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ESTIMATION OF THE OXIDE CATALYST VOLUME AND THE CELLS QUANTITY INFLUENCE ON CO, HC AND NO_x CONVERSION IN THE AVL BOOST COMPUTING APPLICATION

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Abstract

The article contains the results of the simulation tests of oxidizing catalytic reactor obtained by use of the AVL Boost simulation application. The chemical reactions and the reactions rates on which computations were based are specified in this paper. The simulations were related to the influence of the catalytic reactor volume and reactor's cells quantity influence on the carbon oxide, hydrocarbons and nitric oxides conversion levels. The influence on the nitric oxides conversion was presented in this paper as the content of NO and NO_2 in NO_X. The simulated computations were performed separately for the variable reactor volume ranging from 1 to 2.2 dm^3 with a step of 0.4 dm^3 and for the variable reactor cells quantity ranging from 200 to 600 cells per square inch with a step of 100 cpsi. As the input data for the simulation computations the actual values of the toxic compounds concentrations in the exhaust gases at the outlet of the Diesel engine were used. The measurements of the toxic compounnds were made at the chosen engine steady state work points and are presented in this paper as a graph of the toxic gases concentrations in the form of the function of the engine torque. The simulation computaitons were performed for the same points and their results are also presented in the form of the function of the engine torque. The Results presented in this paper have shown that the increase in the CO, HC and NO_X conversion in the case of the oxide catalyst can be obtained both by increasing the reactor volume and its cells quantity. It also have been observed that the increase in the reactor cells quantity and volume is not proportional as regards the toxic gases conversion increase and lowers in the case of higher values of the simulated reactor parameters.

Keywords: *combustion engines, catalytic reactors, simulation, air pollution, environmental protection*

1. Introduction

Together with the development of computing technology, new software was gradually introduced to support the engineering and design works. The first applications were mainly intended for engineering computations connected with the design and computations for the machinery and structure components. Over time, the professional software was introduced into the majority of technology fields including the applications used for the broadly defined modelling of the combustion engines. Currently, there are several applications available on the above-specified software market, which is mainly intended for modelling, and simulation computations connected with the combustion engine components mechanics and kinetics, physical and chemical and thermodynamic processes in the engine as well as the catalytic processes in the exhaust gas treatment systems. The tool in the form of simulation software combining a number of the phenomena in the engine enabled the designers and constructors to verify the design bases at the very initial phase of manufacture of the individual engine components including the catalytic systems. One of the leading manufacturers of software supporting the works connected with designing the combustion engines is AVL, the company that launched a series of applications including such applications as AVL Boost, AVL Fire and AVL Concerto. The AVL Boost application includes four modules to simulate the engine performance, acoustic phenomena in the

individual engine inlet and outlet system components and the catalytic phenomena in the exhaust gas treatment systems. The last AVL Boost application module of those mentioned above was used for simulation tests of the oxidation catalytic reactor of the particulate filter trap system.

The purpose of the work was a simulation aimed at determining the influence of volume and the number of the cells of the oxidation catalytic reactor in the particulate filter trap system on the CO and HC conversion levels obtained and the content of NO and NO_2 in NO_x.

2. Reactor model and simulation parameters

The chemical reactions model which is used in the AVL Boost application [1] for simulation computations connected with the Diesel engine oxidation catalytic reactor includes the following carbon oxide, hydrocarbon and nitric oxide oxidation reactions:

$$\mathrm{CO} + \frac{1}{2}\mathrm{O_2} \rightarrow \mathrm{CO_2}, \tag{1}$$

$$\mathrm{C_3H_6} + \frac{9}{2}\mathrm{O_2} \rightarrow 3\,\mathrm{CO_2} + 3\,\mathrm{H_2O}, \tag{2}$$

$$2\,\mathrm{NO} + \mathrm{O_2} \leftrightarrow 2\,\mathrm{NO_2}, \tag{3}$$

The computation simulation application uses the following reaction rates and kinetic parameters [2, 3]:

