

Hybrid 2-Zone Diesel Combustion Model for NO Formation

Klaus S. Oppenauer¹ and Luigi del Re

Institute for Design and Control of Mechatronic Systems, Johannes Kepler University Linz

Copyright © 2009 SAE International

ABSTRACT

This paper presents a methodology which is able to calculate emissions over crank angle (CA) using the measured cylinder pressure. The models are based on a 2-zone Diesel combustion process calculation combined with data based methods to fulfill the objective of a wide operating range, for a later possible use in transients – differently from the standard methods, which usually work accurate only in a small range. The resulting hybrid or grey box oriented model structure offers many advantages when purely physical modeling is too complicated and the combination with data based methods allow to obtain better results. The workflow of CA based emission models on the basis of a 2-zone calculation is presented. The focus of this paper is to explain the development process of a nitric oxide (NO) formation model, which is accurate over a wide operating range. For future similar data based particulate matter (PM) models the shown workflow could be used too.

INTRODUCTION

All over the world the emission limits for Diesel passenger cars are continuously decreased by the governments to significant lower levels. Especially the reduction of PM- and NO_x-emissions in transient operation modes is getting more important, because the transient emission peaks have become a main fraction of the total emissions during the standard test cycles (Figure 1). The main reasons for higher emissions are the time delay of the air system caused by the inertia of the turbocharger, as well as the changed EGR-rates in transient. However, a lot of other transient effects are relevant too and they result in a modified combustion, which impacts emissions compared to steady state. Decreasing transient emission peaks with new alternative control strategies for EGR [1], boost pressure and especially combustion itself will be a main topic to reach future limits. To determine the correct control action we require adequate models which need to incorporate our understanding on how NO and PM are formed or oxidized during the combustion process. Diesel engine raw NO_x emissions consist mainly of thermal formed NO emissions, hence the paper focuses on NO.

Only models which depend strictly on the combustion itself are able to make transient effects visible. Thus CA based models depending on the measured cylinder pressure are needed. Previous use of CA based emission models have only focused on steady state operating modes because of the complexity and the range of validity, but actually there is no physical restriction to use the models also in transient states too.

Attention has to be paid on necessary gas conditions in transient. They should be measured or alternatively modeled with fast sensors in the intake and exhaust manifold. Uncertainties in the gas compositions might have an impact on the transient results and have to be checked in the future.

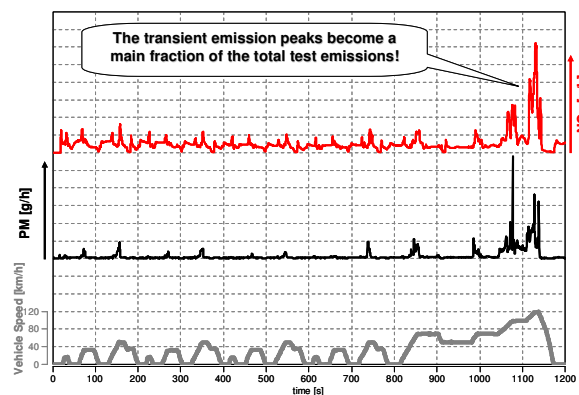


Figure 1: Transient test emissions during NEDC

CA based models could avoid problems with time delays which exist with exhaust gas analyzers. They also could be used more or less as alternative virtual sensors as described in [2]. The models should help to find the combustion cycles which are responsible for the high transient emissions and furthermore to develop optimal control strategies. It is also to assume that the calibrated desired values in the engine control unit (ECU) for injection timing and air path are suboptimal under transient conditions, although they are usually optimized with complex methods, but mainly on a steady state testbench under steady state conditions.

¹ Permanent address: BMW Motoren, Steyr, Austria

Against this background, the paper focuses on the prediction of NO emissions for a wide operating range of the engine. The requirement “wide range” is a condition for a later transient application. Several NO models based on 2-zone combustion models were published by different authors. See [3], [4], [5], [6], [7] and [8]. The main attention has been paid on the energy interaction between the burned and unburned zone, which must be modeled physically or empirically.

Pure physical models are quite complicated to adapt, to predict absolute NO values over a wide range. Trends are often given quite well, but the model accuracy in a wide range is usually not below 20 percent deviation. Especially for modern diesel engines it is getting quite more complicated to predict accurate NO values, because calibration values for injection timing, EGR-rates and other ECU-parameters vary quite a lot over the whole operating range.

