RDE around Seoul.

3.1. Reaction rate

To predict $\dot{m}_{NOx,o}$, Reaction. 2.1 and 2.2 must be considered. In the whole reaction, the amount of $\dot{m}_{NOx,i}$ enters LNT, and some of NOx are adsorbed in it, the amount of $\dot{m}_{NOx,o}$ comes out. So the amount of $\dot{m}_{NOx,i}$ and mass flow rate of adsorbed NOx are need to predict $\dot{m}_{NOx,o}$.[2]

Table 3.1. Target vehicle description

Engine Type	Diesel R2.0 e-VGT
Fuel Type	Diesel
Displacement Volume(cc)	1,995
Max Power(ps/rpm)	186/4,000
Max Torque(kg·m/rpm)	41/1,750～2,750
Combined Fuel Economy(km/L)	13.8
City Fuel Economy(km/L)	12.7
Highway Fuel Economy(km/L)	15.4

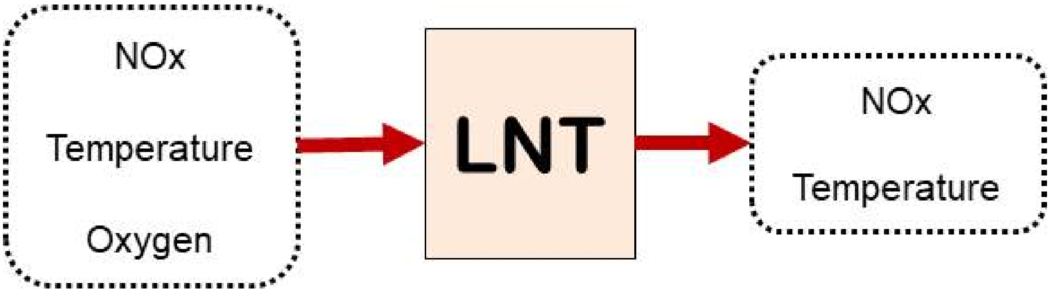

Fig 3.1. Schematic of LNT for modeling

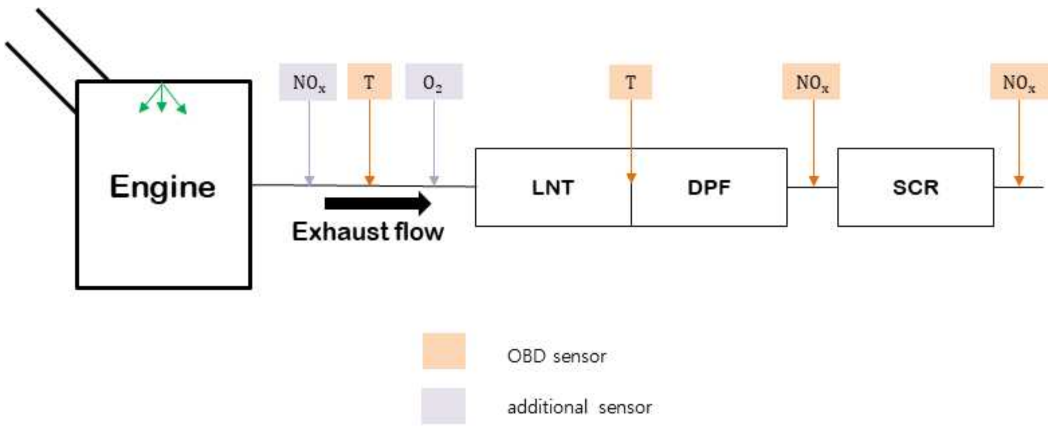

Fig 3.2. Equipped sensors in the after-treatment system

3.1.1. Concentration & Flow rate

$\dot{m}_{N,i}$ is measured by the additional NOx sensor at LNT inlet, but mass flow rate of adsorbed NOx need to be calculated. To do this, the reaction rate of Reaction. 2.1 is come up and indicated below.

$$r_1 = k_1 [NO]^{m_1} [O_2]^{m_2} \qquad (3.1)$$

The mass flow rate of reduced NO can be expressed as Eqn. 3.2 referring to Eqn. 3.1 with non-dimensional coefficient κ.

