PARAMETER ANALYSIS OF NO EMISSIONS FROM SPARK IGNITION ENGINES

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Abstract. Environmental protection, especially a reduction in emissions from vehicles, bears great importance nowadays. Combustion engine manufacturers invest large sums of money in order to cut the emission of carbon monoxide (CO), unburnt hydro carbons (CH or THC), carbon dioxide (CO_2) and nitrogen oxides (NO_x). To variously reduce NO_x emission either inside (e.g. exhaust gas recirculation) and/or outside the engine (like three-way catalyst), different solutions have been elaborated. The most expedient methods are, however, those reducing NO_x during the process of combustion itself. Modelling and parameter analysis of NO_x formation in combustion engines provide a new possibility of optimizing engine combustion and operation. To accomplish the above objective, the author of the article has developed a computer model that calculates the thermo-formation of NO by means of the Zeldowich mechanism and applied a multi-zone model for making calculations.

Keywords: parameter analysis, NO emission, model, simulation.

1. Introduction

The most important form of reactive nitrogen in the air is nitrogen dioxide (NO_2). Nitrogen oxides formed in combustion are the oxidation of molecular nitrogen in the post flame zone (thermal NO), the formation of NO in the flame zone (prompt NO) and the oxidation of nitrogen containing compounds in the fuel (fuel NO) (Warnatz, Maas 1993*)*. As for internal combustion engines, NO mainly arises and oxidizes to NO_2 in the atmosphere (Cheremisinoff, Young 1977) which is hazardous to the environment. Therefore, nitrogen monoxide (NO) and nitrogen dioxide (NO_2) together are called NO_x. Vehicle engines operate at sufficiently high temperatures, which is enough to break down the oxygen molecule.

The current statistical dataset shows that Hungarian transport related to a decrease in NO_x emission is slowing down compared to other transport related gas emissions (Fig. 1) (Zöldy 2009; Tánczos, Török 2007).

Catalytic converters fitted to cars decrease the production of the above introduced harmful compounds. To find out NO_x emissions from internal combustion engines, first, we have to know the mechanism of NO_x formation and possess a set of data that includes all information necessary for calculating the formation mechanism that has been extensively studied (Eyzat, Guibet

1968; Bartels, Mollenhauer 1994; Weisser, Boulouchos 1995; Miller, Bowman 1989*)*.

The present study does not contain the prompt and fuel specific NO formation considering their insignificant character in internal combustion engines. Also, the paper does not include NO_2 formation during combustion or NO oxidation. For this reason, the author has built up a computer model that calculates the thermo formation of NO employing the Zeldovich (1946) mech-
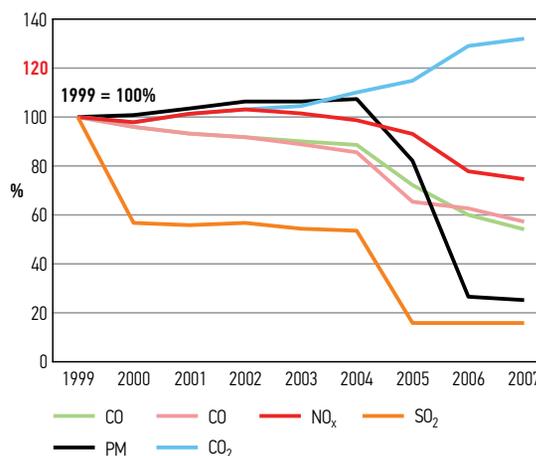

Fig. 1. Transport related emission in Hungary

anism. Due to the applied multi-zone model, the influence of different combustion parameters and boundary conditions (intake pressure, temperature, speed, etc.) of NO emission can be analysed.

2. The Mechanism of Thermal NO Formation

The mechanism of thermal NO formation has been laid by Zeldovich (1946) following the theory of which, O_2 molecules in the air are decomposed into active Oxygen atoms that come to reaction with N_2 molecules in the air and develop NO and N (Komiyama, Heywood 1973; Heywood 1988; Boschán, Meggyes 1989; Raine *et al.* 1995). This induces further chain reactions. Rising O comes to reaction with N_2 molecules in the air or with OH radicals developed from combustion, due to which NO repeatedly arises. At the same time, the reaction of NO decomposition can also start in a reversed way.

