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A Physical Two-Zone NO_x Model Intended for Embedded Implementation

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ABSTRACT

This paper offers a two-zone NO_x model suitable for vehicle on-board, on-line implementation. Similar NO_x modeling attempts have previously been undertaken. The hereby suggested method does however offer clear and important benefits over the previously methods, utilizing a significantly different method to handle temperature calculations within the (two) different zones avoiding iterative computation. The new method significantly improves calculation speed and, most important of all, reduces implementation complexity while still maintaining reasonable accuracy and the physical interpretation of earlier suggested methods. The equations commonly used to compute NO_x emissions is also rewritten in order to suit a two-zone NO_x model. An algorithm which can be used to compute NO_x emissions is presented and the intended contribution of the paper is a NO_x model, implementation feasible for an embedded system, e.g. embedded processor or embedded electronic hardware (FPGA). For that purpose parts of the algorithm can be pre-computed and stored in tables allowing significant acceleration of the computation.

INTRODUCTION

In the automotive industry models are commonly used mainly for three purposes; calibration, analysis and control. The model presented in this paper is intended for engine control and computational ease is hence much more important than maximal accuracy and full physical interpretation. Physical models of different kinds can be used for engine control. Physical models are often preferred over 'black-box' (empirical) models due to their more general nature, provided that assumptions and simplifications are well chosen. If a model successfully captures physical phenomena common for, in this case, engines, the model calibration effort hopefully decreases when adopting the

model in different contexts (on different engines). If so, physical models may well be used out of their proven area of verification, that is of course if the assumptions still are valid in the new context. Physical models can often be used both for prediction and indirect measurement.

Several authors made attempts in finding NO_x models which are physical (or at least semi-physical) and still usable in engine control units, for example [2] and [3], the second being based on the first. Andersson et. al. shows a multi-zone model accelerated using pre-calculation techniques. The claim of [2] is "real-time" performance of the pre-calculated multi-zone model, the platform was however a (for the time) high-spec desktop computer, avoiding many of the obstacles present in on-board computation systems. The main idea with the models of [2] and [3] was to compute adiabatic flame temperatures in the different zones (more than two), these temperatures being compensated in different steps according to partly physical, partly empirical relationships which are pre-computed and stored in tables. These relationships are intended to correct the burned zone temperature for incomplete combustion, wall heat-transfer and dissociation.

Another contribution in the area is given by [4] on which this paper (as well as the work of [2] and [3]) is based. The major difference between this contribution and [4], who utilizes conservation of energy iteratively to find a burned zone temperature, is the observation that it is possible to indirectly compute the temperature of the burned and unburned zones (provided that a two-zone approach is used). The computation of the burned zone temperature is hence exchanged for a physically correct computation which does not require iterations without additional empirical compensation. Computational speed can hence be increased without having to introduce the *ad-hoc* assumptions of for example [2]. It should be stated that there also

are other approaches to speed-up the algorithms of [7]. Egnell partly solves this iterative energy balance in advance and tabulates it as a function of global λ and EGR content. [2] and [3] have altered the method of [4] in different ways and added different kinds of compensations (in the form of tables) in order to take account for observed phenomena and ultimately obtain as correct combustion temperature as possible.

Using the methods described in [4], [6] and [7] and being able to compute the burned zone temperature it is possible to compute burned zone composition, NO_x formation rate and finally total NO_x content. In order to find the burned zone composition a nonlinear equation system has to be solved in each point. Needless to say it is very time consuming to solve this equation system and for embedded implementation some sort of pre-calculated table will have to be used instead. The contribution is a control-oriented model and should be read in the light of on-line on-board modeling, the contribution is *not* an effort to exhaustively model combustion physics and chemistry.

PROBLEM FORMULATION

To this day there are according to [1] no physical time resolved (non-mean value) NO_x model simple enough for on-board application. The reason is that the physical NO_x models generally require a lot of complex computations which frequently are iterative by nature. Current engine controllers often do not have that much 'spare' computation time (obviously) and NO_x computations within an engine cycle is out of the question using conventional implementation platforms and models; this work aims to fill that gap. Since the suggested model is intended for embedded implementation it will not be benchmarked for computational time on a desktop computer since the benchmark as such says very little about the actual performance of the model. The suggested model is *not* an attempt to produce a fully-detailed chemical or fluid-dynamical model and does not aim for spacial resolution. It is rather a control oriented, physically based model able to predict NO_x formation during the cycle as well as NO_x formation trends. The output from the model could for example be used for closed-loop Diesel combustion control.

THE MODEL

OVERVIEW The model in this work is a two-zone model, one burned zone in which the NO_x formation takes place and one unburned zone composed of only air, as explained by Fig. 1. In this work the burned zone temperature was computed using knowledge about the number of moles in the different zones and the global temperature as well as the temperature of the unburned zone (under the assumption of isentropic compression), rather than using the iterative energy balance approach. Using this method the physical interpretation can be maintained while the algorithm is significantly simplified.

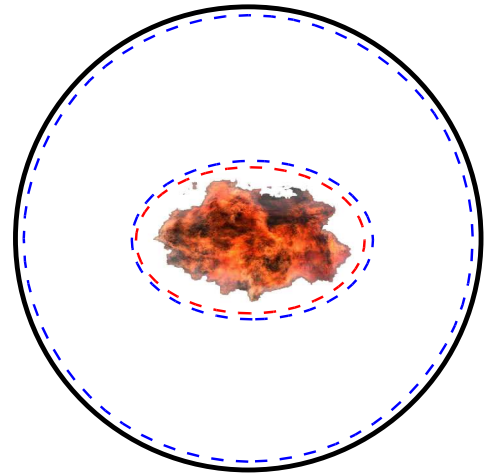


Figure 1: The model works according to a two-zone concept. NO is formed in the inner, burned, zone marked in red. The unburned zone is marked in blue.

