

Modelling diesel engine combustion and NO_x formation for model based control and simulation of engine and exhaust aftertreatment systems

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ABSTRACT

Emissions standards are becoming increasingly harder to reach without the use of exhaust aftertreatment systems such as Selective Catalytic Reduction and particulate filters. In order to make efficient use of these systems it is important to have accurate models of engine-out emissions. Such models are also useful for optimizing and controlling next-generation engines without aftertreatment using for example exhaust gas recirculation (EGR). Engines are getting more advanced using systems such as common rail fuel injection, variable geometry turbochargers (VGT) and EGR. With these new technologies and active control of the injection timing, more sophisticated models than simple stationary emission maps must be used to get adequate results.

This paper is focused on the calculation of engine-out NO_x and engine parameters such as cylinder pressure, temperature and gas flows. A quasi steady gas exchange model (including models for EGR and VGT) is combined with a two-zone zero dimensional combustion model. The combustion model uses fuel flow parameters to generate heat release data and calculates the corresponding pressure trace. The temperature and equilibrium concentrations in the zones are calculated by the simplified combustion model and the corresponding NO_x concentration is given by the original Zeldovich mechanism.

The result is a low complexity complete engine model which requires far less computational effort than a CFD model but which yet shows good agreement between measured and calculated emissions data. The model is appropriate to use for simulation of complete engine and SCR systems and in a simplified form for model based control.

INTRODUCTION

Models of engine-out emissions (and NO_x emissions in particular) are useful in many applications. Exhaust aftertreatment systems including SCR are increasing in popularity because of their ability to reduce emissions while keeping the fuel consumption at a competitive level. To get optimum performance of these systems it is important to have a complete system approach. The engine is not separate from the aftertreatment system when it comes to optimization. This article presents the first step in such an approach: a complete engine model capable of predicting the engine out NO_x flow and exhaust temperature. In order to get reasonable simulation times, it is important that the model is of low complexity and requires little computational effort. Previous work in the area includes a neural network dynamic engine model which offers quick simulation performance [6]. The model presented in this paper is based on the actual physical and chemical reactions rather than the use of neural networks. Other applications include automatic control of next generation engines and on board diagnostics (OBD) applications. In these applications, computational efficiency is even more important. For engine control other parameters such as cylinder pressure, turbine speed and EGR rate are also useful in addition to emissions.

Increasingly complex engines using high EGR rates and advanced fuel injection systems makes low complexity engine modelling challenging. The use of quasi stationary models (i.e. models based on stationary engine maps) was studied in [4] using measurement data from engines certified for Euro 3. Even on these engines (which use primitive engine control and technology compared to upcoming Euro 5 engines) it is clear that more advanced models are needed to simulate NO_x emissions.

The modelled engine is an inline six cylinder experimental engine using cooled EGR. The engine is equipped with a variable geometry turbocharger (VGT) and common rail fuel injection system.

MODELS

The model consists of two parts. The combustion model describes the heat release, pressure and temperature inside the cylinder and NO_x formation. The gas exchange model generates input to the combustion model; inlet manifold pressure and EGR rate.

COMBUSTION MODEL

The combustion model is a further development of the zero dimensional model HRNO_x presented by Egnell [1], [7]. Two zones are used, one unburned and one burned zone. The major difference from HRNO_x is the use of a substantially faster way to calculate the burned zone temperature. This will be discussed further in this section. The model can be either diagnostic (i.e. using a measured pressure trace for input) or predictive. In this application the predictive version is used. A number of assumptions have been made:

- The cylinder content can be described as an ideal gas.
- All combustion takes place at the same local air-fuel equivalence ratio.
- There are no pressure gradients inside the cylinder.
- No air entrainment occurs in the burned zone.
- The zones are compressed isentropically.
- All injected fuel is fully burned.
- Radiative heat losses from the flame only.
- NO_x is formed in the burned zone.
- All NO_x content in the recirculated exhaust gas is neglected.
- All released energy originates from injected fuel.

The ambition has been to use models which are physically based as far possible while keeping the complexity low. In some cases however, for example ignition delay and radiative heat loss calculations, (partially) black box models are used. This does decrease the generality of the model; these submodels have been validated on the test engine only. The gains in computational efficiency over previous combustion models are substantial though.