$$\dot{m}_{NO,red} = \kappa \times \dot{m}_{exh} \, x_{NO}^{m_1} x_{O_2}^{m_2} \qquad (3.2)$$

Comparing Reaction. 2.1 and 2.2, Reaction. 2.2 occurs more easily due to its activation energy. So an assumption that all NO_2 are adsorbed at LNT is applied without considering the effect of temperature. Another assumption is that the ratio of NO and NO_2 is constant with the value of $\dot{m}_{NO_2,i} / \dot{m}_{NOx,i} = c$ and $x_{NO,i} / x_{NOx,i} = c'$. Mass flow rate of exhaust gas is measure by an OBD sensor, is measured by an OBD sensor. Considering these assumptions and Eqn. 3.2, the total reduced mass flow rate of NOx can be indicated by Eqn. 3.3.[10]

$$\dot{m}_{NOx,red} = \dot{m}_{NO,red} + \dot{m}_{NO_2,red} = (\kappa \times c'^m) \times \dot{m}_{exh}\, x_{NOx}^{m_1}\, x_{O_2}^{m_2} + c \times \dot{m}_{NOx,i} \qquad (3.3)$$

Therefore, mass flow rate of NOx at LNT outlet is expressed by

$$\dot{m}_{NOx,o} = (1-c) \times \dot{m}_{NOx,i} - (\kappa \times c'^m) \times \dot{m}_{exh}\, x_{NOx}^{m_1}\, x_{O_2}^{m_2} \qquad (3.4)$$

Eqn. 3.4 shows that a constant ratio of NO_2 among NOx is eliminated, and reduced NO is proportional to $\dot{m}_{exh}$, $x_{NOx}^{m_1}$, and $x_{O_2}^{m_2}$. For fitting the predicted value to the experimental data, Eqn. 3.4 is written as Eqn. 3.5 with undefined coefficients of $\alpha, \beta, \gamma, \delta$.

$$\dot{m}_{NOx,o,CF} = \alpha \times \dot{m}_{NOx,i} - \beta \times \dot{m}_{exh}\, x_{NOx}^{\gamma}\, x_{O_2}^{\delta} \qquad (3.5)$$

3.1.2. Temperature

At low temperature where chemical reaction rate is not fast enough, NOx reduction increases as temperature increases. However there is difference between the temperature of reaction site and exhaust gas due to transience. Nevertheless, the assumption about temperature is that the temperature of exhaust gas can represent the whole reaction. By following the Arrhenius equation, the reaction rate constant is the form of $Ae^{-\frac{E_a}{RT}}$, where A is the pre-exponential factor, E_a is the activation energy for the reaction and R is the universal gas constant. The other effect of temperature is the speed of molecular when adsorbing like Fig. 3.3. If temperature is so high that the molecular speed exceeds a certain limit, NOx don't adsorb but bounce-off rather. Maxwell-Boltzmann distribution is applied to represent the adsorbing probability, shown on Fig. 3.4. When the gas temperature is set, the probability density function and the cumulative function are expressed as Eqn. 3.6 and 3.7 each.[12]

$$f_T(v) = \sqrt{\frac{2}{\pi}}\frac{v^2 e^{-\frac{v^2}{2a^2}}}{a^3} \qquad (3.6)$$

$$F_T(v) = erf\left(\frac{v}{\sqrt{2}\,a}\right) - \frac{ve^{-\frac{v^2}{2a^2}}}{a}\sqrt{\frac{2}{\pi}} \qquad (3.7)$$

a is $\sqrt{\frac{kT}{m}}$ with k is the Boltzmann constant and m is the mass of a molecule. The area where the speed of molecule is lower than $v_{\lim}$ can be proportional to $\dot{m}_{NOx,red}$ and the value of it is $F_T(v_{\lim})$. Therefore, effect of temperature on the reduced mass flow rate of NOx is represented in Eqn. 3.7, that should be multiplied by Eqn. 3.5.

$$EFF_T = \epsilon \times (1 - F_{T_i}(\zeta)) + \eta \times e^{\frac{\theta}{T_i}} \qquad (3.8)$$

Eqn. 3.8 is gained by summing dominating phenomenon of temperature weighted by undefined coefficients of ϵ and η. ζ indicates the factor of $v_{\lim}$ and θ indicates the factor of $-\frac{E_a}{R}$, but all of these coefficients must be fitted by experimental data. The only variable at Eqn. 3.8 is the inlet temperature and it is measured by an OBD sensor.