If the pressure in the cylinder is known (which is a basic condition for much combustion engine related modeling) it is possible to compute the global temperature as well as the temperature of the unburned zone using a number of assumptions. Furthermore it is possible to compute the number of moles in the burned zone using 'conventional' heat release analysis (according to [5]). It is also possible to compute the total number of moles in the combustion chamber and hence the number of moles in the unburned zone. When the number of moles in the unburned zone, burned zone and globally is known as well as the temperature globally and in the unburned zone it is possible to compute the temperature of the burned zone. A more extensive model of the combustion is hence not needed to compute the temperature of the burned zone. It is possible to avoid a direct computation of burned zone temperature and the related complex and iterative numerical solution of an energy balance 'normally' used to determine burned zone temperature and mole content.

In this context a common simplification is that NO_x emissions mainly are composed of nitrogen oxide, NO , [6]. Hence notation is that NO is modeled rather than NO_x and NO emissions is equivalent to NO_x emissions. NO formation results from high temperatures in the gases resulting from the combustion, hence the burned zone temperature of the combustion products is a key variable for computing NO emissions. The methods for computing NO based on known burned zone temperature are fairly well known and straight forward, [4], [6] and [7]. The algorithm from [4] has been used, but it has been significantly rewritten to increase precision and reduce numerical problems. It has also been corrected for varying burned zone volume. The final step is to solve the differential equation which gives the NO content of the burned zone and recalculate the local NO content to a global one.

ASSUMPTIONS All of the assumptions made are listed below and they are mentioned where needed in the model description as well. Their impacts on the result is discussed later on.

- The ideal gas law is valid for each zone separately and for the complete combustion chamber.
- The pressure is uniform throughout the cylinder.
- The gas temperature just after Inlet Valve Close (IVC) is roughly equal to the intake temperature.
- The number of moles in the combustion chamber is not significantly changed by the combustion.
- The temperature of the unburned zone is assumed to vary according to an isentropic relationship.
- The ratio of specific heats, γ is assumed to be constant in the unburned zone.
- The heating value of the fuel is known.
- Iso-octane is used to model Diesel-fuel.
- The combustion efficiency is 100%.
- Combustion takes place at a constant local λ , which is assumed to be known.
- Species in the burned zone are in equilibrium.
- NO_x emissions mainly consist of nitrogen oxide, NO .

ZONE TEMPERATURES AND NUMBER OF MOLES

As stated earlier one of the novel features with this model compared to earlier work is the computation of burned zone temperature. A two-zone approach together with uniform pressure and the ideal gas law for each zone individually as well as for the complete combustion chamber (the sum of both zones) allows computation of the burned zone temperature according to Eq. (2). The proof is formed in two steps; first Eq. (1) is formed by applying the ideal gas law to the burned zone and the unburned zone. Using Eq. (1) and the ideal gas law for the complete combustion chamber together with the observation that the sum of the volumes of the burned and unburned zones must equal the total volume of the combustion chamber it is possible to form Eq. (2). We now have an equation for the temperature of the burned zone that depends on the *number of moles* in the complete combustion chamber, in the burned zone and in the unburned zone and the *global temperature* in the combustion chamber as well as the *temperature* of the unburned zone.

$$\left. \begin{aligned} pV_{bz} &= n_{bz}\tilde{R}T_{bz} \\ pV_{uz} &= n_{uz}\tilde{R}T_{uz} \end{aligned} \right\} \Rightarrow$$

$$n_{uz}T_{uz} + n_{bz}T_{bz} = \frac{pV_{uz}}{\tilde{R}} + \frac{pV_{bz}}{\tilde{R}} = \frac{p(V_{uz} + V_{bz})}{\tilde{R}} \quad (1)$$

$$\left. \begin{aligned} n_{uz}T_{uz} + n_{bz}T_{bz} &= \frac{p(V_{uz} + V_{bz})}{\tilde{R}} \\ V_{uz} + V_{bz} &= V_g \\ pV_g &= n_g\tilde{R}T_g \\ n_{uz} &= n_g - n_{bz} \end{aligned} \right\} \Rightarrow$$

$$\begin{aligned} n_{uz}T_{uz} + (n_g - n_{bz})T_{bz} &= \\ &= \frac{p(V_{uz} + V_{bz})}{\tilde{R}} = \frac{pV_g}{\tilde{R}} = n_gT_g \Leftrightarrow \\ n_gT_g &= (n_g - n_{bz})T_{uz} + n_{bz}T_{bz} \Leftrightarrow \\ T_{bz} &= \frac{n_gT_g - (n_g - n_{bz})T_{uz}}{n_{bz}} \end{aligned} \quad (2)$$

Given the cylinder pressure and assuming that the gas temperature in the cylinder just after Inlet Valve Close (IVC) is roughly equal to the intake temperature it is possible to compute the initial state in the cylinder. The initial state here refers to initial global temperature T_0 and the total number of moles of air in the cylinder at IVC, n_0 . The number of moles in the entire combustion chamber (the global number of moles, n_g) can be computed using the ideal gas law at based on a small number of data-points just after IVC giving the initial number of moles, n_0 . Assuming that the number of moles is not significantly changed by combustion the global number of moles (n_g) is known from n_0 throughout the complete cycle. Furthermore the global temperature (T_g) can be computed from the cylinder pressure and the global number of moles, n_g using the ideal gas law, all according to Eq. (3).

$$\left. \begin{aligned} n_0 &= \frac{p_0V_0}{\tilde{R}T_0} \\ n_g &= n_0 \end{aligned} \right\} \Rightarrow T_g = \frac{pV}{n_0\tilde{R}} \quad (3)$$

The unburned zone temperature (T_{uz}) is computed using a datum point during the cycle and the assumption of an isentropic relationship, Eq. (4), similarly to [4] and [2]. The temperature and pressure datum (T_{g0} and P_{g0}) used to compute the temperature of the unburned zone is acquired just before the combustion has started to reduce the effect of losses, e.g. heat losses and mass loss. The ratio of specific heats, γ is here assumed to be constant.

$$T_{uz} = T_{g0} \left(\frac{p}{p_{g0}} \right)^{\frac{\gamma-1}{\gamma}} \quad (4)$$

The number of moles in the burned zone (n_{bz}) is obtained from heat release analysis which is significantly more complex than computing the other variables mentioned. The global temperature, the unburned zone temperature and the burned zone temperature for one operation point is shown in Fig. 2, corresponding average temperature traces of the different zones are shown in Fig. 3.

