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Diagnosing catalytic converters based on gas temperature measurement

Abstract: The article presents methodology of experimental, simulated catalytic converter deactivation tests and measurements of the temperature changes of the exhaust gases flowing through a tested catalytic converter mounted in the exhaust system of the Rover 1.4 engine and operating in steady conditions. The energy balance of the catalytic converter has been presented, based on the equation which allows to calculate the exhaust gas temperature change in this converter, depending on the intensity of the chemical reactions occurring in it, and its technical condition. This in turn allowed to assess the effectiveness of the catalytic converter and to formulate diagnostic evaluation criteria for the trifunctional catalytic converter.

Keywords: *catalytic converter, monitoring, diagnostic*

Diagnozowanie reaktorów katalitycznych spalin w oparciu o pomiary temperatury spalin

Streszczenie: W artykule przedstawiono metodykę eksperymentalnych, symulacyjnych badań dezaktywacji reaktora katalitycznego oraz pomiary zmiany temperatury spalin przepływających przez badany reaktor katalityczny zamontowany w układzie wylotowym silnika Rover 1,4 pracującego w warunkach ustalonych. Przedstawiono energetyczny bilans reaktora katalitycznego, w oparciu o równanie którego wyznaczono zależność pozwalającą na obliczenie zmiany temperatury spalin w tym reaktorze w zależności od intensywności reakcji chemicznych w nim zachodzących i jego stanu technicznego, co pozwoliło dokonać oceny skuteczności działania reaktora katalitycznego i sformułować kryteria oceny diagnostycznej trójfunkcyjnego reaktora katalitycznego spalin.

Słowa kluczowe: *reaktor katalityczny, monitoring, diagnostyka*

1. Introduction

A commonly used means of reducing emissions of harmful exhaust components of diesel engines, next to systematic improvement of cycle processes' quality, is to apply a catalytic converter in an engines' exhaust system. However, long-term exploitation of catalytic converters, varying quality of engine fuels, complex construction of converters and low concentration of noble metals make catalytic converters vulnerable to deactivation and ageing. Consequently, one can easily note a drastic decrease in the level of oxidation of carbon monoxide and carbohydrates as well as decreased reduction of nitric oxides. That in turn has a marked influence on the general level of emissions of those substances into the atmosphere by the monitored vehicle. Therefore the assessment of efficiency of catalytic converter should be constantly monitored by the system diagnosing performance of the vehicle. The diagnostics of the converter is deemed a manner of collecting information on its real condition, i.e. on its capability to reduce the emissions of toxic substances within the exhaust fumes. Applying on-board diagnostics (OBD) results in the necessity to continuously monitor performance of systems emitting harmful exhausts' components. Europe and the USA have had their criteria specified of inoperability of catalytic converters which always base on the admissible increment in carbohydrates' emission. The criteria in the USA refer to the results of emission measurements acquired in a FTP 75 test whereas in Europe they refer to the results of emission measurements acquired in a UDC+EUDC test [4, 5].

2. Method of diagnosing catalytic converter based on exhausts' temperature measurements.

Method of diagnosing catalytic converter basing on exhaust's temperature measurements is also carried out in an indirect manner. The condition of a converter is assessed basing on measurements of exhausts' temperature before and behind the converter [4].

Pursuant to other method of monitoring thermal condition of the catalytic converter the sensors have been located at the inflow and outflow of exhaust catalytic converter [4]. The sensors have been placed in line with the direction of exhausts' flow (Figure 5.). An experimental simulation of catalytic converter's activeness has been performed over the course of the method. To that end nearly real conditions were assumed of flow of exhausts' through the Rover 1.4 petrol engine fitted with exhaust catalytic converter.

Accordingly, two metal monoliths have been prepared: the active (with a middle layer and a catalytic layer made of noble metals: platinum and rhodium) and inactive one (with no middle layer and catalytic layer made of noble metals). Both of them were divided into eight equal segments. These segments have been mounted to the casing of the converter in the way which guarantees the continuity of overflow of exhausts' as well as tightness between the monolith and converter's wall. The experimental simulation of deactivation was carried out through the replacement of active monolith segments on the front of the converter with the inactive monolith segments (Figure 5.). as in that section the converter loses the most of its activeness. The experiment resulted in two different values of converter activeness (A) from A = 100% to A = 0% with the step of 12.5%. [4]

The exhausts' temperature measurement taken before and behind the converter was carried out for each level of activeness of catalytic converter at engine's rotational speed of n = 2000, 3000 and 4000 $min^{-1} \pm 25\ min^{-1}$ and for three different loads of engine M_e = 36, 46, 56 ±3 N·m. For those parameters of engine's operation the composition of combustible mixture is stoichiometric and the catalytic converter's efficiency in neutralizing the exhausts boasts the greatest values.