The rate of the first $\dot{r}_1$ reaction is as follows:

$$\dot{r}_1 = \frac{\left[K_{r1}\cdot\exp\left(-\frac{E_{r1}}{T_s}\right)\cdot y_{\mathrm{CO}}\cdot y_{\mathrm{O_2}}\right]\cdot\left[1+K_1\cdot\exp\left(-\frac{E_1}{T_s}\right)\cdot y_{\mathrm{CO}}+K_2\cdot\exp\left(-\frac{E_2}{T_s}\right)\cdot y_{\mathrm{C_3H_6}}\right]^{-2}}{T_s\cdot\left[1+K_3\cdot\exp\left(-\frac{E_3}{T_s}\right)\cdot y_{\mathrm{CO}}^2\cdot y_{\mathrm{C_3H_6}}^2\right]\cdot\left[1+K_4\cdot\exp\left(-\frac{E_4}{T_s}\right)\cdot y_{\mathrm{NO}}^{0.7}\right]}. \tag{4}$$

The rate of the other $\dot{r}_2$ reaction is as follows:

$$\dot{r}_2 = \frac{\left[K_{r2}\cdot\exp\left(-\frac{E_{r2}}{T_s}\right)\cdot y_{\mathrm{C_3H_6}}\cdot y_{\mathrm{O_2}}\right]\cdot\left[1+K_1\cdot\exp\left(-\frac{E_1}{T_s}\right)\cdot y_{\mathrm{CO}}+K_2\cdot\exp\left(-\frac{E_2}{T_s}\right)\cdot y_{\mathrm{C_3H_6}}\right]^{-2}}{T_s\cdot\left[1+K_3\cdot\exp\left(-\frac{E_3}{T_s}\right)\cdot y_{\mathrm{CO}}^2\cdot y_{\mathrm{C_3H_6}}^2\right]\cdot\left[1+K_4\cdot\exp\left(-\frac{E_4}{T_s}\right)\cdot y_{\mathrm{NO}}^{0.7}\right]}. \tag{5}$$

The rate of the third $\dot{r}_3$ reaction is as follows:

$$\dot{r}_3 = K_{r3}\cdot T_s^A\cdot\exp\left(-\frac{E_{r3}}{T_s}\right)\cdot\left(c_{\mathrm{NO}}^2\cdot c_{\mathrm{O_2}} - \frac{c_{\mathrm{NO_2}}^2}{K_{eq,1}}\right). \tag{6}$$

The following symbols are used in the above-specified equations:

$K_{r1}, K_{r2}, K_{r3}, K_1, K_2, K_3, K_4$ – Arrhenius equation pre-exponential factors,

$E_{r1}, E_{r2}, E_{r3}, E_1, E_2, E_3, E_4$ – activation temperatures,

$y_{\mathrm{CO}}, y_{\mathrm{O_2}}, y_{\mathrm{C_3H_6}}, y_{\mathrm{NO}}$ – content of the substances in the reactive gaseous phase surface expressed in moles,

$c_{\mathrm{NO}}, c_{\mathrm{O_2}}, c_{\mathrm{NO_2}}$ – substance concentrations on the active surface,

T_s – solid temperature,

A – temperature relationship value.

The $K_{eg,1}$ equilibrium constant contained in the third reaction rate formula is a catalytic reactor carrier temperature function defined as:

$$K_{eq,1} = \left(\frac{p_{atm}}{RT_s}\right)^{-1} \cdot \exp\left[-18.518 + \frac{13607}{T_s} + 0.5582 \cdot \frac{T_s}{1000} - 0.04489 \cdot \left(\frac{T_s}{1000}\right)^2 - 0.8278 \cdot \log\left(\frac{T_s}{1000}\right)\right], \quad (6)$$

where p_{atm} is the atmospheric pressure and R is the universal gas constant.

All factor values are used in AVL Boost as default values and they are not changed for any simulation purposes.

The combustion engine oxidation catalytic reactor used in the application is shown as a single reactor (CAT1) with the possibility to define its inlet (ATB1) and outlet (ATB2) boundary conditions. Such a system, which is used in the application, is shown in Fig. 2.