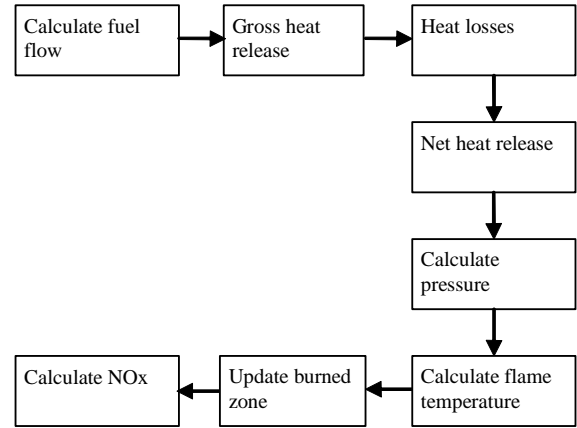


Figure 1 Flowchart of the combustion model

A flowchart of the combustion/NO_x model is shown in Figure 1. First the fuel flow is calculated using measured rail pressure. Using the fuel flow and calculating the heat losses, the net heat release and the corresponding pressure differential are determined. The adiabatic flame temperature of the currently burning fuel mass element is calculated and the burned zone is updated by expanding/compressing the previous contents isentropically and adding the freshly burned charge. The burned zone temperature is compensated for dissociation of the combustion products and finally the amount of NO_x generated in the current timestep is calculated.

This sequence of calculations is performed with a fixed crank angle interval. Typically the burned zone temperature and NO_x concentration calculations are performed more sparsely than the heat release part in order to save time. The model will now be described in more detail.

Fuel flow and heat release calculations

The ignition delay is calculated using a linear black-box model:

$$\alpha_{SOC} - \alpha_{SOI} = f(\delta, n_{eng}, p_{rail}, x_{egr}, p_{im}, \lambda) \quad (1)$$

δ is the injected fuel mass, n_{eng} the engine speed, p_{rail} the injection system rail pressure, x_{egr} the EGR rate, p_{im} the inlet manifold pressure and λ the air-fuel equivalence ratio. Using the fuel mass flow (W_{fuel}), the injected fuel energy at a crank angle θ is calculated:

$$Q_{fuel, inj} = Q_{LHV} \int_{\alpha_{SOI}}^{\theta} W_{fuel}(\theta) d\theta \quad (2)$$

where Q_{LHV} is the lower heating value of the fuel and α_{SOI} the start of injection.

The gross heat release rate is given by:

$$dQ_g = \begin{cases} 0 & \theta < \alpha_{SOC} \\ C_1(Q_{fuel, inj} - Q_g) & \alpha_{SOC} \leq \theta < \alpha_{SODC} \\ C_2(Q_{fuel, inj} - Q_g) & \alpha_{SODC} \leq \theta \end{cases} \quad (3)$$

where α_{SOC} and α_{SODC} indicates the start of combustion and start of diffusion combustion. C_1 is an empirically determined constant. C_2 is a second degree polynomial fitted to engine speed. C_2 will have a larger value at lower engine speeds, and also a slight increase at high speeds. The higher heat release rate per crank angle at lower speeds is expected because the diffusion combustion speed is fairly constant per time step. The increase at higher engine speeds could possibly be related to increased cylinder turbulence. In order to model the higher heat release rate during premixed combustion, C_1 is typically 2-3 times higher than C_2 . The fuel injected during the ignition delay will be added to the injected fuel during a short (fixed) crank angle interval, $\alpha_{SODC} - \alpha_{SOC}$, post the ignition delay. The length of this interval is determined empirically to fit measured heat release rate. More advanced models where the kinetic energy of the fuel spray is taken into account will give better results, especially during longer injection durations [8]. Computational efficiency is critical in this application; therefore this simple model for gross heat release is used.

Convective heat losses are given by:

$$dQ_{ht, conv} = Ah_c(T - T_{wall}) \quad (4)$$

The area A is calculated using the geometric properties of the engine. The gas temperature used is the global in-cylinder gas temperature T (from the previous crank angle step). The wall temperature T_{wall} is fixed at 450K and h_c is calculated using the Woschni expression [5]:

$$h_c = CB^{m-1} p^m w^m T^{0.75-1.62m} \quad (5)$$

B is the cylinder bore, p the cylinder pressure, w the average gas cylinder velocity and C is an empirically determined constant. The flame radiative heat losses are calculated using an approximate flame temperature T_{flame} (from the previous crank angle step):

$$dQ_{ht, rad} = C_{rad}(T_{flame}^4 - T_{wall}^4) \quad (6)$$

The factor C_{rad} is calculated by means of a black box expression (a linear regression model) depending on speed and injected fuel mass. C_{rad} is not a strictly physical parameter, it is used in the final step of the combustion model tuning to fit simulated to measured NO_x .