Considering the net rate (R_i) of chemical reactions (2, 3 and 4), changes in NO concentration can be described in the following way (1):

$$\frac{d[NO]}{d\tau} = \frac{2R_1\left(1 - \frac{[NO]^2}{[NO]_e^2}\right)}{1 + \frac{[NO]}{[NO]_e}\frac{R_1}{R_2 + R_3}}, \quad (1)$$

where:

$$k_1^+[O]_e[N_2]_e = k_1^-[NO]_e[N]_e = R_1; \quad (2)$$

$$k_2^+[N]_e[O_2]_e = k_2^-[NO]_e[O]_e = R_2; \quad (3)$$

$$k_3^+[N]_e[OH]_e = k_3^-[NO]_e[H]_e = R_3, \quad (4)$$

where: [ ] is the concentration of components; [ ]$_e$ means concentration belonging to the equilibrium condition, k_i^+ and k_i^- [cm³/mol] are forward and reverse rate constants of reactions.

3. A Thermodynamic Model

For the model of NO formation, the given pressure, volume, temperature, and time of status are required. In addition, knowledge of the gas component for given space and time is necessary. There are two ways for determining necessary input data on modelling.

The first approach (direct approach) focuses on pressure in the combustion chamber measured or calculated as a function of the crankshaft angle (Stone 1999; Gorenflo 1997). Based on the volume connected to pressure and using the uni- or two-zone model, the temperature of the zones, the combustion function and the ratio of gas components can be calculated. The basic assumption of one zone model is that the pressure and temperature of the gases in the combustion chamber is homogeneous, i.e. only the average temperature can be calculated producing incorrect results of the NO formation model. The two-zone model is more precise and describes the combustion process more adequately (Gorenflo 1997; Heider *et al.* 1998; Merker *et al.* 1993; Zöldy *et al.* 2010). There is significant difference between the two models. The two-zone model consists of two volumes that are thermally separated from each other

(Komiyama, Heywood 1973; Heywood 1988). In one separated volume, gas from the burnt fuel is produced, whereas in the other, the unburnt air-fuel mixture is stored. Temperatures for the volume unit are calculated separately.

The author of the paper used the second approach, a multi-zone model that is an indirect method for calculating the input parameters of NO formation (Raine *et al.* 1995). Input is not an indicator diagram but the combustion function and other boundary parameters (Fig. 2).

The mass of each zone (*i*) is equal to the mass of the air-fuel mixture that burns during $\varphi_{start\ of\ combustion+i}$ and $\varphi_{start\ of\ combustion+i+1}$ crankshaft rotation. In this model, combustion is done in one degree of the crank angle and the number of zones is equal to the length of combustion (end of combustion (EOC) – start of combustion (SOC)), measured in degrees (*i* = 1 to the length of combustion).

The zones are located as ring-base cylinders inside the combustion chamber for simplification. Because of the basic assumption that mass is constant during combustion in each zone and due to thermal inhomogeneity, the zones are moving and their diameters are changing (Fig. 3).
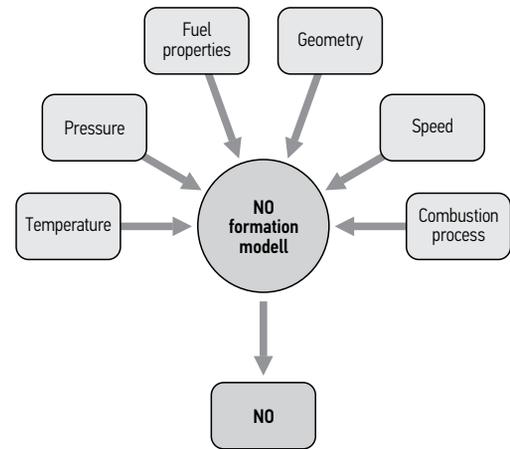

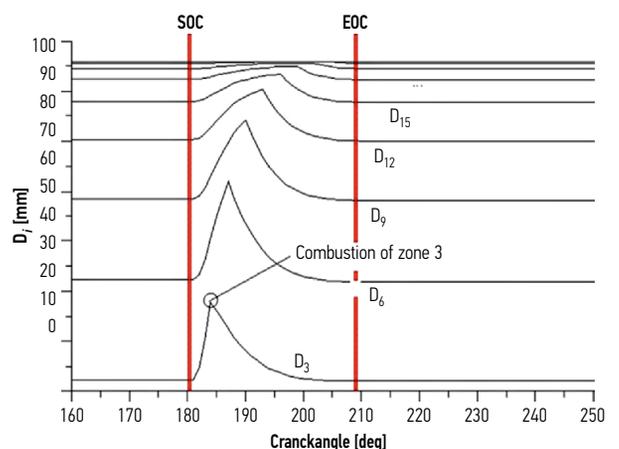**Fig. 2.** The structure of the model (*source*: own edition)