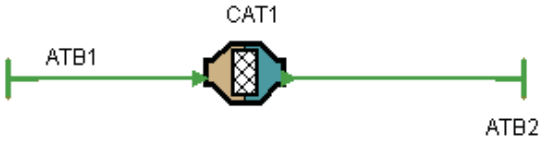

Fig. 1. A simulated oxidation catalytic reactor (CAT1) with the boundary conditions (ATB1, ATB2)

By using the Aftertreatment module of the AVL Boost software, it was possible to skip the process of creating a completely new model of the combustion engine generating the exhaust gases of the specified composition. As regards the module used, the catalytic reactor inlet boundary conditions used for defining the concentrations of the individual exhaust gas components, catalytic conversion temperature and the system inlet pressure have been provided basing on the data obtained from the tests of the Fiat MultiJet supercharged engine with a cubic capacity of 1.3 dm^3. During the tests, the engine was operating at a constant rotational speed of 2,000 rpm. Fig. 2 presents the concentrations of the toxic compounds analysed and the reactor temperature in the form of an engine-generated torque function.

The pressure behind the catalytic reactor is the only reactor outlet boundary condition used by the application and it is assessed during the bench test. The pressure values are given in Tab. 1.

Tab. 1. A catalytic reactor outlet boundary condition

		Engine torque [Nm]						
		40	60	80	100	120	140	160
Pressure behind DOC	[bar]	1.02	1.02	1.03	1.04	1.05	1.05	1.06

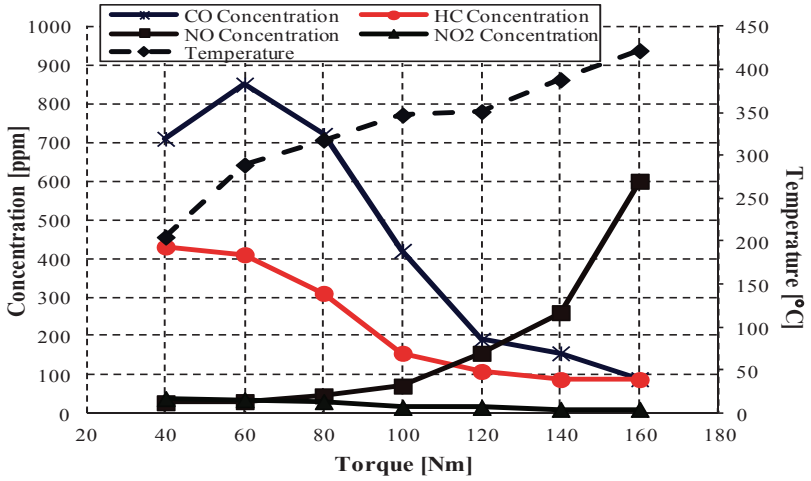

Fig. 2. The toxic compound concentrations measured and the reactor temperature used as the input simulation boundary conditions

The initial tests performed with the AVL Boost application have shown that the simulation results are already defined after about 15 seconds. The period of 100 seconds and the sampling frequency of 0.5 second have been specified as the total simulation time. To obtain more accurate

simulation results when determining the reactor inlet gas concentrations apart from the values shown in Fig. 2 the gas composition has been expanded with the CO_2, O_2 and N_2 concentrations measured during the same experiment.

3. Simulation computation results

The simulation computations performed aimed at determining the influence of both the catalytic reactor volume and this reactor cell packing density on the toxic compound conversion levels obtained. To do this we used computations performed for 9 parameter configurations concerning the structure of the catalytic reactor simulated. Reactor volume as well as the reactor cell packing density set in the application is shown in Tab. 2.

Tab. 2. The examined reactor structure parameter configurations

No.	1	2	3	4	5	6	7	8	9
	CPSI								
	400				200	300	400	500	600
reactor volume [dm^3]	1.0	1.4	1.8	2.2	1.4				

Figures 3-6 show the results of the simulation computations performed at a constant reactor solid cell packing density and a variable volume of the solid (positions 1 - 4 in Tab. 2).

