Development of the model for a diesel engine catalytic converter

Artem Blinov*, Nikolay Malastowski and Leonid Myagkov

Bauman Moscow State Technical University, 2-ya Baumanskaya Street, 5, Moscow, Russia, 105005

Abstract. One of the key issues of the modern engine development is to comply with today's stringent emission standards. It forces the manufacturers to enhance in-engine and aftertreatment emission reduction technologies continuously. The selective catalytic reduction (SCR) is still the most effective technique for nitrogen oxides removal from exhaust gases of vehicles with diesel engines. Numerical modelling is widely used for SCR systems development and assessment. In this paper, a simplified one-dimensional numerical model of diesel SCR catalyst, which was implemented in Matlab, is described. The algorithm for automatic mesh generation describing real cross-section geometry of the catalyst block and the calculation procedure allowing to take into account non-uniform distribution of the gas flow parameters at the catalyst inlet are presented. Model was validated by the experimental data available in the literature. Numerical simulations for the full-scale modern SCR catalyst were carried out. The effect of the gas velocity non-uniformity at the catalyst inlet on the overall NO_x reduction efficiency was evaluated.

1 Introduction

Diesel engines are a significant source of pollutant emissions [1], especially nitrogen oxides (NO_x). The most approaches include reducing formation of pollutants within the engine [2-4] or control of the emissions in the exhaust gases using aftertreatment technologies.

One of the way for reduction nitric oxides (NO_x) emissions to comply with today's stringent emission standards is selective catalytic reduction technology. SCR becomes the part of diesel aftertreatment system universally applied from Tier 4f/Stage IV standard (Table 1) [5].

SCR system introduces ammonia (NH₃) to react with

NO_x over a catalytic surface, producing nitrogen and water. The introduction of the ammonia in the exhaust systems takes place upstream the SCR catalyst by injecting an aqueous urea solution. The injected urea-water droplets convert into ammonia, carbon dioxide and vapor. Ammonia adsorbs at the SCR catalyst surface or desorbs from it. The reduction of nitric oxides takes place through reactions where ammonia gets consumed and nitrogen and water are produced [6].

A wide range of different numerical models in terms of accuracy, capabilities and computational efficiency are available today in literature [7–21]. They vary from simple distributed models [7–14] to one's based on computational fluid dynamics (CFD) methods [15–21].

It should be noted that the physical and chemical

Table 1. Technology pathway for diesel engines.

	(Tier 3/Stage IIIA)	Tier 4i/Stage IIIB		Tier 4f/Stage IV	Stage V (Tier 4f/Stage IV w/DPF)
		SCR	EGR		
Engine-out emissions and air/ fuel controls	Wastegated turbocharger	Wastegated turbocharger	Wastegated turbocharger	Wastegated turbocharger	Wastegated turbocharger
	Electronic direct fuel injection	Common rail fuel injection	Common rail fuel injection	Common rail fuel injection	Common rail fuel injection
	Cooled EGR	Electronic control unit	Cooled EGR	Cooled EGR	Cooled EGR
	Electronic control unit	-	Electronic engine control	Electronic control unit	Electronic control unit
Aftertreatment systems	None	NOX control through SCR system	PM control through DOC and DPF	PM control through DOC	PM control through DOC
		Ammonia slip catalyst	-	NOX control through SCR system	NOX control through SCR system
		-	-	Ammonia slip catalyst	Ammonia slip catalyst

* Corresponding author: as_blinov@bmstu.ru

phenomena that occur in SCR system can be divided into two main processes [22]. First, the injection and decomposition of urea-water solution within engine exhaust channel and second nitric oxides reduction in catalytic converter. It means that it is possible to split the simulation procedure into the two stages. For the first one is strictly recommended to use 3D CFD simulations, but for catalytic converter processes due to its honeycomb structure possible to reduce model up to 1D case [21].

In this study, a 1D model of SCR converter model was described and the algorithm considered non uniform parameters on inlet surface to prediction of NO_x emissions rate was suggested.

2 Methods

2.1 Catalyst block spatial discretization

In this study honeycomb type catalytic converter is investigated (Fig 1). It consists of individual square channels formed by a solid substrate. The inner channel walls are coated with thin porous washcoat layer containing catalytic sites [13].

Using MATLAB® an algorithm for automatic mesh generation describing real cross section geometry of the catalyst block was created. The input parameters such as number of cells per square inch (cpsi), walls thickness (δ) and outer diameter (D) of the catalyst block determine channels dimensions and cross section area.

2.2 Governing equations and assumptions

A well known approach based on a single channel model was applied to current simulation [23]. The validity of this assumption is justified by the fact that processes occurring in channels are generally identical. In this case, the calculation procedure for the entire converter consists of sequential modeling of each channel, taking into account possible changes in the geometry and / or boundary conditions at their inlet surface.

To simplify the model [24], only four dominant reaction pathways such as adsorption(a), desorption(d), reduction(r), and oxidation(o) are included in 1D model [25]: Corresponding reaction rates were taken from [26].

In general, within the catalyst channel several physical and chemical phenomena occur [27]. It can be distinguished between convective and conductive transport phenomena in axial direction in the gas and converter material.

