



# Air-fraction modeling for simultaneous Diesel engine NO<sub>x</sub> and PM emissions control during active DPF regenerations



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## HIGHLIGHTS

- A control-oriented air-fraction model during DPF regenerations.
- Diesel engine air-path oxygen concentration prediction with incomplete combustion.
- Experimental validation of the air-fraction dynamic model.

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## ABSTRACT

This study develops a control-oriented air-fraction model which can accurately predict the air-fraction dynamics for a Diesel engine and the coupled aftertreatment system (mainly Diesel oxidation catalyst (DOC)) during active DPF regenerations. NO<sub>x</sub> and particulate matter (PM) emissions are the two main concerns for modern Diesel engine development. Diesel particulate filters (DPFs) have become a standard device for reducing the PM emissions from Diesel engine powertrains. To maintain high filtration efficiencies and avoid high back pressures, active DPF regenerations have to be implemented periodically by significantly elevating the exhaust gas temperatures. However, during active DPF regenerations, the selective catalytic reduction (SCR) deNO<sub>x</sub> performance may be significantly decreased, while the high temperature durability and total hydrocarbon (THC) poisoning of SCRs may be potential issues. To simultaneously meet the NO<sub>x</sub> emission standard, high-pressure loop EGR needs to be applied. Since in-cylinder NO<sub>x</sub> reduction relies heavily on the in-cylinder oxygen content, an accurate air-fraction model is necessary, and the effects of recycled THC and CO emissions should be considered. The developed air-fraction model has been experimentally validated to show its capability of capturing the actual air fraction dynamics accurately. Such a model can be instrumental in simultaneous NO<sub>x</sub> and PM emission control during active DPF regenerations and in advanced combustion mode control.

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## 1. Introduction

Diesel powertrains with low NO<sub>x</sub> and particulate matter (PM) emissions have become the trend of Diesel engine development in the future due to the growing concerns of Diesel emissions to the environment and public health. To reduce tailpipe NO<sub>x</sub> emissions, various techniques have been proposed which can be classified into two groups: in-cylinder techniques and aftertreatment systems. One of the most popular in-cylinder measures for engine-out NO<sub>x</sub> reduction is the exhaust gas recirculation (EGR) system which recycles part of the exhaust gas back into cylinders such that the flame temperature and oxygen concentration can be lowered [1,2]. Since in-cylinder NO<sub>x</sub> generation typically increases

with the flame temperature and oxygen concentration, the engine-out NO<sub>x</sub> concentration can be substantially reduced via EGR. The aftertreatment systems for reducing Diesel NO<sub>x</sub> emissions include lean NO<sub>x</sub> traps (LNTs), selective catalytic reduction (SCR) systems, and others [3,4]. In specific, urea-based SCR systems have proven to be promising in controlling the tailpipe NO<sub>x</sub> emissions from medium-to-heavy-duty Diesel engines [5].

On the other hand, Diesel particulate filters (DPFs) have become standard components for PM emission control [6]. Wall-flow DPFs are designed such that the soot in the raw Diesel exhaust can be effectively filtered. In order to make the DPFs function consistently and avoid high back-pressures across DPFs which can result in engine power losses, the accumulated soot inside the filters should be burned off via passive or active regenerations. The passive regeneration relies on the continuous NO<sub>2</sub>-assisted soot oxidation which requires relatively low DPF inlet temperature, while the active

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## Nomenclature

### Variables and constants

|                  |                                                        |
|------------------|--------------------------------------------------------|
| $A_{negr}$       | effective flow area for HPL-EGR valve ( $m^2$ )        |
| $C_i$            | molar concentration of species $i$ ( $mol/m^3$ )       |
| $F_i$            | air fraction at point $i$ (–)                          |
| $\dot{m}_{eo}$   | mass flow rate from engine cylinders ( $kg/s$ )        |
| $N_e$            | engine speed (rpm)                                     |
| $P_i$            | gas pressure at point $i$ (Pa)                         |
| $R$              | specific gas constant ( $J/kg/K$ )                     |
| $T_i$            | gas temperature at point $i$ (K)                       |
| $V_i$            | control volume at point $i$ ( $m^3$ )                  |
| $V_d$            | volume displacement of engine ( $m^3$ )                |
| $\dot{W}_i$      | volume flow rate through component $i$ ( $m^3/s$ )     |
| $\lambda_{stoi}$ | stoichiometric air-fuel ratio (–)                      |
| $\eta_{post,i}$  | combustion efficiency of the $i$ th post injection (–) |
| $\eta_v$         | engine volumetric efficiency (–)                       |

### Abbreviations

|      |                       |
|------|-----------------------|
| ATDC | after top dead center |
|------|-----------------------|

|      |                                        |
|------|----------------------------------------|
| CAD  | crank angle degree                     |
| DOC  | diesel oxidation catalyst              |
| DPF  | diesel particulate filter              |
| ECU  | engine control unit                    |
| EGR  | exhaust gas recirculation              |
| HCCI | homogenous charge compression ignition |
| LNT  | lean $NO_x$ trap                       |
| LTC  | low temperature combustion             |
| PM   | particulate matter                     |
| SCR  | selective catalytic reduction          |
| SOI  | start of injection                     |
| THC  | total hydrocarbon                      |
| VGT  | variable geometry turbocharger         |