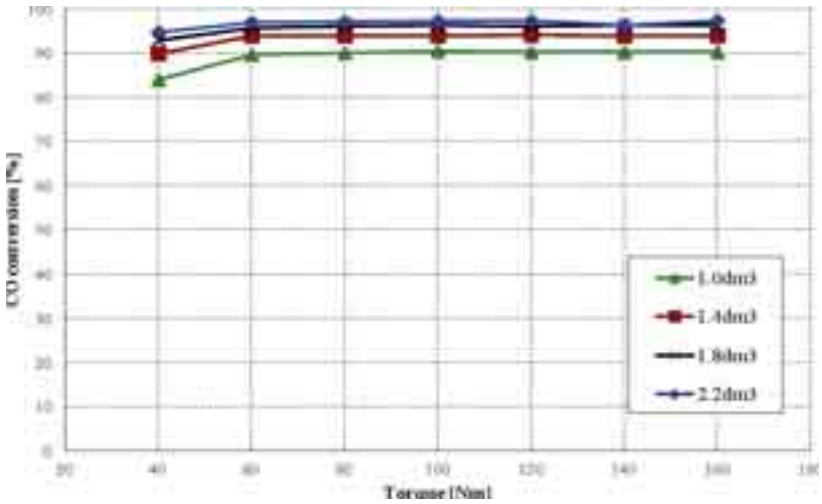

Fig. 3. The simulation computations concerning the influence of the change in the reactor solid volume at a constant cell packing density of 400 on the change of the CO conversion

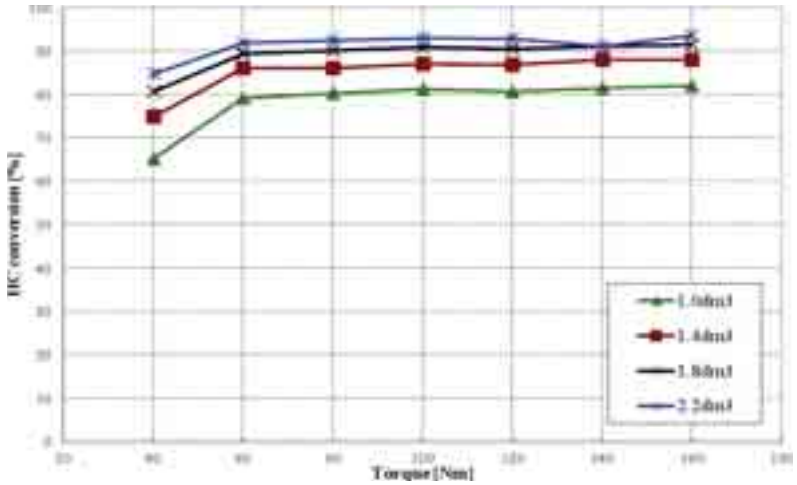

Fig. 4. The simulation computations concerning the influence of the change in the reactor solid volume at a constant cell packing density of 400 on the change of the HC conversion

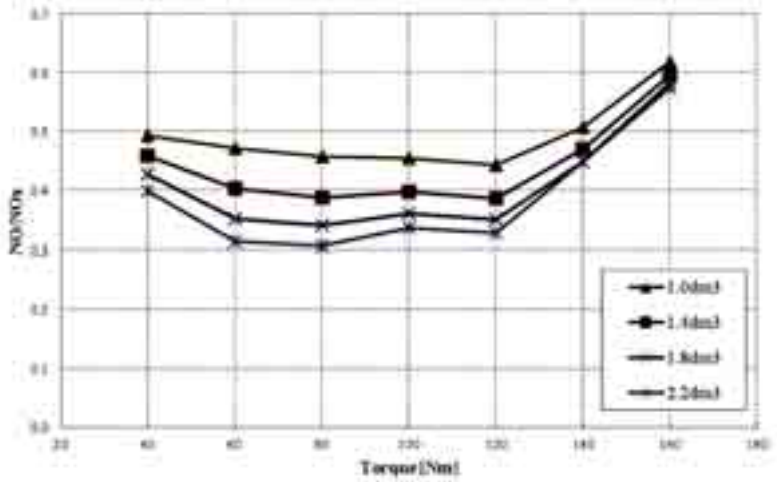

Fig. 5. The simulation computations concerning the influence of the change in the reactor solid volume at a cell packing density of 400 on the change of the content of NO in NO_x