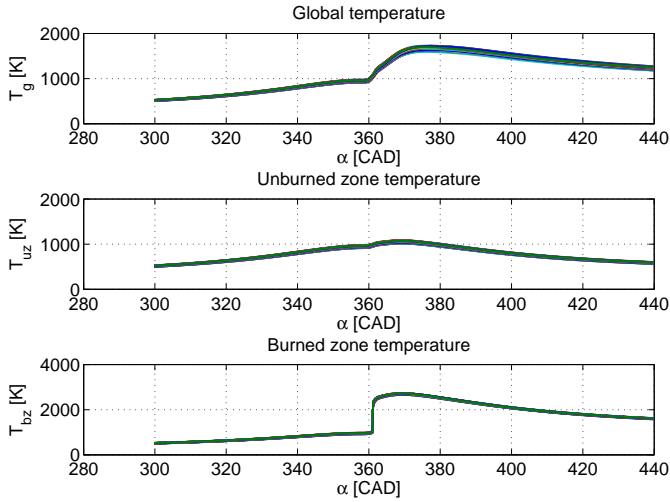


Figure 2: In-cycle zone temperatures of the three different zones resulting from the method described, 100 cycles.

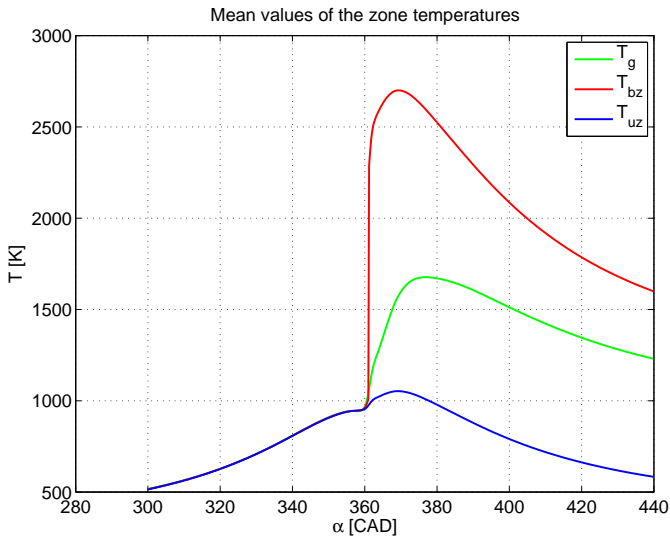


Figure 3: 100 cycle average in-cycle zone temperatures of the three different zones resulting from the method described.

Number of moles in the burned zone One way to compute the number of moles in the burned zone is to use heat-release to compute the amount of released energy. Assuming that combustion does not change the number of moles significantly, it just 'moves' moles from the unburned zone to the burned zone it is possible to compute the number of moles in the burned zone from the heat-release. It does however require some further assumptions, the heating value of the fuel must be known and the combustion efficiency is assumed to be 100%. The local air/fuel ratio, λ , must also be known. Knowing the exact local λ is difficult, λ is hence introduced as a tuning parameter in the model in a fashion similar to [4], hence combustion is assumed to take place at a constant λ .

The heat release equation, Eq. (5), used in this work represents an integrated version of the apparent heat release equation in [5] assuming constant γ . It was first presented in [10] and has been applied in e.g. [9].

$$Q = \frac{1}{\gamma - 1} p(\alpha) V(\alpha) + \int_{\alpha_{start}}^{\alpha} p(\alpha) \frac{dV}{d\alpha} d\alpha - \frac{1}{\gamma - 1} (p(\alpha_{start}) V(\alpha_{start})) \quad (5)$$

Both heat losses to the combustion chamber walls and the effect of varying γ is neglected in this step in order to decrease the computational load. The entire heat release was then normalized against the energy content of the injected fuel (assuming 100% combustion efficiency), in this way the 'shape' of the heat-release is maintained as well as a full physical interpretation, while still avoiding extensive models for varying γ and heat losses.

Having a accurate heat-release analysis, it is possible to compute the number of moles in the burned zone from Eq. (6) which uses average molar masses of fuel and air together with local, burned zone, λ and the stoichiometric air fuel ratio (α_{safr}).

$$\left. \begin{aligned} n_{bz} &= n_f^{bz} + n_a^{bz} = \frac{m_f^{bz}}{M_f} + \frac{m_a^{bz}}{M_a} \\ m_a^{bz} &= m_f^{bz} \lambda \alpha_{safr} \\ m_f^{bz} &= \frac{Q}{Q_{LHV}} \\ n_{bz} &= \frac{Q}{Q_{LHV} M_f} \left(1 + \frac{M_f \lambda \alpha_{safr}}{M_a} \right) \end{aligned} \right\} \Rightarrow \quad (6)$$

Resulting mole content of the burned zone and unburned zone together with the corresponding heat-release are shown in Fig. 4 and every variable needed to compute the burned zone temperature (T_{bz}) is hence available.

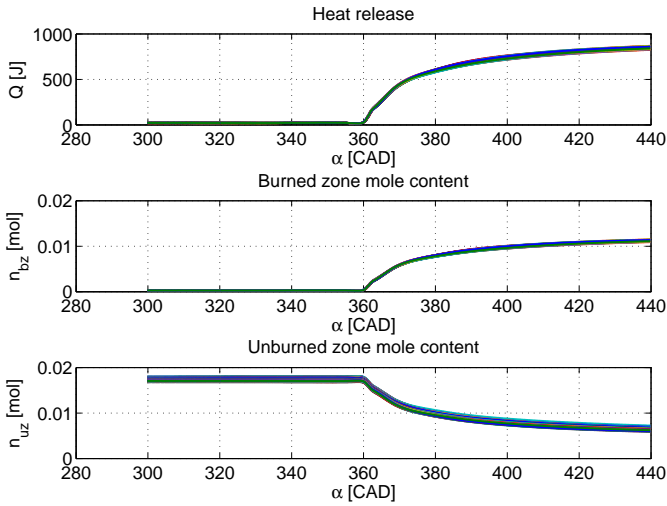
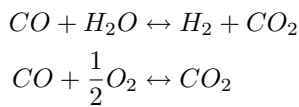


Figure 4: The heat release and number of moles in the burned and unburned zones for 100 cycles.