- The energy conservation laws for gas and converter body are modeled according to following equations:

$$\rho_g A_g C_{p,g} \left(\frac{\partial T_g}{\partial t} + U \frac{\partial T_g}{\partial x} \right) = h \cdot P (T_w - T_g) \quad (5)$$

$$\rho_w A_w C_{p,w} \frac{\partial T_w}{\partial t} = -h \cdot P (T_w - T_g) + k_w \frac{\partial^2 T_w}{\partial x^2} \quad (6)$$

here subscript g and w - inflow and wall parameters respectively, x is the cartesian coordinate in the axial direction, U - the mean flow velocity, ρ is the density, T - temperature, C_p - heat capacity, A - surface area, h - heat transfer coefficient according to [28], k - thermal conductivity of a material, P - perimeter of channel.

- The corresponding transport equations for species NH₄ and NO_x in a channel:

$$\frac{\partial NH_3}{\partial t} = \frac{s}{A_g U} (-R_a + R_d) \quad (7)$$

$$\frac{\partial NO}{\partial t} = \frac{s}{A_g U} (-R_r) \quad (8)$$

here NH and NO - concentration of species, s - refers to the total NH₃ adsorption capacity of the specific catalyst sample, R - reaction rates.

- The extra species equation of adsorbed ammonia on the surface:

$$\frac{\partial \theta}{\partial t} = (R_a - R_d - R_r - R_o) \quad (9)$$

Fig. 1. Catalyst block spatial discretization.

where, θ - the fractional NH_3 loading.

The addition assumptions are made:

- Chemical reactions in gas phase are negligible;
- Heat generation from chemical reactions (1-4) is assumed to be small compared to convective heat transfer.

The upwind difference scheme is employed for approximate space derivatives of the equation system (5-9). Resulted ordinary differential equations were solved using MatLab ode23s algorithm of second order discretization, which is based on a modified Rosenbrock formula [29].

3 Results and discussion

The validation procedure of the proposed catalyst mathematical model was carried out on the base of experimental data [26]. Experimental setup represents aluminum-oxide sample-size reactor with a diameter and length around 1 inch (Fig.2). The catalyst cells per square density was 400. The inlet gas flow containing NH_3 and NO species was supplied into the catalyst at fixed space velocity of 30000 1/Hr. The dynamic experiments were conducted at fixed input concentration of NO and various input concentration of NH_3 and gas temperature (Fig.3).

Fig. 2. Schematic representation of the experimental setup [26].

Fig. 3. Catalyst inlet boundary conditions [26].

Fig. 4. Comparison of numerical and experimental results.

Numerical simulations were carried out for reproduction of the experimental work [26] and numerical results were compared to experimental ones (Fig.4).

The comparison showed reasonable agreement between the model predictions and experiments.

Nevertheless we should take into account the real-working converter's conditions, then the gas flow parameters at the catalyst inlet may have distribution by the inlet surface. To evaluate the effect of non-uniform inlet velocity on catalyst overall NO_x reduction efficiency two numerical experiments for the full-scale modern catalyst used in heavy-duty diesel engine were carried out.

In the first one, uniform velocity distribution at the inlet of the block was assumed, in the second, there was a parabolic velocity profile with the maximum value at the middle point of inlet surface (Fig. 5). For SCR systems without any specific mixing devices this is a widespread conditions. Initial gas flow composition as well as the gas temperature were assumed identical for all catalyst channels in both cases.

In these simulations the aluminum-oxide block with copper-zeolite catalyst had length 0.3 meter and outer diameter was 0.278 meter. The wall thickness was 0.0002 meter with cells density 100 cpsi. The thickness of the washcoat layer was 10 μm . Inlet boundary conditions used in the simulation are presented in Table 2.

Fig. 5. Catalyst inlet velocity profile.

Table 2. Catalyst inlet boundary conditions.

Concentration of NO, [mol/m ³]	0.2
Concentration of NH ₃ , [mol/m ³]	0.2
Concentration of O ₂ , [mol/m ³]	2.7
Concentration of N ₂ , [mol/m ³]	10.6
Gas temperature, [K]	600
Space velocity, [1/Hr]	30000

The overall NO_x reduction efficiency has been decreased by 40% due to radial distributions of inlet velocity (Fig. 6) compared to the case with uniform inlet velocity. At the middle of catalyst block there is less time for chemical reactions compare to outer regions. The level of uniformity has a direct influence on the achievable degree of efficiency. We will have same results for other parameters such as temperature distribution and non-stoichiometric NH₃ to NO_x ratio distribution at the catalyst inlet surface.

Fig. 6. Concentration of NO at the catalyst outlet.

4 Conclusions

This paper has outlined a 1D model for prediction of SCR convertor. The validation with the transient experimental data have revealed an acceptable prediction quality for the NO_x conversion and NH₃ slip of the SCR catalyst.

Steady state simulations have been carried out for the full-scale modern SCR catalyst. Significant radial distributions for flow, species fractions and temperature cannot be neglected during detailed SCR system optimization. In this case the suggested algorithm will allow to connect 3D modeling of injection and decomposition of urea-water solution within engine exhaust channel with described 1D model for improving simulation whole SCR system of diesel engine. The algorithm will help to supports the design and optimization of real systems.

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