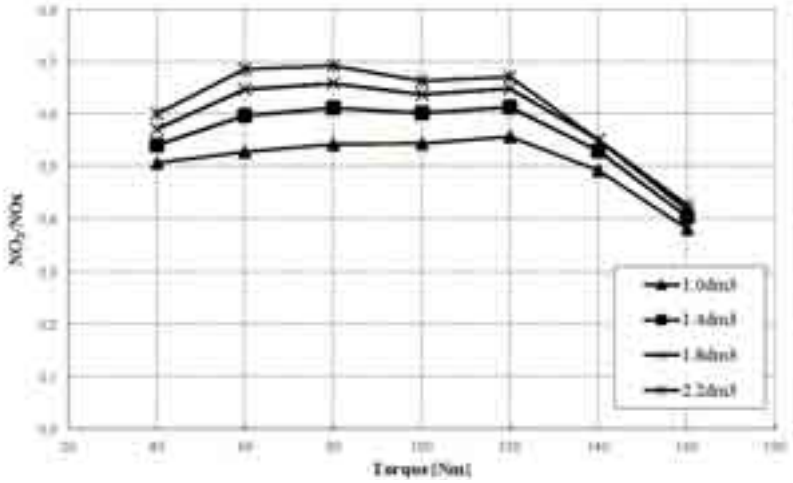

Fig. 6. The simulation computations concerning the influence of the change in the reactor solid volume at a constant cell packing density of 400 on the change of the content of NO_2 in NO_x

Figures 7-10 show the results of the simulation computations performed at a constant reactor volume and a variable reactor cell packing density (positions 5 - 9 in Tab. 2).

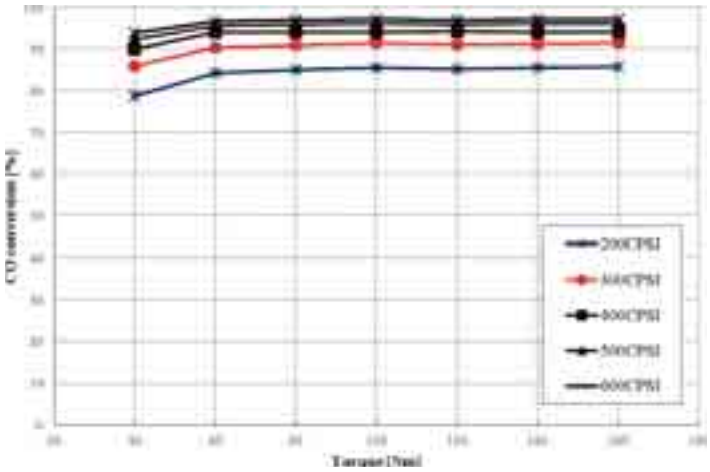

Fig. 7. The simulation computations concerning the influence of the change in the solid cell packing density at a constant solid volume of 1.4 dm^3 on the change of the CO conversion

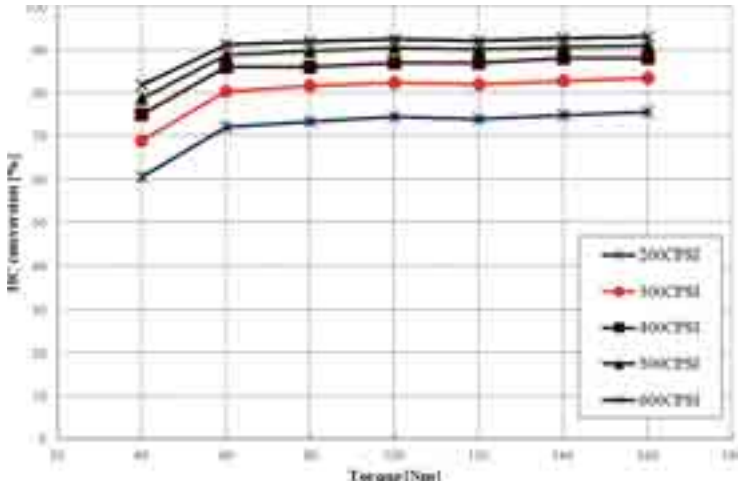

Fig. 8. The simulation computations concerning the influence of the change in the solid cell packing density at a constant solid volume of 1.4 dm^3 on the change of the HC conversion