The percentage value of catalytic converter's activeness has been defined as a ratio of active segments' volume V_a to the entire converter's volume V_k [4].

$$A = \frac{V_a}{V_k} \tag{1}$$

The experiments have been carried out at a constant environment temperature of 298 K. It has been assumed that the exchange of heat between the catalytic converter and the environment takes place through a convective heat transfer. Each measurement was initiated after 120 s calculated from the moment of arriving at stable engine working conditions (rotational speed and load). The values of exhausts' temperature measurements before and behind the converter are constantly changing. That can result in false readings of temperature differences. Over the course of experiments converter walls' temperature was measured as well. The measurement was made using thermo elements deployed in three points on the converter's surface. The temperature of the converter's wall was defined as an arithmetic mean obtained basing on the measurements made. During each measurement the volumes of consumed fuel were equal at 50 cm^3 [4].

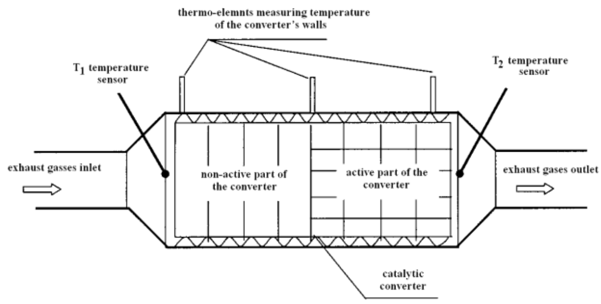

Fig. 1 Diagram of the catalytic converter 50% active [4]

2.1. Evaluation of the converter's condition based on the experimental tests.

The efficiency of catalytic converter has been assessed basing on the level of conversion of carboxide, carbohydrates and nitric oxides making up the exhausts flowing through the converter. The composition of the exhausts before and behind the catalytic converter served to calculate the value of conversion of harmful components: k_{CO}, k_{HC}, k_{NOx} [4].

Conversion translates into a ratio of drop in value of concentration of exhausts' component measured at the inflow and outflow of the converter ($C_{x1} - C_{x2}$) to the value of concentration of the component at the outflow of the converter (C_{x1}). A drop in the value of concentration of exhausts' components in the converter results from chemical reactions occurring within the converter.

The value of component conversion (C) within the converter has been calculated using the following pattern:

$$k_X = \frac{C_{x1} - C_{x2}}{C_{x1}} \tag{2}$$

In the method based on the measurement of the exhausts' temperature difference the diagnostic signal ΔT has been defined as a difference in exhausts' temperature measured before and behind the converter. The difference in the exhausts' temperature is caused by the exothermal reactions of oxidizing carboxide and carbohydrates; reductions of nitric oxide within the converter as well as by convective transfer of heat within the converter [4]:

$$\Delta T = T_2 - T_1 \tag{3}$$

Figure 2 presents the dependency of conversion of carboxide k_{CO}, carbohydrates k_{HC} and nitric oxides k_{NOx} with the use of a function of an experimentally simulated catalytic converter activeness (A). Increase in the activeness of converter is accompanied by the increase of conversion of carboxide k_{CO}, carbohydrates k_{HC} and nitric oxides k_{NOx}. The following diagram demonstrates that with the activeness at the level of 12.5%, the conversion rate of the three components is relatively high and accounts for about 70%. That is caused by the principles of selecting converters for the engines, which take into account their deactivation over the course of exploitation [4].