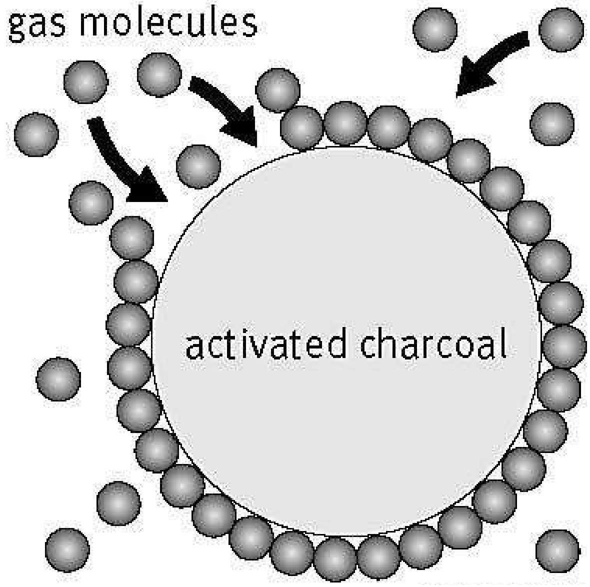

Fig. 3.3. Adsorption of gas molecules

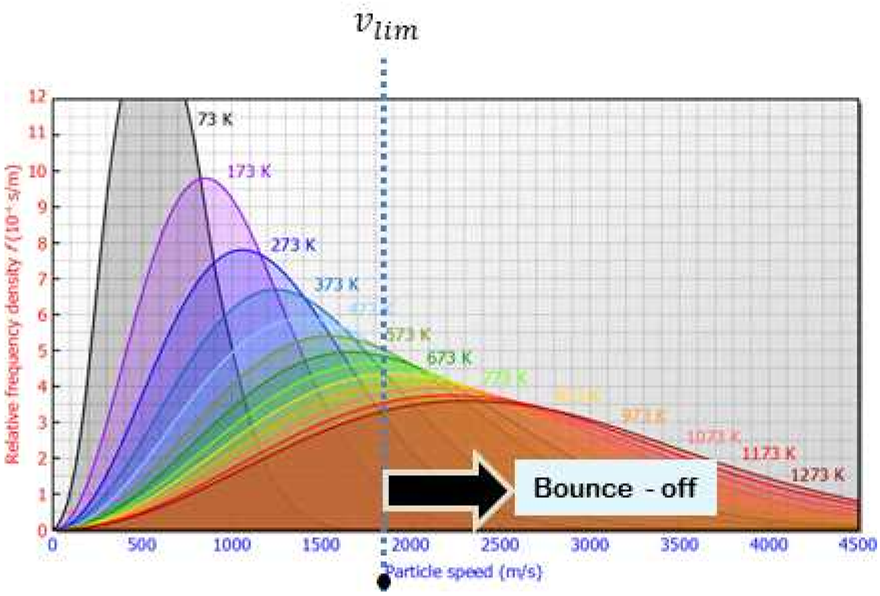

Fig. 3.4. Maxwell-Boltzmann distribution and bounce-off speed

3.2. Degradation

To consider the degradation of LNT, temperature change through LNT has been analyzed first. It can be divided as Eqn. 3.9.

$$\triangle T = \triangle T_{reac} + \triangle T_{tran} \qquad (3.9)$$

Temperature change by reaction occurs by the enthalpy difference of reactants and products. Comparing Reaction. 2.1 and 2.2, enthalpy difference of the latter is larger by about an order, and they are both exothermic. It means that chemical reaction at LNT cause temperature rise with adsorption step dominant. Eqn. 3.10 indicates the temperature difference.