Therefore, this paper presents a new approach where the well known empirical 2-zone model described in [3] is extended by a phenomenological description of a parallel mixing flow. This flow depends on global homogenous in cylinder turbulence analog to [7] and [9]. As the main novelty, the empirical description of the temperature difference between unburned and burned zone is improved by data based methods to yield a better model accuracy. NO formation is described by the extended Zeldovich mechanism [10]. The grey box modeling structure obtained by the combination of physical equations and data based methods is calibrated by adapting the model predicted values at exhaust valve opening (EVO) with measured NO in the exhaust system. The model has similar limitations in steady state in terms of absolute accuracy, as published mean value models [11] or [12].

A main advantage of CA based models is the ability to extrapolate. Changed NO emissions caused by changed combustion can be predicted correctly because the main input is the measured cylinder pressure which inherently takes into account combustion changes.

Model evaluation and development is assisted by an optical global 2 color spectroscopy. The optical endoscope sensor is applied on the engine through the glow plug bore. The global 2 color spectroscopy determines burning soot temperature by measuring the intensity of the radiation at two discrete wavelengths (750nm and 900nm) over crank angle. With the Hottel and Broughten analogy [13] and some assumptions it is also possible to derive the soot concentration in the cylinder. Detailed information about the 2 color spectroscopy can be found in [7], [14], [15], [16] and [17].

Model end values at EVO are compared with conventional exhaust gas analyzers in the tailpipe.

The workflow of the model includes 3 steps (Figure 2):

- First a classical thermodynamic 1-zone process calculation is performed based on the measured cylinder pressure
- Next step is a post 2-zone model depending on the 1-zone results
- Last step are the emission models which use the results from the 2-zone calculation

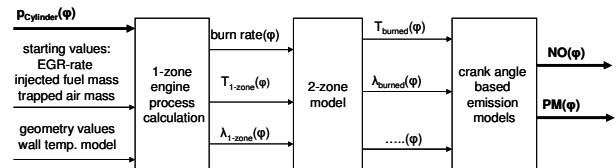


Figure 2: Model workflow for CA based emission models

Finally, a new data based description for the empirical A-value which describes maximum temperature between burned and unburned zone according to [3] is performed with quite better results in terms of NO accuracy.

APPLIED ENGINE

A 4-cylinder DI Diesel EU4 engine was used for the model development. This engine has a common rail injection-system with maximum 1600 bar rail pressure and magnet injectors with a 6 holes nozzle. Only one pilot injection was used in the tests.

Further hardware details:

- variable turbine geometry turbocharger
- EGR-cooler
- air intercooler
- inlet valve deactivation which varies the swirl value

Measurements were performed at the test bench of the Institute for Design and Control of Mechatronical Systems at Johannes Kepler University Linz.

1-ZONE PROCESS CALCULATION

The workflow starts with a classical thermodynamic 1-zone process calculation based on the measured cylinder pressure. See [18].

The calculation is based on 3 equations:

- mass conservation
- energy conservation
- ideal gas equation

We have 4 unknown variables $p(\varphi)$, $T(\varphi)$, $\lambda(\varphi)$, $dQ_B/d\varphi(\varphi)$ and only 3 equations. By measuring the pressure $p(\varphi)$ the system could be solved. Alternatively for combustion studies a given $dQ_B/d\varphi(\varphi)$ could be used to calculate $p(\varphi)$ and the other values. But in our case the burn rate is unknown and we can only measure the pressure.

After some modifications and simplifications we get 3 linear explicit coupled differential equations for $\lambda(\varphi)$, $dQ_B/d\varphi(\varphi)$ and $T(\varphi)$.

$$\begin{aligned} \frac{dm(\varphi)}{d\varphi} &= \frac{dm_B(\varphi)}{d\varphi} = \frac{1}{H_u} \cdot \frac{dQ_B(\varphi)}{d\varphi} \\ \rightarrow \frac{d\lambda(\varphi)}{d\varphi} &= -\lambda \cdot \frac{1}{m_B(\varphi = IVC) + m_B(\varphi)} \cdot \frac{dm_B(\varphi)}{d\varphi} \end{aligned} \quad (1)$$

$$\frac{dQ_B(\varphi)}{d\varphi} = \frac{N1 + N2 + \frac{dQ_w(\varphi)}{d\varphi}}{1 + \frac{u(\varphi)}{H_u} + \frac{T(\varphi)}{H_u} \cdot \frac{\delta u}{\delta T}(\varphi) + D1}$$

with

$$N1 = p(\varphi) \cdot \frac{dV(\varphi)}{d\varphi} \cdot \left(1 + \frac{1}{R(\varphi)} \cdot \frac{\delta u}{\delta T}(\varphi)\right) \quad (2)$$

$$N2 = \frac{dp(\varphi)}{d\varphi} \cdot \left(\frac{V(\varphi)}{R(\varphi)} \cdot \frac{\delta u}{\delta T}(\varphi) + m(\varphi) \cdot \frac{\delta u}{\delta p}(\varphi)\right)$$