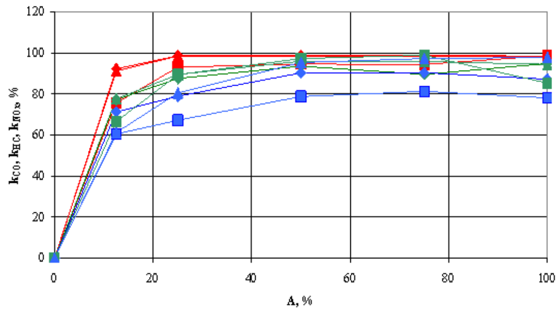

Fig. 2. Dependency of the conversion of carboxide k_{CO}, carbohydrates k_{HC} and nitric oxides k_{NOx} according to the experimentally simulated activeness of exhausts' catalytic converter A [4]

k_{CO} = f(A) at n =2000 rpm
k_{CO} = f(A) at n =3000 rpm
k_{CO} = f(A) at n =4000 rpm
k_{HC} = f(A) at n =2000 rpm
k_{HC} = f(A) at n =3000 rpm
k_{HC} = f(A) at n =4000 rpm
k_{NOx} = f(A) at n =2000 rpm
k_{NOx} = f(A) at n =3000 rpm
k_{NOx} = f(A) at n =4000 rpm

Picture 3 presents the dependency of the experimental increment of the exhausts' temperature difference ΔT_b at the inflow and outflow of the converter according to the experimentally simulated activeness of the catalytic converter (A).

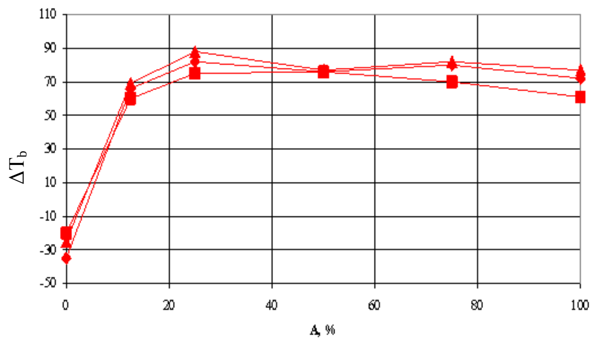

Fig. 4. Comparison of experimental increment of temperature difference ΔT_b at the inflow and outflow of the converter depending on the experimentally simulated activeness of exhausts' catalytic converter (A) [4].

ΔT_b = f(A) przy n =2000 obr/min
ΔT_b = f(A) przy n =3000 obr/min
ΔT_b = f(A) przy n =4000 obr/min

3. Energy balance of the trifunctional exhausts catalytic converter

When preparing the energy balance of the trifunctional catalytic converter, the following assumptions were made [4]:

- converter is operating at steady operating conditions of the internal combustion engine,
- flow of exhausts of known composition at the inlet and outlet of the converter is an l-dimensional flow
- exhaust gas flow takes place in a single channel, in which the convection heat exchange takes place between the exhausts and the walls of the channel, inside the reactor there are four basic reactions taking place: oxidation of carbon monoxide, hydrocarbons and hydrogen and the reduction of nitrogen oxides for which thermal effects are being determined.

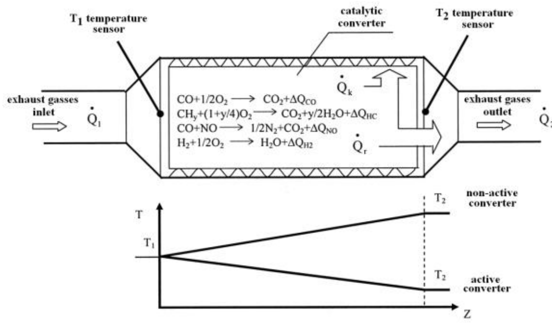

Fig. 5 Diagram of the trifunctional catalytic converter [4]:

$\dot{Q}_1$ - The power of the stream of heat supplied to the converter together with the exhaust gases (heat stream created by the processes occurring in the engine directed further with the exhausts to the converter);

$\dot{Q}_r$ - The power of the internal heat source stream in the catalytic converter (stream formed by an exothermic reaction, oxidation of carbon monoxide, hydrogen and hydrocarbons and reduction of nitrogen oxides);

$\dot{Q}_k$ - The power of heat flux convectionally transferred to the catalytic converter substrate (the heat flux transferred from the exhaust gases to the catalytic converter substrate and further to the walls of the converter);

$\dot{Q}_2$ - The power of the heat flux carried away with the exhaust gases flowing out from the converter.