$$\triangle T_{reac} = \frac{\triangle h_{R_2} \times \triangle n_{NOx}}{C} = \frac{\triangle h_{R_2} \times \triangle \frac{\dot{m}_{NOx}}{M_{NOx}}}{c \times \dot{m}_{exh}} = \frac{\frac{\triangle h_{R_2}}{M_{NOx}}}{c} \times \triangle x_{NOx} \qquad (3.10)$$

$\triangle h_{R_2}$ is the enthalpy difference of Reaction. 2.2, $\triangle n_{NOx}$ is the difference of the number of mole of NOx, C_h is the heat capacity, M_{NOx} is the molecular weight of NOx, c_h is the specific heat. $\triangle T_{reac}$ seems to be proportional to $\triangle x_{NOx}$ because other values are constant. Mole fraction of NOx at LNT inlet and outlet are measured by an additional sensor and

OBD sensor.

$\triangle T_{tran}$ occurs by heat transfer, especially convection, due to the transiency of gas temperature, which causes the difference of temperature of exhaust gas and LNT wall. Convection heat transfer is proportional to $T - T_s$, and this energy contribute to the decrease of gas temperature. Therefore it can be written as Eqn. 3.11 considering thermal capacity where T_{avg} is the average of T_i and T_o, and T_s is the surface temperature assumed to be constant with the value of 537.68 K in the experimental data.

$$\triangle T_{tran} \propto \frac{T_{avg} - T_s}{\dot{m}_{exh}} \qquad (3.11)$$

As a result of Eqn. 3.9, 3.10, and 3.11, the total temperature difference can be expressed including $\triangle x_{NOx}$. To acquire EFF_D to be multiplied to Eqn. 3.5 together with EFF_T, Eqn. 3.12 is needed.[13]

$$\frac{\dot{m}_{NOx,o}}{\dot{m}_{NOx,i}} = \frac{x_{NOx,o}}{x_{NOx,i}} = 1 + \frac{\triangle x_{NOx}}{x_{NOx,i}} \qquad (3.12)$$

By combining Eqn. 3.9, 3.10, 3.11, and 3.12, EFF_D is shown below.

$$EFF_D = 1 + \frac{\lambda \times \triangle T + \mu \times \frac{T_{avg} - 537.68}{\dot{m}_{exh}}}{x_{NOx,i}} \qquad (3.13)$$

Temperature of LNT inlet and outlet, mass flow rate of exhaust gas, and mole fraction of NOx at LNT inlet are measured by OBD sensors and additional sensors.

3.3 Entire model and validation method

The entire model considering both concentration, flow rate, temperature, and degradation is expressed in Eqn. 3.14.

$$\dot{m}_{NOx,o} = \dot{m}_{NOx,o,CF} \times EFF_T \times EFF_D \qquad (3.14)$$

To explain in detail, $\dot{m}_{NOx,o,CF}$ is the predicted flow rate of NOx at LNT outlet when only concentration and flow rate are considered. EFF_T and EFF_D are factors to include the effect of temperature and degradation, so multiplying $\dot{m}_{NOx,o,CF}$, EFF_T, and EFF_D is the final prediction model of LNT.

All coefficients – $\alpha, \beta, \gamma, \delta, \epsilon, \zeta, \eta, \theta, \lambda, \mu$ – have been fitted by method of least squares. Other parameters are measured by OBD sensors and additional sensors. The validation and calibration is done by limiting the coefficients to be appropriate value, and the coefficients were multiplied by proper number to reduce the calculation time.

4. Result and Discussion

In this section, final fitted result of Eqn. 3.14 is introduced which can be used to predict the flow rate of NOx at LNT outlet. The model of which correlation is 0.80898 is shown in Fig. 4.1 together with the measured data. Additionally the comparison of the model and the measured data is indicated in Fig. 4.2, more useful to estimate the tendency of the result.
At the region of low value of the measured data, the prediction doesn't match well comparing to that of high value of the measured data in Fig. 4.1. The more high the measured data, the more accurate the model. However some path deviate the prediction result at the point of high measured value. In Fig. 4.2, in the points of high NOx value, the model predicted relatively lower than the measured data, but the tendency of the model well matches with the measured data.[7]