Fig. 3. The diameter of the zones in the function of the main crankshaft angle (SOC – Start of Combustion, EOC – End of Combustion, *source*: calculations were done by the author)

For calculation purposes it is accepted that during initial compression in individual volume parts, adiabatic compression and isochoric heat transfer (5) can be expressed as:

$$\frac{dT_{i,\varphi}}{d\varphi} = \frac{1}{c_{v,i,\varphi}m_i}\left(\frac{dQ_{i,\varphi}}{d\varphi} - p_\varphi\frac{dV_{i,\varphi}}{d\varphi}\right), \qquad (5)$$

where: $T_{i,\varphi}$ and $V_{i,\varphi}$ are the temperature and volume of zone 'i' in the function of crank angle (φ), $c_{v,i,\varphi}$ is the isochoric heat capacity of zone 'i' in the function of the crank angle, m_i is the mass of the zone. Also, reckoning with the contact surfaces of each zone with wall (6) equals:

$$dQ_{w,i,\varphi} = A_{i,\varphi}\alpha_\varphi(T_{w,\varphi} - T_{i,\varphi})d\tau, \qquad (6)$$

where: heat transfer coefficient (α) is calculated applying the Woschni method (Woschni 1965, 1970); $A_{i,\varphi}$ is the area of zone 'i', $T_{w,\varphi}$ is wall temperature in the function of the crank angle (φ), $T_{i,\varphi}$ is the temperature of zone 'i' in the function of the crank angle. During combustion, the flame moves successively in the zones. The temperatures of the zones can be determined from enthalpies. Flame temperature is calculated as equilibrium adiabatic flame temperature (Olikara, Borman 1975). After combustion, the zones can get more compressed (burning before the top dead centre (TDC) is reached) or expand (burning after the top dead centre); heat transmission is also considered (6). The results fit well with the values obtained from other local temperature measurements using different techniques (Rhee, Chang 1985; Bach *et al.* 1996).

When a multizone model is used, the following parameters are supposedly known: the geometry of the combusting chamber, the quality of the mixture (air-to-fuel ratio), the temperature of the air and pressure in the combustion chamber after the intake valve closes, the speed and combusted fuel proportion in the function of time/degree (combustion law) (Fig. 2). The combustion process can be described with reference to the Vibe function (7) (Vibe 1970):

$$x_b = 1 - e^{-6.809\left(\frac{\varphi - \varphi_{SOC}}{\varphi_{EOC} - \varphi_{SOC}}\right)^{m_e}}, \qquad (7)$$

where: x_b – burned mass fraction [–]; φ_{SOC} – the crank angle at the start of combustion [deg]; φ_{EOC} – the crank angle at the end of combustion [deg]; φ – the actual camshaft angle [deg]; m_e – is the shape factor or the Vibe exponent [–].

The Vibe exponent controlling the shape of the Vibe curve is shown in Fig. 4.

4. Results of the Model and Parameter Analysis

For model calculations, six different combustion processes from preliminary experiments were chosen. These processes have a different start and length of combustion, though the same shape factor was assumed (see Table).

During modelling, only one parameter has been changed once (*caeteris paribus*). In reality, a change in
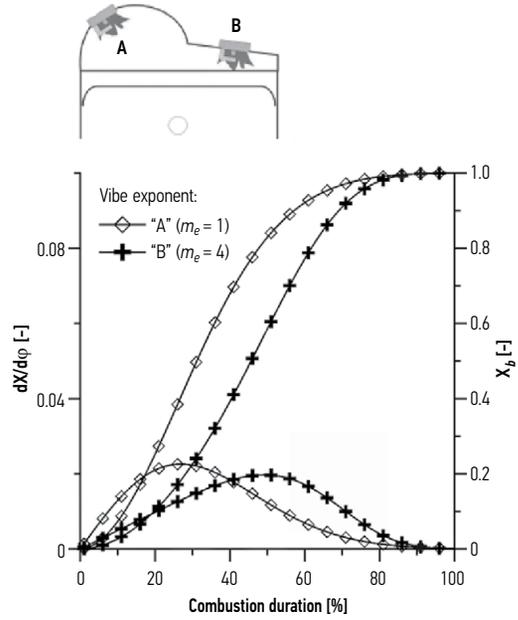

Fig. 4. Burned mass fraction and burn rate in the function of combustion duration at two different ignition points A and B (*source*: own calculations)

one parameter certainly modifies other parameters of combustion. An increase in the initial pressure of compression (e.g. load increase) results in shortening, for example, combustion. On the other hand, the applied method enables the determination of the influencing degree, which helps with understanding processes deeper, and thereby leads to cutting NO emissions.