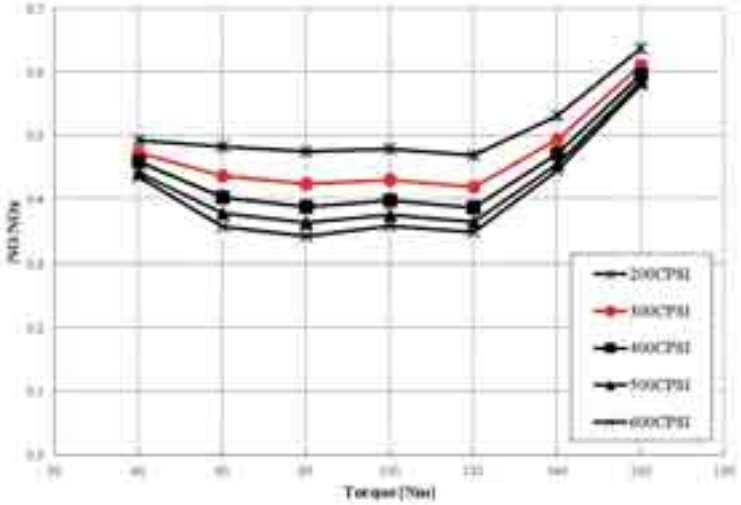

Fig. 9. The simulation computations concerning the influence of the change in the solid cell packing density at a constant solid volume of 1.4 dm^3 on the change of the content of NO in NO_x

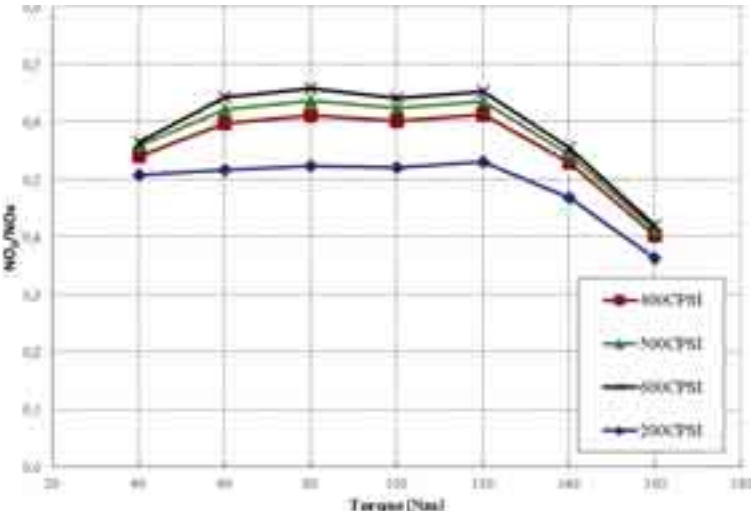

Fig. 10. The simulation computations concerning the influence of the change in the solid cell packing density at a constant solid volume of 1.4 dm^3 on the change of the content of NO_2 in NO_x

4. Conclusions

Basing on the simulation computation results obtained from the AVL Boost application, the following conclusions could have been drawn:

- the used Aftertreatment module of the AVL Boost application allows for easy simulation of the sole processes that take place in the exhaust gas treatment systems without the need to design the entire combustion engine,
- The highest CO and HC conversion levels as well as the highest content of NO_2 in NO_x have been obtained in the case of the reactor of the highest simulated volume of 2.2. dm^3. At the same time, this reactor featured the lowest content of NO in NO_x of all simulated reactors of the cell packing density of 400 cpsi,
- if the simulated cpsi value is constant and equals to 400 and the reactor volume is increased the CO and HC conversion is also higher as well as the content of NO_2 in NO_x but the content of NO in NO_x is lower whereas rate at which these parameters raise decreases as the reactor volume is increased,
- The highest CO and HC conversion levels as well as the highest content of NO_2 in NO_x have been obtained in the case of the reactor of the highest simulated cell packing density of 600 cpsi. At the same time, this reactor featured the lowest content of NO in NO_x of all simulated reactors of the solid volume of 1.4 dm^3,
- if the simulated reactor solid volume is constant and equals to 1.4 dm^3 and the cell packing density is increased the CO and HC conversion is also higher as well as the content of NO_2 in NO_x but the content of NO in NO_x is lower whereas rate at which these parameters raise is clearly decreased as the cell packing volume is increased,

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