Computation trigger The computation of the number of moles in the burned zone can not be started directly after IVC and this is the case for some of the other computations as well. The reason is that the burned zone contains zero moles until combustion has started and for example Eq. (2) will hence include a divide by zero. A computation trigger hence has to be introduced in order to avoid numerical problems before combustion has started. For that purpose the time instance when 10% of the total heat has been released (CA10%) was used.

BURNED ZONE COMPOSITION To be able to compute NO formation rate (using Eq. (21)) the concentrations of a number of species in the burned zone have to be known. It is possible to compute those based on the assumption that corresponding species have reached chemical equilibrium. To compute NO emissions using the Zeldovich mechanism the equilibrium concentration of free oxygen (O), nitrogen (N_2) and nitrogen oxide (NO) must be known (see Eq. (21)). These concentrations can be computed as functions of temperature, pressure-ratio and local λ by taking dissociation reactions into account. The dissociation reactions (meaning the 'backwards' reactions) are considered important since they provide the most important source of free oxygen available for NO formation after the combustion event. Dissociation reactions are taken into account through modeling the two chemical reactions shown below;



The approach of [4] and [7] was used, two reactions, relative Gibbs energy and carbon, hydrogen, oxygen and nitrogen balances are put together to form the nonlinear equation system with six unknown variables shown in Eq. (7)-Eq. (12).

$$\frac{a_{CO_2}a_{H_2}}{a_{CO}a_{H_2O}} = K_{p1} \quad (7)$$

$$\frac{1}{a_{O_2}} \left(\frac{a_{CO_2}}{a_{CO}} \right)^2 =$$

$$= \frac{P}{a_{CO_2} + a_{CO} + a_{H_2O} + a_{H_2} + a_{O_2} + a_{N_2}} K_{p2} \quad (8)$$

$$n = a_{CO_2} + a_{CO} \quad (9)$$

$$m = 2(a_{H_2O} + a_{H_2}) \quad (10)$$

$$2\lambda \left(n + \frac{m}{4} \right) = 2a_{CO_2} + a_{CO} + a_{H_2O} + a_{O_2} \quad (11)$$

$$2\lambda \left(n + \frac{m}{4} \right) = \frac{a_{N_2}}{3.773} \quad (12)$$

n is the number of carbon atoms and m is the number of hydrogen atoms in an arbitrary fuel; C_nH_m (iso-octane was used with $n = 8$ and $m = 18$). P is normalized (cylinder) pressure ($P = \frac{P}{P_0}$, $P_0 = 1.013 \cdot 10^5 [Pa]$) and a_{XX} is a dimensionless number describing the equilibrium concentration of species XX . The two equilibrium constants, K_{p1} and K_{p2} can be computed from polynomials (the algorithm is explained in detail in [7]). The fact that the partial pressure of each species has a relation to K_{p1} and K_{p2} gives Eq. (7) and Eq. (8). It is also a fact that the number of carbon, hydrogen, oxygen and nitrogen atoms involved in the reactions should remain unchanged. Hence it is possible to state in total six equations Eq. (7)-Eq. (12) which would have to be solved, either at runtime or in advance using pre-computation/tabulation.

In order to enable the solver to find a good solution Eq. (7)-Eq. (12) were significantly rewritten using basic algebra. Performing this action gives Eq. (13) and Eq. (14) which, for the solver, has a more suitable format than the previous six equations. In this way the solver can produce a more accurate solution in much shorter time.

$$\frac{a_{CO_2} \left(\frac{m}{2} - a_{H_2O} \right)}{(n - a_{CO_2}) a_{H_2O}} = K_{p1} \quad (13)$$

$$\left(\frac{a_{CO_2}}{n - a_{CO_2}} \right)^2 = \frac{1}{\left(n + \frac{m}{4} \right) \lambda - \frac{1}{2} a_{CO_2} - \frac{1}{2} n - \frac{1}{2} a_{H_2O}} =$$

$$= \frac{PK_{p2}^2}{\frac{1}{2}(3n + m - a_{CO_2} - a_{H_2O}) + 8.546 \left(n + \frac{m}{4} \right) \lambda} \quad (14)$$

Solving Eq. (13) and Eq. (14) gives the dimensionless equilibrium concentrations of CO_2 and H_2O from which CO , H_2 , O_2 and N_2 can be computed.

All of the variables needed to compute dNO/dt are however not yet known. N_2 is known but O and NO have to be found. This requires models for the reactions forming O from O_2 (Reaction 15) and NO from O_2 and N_2 (Reaction 17). Eq. (16) and Eq. (18) represent a similar approach to [4].

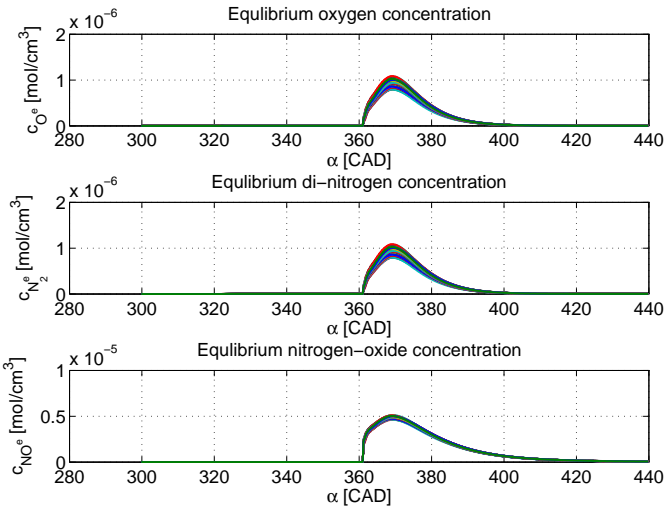


Figure 5: Equilibrium concentration of the three different species, needed to compute NO formation rate.



$$c_O^e = \frac{K_{pO} \sqrt{c_{O_2}^e}}{\sqrt{RT}} = [K_{pO} = 3.6 \cdot 10^3 e^{(-\frac{31090}{T})}] = \frac{3.6 \cdot 10^3 e^{(-\frac{31090}{T})} \sqrt{c_{O_2}^e}}{\sqrt{RT}} \quad (16)$$



$$c_{NO}^e = \sqrt{K_{pNO} c_{O_2}^e c_{N_2}^e} = [K_{pNO} = 20.3 e^{(-\frac{21650}{T})}] = \sqrt{20.3 e^{(-\frac{21650}{T})} c_{O_2}^e c_{N_2}^e} \quad (18)$$

All equilibrium concentrations were computed with an angular resolution of 0.2 CAD within each cycle, the resulting values are shown in Fig. 5. Knowing equilibrium concentrations of O , NO and N_2 allows computation of dNO/dt .