Let us examine NO emission during the selected (e.g. 'c') combustion process, which shows arising NO concentrations in each zone.

Fig. 5 indicates that in the combusting zones before the top dead centre, temperature keeps rising due to increased compression after combustion. This increases NO concentration at the beginning, but with a small delay, following the upper dead centre, NO starts decomposing. Its concentration falls continuously until temperature goes down below 2200 K where reactions freeze. The later the zone combusts, the shorter is the period during which the temperature of the medium is above 2200 K, and at the same time, the smaller is the quantity of arising NO. The reason is related to geometry (e.g. *r/l* ratio).

Table. Combustion processes applied for parameter analysis (*source*: measurements were done by the author)

Sign	Combustion start	Combustion length	Shape factor
a.	130	90	2
b.	140	110	2
c.	150	120	2
d.	160	125	2
e.	170	130	2
f.	180	130	2

Taking into account the NO concentration of (NO_i) zones and the mass of the zone (Eq. 7), the NO concentration of the combustion process can be calculated (Heywood 1988).

A rise in the beginning temperature of compression makes NO emission significantly higher (Fig. 6).

The extent of the rise depends on ignition advance and the starting pressure of compression. In case it starts with low pressure (0.3 bar), an average rise is 20%, while the starting pressure of 0.6 bar makes 52%, and that of 0.8 bar – a 60% increase. On the basis of the above data, it can be concluded, that higher commencing pressure makes a stronger effect of temperature.

If the starting pressure of compression grows, NO emissions fall due to a decrease in dissociation. The influence of a decrease in NO depends on combustion

start: when decreasing 0.8 bar pressure by 25% (0.6 bar), 180 degree-combustion start results in 45% rise in NO emission, while 130 degree-combustion start results only in 7.8% rise in NO emission. A further decrease in pressure, which makes 63% (0.3 bar), indicates that the rise of NO emission is 170% in case of 180 degree- combustion start and 16% if combustion start reaches 130 degrees.

In case compression commences with high temperature (e.g. 400 K), the effect of pressure increase is reduced by an average of 5÷7%.

NO emission grows due to a decrease in combustion length. An increase in emission depends on combustion start (Fig. 7). If combustion commences at 170 degrees and combustion length is decreased by 30%, an increase in NO emission makes 0.7%, whereas a rise is
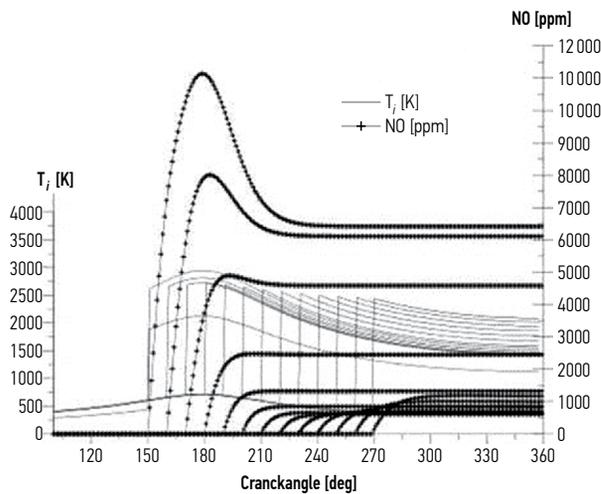

Fig. 5. The temperature and NO concentration of the zones as a function of the crank angle and NO emissions of the zones (*source*: own calculations)
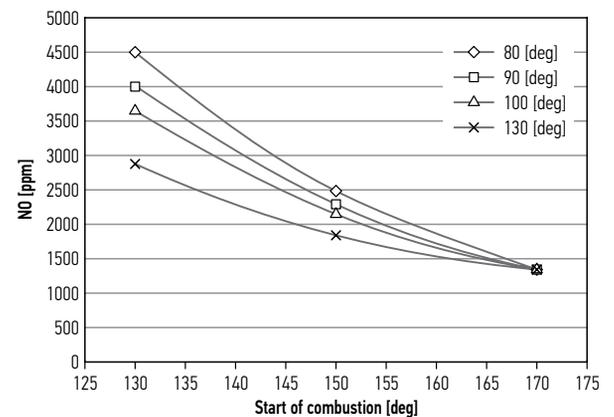