The radiative heat losses are thus implemented as a way of compensating some of the simplifications in the model. The wall temperature is usually small compared to the flame temperature, therefore it can be neglected. The resulting expression is:

$$dQ_{ht, rad} = C_{rad}(n_{eng}, \delta) T_{flame}^4 \quad (7)$$

where $C_{rad} = c_0 + c_1 \cdot n_{eng} + c_2 \cdot \delta$

Combining the equations, the net heat release is:

$$dQ_n = dQ_g - dQ_{ht, conv} - dQ_{ht, rad} \quad (8)$$

Finally, the pressure is calculated by rearranging the first law of thermodynamics (assuming that the gas composition is constant between two crank angle steps):

$$\frac{dp}{d\theta} = \left(\frac{dQ_n}{d\theta} - \frac{\gamma}{\gamma-1} P \frac{dV}{d\theta} \right) \left(\frac{\gamma-1}{V} \right) \quad (9)$$

Combustion

A complex iteration loop based on the minimization of Gibbs free energy is performed in each crank angle step in HRNOx [1]. The iteration determines the gas composition and the burned zone temperature. This type of model requires too much computational power in order to be used for engine control and transient simulation applications. A simplified method of calculating burned zone temperature in a multi-zone model is presented in [3]. A variation of this method has been implemented in this two-zone combustion model.

Locally stoichiometric combustion is assumed ($\lambda_{local} = 1$) and no air entrainment in the burned zone occurs.

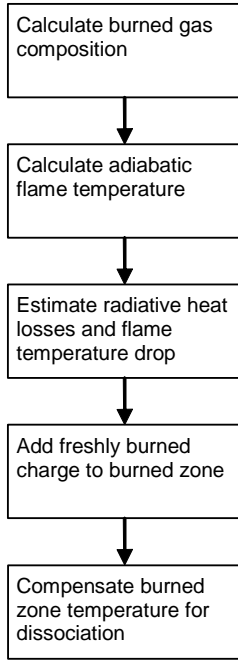


Figure 2 Burned zone temperature calculation

A flow chart of the simplified method is shown in Figure 2. First the gas composition of the unburned zone is calculated. The content of the recirculated exhaust is assumed to be the result of perfect (complete) combustion.

The gas composition is stored in a vector containing the following species: fuel, N_2 , O_2 , CO_2 and H_2O . The burned zone will consist of N_2 , CO_2 and H_2O only at all times due to the stoichiometric assumption. A fraction of the unburned charge is mixed with liquid fuel to stoichiometric conditions and instantaneously combusted to N_2 , CO_2 and H_2O .

The adiabatic flame temperature $T_{flame,ad}$ is calculated with an iteration loop (enthalpy balance between an unburned mass element and a perfectly burned mass element). The enthalpy and specific heats in the iteration are calculated using thermodynamic curve fit coefficients [9].

In order to compensate for dissociation of the (perfect) combustion products, tabulated data is used. This table describes the temperature drop ΔT which would occur if the combustion products (CO_2 , H_2O and N_2) dissociate adiabatically to CO , CO_2 , H_2 , H , OH , O , O_2 , NO , H_2O , N_2 and N . It is a function of pressure, temperature and local air-fuel equivalence ratio:

$$\Delta T = f_{eq}(p, T, \lambda_{local}) \quad (10)$$

The table is generated using a Gibbs free energy minimization approach analogously to Egnell [1]. Using this table, an estimation of the flame temperature (for radiative heat loss calculations only) is calculated:

$$T_{flame} = T_{flame,ad} - f_{eq}(p, T_{flame,ad}, \lambda_{local}) \quad (11)$$

$$dQ_{ht,rad} = C_{rad}(n_{eng}, \delta) T_{flame}^4 \quad (12)$$

A new flame temperature which is compensated for radiative heat losses can be calculated according to:

$$T_{flame,ht} = T_{flame,ad} - \frac{dQ_{ht,rad}}{C_p} \quad (13)$$

The flame temperature compensation is illustrated in Figure 3.

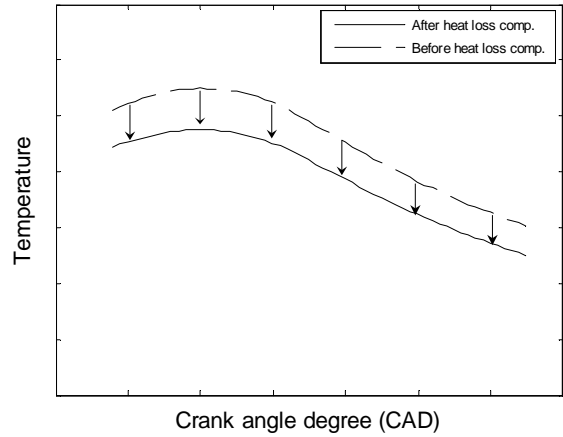


Figure 3 Illustration of flame temperature before and after heat loss compensation

