System catalytic neutralization control of combustion engines waste gases in mining technologies

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Abstract. The paper presents the problems solution of the atmospheric air pollution with the exhaust gases of the internal combustion engines, used in mining technologies. Such engines are used in excavators, bulldozers, dump trucks, diesel locomotives in loading and unloading processes and during transportation of minerals. NOₓ, CO, CH emissions as the waste gases occur during engine operation, the concentration of which must be reduced to the standard limits. The various methods and means are used for the problem solution, one of which is neutralization based on platinum catalysts. A mathematical model of a controlled catalytic neutralization system is proposed. The simulation results confirm the increase in efficiency at start-up and low engine load and the increase in the catalyst lifetime.

1. Introduction

The catalytic converters [1] are used to reduce the level of the harmful waste gases (WG) of internal combustion engines. The increase of the chemical neutralization processes rate of WG is achieved using special catalyst constructions. Three basic processes occur when gases pass along surfaces covered with an active catalytic layer: adsorption, actual chemical reactions and desorption.

The rates of the reactions of the CH and CO to CO₂ and H₂O conversion increase in the oxidative neutralizers. Free oxygen is required to operate such neutralizer. Therefore, the additional amount of oxygen is introduced before the neutralizer into the WG flow (with secondary air) in an engine with a spark ignition for α<1. The catalysts operate at a temperature of 300...600°C, and basically platinum and also palladium are used in them.

The operation of catalysts without the catalysis process controlling based on the amounts of CO, NOₓ, CH measured using stoichiometric coefficients does not ensure their rational application in efficiency and resource. The considered control system for neutralization of WG allows one to increase the rate of neutralization chemical reaction of the harmful substances; that is why, the level of WG of the engine will be reduced.
2. Catalyst controlled heating

As a control mode, it is proposed to use the process of electric catalyst controlled heating to its operating temperatures in addition to the uncontrolled process of heating the catalyst with hot gases.

An analysis of the results [1, 2] of experimental studies of open WG neutralization systems with the catalyst produced by Continental Emitec GmbH [3] according to the MNEDC (Modified New European Driving Cycle) method allowed one to obtain the temperature dependence of the catalyst heater as a function of time in the form \( T^\circ = 0.0002t^3 - 0.0499t^2 + 4.7519t + 26.567 \) (Figure 1).

![Figure 1. Dependence of temperature of catalyst heating on time](image)

The curve showed that the output of the catalyst to the operating modes occurs in 100-120 s.

3. Mathematical model of catalyst

The measured WG concentrations are transferred to the controller in the catalytic converter system which controls the heater located in the catalyst, leading it to the optimum operating temperature in the automatic control mode. At the same time, the WG concentration is minimized in accordance with the maximum permissible concentration in the automatic stabilization mode. The evaluation of the system indicators is based on the modeling of the system [4, 5] in accordance with the principles outlined in [6, 7].

The catalyst behavior is described by a system of nonlinear differential equations [2]:

\[
\frac{dX_O}{dt} = -k_1 X_O Q^n + k_0 Q^{n+} \\
\frac{dQ}{dt} = -k_1 X_O Q^n + k_4 Q^{n+} - k_2 X_{CO} Q^n + k_3 Q_{pCO} + k_3 Q_{pCO} Q^{n-} \\
\frac{dQ_{pCO}}{dt} = k_6 X_{CO} Q^n - k_4 Q^{n+} - k_3 Q_{pCO} Q^{n-} \\
\frac{dX_{CO}}{dt} = -k_2 X_{CO} Q^n + k_4 Q_{pCO} \\
\frac{dQ_{pCO}}{dt} = k_6 X_{CO} Q^n - k_4 Q^{n+} - k_3 Q_{pCO} Q^{n-} \\
\frac{dX_{CO_2}}{dt} = k_3 Q_{pCO} Q^{n-}
\]

where

\( X_O, X_{CO}, X_{CO_2} \) – molar concentration \( O_2, CO, CO_2, \) mol/m³.
$Q_{Pt}$, $Q_{PtO}$, $Q_{PtCO}$ – surface concentration Pt, PtO, PtCO, mol/m$^2$;

$k_{\text{i}}$ - the rate coefficients for the forward reaction of the second order for the surface environment, m$^3$/mol*s;

$k_{\text{-i}}$ - the rate coefficients for the reverse reaction of the second order for the surface environment, m$^3$/mol*s;

$k_{\text{1}}$ - the rate coefficients for the forward reaction of the second order for a gaseous medium, m$^3$/mol*s;

$k_{\text{2}}$ - the rate coefficients for the forward reaction of the second order for a gaseous medium, m$^3$/mol*s;

$k_{\text{1}-}$ - the rate coefficients for the reverse reaction of the first order, 1/s;

$k_{\text{3}}$ - the rate coefficients for the forward reaction of the third order for the surface environment, m$^3$/mol*s;

$k_{\text{3}-}$ - the rate coefficients for the forward reaction of the second order for the surface environment, m$^3$/mol*s.

The general view of the model in the Simulink is:

Figure 2. General view of the model in the Simulink

The constants and the solution of the system are implemented using subsystems. All subsystems used are shown below.
Figure 3. The definition of constant values
Figure 4. The decision system is implemented using subsystems: a – equation (1); b – equation (2); c - equation (4) and (5); d - equation (3) and (6).

4. The simulation results
The analysis of the catalytic process dynamics based on the mathematical model of the catalyst was performed by the method of mathematical modeling in Simulink. The purpose of this analysis is to determine the dependence of the concentration of WG on temperature changes in the catalyst and the concentration minimization time of harmful emissions to the standard limits.

The solution of the system of differential equations (1) ÷ (6) with the initial conditions $X_{O_2}(0), Q_{Pt}(0), Q_{PtO}(0), X_{CO}(0), Q_{PtCO}(0), X_{CO_2}(0)$ is carried out with frozen coefficients at discrete values of T. The discrete temperature values are selected in the operating range of the catalyst operating temperatures of $200 ^\circ C < T < 700 ^\circ C$.

The temperature change in the catalyst as a function of time is known from experimental data [8]. Figure 5 shows these relationships for catalysts without electrical heating.

Figure 5. The change in exhaust gas temperature before and after the catalyst over time
The obtained graphic dependences illustrate the CO concentration decrease and the CO\textsubscript{2} concentration increase with temperature increasing.

The analysis of the time values corresponding to the output values of PtCO, PtO, O\textsubscript{2}, CO, CO\textsubscript{2} which correspond to maximum permissible limit of CO could be fulfilled on the basis of the graphs for fixed T with a step of 50°K. It is possible to present the same dependences for other harmful substances.

5. Conclusion
The solution of system of equations allows analysing the dynamics of changes in concentrations of CO, CO\textsubscript{2} and related parameters at a fixed temperature of WG in function of time. Both increasing the efficiency of work and resource of the catalyst with increasing temperature and the required temperature mode for the concentration outlet of CO, CO\textsubscript{2} were revealed in a given regulatory corridor for the minimum time.

To maximize the speed of the process it is necessary to increase the temperature of the electrical heating in modes of low engine load or idle running. This will allow one to reduce the WG concentration according to [9, 10] with the controlled heating application when loading and unloading processes and transportation of minerals are performed and to increase the lifetime of the catalyst.

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