Fig. 7. The quantity of NO concentration as a function of combustion starting at a different length of combustion (*source*: own calculations)
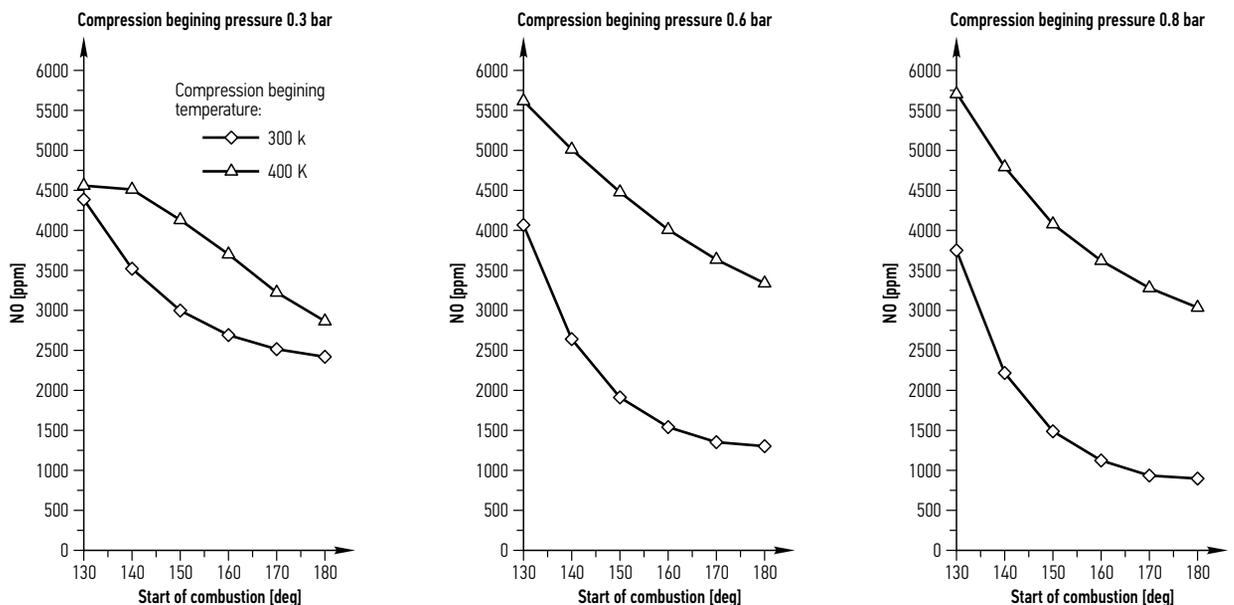

Fig. 6. NO emission as a function of combustion starting at different commencing pressures of compression (*source*: own calculations)

only 2% if combustion length is decreased by 40%. On the other hand, if combustion starts at 130 degrees and combustion length is decreased by 30%, NO emission increases by 40%, whereas a 40% decrease in combustion length induces a 55% rise.

Speed as the time parameter of NO formation holds a significant influence on emission. If speed increases, NO emission does not reach equilibrium concentration in exhaust gas, but tends towards equilibrium concentration typical of the given temperature. Fig. 8 shows that emission is always higher in lower speed ranges, except for 130 degrees and 0.3 bar combustion. This is due to increased decomposition, which can be led back to accelerating reactions in lower pressure. Emission difference grows in the function of combustion start.

The reason for explaining the above situation is that a growth in combustion start steps up the number of the zones where formation rather than decomposition grows due to a longer period.

