

Architecture Design and Analysis of Diesel Engine Exhaust Aftertreatment System and Comparative Study with Close-coupled DOC-DPF System

Anand Gurupatham

General Motors Powertrain - India

Yongsheng He

General Motors Research and Development

Copyright © 2008 SAE International

ABSTRACT

In response to the emissions standards for diesel engines, it is essential to have separate aftertreatment devices for controlling the specific tailpipe emissions like HC, CO, NO_x, and particulate matter. An advanced diesel exhaust aftertreatment system consists of channel-flow catalytic converters such as diesel oxidation catalyst (DOC), selective catalyst reduction (SCR) and wall-flow diesel particulate filters (DPF) each with discrete functions. Because of this multi-component aftertreatment system configuration, there are an increase in system complexity, development time and cost for doing experiments in order to evaluate various options and find the optimum aftertreatment system architecture.

The objective of this work is the development and application of an integrated aftertreatment system model including DOC, SCR, DPF and all connecting pipes. The study includes the baseline system performance, i.e. SCR forward system (DOC-SCR-DPF), DPF forward system (DOC-DPF-SCR), and DPF forward (DOC-DPF-SCR) aftertreatment system when DOC and DPF were closely coupled. Basically all component models were 1-D, quasi-steady with global kinetic approach. All component models are incorporated and integrated into a diesel exhaust aftertreatment simulation tool in Matlab / Simulink platform. The developed model was used for designing and analyzing different aftertreatment system architectures for a light-duty diesel engine. Both temperature and emissions reduction efficiency of each component were considered to improve the overall aftertreatment system performance to reduce tailpipe emissions.

INTRODUCTION

More stringent emission regulations are enforced worldwide in order to control engine tailpipe emissions,

primarily carbon monoxide (CO), unburned hydrocarbons (HC), oxides of nitrogen (NO_x), and particulate matter (PM). In response to the more stringent emissions standards for diesel engines, it is essential to have separate aftertreatment devices for controlling the specific tailpipe emissions like HC, CO, NO_x, and particulate matter. Diesel oxidation catalysts (DOC) have been widely used to remove CO and HC, and also oxidize some soluble organic fractions (SOF) of PM. Wall-flow diesel particulate filters (DPF) have become standard devices to filter PM from the exhaust. Common NO_x aftertreatment devices include selective catalytic reduction (SCR) and lean NO_x traps (LNT).

Because of this multi-component aftertreatment system configuration, there are an increase in system complexity, development time and cost for doing experiments in order to evaluate various options and find the optimum aftertreatment system architecture.

Therefore, modeling tools are needed and necessary in the exhaust system development and optimization process. System-level simulations are crucial to optimize the size, position, and architecture of the aftertreatment system, which allow effective and efficient evaluation and screening of numerous design concepts and new technologies to reduce engineering time and cost.

In earlier studies [1-2], an integrated diesel exhaust aftertreatment simulation tool has been developed for diesel aftertreatment system architecture design. The developed aftertreatment system simulation tool was demonstrated to evaluate and analyze different architectures of a characteristic advanced diesel engine exhaust aftertreatment system that consists of DOC, LNT, and DPF.

This paper incorporates a SCR model into the system model, and presents the development and application of the integrated model of a typical advanced diesel engine

exhaust aftertreatment system that consists of DOC, SCR, and DPF. In the following sections, the models for various exhaust aftertreatment components will be briefly reviewed first. Next, the detailed results of applying the integrated system model are discussed, which include the thermal response study of the aftertreatment system, the overall emissions reduction performance, and the assessment of various architecture designs such as DOC-SCR-DPF system versus DOC-DPF-SCR systems which includes close-coupled DOC-DPF system also. Finally, the conclusions and future work of this study will be given.

COMPONENT MODEL DESCRIPTION

A typical diesel exhaust aftertreatment system consists of exhaust pipes (including down pipes and tailpipes), channel-flow catalytic converters (such as the DOC, the LNT, the SCR), and wall-flow diesel particulate filters (DPF). The details of component models used in this study are given as follows.