NO FORMATION Once the equilibrium concentrations of the different species are known it is possible to compute the NO_x formation rate using the Zeldovich mechanism shown in Eq. (21). The Zeldovich mechanism which models Reaction 19 and Reaction 20 is commonly used for NO_x modeling.



$$\frac{\partial c_{NO}}{\partial t} = \frac{15.2 \cdot 10^{13} e^{-\frac{38000}{T}} c_O^e c_{N_2}^e (1 - (\frac{c_{NO}}{c_{NO}^e})^2)}{1 + \frac{7.6 \cdot 10^{13} e^{-\frac{38000}{T}} c_O^e c_{N_2}^e}{1.5 \cdot 10^9 e^{-\frac{19500}{T}} c_{NO}^e c_O^e} (\frac{c_{NO}}{c_{NO}^e})} \quad (21)$$

During this work it was however unveiled that the original Zeldovich mechanism (which equals Eq. 21) as presented by [4] and [6] actually is not valid if the volume of the zone it is applied to varies! For a two-zone model it is obviously the case that the volume of the burned zone increases as combustion progresses and more and more moles are included in the burned zone. Eq. (21) hence had to be rewritten according to Eq. (22) (which from now on is denoted the *modified Zeldovich mechanism*) in order to be valid even when the volume of the burned zone varies.

$$\left. \begin{aligned} \frac{dc_{NO}}{dt} &= \frac{\partial c_{NO}}{\partial t} + \frac{\partial c_{NO}}{\partial V} \frac{dV}{dt} \\ \frac{\partial c_{NO}}{\partial V} &= -\frac{n_{NO}}{V^2} = -\frac{c_{NO}}{V} \\ c_{NO} &= \frac{n_{NO}}{V} \end{aligned} \right\} \Rightarrow \frac{dc_{NO}}{dt} = \frac{\partial c_{NO}}{\partial t} - \frac{c_{NO}}{V} \frac{dV}{dt} \quad (22)$$

$\frac{\partial c_{NO}}{\partial t}$ is given by the original Zeldovich mechanism in Eq. (21), $\frac{dV}{dt}$ and V represent volume derivative and volume, respectively, of the *burned zone* computed using the ideal gas law and the previously computed temperatures and mole numbers of the burned zone. Solving the *modified Zeldovich* in Eq. (22), which can be done for example using a simple Newton method, gives the NO concentration (the unit is [$mole/cm^3$]) of the *burned zone*! Typical NO formation and NO concentration 'traces' belonging to 100 consecutive engine cycles can be viewed in Fig. 6.

It is however the concentration of NO in the exhaust gases that is to be determined by the model. To compute the *overall* NO fraction the 'size' of the burned zone must be divided by the 'size' of the total combustion chamber. Since NO tail-pipe emissions commonly are measured as a mole-based fraction the best way to compute overall NO is to compute the number of moles of NO in the burned zone and divide it by the total, global, number of moles. The procedure is shown in Eq. (23).

$$X_{NO} = \frac{V_{bz} c_{NO}}{n_g} \quad (23)$$

This actually is the final step of the NO algorithm or model. The fraction of NO in the exhaust gases is now known throughout the engine cycle, a typical NO formation case for the same 100 cycles as shown in Fig. 6 is shown in Fig. 7.

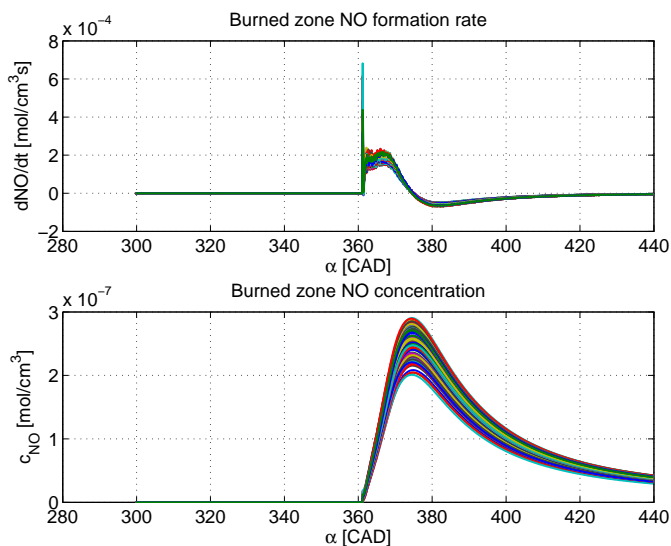


Figure 6: Burned zone NO formation rate and concentration belonging to 100 consecutive cycles.

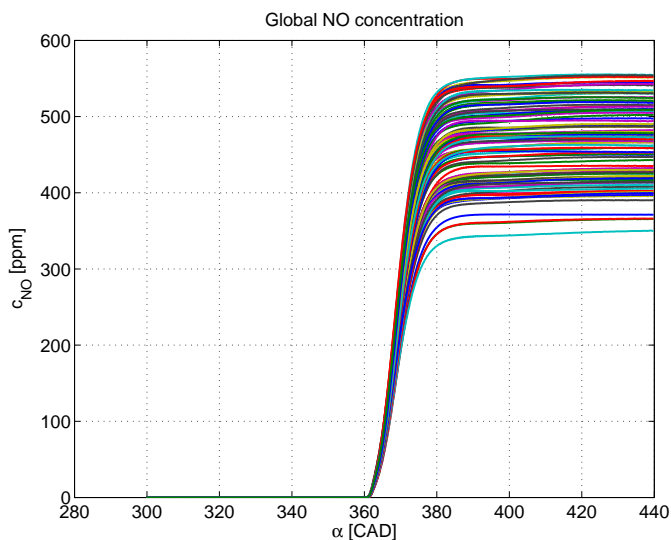


Figure 7: Total fraction of NO within 100 engine cycles.