Recalling that this model is created to reduce NOx emissions, by controlling LNT inlet condition to elevate the efficiency of LNT, points inside the black dotted circle in Fig. 4.1 is not that important. However, if the real value is low but the model predicts significantly high, the control will severely proceed to increase the efficiency that could lead to worse emission rather. Or in the case that the real value is so high that NOx control is necessary but the model doesn't notice, large amount of NOx emission can occur instantly. In this perspective, the developed model in this research can be applicable in control method of reducing NOx emission, despite the discrepancy at points inside the black dotted circle in Fig. 4.1.

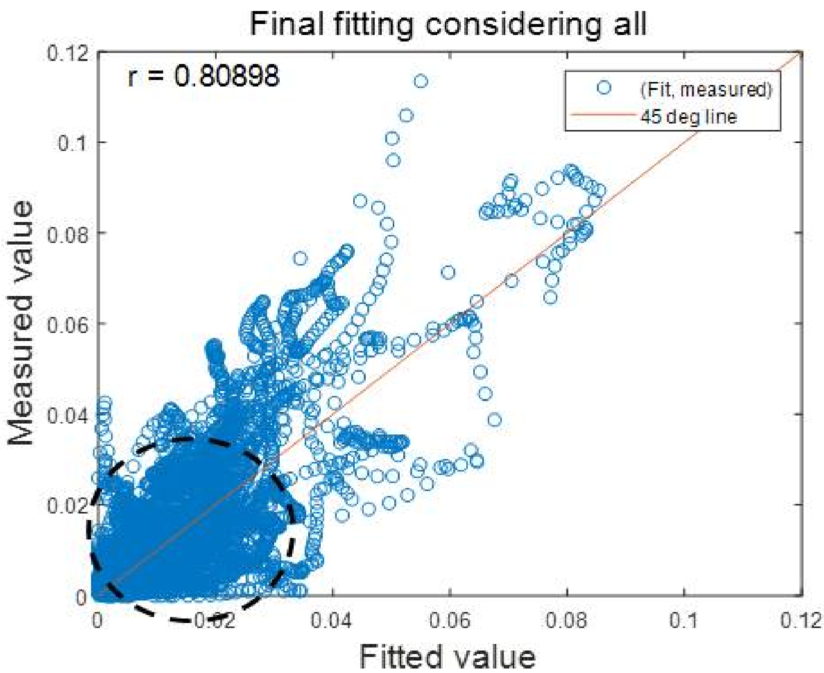

Fig. 4.1. Final prediction result and the measured data

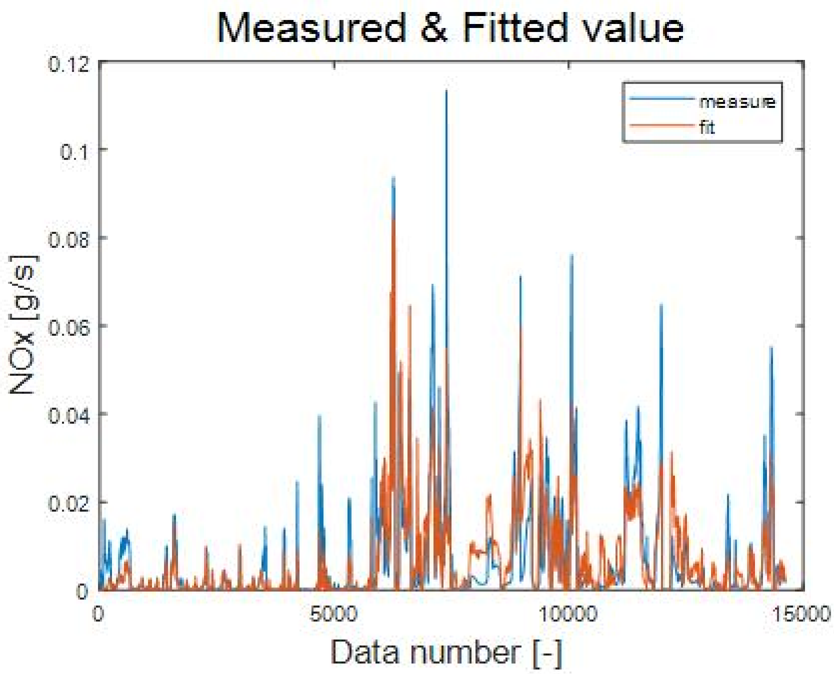

Fig. 4.2. Comparison of the model and the measured data by data number

5. Conclusion

Predicting LNT operation is completed in this research by several physical models and validated by the values of OBD and additional sensors in real driving situation. First, adsorption process is analyzed by two simple reaction steps. Because the step of NO_2 adsorption arise easily, NO oxidation rate is calculated by the concentrations of species and the flow rate of NOx. Second, the effect of temperature is considered because temperature can cause the reaction rate of NO oxidation and NO_2 adsorption to be changed. If temperature is too low, overall reaction rate is low due to deficiency of molecular energy. On the opposite condition, molecular speed can be too high to adsorb, rather molecules bounce off the adsorbers. So these two effects are considered and the factor of EFF_T is presented. Lastly, since the number of available sites decreases as time passes before regeneration process called degradation in this research, LNT operation could be poorer. The temperature difference through LNT is thought to be result of this phenomena. It is devided as two : changes due to exothermic reaction and convective heat transfer. Because the change of NOx mole fraction is the parameter in temperature difference by chemical reaction, summing two temperature changes is useful when the change of NOx mole fraction is expressed another way. This result is substituted to the efficiency of LNT that could led to EFF_D. Therefore the final model has been developed by multiplying flow rate of NOx at