### Unit

|            |                           |
|------------|---------------------------|
| mg/stk/cyl | milligram/stroke/cylinder |
|------------|---------------------------|

DPF regeneration, triggered by the back pressure signal across DPF, is based on  $O_2$ -assisted soot oxidation which requires much higher DPF inlet temperature (550 °C or higher) [7,8]. Since Diesel exhaust temperature under normal operating conditions is typically lower than the desired temperature in the case of active DPF regeneration, additional measures are needed to maintain high DPF temperature. With the introduction of high-pressure common-rail fuel injection systems, post fuel injection in combination with a Diesel oxidation catalyst (DOC) has become a popular technique in elevating the DPF inlet temperature [9]. The main strategy is to generate a large quantity of total hydrocarbon (THC) emissions by retarding the post fuel injection timing to the late phase of power stroke. These THC emissions can later be oxidized by the DOC downstream, substantially raising the DOC-out temperatures. As the DOC is typically installed upstream of DPF, DPF temperature can be considerably increased as well via appropriate post injection strategy. To ensure the DOC functions appropriately, a comparatively early post injection may also be needed to achieve the desired DOC temperature before it is fed with a large amount of THC emissions [10].

Simultaneous  $NO_x$  and PM emissions reductions for Diesel engines have received growing attention in the past decade [11–14]. Nevertheless, due to the tradeoff between the engine-out  $NO_x$  and PM emissions, it is of great challenge to meet both emission standards via only in-cylinder techniques without significantly sacrificing the engine fuel economy. Advanced combustion concepts, such as low temperature combustion (LTC) and homogenous charge compression ignition (HCCI), have been reported to be capable of simultaneously lowering engine-out  $NO_x$  and PM emissions [15,16]. As a side effect, advanced combustion modes may result in ultra-high CO and THC emissions [15,17,18]. To alleviate the problems,  $deNO_x$  devices, such as SCRs, and DPFs for PM control, have been applied to modern Diesel engines. One of the main concerns for integrated Diesel engine and aftertreatment system operation is the simultaneous  $NO_x$  and PM emissions during active DPF regenerations. In this circumstance where high exhaust temperatures up to 700 °C can be expected in the exhaust line,  $NO_x$  reduction capability from the urea-based SCR systems, downstream of DPF, may be quite limited due to the following reasons. First, a large portion of ammonia may be oxidized into nitrogen at high SCR temperature [19,20]. Secondly, the  $NO_x$  conversion from SCR may decrease because of the reduced oxygen concentration due to the oxidations of THC and CO by the DOC and active DPF

regeneration [21]. In addition, at high exhaust temperatures, the SCR catalyst may be severely aged due to the thermal deactivation from active DPF regenerations [22]. Furthermore, it was found recently that SCR catalysts could be poisoned by the excess THC emissions during active DPF regenerations [3,23–25]. In the case that LNTs are installed after DPFs for  $NO_x$  reduction, the performance of LNTs can be deteriorated significantly in high catalyst temperature range [22]. To simultaneously reduce the tailpipe  $NO_x$  and PM emissions under this situation, the combined EGR–DPF system should be applied.

The modeling of air-fractions of Diesel engines equipped with EGR systems have been intensively studied in the past decade. Modeling of air-fractions for Diesel engines equipped with DOC/DPF and dual-loop EGR systems can be found in several studies [2,26–28]. In most of these papers, only complete combustion of pilot fuel injection and main fuel injection was considered regarding the air fraction reduction inside the cylinders. However, in the case of active DPF regeneration, the aforementioned air-fraction models may not be capable of well predicting the actual air-fraction dynamics due to the following reasons. First, since the combustion of post injected fuel may be rather incomplete, the assumption of complete combustion may be invalid. Secondly, since a large quantity of THC and CO emissions can be generated from post injection and be recycled into cylinders via EGR under such situations, in-cylinder air-fraction can be reduced drastically because of the oxidations of recirculated THC and CO emissions. Last but not the least, with heavy EGR, advanced combustion modes, such as LTC and HCCI, can lead to very low engine-out  $NO_x$  and PM emissions [15]. However, LTC mode and HCCI mode may be accompanied with ultra-high CO and THC emissions [17,18]. Therefore, the oxidations of recirculated THC and CO emissions also need to be considered in the in-cylinder air-fraction model suitable for advanced combustion modes even without post injection.

The main contribution of this study is to develop a control-oriented Diesel engine air-fraction model with the combustion of post injected fuel and the oxidations of recirculated THC and CO emissions being taken into account. Such a model will be instrumental in simultaneous  $NO_x$  and PM emission control during active DPF regenerations. Furthermore, such a model can be beneficial in advanced combustion mode control in the future.

The remaining part of this paper is organized as follows. First of all, the experimental setup and measurement instruments are

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