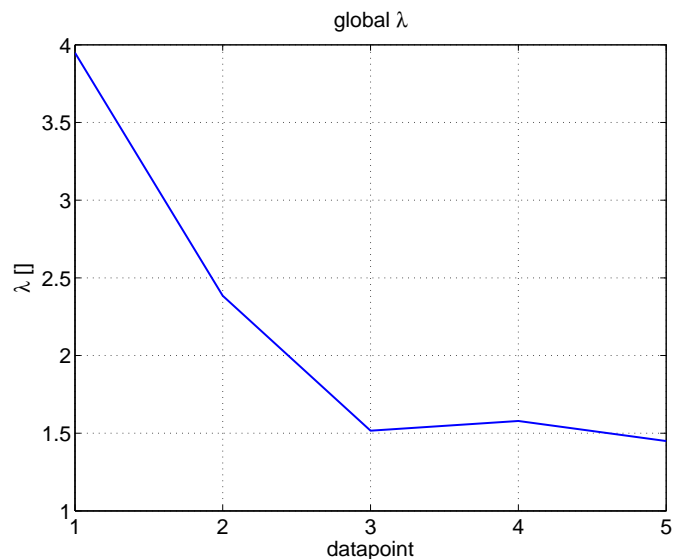


Figure 8: Actual measured, global, λ .

EXPERIMENTAL PLATFORM

Unfortunately no suitable extensive dataset was available to the authors at the time of development, a mere five data points consisting of some 150 cycles each has hence been used for the validation of the algorithm. The data was obtained on a single-cylinder version of a passenger-car sized Volvo 'D5' diesel engine (0.5l displacement per cylinder). The setup is presented in detail in [11]. The data points were taken at increasing loads with varying intake-pressure, no external or internal Exhaust Gas Recirculation was present. The fuel was standard (Swedish MK1) Diesel fuel and the injection strategy was single injection with constant End Of Injection and varying Start of Injection. Global λ hence varied between about 4 and 1.5 according to Fig. 8. The reader should note that even though the three last data-points had the same lambda, the load varied between the points since the intake pressure differed (due to turbo-charging). One could probably say that the data-points represent a common Diesel load sweep.

All computations and simulations were carried out using Matlab.

RESULTS AND PERFORMANCE

So far only the derived equations and algorithm (model) concept has been presented, even though they represent the actual work performed they had to be tested on real-world data to show their validity. The five data points described above were used to test the performance of the model. There was one parameter available for 'tuning' of the model namely the burned zone λ which was swept with high resolution between 0.95 and 1.2 and the results are shown in Fig. 9. Also included in the figure are dots indicating the actual measured NO emission for each data-point and a vertical line indicating the average local ' λ ' giving the highest agreement with the measured values of all five data points. For these five data points the av-

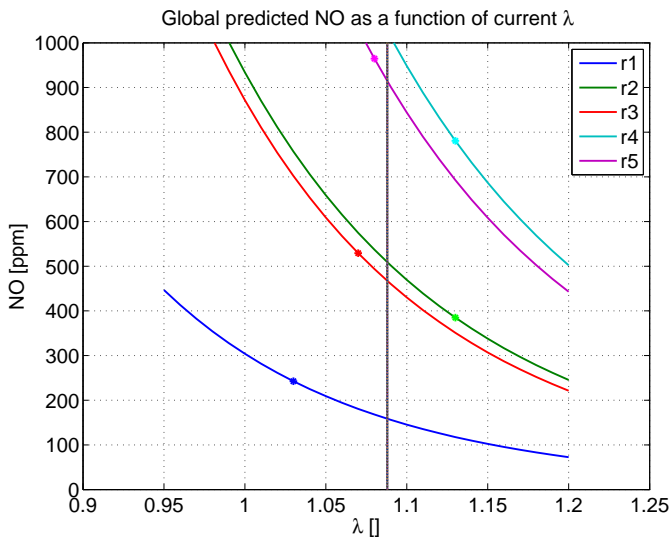


Figure 9: The exhaust gas NO content as a function of current λ used by the model.

verage local λ giving best agreement between measured NO emission and those computed by the model is 1.088. Using a model λ value of 1.088 gives a maximum error of about 30% and an absolute average error of roughly 20%. Considering the coarse nature of the model and the very complex nature of the physical process this must be considered acceptable at least for qualitative control and diagnostics purposes.

All the figures previously presented in the form of crank angle resolved plots, originate from data point 3 (which was randomly selected) using the average lambda of 1.088.

DISCUSSION

Models are, naturally, rarely perfect. Assumptions which have to be made represent simplifications of the real world and will hence infer errors. How large errors can be tolerated varies depending on the purpose of the model. The errors reported for this model are considered as acceptable for control and embedded applications. Similarly to the physical world where NO formation depends exponentially on combustion λ , the model NO formation depends exponentially on the 'calibration' lambda as seen in Fig. 9. The NO model is thus very sensitive to this setting which explains the maximum absolute error of 20% even though best calibration λ only differs at most by 0.1 between the different points. In the light of the exponential dependence between NO and calibration λ and considering the relatively coarse nature of the model the 20% average error must be considered as a very good result.

SENSITIVITY TO ASSUMPTIONS It is very difficult to state which of the assumptions that has the largest impact on the performance of the model. During the work it was however obvious that the model is very sensitive to variables that affect the total number of moles included in the burned zone, for example local λ to which model out

NO shows exponential dependence. The total heat release (giving the number of moles in the burned zone) is also very important in order to get acceptable results from the model, which was the reason for normalizing the heat release with the total energy content of the injected fuel.

The error coming from assuming that combustion does not change the number of moles in the combustion chamber are regarded as very small. Egnell quantifies the error coming from neglecting the combustion effect on the number of moles to about 1.5% @ $\lambda = 1$.

Assuming 100% combustion efficiency and a known heating value of the fuel are reasonable assumptions which should have a very small impact on the final result. Diesel engines commonly have a very high combustion efficiency and they are frequently run on Diesel fuel.