Carbon monoxide, hydrocarbons, and hydrogen are oxidized by oxygen, while nitrogen oxides are reduced by carbon monoxide. Inside the converter, there are four basic reactions that are taken into consideration:

$$CO + 0,5O_2 \rightarrow CO_2 + \dot{Q}_{CO} \qquad (4)$$

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O + \dot{Q}_{HC} \qquad (5)$$

$$H_2 + 0,5O_2 \rightarrow H_2O + \dot{Q}_{H_2} \qquad (6)$$

$$CO + NO \rightarrow CO_2 + 0,5N_2 + \dot{Q}_{NO} \qquad (7)$$

In the reaction (5) propane (C_3H_8) represents hydrocarbons - because this compound is most prolific in the exhaust gases. In the reaction (7) nitric oxide represents nitrogen oxides contained in the exhaust gases. This oxide is formed as the only one, as a result of direct synthesis of oxygen and nitrogen.

The observed temperature rise is caused by the sum of heats emitted during the oxidation reaction of CO, HC and H_2 and reduction of NO_x (4 ÷ 7). Temperature increase of exhaust gases flowing through the reactor is a measure of the total activity of the catalytic converter.

The heat balance equation in the converter is as follows:

$$\dot{Q}_1 + \dot{Q}_r - \dot{Q}_k - \dot{Q}_2 = 0 \qquad (8)$$

1) Power of the exhaust heat flux $\dot{Q}_1$ at the converter inlet is calculated in relation to the temperature T_o:

$$\dot{Q}_1 = \dot{M}_s \cdot \mu c_{p1} \cdot \Big|_{T_o}^{T_1} (T_1 - T_o), \mathrm{W} \qquad (9)$$

2) Power of the internal heat source stream $\dot{Q}_r$ in the catalytic converter:

$$\dot{Q}_r = \Delta \dot{M}_{CO} \cdot Q_{pCO} + \Delta \dot{M}_{HC} \cdot Q_{pHC} + \Delta \dot{M}_{H_2} \cdot Q_{pH_2} + \Delta \dot{M}_{NO} \cdot Q_{pNO}, \mathrm{W} \qquad (10)$$

3) Power of heat flux $\dot{Q}_k$ transferred to the catalytic converter:

$$\dot{Q}_k = \pi \cdot D_z \cdot L \cdot \alpha_p \cdot \left(\frac{T_2 + T_1}{2} - T_{sc} \right), \mathrm{W} \qquad (11)$$

4) Power of heat flux $\dot{Q}_2$ carried away with the exhaust gases flowing out from the converter are calculated in relation to the temperature T_o:

$$\dot{Q}_2 = \dot{M}_s \cdot \mu c_{p2} \cdot \Big|_{T_o}^{T_2} (T_2 - T_o), \mathrm{W} \qquad (12)$$

Where:

D_z – substitute diameter of the converter, m

L – length of the converter, m

$\dot{M}_s$ – molar expenditure of the exhausts flowing out of the engine, kmol / s

$\Delta \dot{M}_{CO}$, $\Delta \dot{M}_{HC}$, $\Delta \dot{M}_{H2}$, $\Delta \dot{M}_{NO}$ – molar expenditure of the oxidizable reactants CO, HC, H_2 and reducing the NO in the catalytic converter, kmol/s

Q_{pCO}, Q_{pHC}, Q_{pH2}, Q_{pNO} – thermal effects of oxidation of CO, HC, H2 and reduction of NO taking place in the converter, J/kmol

T_{sc} – average surface temperature of the catalytic converter walls acquiring heat, K

T_1 – temperature of the exhaust gases at the inlet to the converter, K

T_2 – temperature of the exhaust gases at the outlet from the converter, K

T_o – ambient temperature, K

α_p – heat transfer coefficient, $W/m^2 \cdot K$

μc_{p1} – average molar specific heat of the exhaust gases at constant pressure at the inlet into the converter, J/kmol·K

μc_{p2} – average molar specific heat of the exhaust gases at a constant pressure at the outlet from the converter, J/kmol·K.

Block diagram of the algorithm used to determine the gas temperature difference (T2-T1), being a diagnostic signal, is shown on the Figure 5.

Data:
- engine technical specifications: D_c, S, ε, z,
- fuel characteristics: ρ_{pal}, W_u,
- engine operating conditions: n, M_e, V_p, t_p, ΔT_{ss}, Δp_{ss},
- measurement results of the concentrations of CO, O_2, CO_2, HC, NO_x.

↓

Calculation of:
- fuel dose per one engine cycle q_c,
- amount of the working medium performing M_{czr} engine cycle,
- air excess coefficient of the fuel mixture λ.