EXHAUST PIPES

A one-dimensional quasi-steady thermal model has been developed to simulate the heat transfer phenomenon in exhaust pipes, which is based on the assumption that the characteristic time constant of the flow rate and temperature is much higher than the residence time of the flow. The exhaust pipe model also assumes incompressible flow and negligible impact of pressure variations.

The modeling of the heat transfer in the exhaust pipe considers the axial heat conduction within the pipe (q_{cond}), the heat convection between the exhaust gas and the pipe (q_{conv}), and the external heat loss of the pipe to the environment (q_{loss}). The details could be found in [1-2].

CHANNEL-FLOW CATALYTIC CONVERTERS

One-dimensional global kinetic approach has been widely used in modeling channel-flow catalytic monoliths [3-6]. The monolith model generally assumes the species concentration and temperature profiles in all channels of the monolith to be identical. The modeling of the heat transfer in the monolith considers the axial heat conduction in the solid phase, the radial heat convection between the gas and the solid, and the heat generation by chemical reactions. The heat loss of the monolith to the ambient is usually regarded as negligible.

For the mass balance, the gas species concentration (C_g) and surface species concentration (C_s) are governed by:

$$e \cdot \frac{\partial C_g}{\partial t} + U_g \cdot \frac{\partial C_g}{\partial x} = -k_m \cdot G_a \cdot (C_g - C_s) \quad (1)$$

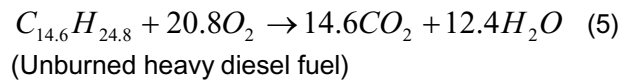
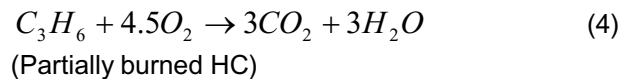
$$(1 - e) \cdot \frac{\partial C_s}{\partial t} = k_m \cdot G_a \cdot (C_g - C_s) + R_s \quad (2)$$

where e is the void fraction of the catalyst, U_g is the bulk gas velocity in the flow direction x , k_m is the mass transfer coefficient, G_a is the geometric catalyst surface to volume ratio, and R_s is the production rate of the surface species due to chemical reactions on the surface.

The reaction rates of catalytic reactions for various channel-flow catalysts are described in different kinetic forms, as illustrated in the following sections. In this study, only the SCR is shown for NOx aftertreatment devices.

DOC Kinetics

The DOC model considers the following major reactions, which include CO and HC oxidation, and NO oxidation to NO₂:



Two hydrocarbons were chosen to represent the typical hydrocarbon species in diesel exhaust: partially burned HC represented by C_3H_6 and unburned heavy diesel fuel represented by $C_{14.6}H_{24.8}$. Langmuir-Hinshelwood kinetic expressions are used to model the reactions. The kinetic parameters (i.e., the pre-exponential factor and the activation energy) of each reaction were obtained by calibrating the model against steady-state flow reactor data. Good agreement between simulations and reactor experiments were reported [3].

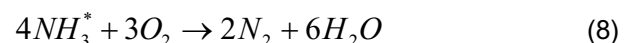
SCR Kinetics

These are the set of reactions and associated rate expressions involved in the NH₃-NO/NO₂ reacting system of SCR:

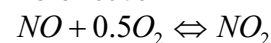
Ammonia adsorption-desorption



Ammonia oxidation



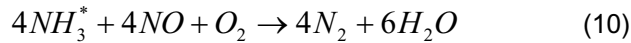
NO oxidation



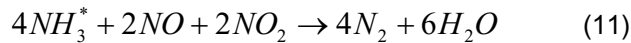
Documents

Document Sharing Hub

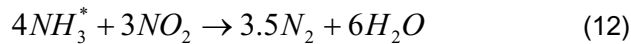
Standard SCR reaction



Fast SCR reaction



Slow SCR reaction



The SCR kinetic model was developed based on a broad range of experimental conditions for ammonia adsorption/desorption, NO oxidation, standard/fast/slow SCR reactions with different NO/NO₂ ratios. The SCR kinetic parameters were adjusted to minimize the difference between the simulated and experimental species concentrations at the SCR outlet for a range of steady state engine conditions. The SCR model has been extensively validated with transient experiments with varying temperatures, NO and NH₃ concentrations, and a very good model predictive accuracy was achieved [6].