Using a combustion trigger might have some impact on the results, the best candidate for computation trigger would obviously be CA5% which however proved to be too sensitive to noise to be used. Instead CA10% was selected as a more stable approach with the drawback of reduced accuracy during the early combustion. Giving a general answer regarding the impact of using CA10% instead of CA5% is difficult. Considering the very small 'size' difference (difference of the number of moles) of the burned zone between CA5% and CA10% the authors consider the impact of the 'late' trigger point of the computation as very low.

These are some of the assumptions which could have an effect on the performance of the model. Some of the model assumptions are not discussed further since they belong to 'common practice' in the field, these are for example assuming chemical equilibrium, assuming that the ideal gas law is valid and assuming the NO_x mainly consists of NO .

It should be pointed out that the impact of errors and assumptions in the model is that the 'best calibration' λ is shifted away from its physically correct value which is considered to be one. The fact that the best calibration λ is very close to one strongly indicates that the assumptions made are reasonable.

CALIBRATION LOCAL λ Commonly some variable(s) are introduced in models which allows calibration of a model output, meaning that the model output can be adjusted to fit empirical data. If the number of parameters that are introduced can be kept small it is beneficial for the validity of the model and for the model calibration effort. In the suggested approach actually only one variable is available for calibration, the modeling local λ . It is very important to point out that the calibration λ used in the model is *not* the same as the global λ for the engine. Calibration λ is nor the same as the actual *physical* local λ categorized by [8]. The 'calibration' local λ has a physical interpretation even though it is a calibration vari-

able though. It can be said to reflect the 'average' lambda at which combustion takes place, or rather the average λ of the gases which enter the burned zone. Turbulence will introduce gases which do not take part in combustion (not adding to the heat-release) into the burned zone and since there is no account for turbulence in the model this phenomenon will be accounted for through a slightly leaner model average λ . A calibration λ of 1.088, which is the 'best on average' calibration value according to Fig. 9, holds some promise regarding the validity of the model considering that it is significantly richer than the real measured global lambda in all of the five data-points. It is also not very far from 1.0 which according to [8] is the *physical* λ maintained during Diesel diffusion combustion.

Clearly calibration λ can not be expected to *exactly* match the values physically expected, the calibration λ will be affected by the validity of many different assumptions and will include many effects. Hence even though calibration λ has a full physical interpretation it will not obtain fully physically correct values! It is important to note that calibration λ should *not* exceed the *global* λ , shown in Fig. 8. If it exceeded the global λ the use of a stratified, two-zone, model would have been questionable. Such a case would probably indicate that some of the assumptions or computation (for example the heat-release analysis) were erroneous.

HEAT RELEASE AND MOLE NUMBERS The format of the heat release needed to compute the number of moles in the burned zone differs significantly from the 'standard' heat release equation (see [6]). With this heat release equation the accumulated heat release is obtained directly without any need for a cylinder pressure derivative. This improves the numerical accuracy particularly at high sample rates and with limited numerical precision.

Using a heat release analysis which neglects all the effects of losses (heat losses, crevice losses and losses due to combustion inefficiency) and neglects the varying γ of the combustion zone has the drawback that the value of the result may differ significantly from the value expected from the amount of fuel injected. During the work the precision of the heat release actually appeared to be a severe problem since it is very important to be able to compute the number of moles in the combustion zone with reasonable accuracy. This issue was solved by normalizing the output of the heat release against the amount of fuel actually injected. The amount of fuel actually injected was computed using fuel flow, it could also be computed from the injector signals with high accuracy. Normalizing the heat release proved to be an efficient method to keep the 'shape' of the heat release while obtaining reasonable values. The normalization is a very efficient way to significantly reduce the effects that heat losses and a varying γ (which is very difficult and time consuming) have on the computations using one very simple value already available in an engine systems (the injector signal).

SENSITIVITY TO γ The ratio of specific heats, γ , is an important variable in these modeling contexts. The true and correct way to handle γ is a matter of dispute in modeling communities. Assuming an ideal gas γ is a function of current temperature and it is in many contexts important to include this dependence of temperature.

In this work the fluid are assumed to be ideal gases, γ is however assumed to have a constant value! The reason for doing so in this case is to spare computation time and memory. γ was used in two places in the model, one place is in the heat release which is considered to be the place where a varying γ has its largest impact since the temperature in the burned zone is high. The issue with varying γ in this case is however solved by normalizing the heat release with the amount of injected fuel.

γ was also used to compute the temperature of the unburned zone. The unburned zone is however significantly colder than the burned zone. In the temperature regions of the unburned zone γ does not vary enough to affect the results. The model as such is hence not significantly affected by the assumption of a constant γ and being able to assume a constant γ actually was one key issue obtaining a fast model.

MODIFIED ZELDOVICH Realizing that a modification to the commonly used and well known Zeldovich mechanism causes some confusion a short motivation in the form of logic reasoning follows. Consider a volume containing a certain number of moles of *NO*. Let us assume that, at current conditions, no *NO* is either formed or consumed meaning that $\frac{dc_{NO}}{dt} = 0$ according to the original Zeldovich mechanism. At such a situation we have a fixed number of *NO* molecules in a fixed volume. If the volume changes but the formation of *NO* molecules still is zero an issue with the original Zeldovich mechanism arises. In such a case the *actual physical concentration* will decrease but the original Zeldovich mechanism as presented in Heywood will still compute the *NO* concentration change to zero since the difference in volume is not included in the Zeldovich mechanism!

From this reasoning it undoubtedly follows that the original Zeldovich mechanism is only valid for constant volume. If the volume varies it has to be complemented with a term describing the concentration change due to volume change. This explains the development of the *modified* Zeldovich mechanism.

Since previous contributions in the area use a multi-zone approach it is highly likely that each zone does not vary significantly in volume, the number of zones just increases. The original Zeldovich mechanism has hence been valid in those cases.