↓

Determining:
- temperature of the end of the cylinder filling process T_a,
- temperature of the end of the compression process T_c,
- maximum combustion temperature of the fuel mixture T_z,
- expansion process temperature T_w,
- exhaust gases temperature at the inlet to the catalytic converter T_1.

↓

Determining:
- exhausts flow rate through the catalytic converter $\dot{M}_s$,
- volumetric exhausts flow intensity SV,
- difference in molar expenditure of carbon monoxide $\Delta\dot{M}_{CO}$, hydrocarbons $\Delta\dot{M}_{HC}$, nitrogen oxides $\Delta\dot{M}_{NOx}$ and hydrogen $\Delta\dot{M}_{H2}$,
- thermal effects of the oxidation reaction of CO, HC and H_2 and reduction of NO_x occurring in the catalytic converter.

Determining:
- power of the exhausts heat stream $\dot{Q}_1$ at the inlet to the converter,
- power of the internal heat source stream $\dot{Q}_r$ in the catalytic converter,
- power of the exhausts heat stream $\dot{Q}_k$ transmitted to the substrate of the catalytic converter,

Calculating:
- exhausts temperature T_2 at the outlet of the catalytic converter,
- exhausts temperature difference $(T_2 - T_1)$ which is a diagnostic signal for the catalytic converter,
- diagnostic index $I_T = \frac{|\Delta T|}{T_o} = \frac{|T_2 - T_1|}{T_o}$.

Fig. 5. Block diagram of the algorithm used to determine the gas temperature difference (T2-T1) being a diagnostic signal [4].

Figure 6 shows the dependence of the total amount of heat expenditure resulting from the oxidation reaction of carbon monoxide, hydrocarbons and nitrogen oxides reduction, depending on the experimentally simulated activity A and for three different load-velocity conditions of the engine. With the increase in the activity of the converter total heat expenditure resulting from the oxidation reaction of carbon monoxide, hydrocarbons and nitrogen oxides reduction increases. This is due to the fact that as a result of chemical reactions occurring within the converter and increasing activity of the converter, the amount of released heat increases.

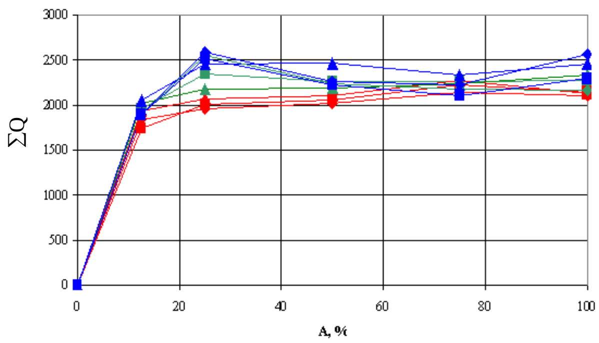

Figure 6. Dependence of amount of heat expenditure $\sum\dot{Q}$ generated in the reactor due to the oxidation reaction of carbon monoxide, hydrocarbons, hydrogen and nitrogen oxides reduction as a function of the experimentally simulated activity of the converter A, and three crankshaft rotational speeds of the engine [4].

- $\sum\dot{Q} = f(A)$ at M_e = 36 Nm and n = 2000 RPM
- $\sum\dot{Q} = f(A)$ at M_e = 45 Nm and n = 2000 RPM
- $\sum\dot{Q} = f(A)$ at M_e = 60 Nm and n = 2000 RPM
- $\sum\dot{Q} = f(A)$ at M_e = 36 Nm and n = 3000 RPM
- $\sum\dot{Q} = f(A)$ at M_e = 45 Nm and n = 3000 RPM
- $\sum\dot{Q} = f(A)$ at M_e = 60 Nm and n = 3000 RPM
- $\sum\dot{Q} = f(A)$ at M_e = 36 Nm and n = 4000 RPM
- $\sum\dot{Q} = f(A)$ at M_e = 45 Nm and n = 4000 RPM
- $\sum\dot{Q} = f(A)$ at M_e = 60 Nm and n = 4000 RPM