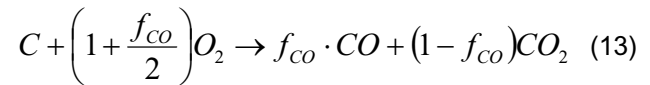
Wall-flow Particulate Filters

The one-dimensional single-channel catalyzed wall-flow DPF model [8] solves mass, momentum, and energy equations across the inlet and outlet channel for the flow field. The pressure drop across the porous wall of the DPF is modeled using the Darcy law, considering both the deep-bed filtration in the wall and the cake filtration on the wall as follows:

$$\Delta P = \frac{\mu_w}{k_w} u_w w_w + \frac{\mu_w}{k_s} u_w w_s \quad (13)$$

where μ_w is the gas viscosity in the wall, k_w and k_s are the wall and soot permeability, u_w is the gas velocity in the wall, w_w and w_s are the wall and soot layer thickness. Note that the pressure drop across the whole filter also includes the pressure drop due to the contraction of the exhaust gas at the channel inlet, the expansion of the exhaust gas at the channel outlet, and the friction between exhaust gas and channel walls. The filtration efficiency of the porous wall is calculated based on the unit collector concept, which assumes that the soot uniformly deposits on identical spherical unit cells. Brownian diffusion and direct interception are the main mechanism for particle captures by individual unit collectors.

Both thermal and catalytic oxidations of the trapped soot are modeled. The following global oxidation reactions are used (with different reaction rate constants for thermal and catalytic oxidation):



where f_{co} is CO selectivity. The DPF model was calibrated using engine dynamometer data at various engine operating conditions, and a good agreement between simulations and experiments was obtained [9].

INTEGRATED DIESEL AFTERTREATMENT SYSTEM MODEL DESCRIPTION

Based on the same framework of previous work [1-2], all above-mentioned component models are integrated into a single global model to represent a characteristic advanced diesel exhaust aftertreatment system that consists of a DOC, a SCR, a DPF, and exhaust pipes. The DOC model, the SCR model, the DPF model, and the pipe model are converted into S-Functions and incorporated with uniform I/O in MATLAB/Simulink.

In this paper, an advanced diesel aftertreatment system for a light-duty application is modeled and studied. It is assumed that the DOC oxidizes all the soluble organic fractions (SOF) of PM, and only the elemental carbon fraction (i.e., soot) of PM is considered in the filtration and oxidation process of the DPF.

Table 1 lists the specifications of each aftertreatment device used in this study. The specifications of aftertreatment devices were chosen based on the devices used in engine test cell. In this study, the integrated diesel aftertreatment system model has been utilized to evaluate various aftertreatment system architectures and optimize the overall system performance of emissions reduction. The detailed results are discussed in the next section.

Table 1: Specifications of diesel aftertreatment devices

Device	Volume (Liter)	PGM Loading (g/ft ³)	Cell Density (cpsi)
DOC	2.87	40	400
SCR	7.24	-	400
DPF	8.69	5	100

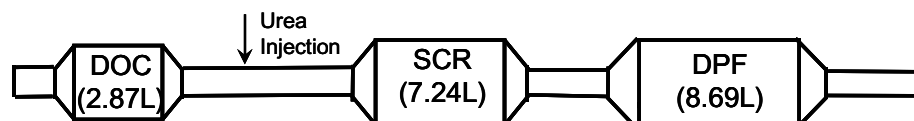


Figure 1 Schematic of an advanced diesel aftertreatment system architecture (baseline)