LNT outlet with considering only concentration and inlet flow rate, EFF_T, and EFF_D. The undefined coefficients are derived with limiting the values to be appropriate.

The correlation of the model is 0.80898, and the tendency of result matched well with the measured data. But the prediction is not that correct if the real value is relatively low. Nevertheless in that this model is developed to be applied to control the LNT inlet condition for NOx reduction, that range of NOx value is not that critical, since predicting well when the real value is high is more effective to reduce NOx emission. In this perspective, fitting the model to the influential measured data rather than entire measured data can be more applicable to NOx emission control.

References

1. Timothy V. John, 2015, Review of Vehicular Emissions Trends, SAE Int. J. Engines, 8, pp. 1152-1167.

2. Charlton, S., 2015, Developing Diesel Engines to Meet Ultra-low Emission Standards, SAE Technical Paper, 2005-01-3628.

3. Marek Vaclavik, Vladimir Novak, Jan Brezina, Petr Koci, Gregory Gregori, David Thompsett, 2016, Effect of diffusion limitation on the performance of multi-layer oxidation and lean NOx trap catalysts, Catalysis Today, vol. 273, pp. 112-120.

4. Bastian Holderbaum, Michael Kind, Christoph Menne, Thomas Wittka, Giovanni Vagnoni MSc, Dirk Bosteels MSc, MBA, Cecile Favre, John BSc, 2015, Potential for Euro 6 Passenger Cars with SCR to meet RDE Requirements, Internationales Wiener Motorensymposium.

5. Cha-Lee Myung, Wonwook Jang, Sangil Kwon, Jinyoung Ko, Dongyoung Jin, Simsoo Park, 2017, Evaluation of the real-time de-NOx performance characteristics of a LNT-equipped Euro-6 diesel passenger car with various vehicle emissions certification cycles, Energy, 132, pp. 356-369.

6. Yanying Wang, S. Raman, J.W. Grizzle, 1999, Dynamic modeling of a lean NOx trap for lean burn engine control, Proceedings of the 1999 American Control Conference.

7. L. Cao, J.L. Ratts, A. Yezerets, N.W. Currier, J.M. Caruthers, F.H. Ribeiro, W.N. Delgass, 2008, Kinetic Modeling of NOx Storage/Reduction on Pt/BaO/Al2O3 Monolith Catalysts, Industrial & Engineering Chemistry Research, 47, pp. 9006-9017.