$$D1 = \frac{m(\varphi) \cdot \lambda(\varphi)}{H_u(m_B(\varphi = IVC) + m_B(\varphi))} \cdot \frac{\delta u}{\delta \lambda}(\varphi)$$

$$\frac{dT(\varphi)}{d\varphi} = \frac{N3 - N4}{m(\varphi) \cdot R(\varphi)}$$

with

$$N3 = p(\varphi) \cdot \frac{dV(\varphi)}{d\varphi} + V \cdot \frac{dp(\varphi)}{d\varphi} \quad (3)$$

$$N4 = m(\varphi) \cdot T(\varphi) \cdot \frac{dR(\varphi)}{d\varphi} + R(\varphi) \cdot T(\varphi) \cdot \frac{dm(\varphi)}{d\varphi}$$

Some starting values are also needed based on measured EGR-rate, injected fuel mass and fresh air mass.

The volume and volume changing work calculation is done by the following crank equations

$$\lambda_c = \frac{L_s}{L_c} \quad (4)$$

$$V(\varphi) = V(\varphi = TDC) + \frac{V_D}{L_s} \cdot \left[\frac{L_s}{2} \cdot (1 - \cos(\varphi)) + T1\right] \quad (5)$$

$$T1 = L_c \cdot (1 - \sqrt{1 - (\lambda_c)^2 \cdot \sin^2(\varphi)})$$

$$\begin{aligned} p(\varphi) \cdot \frac{dV(\varphi)}{d\varphi} &= p \cdot V_D \cdot \left(\frac{\sin(\varphi)}{2} + T2\right) \\ T2 &= \frac{\lambda_c}{4} \cdot \frac{\sin^2(\varphi)}{\sqrt{1 - (\lambda_c)^2 \cdot \sin^2(\varphi)}} \end{aligned} \quad (6)$$

A heat transfer multiplier according to [19] is used for wall temperature losses. Equation (7) was chosen because it was developed especially for Diesel engines. Alternatively more complicated models could be used.

$$\alpha(\varphi) = 130 \cdot V(\varphi)^{-0.06} \cdot p(\varphi)^{0.6} \cdot T(\varphi)^{-0.4} \cdot (c_m + 1.4)^{0.8} \quad (7)$$

$$\frac{dQ_w(\varphi)}{d\varphi} = \alpha(\varphi) \cdot A \cdot (T - T_w) \quad (8)$$

The following caloric parameters are calculated with the algorithm described in detail by [9] and [20]:

$u(\varphi)$, $R(\varphi)$, $\frac{\delta u}{\delta T}(\varphi)$, $\frac{\delta u}{\delta p}(\varphi)$. This is done by a chemical

equilibrium calculation for 11 components (CO_2 , CO , O_2 , H_2O , H_2 , OH , H , O , N_2 , N , NO). The equilibrium concentrations which are also calculated for the burned and unburned zone are used for the following emission model as inputs.

2-ZONE MODEL

Based on the burn rate calculated in the 1-zone model, a post 2-zone model is used to derive temperature and λ in the burned and unburned zone for the following emission models. The combustion chamber must be divided into two zones, because the mean temperature from the 1-zone model is too low for an adequate NO model. The temperature in the modeled burned zone should reflect the temperature behind the flame where NO is formed.

Mass transport between the zones is done by the flame front, where the fuel is burned with air and λ_{Flame} values which start at 0.8 and rise up to 1. Furthermore, there is also a parallel mixing flow based on global turbulence from the unburned directly to the burned zone. This flow is also implemented into the model. See Figure 3 and equation (13).

The empirical 2-zone model published by Heider and Woschni [3] is extended with a parallel mixing flow based on global turbulence. The big advantage of the empirical energy transport formulation is that the energy equations are not required for both zones. The energy interaction between the two zones is quite complicated to model and not measurable. Fully physical modeled 2-zone models like described in [7] have usually problems with convergence in some points, need starting masses and are difficult to adapt for a wide operating range. The second big advantage of the Heider formulation is a simple A-value to model the temperature difference between the two zones. This factor has a physical meaning and a new data based function structure for the

A-value description is developed using the measured data with sensible physical inputs.