3.1. Evaluation of the effectiveness of catalytic converter diagnosing methodology.

Based on the analysis of experimental tests results and the calculations made, it can be concluded that with the decrease in activity of the converter is followed by the fall in the value of the converter temperature increase of the exhaust gases flowing through the converter. This is due to a smaller amount of heat released in the converter at the time of the exothermic reactions taking place and resulting in neutralization of harmful exhaust gasses content. If the converter is active, the chemical reactions occurring in it result in the production of more heat in the reactor, causing a significant increase in the temperature of the exhaust gases flowing through. The paper states that in order to regard catalytic converter as an inactive, its activity should be less than the activity of about 20%. With this activity the temperature difference ΔT is still about 70K (Fig. 7) The calculated value of the temperature difference ΔT for the reactor with activity greater than 20% was ΔT = 80K. Thus, from the analysis of ΔT determined experimentally and numerically, with the activity of the converter of about 20% it appears that the ΔT value error obtained based on the proposed catalytic converter energy model solution, is approximately 14%. The value of this error depends on the number of chemical reactions taken into consideration, that occur in the converter and the accuracy of determining the thermal effects of these reactions as well as the accuracy of the calculations of the amount of heat convectionally transferred by the exhaust gases to the catalytic converter substrate. With a further decrease in activity of the converter, the exhaust temperature increase slows down below 70K, and can even achieve a negative value. This means that the exhaust gases temperature behind the converter is lower than the exhaust gases temperature upstream of the converter. This can be explained by the fact that, with the quantity of heat generated in the reactor striving towards zero, the heat transmitted by the exhaust gases to the catalytic converter substrate, causes cooling of the exhaust gases, and so the difference $T_2 - T_1$ takes the negative values. Catalytic converter in this case should be considered inactive and be replaced.

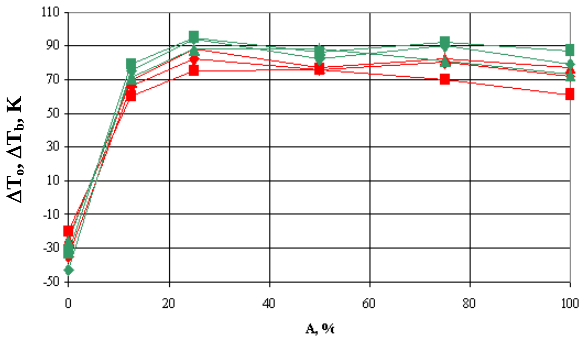

Figure 7. Comparison of experimental ΔT_b and calculated ΔT_o of the increase in the difference of the exhaust gases temperatures at the inlet and outlet of the converter according to the experimentally simulated exhausts catalytic converter activity - A [4].

ΔT_b = f(A) at n =2000 RPM
ΔT_b = f(A) at n =3000 RPM
ΔT_b = f(A) at n =4000 RPM

ΔT_o = f(A) at n =2000 RPM
ΔT_o = f(A) at n =3000 RPM
ΔT_o = f(A) at n =4000 RPM

4. Summary.

The paper presents the methodology and results of experimental studies and the results of calculations enabling evaluation of the functionality of trifunctional catalytic converter operation. To assess the functionality of the aforementioned converter and its technical condition, the diagnostic signal was used, which was the exhausts temperature difference determined at the inlet and outlet of the exhaust gases from the converter. The difference of the above mentioned exhaust gas temperatures were determined in two ways: experimentally and computationally based on the energy balance of the catalytic converter. The determined temperature difference depends on the amount of harmful components in the exhaust gases flowing through the converter and from the completeness of the exothermic reactions taking place within the converter. Chemical reactions in an active converter cause the raise of the exhaust gases temperature at the outlet of the converter, when the amount of heat evolved during the exothermic reactions occurring in the converter is greater than the amount of heat convectionally transferred by the exhaust gases to the catalytic converter.

The measurement of the temperature differences $\Delta T = T_2 - T_1$, which is a diagnostic signal, requires an accurate, durable temperature sensor of low thermal inertia, adapted to the measurement of high temperatures in a chemically aggressive exhaust gases. Durability of these sensors should correspond to about 100 thousand km of the car mileage.

The methodology, developed and presented in this paper can be applied to evaluation of the technical condition of the catalytic converter only in the steady operating conditions of the engine. Temperature measurements made under transient engine operating conditions may cause quite significant errors in determining the value of the temperature difference ΔT. In practice, in order to improve the accuracy of diagnosing trifunctional catalytic converter, this method can be used in combination with the method of diagnosis based on the measurement of oxygen concentration. The combination of these two methods will allow more reliable assessment of functionality of the catalytic converter tested.

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