8. Yang. H., 2010, LNT NOx Storage Modeling and Estimation via NARX, SAE Technical Paper, 2010-01-1937.

9. James Edward McCarthy, Erik Dykes, Evan Ngan, Vadim O. Strots, 2010, Aftertreatment System Performance of a Fuel Reformer, LNT and SCR System Meeting EPA 2010 Emissions Standards on a Heavy-Duty Vehicle, SAE Int. J. Commer. Veh, 3, pp. 130-142.

10. David Marie-Luce, Damiano Di-penta, Pierre-Alexandre Bliman, Michel Sorine, 2011, Control-Oriented Modeling of a LNT-SCR Diesel After-Treatment Architecture, SAE Int. J. Engines, 4, pp. 1764-1775.

11. Maurer, M., Fortner, T., Holler, P., Zarl, S., & Eichlseder, H., 2017, Impact of phosphorus on a conventional lean NOx trap for Diesel cars, Internationales Stuttgarter Symposium in 17, pp. 1183-1201.

12. Charlton, S., 2015, Developing Diesel Engines to Meet Ultra-low Emission Standards, SAE Technical Paper, 2005-01-3628.

13. Zhen-yu Zhang, Yan-ten Lu, Horia Metiu, 1991, Adsorption and diffusion sites of a Si atom on a reconstructed Si(100)-(2×1) surface, Surface Science, 248, pp. 250-254.

요약

접근성 높은 변수 기반의 디젤 차량 실도로 주행 질소산화물 제어를 위한 희박 질소산화물 트랩의 효율 예측

서울대학교 대학원
기계항공공학부
현재우

대한민국에서는 2019년 9월부터 Euro 6D-TEMP가 적용되었으며 여기에는 실도로 주행 배출가스(Real Driving Emission)테스트가 포함된다. 차대동력계에서 수행되는 기존의 배출가스 측정과 달리 실제 도로 측정은 외부 온도, 운전자 경향 및 도로 조건에 따라 매우 높을 수 있다. 따라서 차량 배출물을 줄여주는 후처리장치의 측면에서, 온도에 따른 정화 효율과 같은 후처리장치 자체의 성능뿐만 아니라 후처리장치가 작동하기 위한 엔진 작동 조건 제어 또한 중요하다. 디젤 차량의 경우 질소산화물(NOx)을 환원시키기 위해 후처리장치인 희박 질소산화물 트랩(LNT) 및 선택적 환원 촉매 장치(Selective Catalytic Reduction)가 사용되지만 실제 도로주행은 운전자의 성향과 교통 상황, 작동 온도의 영향을 받으므로 후처리장치의 작동온도가 항상 만족될 수는 없다. 특히 SCR은 주행 초기 또는 긴 정지 구간에서 작동하지 않으므로

LNT만이 NOx를 줄이게 되며, RDE 데이터에 따르면 이 구간에서의 NOx 배출량이 총 NOx 배출량의 40 %를 차지하는 것으로 나타났다. 이는 실제 도로주행에서 LNT의 효율 변화가 NOx 배출에 큰 영향을 미친다는 것을 의미한다. 따라서 본 논문에서는 최대한 적은 개수의 변수를 이용하였고, 온보드 진단(OBD)과 같이 접근 가능한 변수들을 위주로 LNT 효율을 예측하여 실시간 실도로 주행 배출물 제어에 적용시킬 수 있는 모델이 개발되었다. 먼저 LNT 효율을 모델링하기 위하여 LNT 입구에서의 질소산화물과 산소의 농도와 유량이 고려된 예측 식을 구하였다. 다음으로 온도가 LNT 효율에 미치는 두 가지의 영향을 포함시키기 위하여 앞의 식을 보정시키는 변수로서 사용되었다. 마지막으로는 LNT의 용량 감소가 LNT를 지나는 배기가스의 온도변화에 영향을 준다는 것을 고려한 식이 표현되었고, 이 식에서 NOx 몰분율의 변화를 전체 온도 변화와 대류 열전달의 항으로 나타낸 후 이 값을 LNT 효율에 대입하였다. 따라서 최종 모델이 만들어졌으며, 최소 제곱법에 의하여 피팅 계수들이 정해졌다. 그 결과 측정값과의 상관계수는 0.80898이 나왔으며 예측값이 측정값의 경향을 잘 반영한다는 것을 마지막 그림을 통해 나타냈다.