Modifying the shape factor of the Vibe function induces a slight change in NO concentration evolved in individual mass units (Fig. 9). A significant change in NO emission is caused by mass difference in individual units. If combustion start is 180 degrees and the shape factor is decreased from $m_e = 2$ to $m_e = 1$, it makes a 1.4% decrease in NO emission; while increasing the shape factor to $m_e = 4$, emission steps up in 9%. On the other
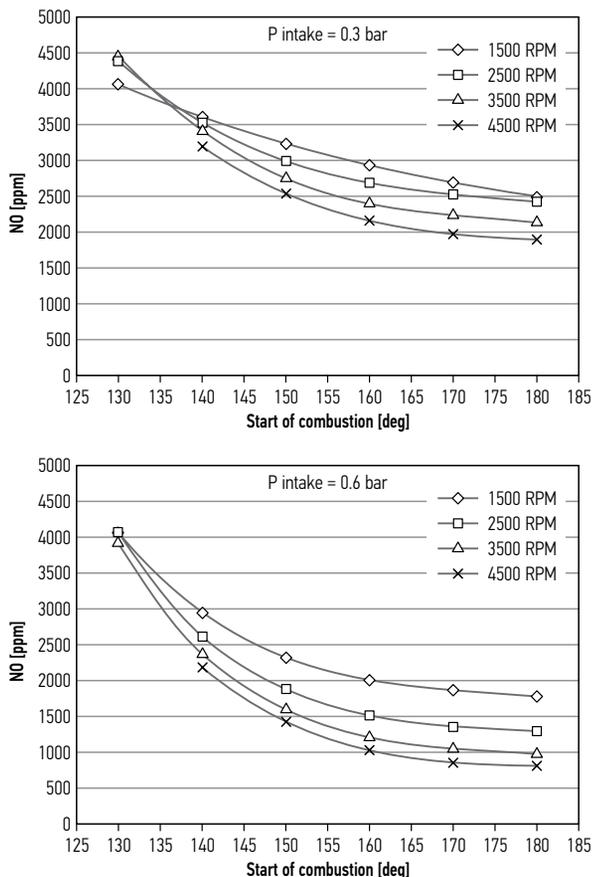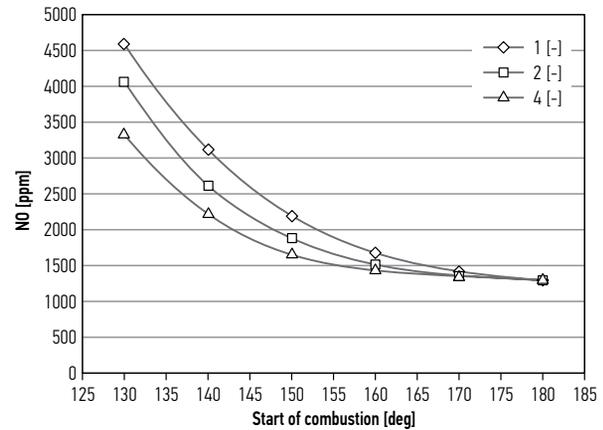

Fig. 9. NO emission as a function of combustion starting at a different shape factor of the Vibe function (*source*: own calculations)

hand, if combustion start is 130 degrees and the shape factor is decreased from $m_e = 2$ to $m_e = 1$, NO emission decreases in 13%; however, considering the shape factor of $m_e = 4$ it grows in 25%.

5. Summary

The model is a relatively simple one containing approximations, contributes to a system capable of revealing novel interrelations and provides a possibility of simultaneously examining not only NO but also a larger amount of components depending on the complexity of the mechanism. Moreover, the model is capable of analyzing efficiency and emissions at the same time.

The author of the article has investigated the influence of different parameters thus keeping other factors constant. In conclusion, the following points can be emphasized:

- high NO_x emission is caused by the zones combusted before TDC due to the fact that high temperature evolves in these zones for a considerable time;
- in case of increased spark advance, the amount of zones combusted before TDC increases, and thus emission considerably increases;
- in case of low Vibe exponent, a higher amount of the mixture burns at the beginning of the combustion process, and therefore emission increases;
- in case of the elongation of the combustion process, NO_x emission decreases because less mixture is able to burn close to TDC, thus emission decreases. However, this phenomenon is influenced by spark advance;
- in case of increased speed, duration time at high temperature decreases along with emission; nevertheless, this phenomenon is also influenced by spark advance;
- in case of an increased initial temperature of compression, emission considerably increases.

The model needs the further development of applying compression ignition engine, however, several achievements have already been utilized, e.g. alcohol–diesel fuel blends (Raslavičius, Bazaras 2010).

Fig. 8. NO emission as a function of combustion starting at different speeds and starting pressures (*source*: own calculations)

High evaporation heat of alcohol has a cooling effect on the mixture, and therefore emission decreases; in case of certain mixing ratios, alcohol combusts in the kinetic phase close to TDC (Lujaji *et al.* 2011), and therefore NO_x emission increases.

Acknowledgement

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