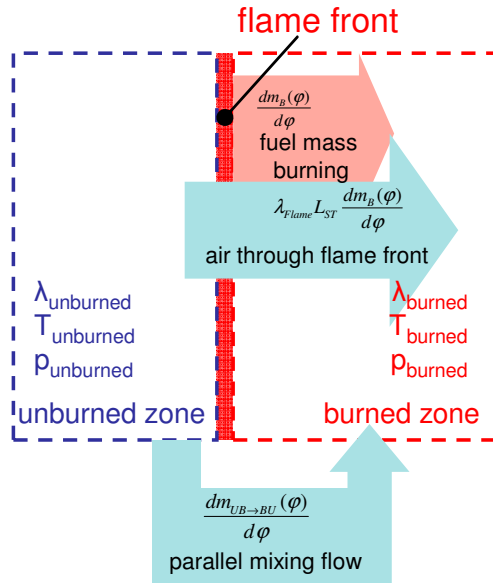


Figure 3: Mass transport between the zones

3 conditions for the 2-zones are:

$$p(\varphi) = p(\varphi)_{burned} = p(\varphi)_{unburned} \quad (9)$$

$$V(\varphi) = V(\varphi)_{burned} + V(\varphi)_{unburned} \quad (10)$$

$$m(\varphi) = m(\varphi)_{burned} + m(\varphi)_{unburned} \quad (11)$$

The pressure in both zones must be the same and the sum of the masses and volumes must be equal to the values from the 1-zone model.

Mass transport through the zones and the flame front is done by the following equations. In equation (13) a parallel mixing flow is implemented. The term is modeled similar to [7] and is described in the next chapter.

$$m_B(\varphi) = \frac{1}{H_U} \cdot \int \frac{dQ_B(\varphi)}{d\varphi} \cdot d\varphi + m_B(\varphi = IVC) \quad (12)$$

$$m_{burned} = m_{burned0} + m_B(\varphi) + \lambda_{Flame} \cdot L_{ST} \cdot m_B(\varphi) + m_{UB \rightarrow BU} \quad (13)$$

$$m_{UB \rightarrow BU} = \int \frac{dm_{UB \rightarrow BU}(\varphi)}{d\varphi} \cdot d\varphi$$

$$\rightarrow m(\varphi)_{unburned} = m(\varphi) - m(\varphi)_{burned} \quad (14)$$

Now we have 4 unknown variables (T_{burned} , $T_{unburned}$, V_{burned} , $V_{unburned}$) and only 3 physical equations are left.

$$p(\varphi) \cdot V(\varphi)_{burned} = m(\varphi)_{burned} \cdot T(\varphi)_{burned} \cdot R(\varphi)_{burned} \quad (15)$$

$$p(\varphi) \cdot V(\varphi)_{unburned} = m(\varphi)_{unburned} \cdot T(\varphi)_{unburned} \cdot R(\varphi)_{unburned} \quad (16)$$

$$V(\varphi) = V(\varphi)_{burned} + V(\varphi)_{unburned} \quad (17)$$

To solve the equation system Heider found the following empirical description for the temperature difference between the two zones.

$$T(\varphi)_{burned} - T(\varphi)_{unburned} = B(\varphi) \cdot A \quad (18)$$

$B(\varphi)$ is a function over crank angle and describes the timeline of the temperature difference. It begins with one at combustion start and ends with zero when combustion is finished. That is near the physical behavior, because if combustion starts the difference must be a maximum and it goes down by the energy interaction between the two zones described by the pressure difference which is caused by combustion. A similar formulation was used by Woschni to model the heat transfer multiplier.

$$B(\varphi) = \frac{K - \int_{\varphi_{CombustionStart}}^{\varphi} (p(\varphi) - p_{woComb}(\varphi)) \cdot m(\varphi)_{burned} \cdot d\varphi}{K} \quad (19)$$

$$K = \int_{\varphi_{CombustionStart}}^{\varphi_{EVO}} (p(\varphi) - p_{woComb}(\varphi)) \cdot m(\varphi)_{burned} \cdot d\varphi \quad (20)$$

The A-value is fixed over the combustion cycle and describes the maximum temperature difference between the two zones. The absolute temperature in the burned zone could be derived out of the above equations and is a function of the mass in the burned zone, the B-value and the burn rate. All these inputs have a physical influence and that is why this simple empirical description has shown his capableness. For the A-value Heider defined the following formulation.

$$A = A_{ES} \cdot \frac{1.2 + (\lambda - 1.2)^{C_{gl}}}{2.2 \cdot \lambda_{Flame}} \quad (21)$$

Only one engine specific parameter (A_{ES}) must be defined for one engine and is constant for the whole operating range. The C_{gl} value is defined with 0.15 for 4 valve engines and 0.07 for 2 valve engines. For engines with swirl λ_{Flame} is 1. Several engines were tested by Heider and the model is able to predict the emissions in wide range below 20% deviation between the measured and modeled NO, which is not bad. The model gives the trends quite well, which is most important. [3]

This simple formulation was now applied on a modern passenger car common rail Diesel engine which fulfills the EU4 regulation. The increased degree of freedom for such a modern engine results in a differently ECU calibration for the air path and injection parameters in the whole operation range. However, for a later transient use the absolute accuracy over a wide range is too low. Thus a new modified formulation (54) is developed based on