감사의 글

석사 논문을 마무리하며 감사의 글을 남기는 지금 순간, 되돌아보면 후회도 많이 남지만 공식적으로 석사 학위라는 자격을 부여받을 수 있다는 것이 정말 감격스럽습니다. 어드밴스드 에너지 시스템 연구실에 들어온 초기를 생각해보면 저는 남들보다 대학원 진학을 결정한 시기도 늦었고 연구하고 싶은 분야도 뚜렷하지 않았습니다. 이런 제게 많은 도움과 조언을 주고 같이 연구해나갔던 분들에게 하고 싶었던 얘기를 적어보려 합니다.

제게 연구 방향을 제시해주고 공학자로서의 자세 및 인간으로서의 성품에 귀감이 되어주신 송한호 교수님, 정말 감사드립니다. 제가 나태해지거나 무기력할 때마다 건네주셨던 따뜻한 말씀들은 제게 많은 용기를 불어넣었습니다. 그리고 사소한 고민이라도 귀 기울여주시고 공감해주시고 관심을 가져주셔서 감사드립니다. 항상 학생들에게 도움이 되기 위해 노력하시면서도, 그것이 오히려 부담을 주지 않을까 배려하시는 모습을 보고 스승으로서 누구보다도 존경받을 분이라는 생각이 듭니다.

또 김찬중 교수님과 차석원교수님, 도형록 교수님, 민경덕 교수님께 감사드립니다. 김찬중 교수님과 차석원 교수님은 제 학위 논문 심사에서 연구 내적인 면뿐만 아니라 학교를 졸업하고 더 이상 학생이 아니게 될 때에 직면할 수 있는 상황에 대한 조언을 많이 해주셨습니다. 도형록 교수님은 스크램젯 과제를 통해서 저의 연구 분야가 자동차뿐만 아니라 다른 분야에도 적용될 수 있다는 인상을 갖게 해주셨습니다. 민경덕 교수님은 고급내연기관 수업과 여러 세미나 등을 통해 열공학자로서의 깊은 지식과 통찰을 갖게 해주셨습니다.

다음으로 대학원 생활동안 가장 많은 시간을 보내고 많은 힘이 되어주신 연구실 선배, 동기, 후배 분들에게 감사드립니다. 이룹, 원재, 정우, 은지, 태경, 재현, 세철, 은수, 재영, 형은, 용태, 현호, 명수, 우재, 창현, 민규, 준표, 종호, 예임, 그리고 호영, 모두 잊지 않겠습니다. 특히 조교 활동 및 제가 참여했던 모든 과제에 같이 배정되어 시너지를 발휘하여 서로 부족한 점을 채워준 창현이에게 다시 한 번 감사드립니다. 그리고 비록 다른 연구실이지만 스크램젯 과제를 같이 하며 많은 도움 고민을 같이 했던 성익이에게도 감사합니다.

마지막으로 저처럼 키우기 어려운 아들을 어언 30년 간 보살펴주신 부모님께 감사드립니다. 워낙에 고집이 세고 자존심이 강한 아들이라 속을 많이 썩였을텐데, 또 특히 석사 학위 준비기간에는 너무나 예민해했던 점에 대해 정말 미안한 마음이 듭니다. 점점 나이를 먹어가는 만큼 더 자랑스럽고 다정한 아들이 되겠습니다. 그리고 비록 의견 차이가 심해 서로 서먹해하는 여동생 정아에게는 먼저 다가가서 남매로서의 온정을 나누고 싶다는 얘기를 하고 싶습니다. 또 어렸을 때부터 누구보다 많은 관심과 보살핌을 주신 할머니와 할아버지께 감사드립니다. 지금보다 더 많이 할머니와 할아버지를 떠올리고 찾아뵙겠습니다. 엄마, 아빠, 정아, 할머니, 할아버지! 정말 사랑합니다.

2020년 1월

301동 214호 연구실에서

현재우