PRE-CALCULATION AND TABULATING Since the developed model was intended for embedded implementation, solving the previously described nonlinear equation system (Eq. (7)-Eq. (12)) at runtime must be avoided. Even though it may be possible to implement a really fast solver in some sort of electronic hardware it would be much easier and probably faster to tabulate the result. Some sort of tabulation technique should hence be used which stores the solution as a function of its input variables.

$$\begin{aligned}\frac{\partial c_{NO}}{\partial t} &= f(T_{bz}, c_{NO}, c_{NO}^e, c_{N_2}^e, c_O^e) = \\ &= [c_{N_2}^e, c_O^e, c_{NO}^e = f(P, T_{bz})] = \\ &= f(T_{bz}, P, c_{NO})\end{aligned}\quad (24)$$

In Eq. (24) it is shown that dc_{NO}/dt is a function of three variables; burned zone temperature, the pressure ratio in the cylinder and NO concentration! Since the number of inputs is not too large it is possible to use some sort of pre-computation to avoid solving the nonlinear equations online. Such an approach would potentially speed up calculations and it would probably be possible to compute the NO content in the cylinder within the cycle.

MODELING EGR Modern Diesel engines commonly use Exhaust Gas Recirculation (EGR) to reduce emissions of among others NO_x . Any NO_x model should hence capture the impact of EGR on NO emissions. It is interesting to know if the developed model could easily be changed to include the effects of EGR. The answer to this question is that it would not take much effort to include EGR. The use of EGR will basically have an impact on three places in the algorithm.

The estimation of the global number of moles, n_g , would have to be changed. The current estimation is based on a start temperature, which is assumed to equal the intake temperature, and the ideal gas law. The start temperature of the charge would change by the use of EGR and the start temperature estimation would have to be changed accordingly. The second place in the algorithm where EGR would have an impact is when computing the burned zone species composition. The equation system describing burned zone composition would have to be changed to reflect the use of EGR. The changes are however not large and the basic principle is the same as without EGR. Considering the approach with a tabulated solution of dc_{NO}/dt an additional input describing EGR ratio would probably be the only modification needed. The last variable affected by the use of EGR is the computation of the number of moles in the burned zone. The corresponding equations would have to be altered so that they reflect the number of moles of EGR which enters the burned zone together with the air.

CONCLUSIONS

The paper has presented a model which can be used to compute the NO emissions of a Diesel engine. The model, or algorithm, presented implements a physically correct NO model which use a two zone approach to model the stratified nature of Diesel combustion. Computing the temperature of the burned zone has previously required complex and iterative energy balance computations or *ad-hoc* assumptions. This contribution shows a novel approach for computing the temperature of the burned zone, which is the 'effective' temperature 'active' in the NO formation. The novel temperature computation approach is based on the ideal gas law applied to the different zones in combination with assumption of isentropic compression of the unburned zone. A heat-release computation is needed in order to compute the mole content of the different zones also needed to compute burned zone temperature.

Knowing the temperature of the burned zone it is possible to compute the NO formation rate. The well-known 'Zeldovich mechanism' has for that purpose been modified in order to be correct when the control volume (burned zone) changes its volume. Solving the differential equation describing NO formation rate, the total NO fraction in the exhaust gases can be computed since the number of moles in the different zones is known and (NO is formed only in the burned zone).

The only 'tuning-parameter' within the model is the local λ and the model provides best agreement with measured data when the local λ is within physically reasonable values (λ is close to one). The local λ is also well below the global, measured, λ indicating that the model mirrors the stratified conditions during Diesel combustion.

The performance of the model has been screened showing that the model gives sufficiently accurate results considering the coarse nature of the model. On the five data points available an absolute average error of 20% was obtained, the maximum error using a fixed local λ of 1.088 was about 30%.

Even though this number is not to be considered as a very good result compared to extensive multi-zone models it is, using the model, possible to get quantitative information regarding the instantaneous NO content in the cylinder. This contribution should be read in the context of control oriented, on-board (embedded) implementable models. Comparing with complex multi-zone models is unfair considering the computation times needed to complete the different models. Using the suggested algorithm with pre-computed parts it is most likely possible to obtain information regarding the NO content during the cycle! Information that might prove useful when implementing for example feedback Diesel combustion control.

FUTURE WORK AND OUTLOOK

Even though it seems possible to implement the suggested NO_x model in some sort of embedded system (e.g. engine control units) some work does remain. First of all the model should be proven using a much larger dataset than used in this contribution. The reason is to find out how the model behaves and if some sort of adaptability has to be developed when applying the model over large operating ranges. Secondly the model shall be modified so that it includes the use of EGR. The tabulation and pre-calculation techniques should be developed and proven in order to actually implement the model in an embedded system. Finally but not least importantly (or difficult), the model should be implemented in an actual embedded system such as an embedded processor or FPGA and the performance should be quantified.

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NOMENCLATURE

α	Engine crank position (crank angle degree)
α_{safr}	Stoichiometric air fuel ratio
γ	Isentropic constant
λ	Relative air-fuel ratio
a_{XX}	Fraction of species XX
$CAXX\%$	The time instance for XX% of total heat release
c_{NO}	Concentration of NO
c_{XX}^e	Equilibrium concentration of species XX
EGR	Exhaust Gas Recirculation
IVC	Inlet Valve Close
K_{pX}	Equilibrium constant X
m	Number of hydrogen atoms in arbitrary C_nH_m
M_a	Mole mass of air
m_a^{bz}	Mass of air
M_f	Mole mass of fuel
m_f^{bz}	Mass of fuel
n	Number of carbon atoms in arbitrary C_nH_m
NO	Nitrogen Oxide
NO_x	Nitrogen Oxides including both NO and NO_2
n_0	Number of moles at a zero datum point
n_a^{bz}	Number of moles of air
n_{bz}	Mole number of the burned zone
n_f^{bz}	Number of moles of fuel
n_g	Global number of moles
n_{uz}	Mole number of the unburned zone
P	Pressure ratio
p	Cylinder pressure
p_0	Pressure at a zero datum point
p_{g0}	Global pressure at a zero datum point
Q	Released energy
Q_{lhv}	Lower heating value (of fuel)
\tilde{R}	Universal gas constant on mole basis
T_0	Temperature a zero datum point
T_{bz}	Temperature of the burned zone
T_g	Temperature of the total combustion chamber
T_{g0}	Global temperature at a zero datum point
T_{uz}	Temperature of the unburned zone
V_0	Volume at a zero datum point
V_{bz}	Volume of the burned zone
V_g	Volume of the total combustion chamber
V_{uz}	Volume of the unburned zone
X_{NO}	Fraction of NO (on mole base)

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