The burned zone temperature is given by (isentropic expansion/compression using a fixed gamma value):

$$T_{exp} = T_{burn,perf}(\theta - 1) \left(\frac{p(\theta)}{p(\theta - 1)} \right)^{\frac{\gamma - 1}{\gamma}} \quad (14)$$

$T_{burn,perf}$ is the burned zone temperature before taking dissociation into account. The freshly burned mass element is added to the burned zone and the following energy balance can be calculated:

$$\begin{aligned} T_{burn,perf}(\theta) m_{burn}(\theta) C_p(T_{burn,perf}) &= \\ &= T_{exp} m_{burn}(\theta - 1) C_p(T_{exp}) + \\ &+ T_{flame,ht} m_{flame} C_p(T_{flame,ht}) \end{aligned} \quad (15)$$

where m_{burn} denotes the mass in the burned zone and $m_{flame} = m_{burn}(\theta) - m_{burn}(\theta - 1)$ is the mass of the freshly burned element (flame). In order to solve the new burned zone temperature, an iteration loop is needed.

Using the previous assumption that the burned zone (and the mass of the flame after combustion) consists of results of perfect combustion (N_2 , H_2O and CO_2 only), the specific heat value has weak temperature dependence in the temperature range. Assuming that the specific heats are equal, the burned zone temperature is:

$$T_{burn,perf}(\theta) = \frac{T_{exp} m_{burn}(\theta-1) + T_{flame,ht} (m_{burn}(\theta) - m_{burn}(\theta-1))}{m_{burn}(\theta)} \quad (16)$$

Finally, the burned zone temperature is compensated for dissociation:

$$T_{burn} = T_{burn,perf} - f_{eq}(p, T_{burn,perf}, \lambda_{local}) \quad (17)$$

This temperature is used for the NO formation calculations.

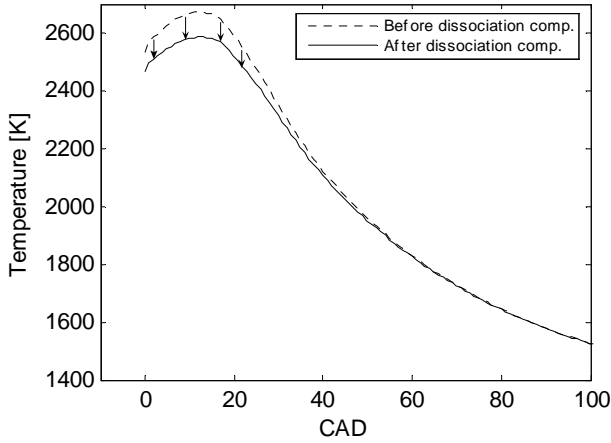


Figure 4 Typical burned zone temperature before and after dissociation compensation

A typical full load burned zone temperature trace before and after dissociation compensation is shown in Figure 4. Note that the temperature compensation is most substantial at high temperatures and close to zero at lower temperatures. This is expected since the dissociation is highly temperature dependent.

The exhaust (manifold) temperature is calculated using a black box expression [10]:

$$T_{em} = T_{im} + \frac{Q_{LHV} f(W_{fuel}, n_{eng})}{C_p (W_{eng,in} + W_{fuel})} \quad (18)$$

where T_{im} is the inlet manifold temperature, W_{fuel} the fuel mass flow, $W_{eng,in}$ the total mass flow (EGR + charge air) into the engine. f is a look-up table.

NO formation

The NO formation is modelled using the Zeldovich mechanism equilibrium approach [5]. The equilibrium approach assumes that the residence time in the flame is short; therefore the NO formation takes place in the burned zone only. The nitrogen concentration is small, compared to the NO concentration; because of this we can assume that

$$\frac{d[N]}{dt} = 0 \quad (19)$$

Using these assumptions, the following expression is derived:

$$\frac{d[NO]}{dt} = \frac{2R_1 \{1 - ([NO]/[NO]_e)^2\}}{1 + ([NO]/[NO]_e)R_1/R_2} \quad (20)$$

where

$$R_1 = k_1^+ [O]_e [N_2]_e \quad (21)$$

$$R_2 = k_2^- [NO]_e [O]_e \quad (22)$$

The rate constants are given by (parameter values from [5]):

$$k_1^+ = 7.6 \cdot 10^{13} e^{\frac{-38000}{T}} \quad (23)$$

$$k_2^- = 1.5 \cdot 10^{-9} e^{\frac{-19500}{T}} \quad (24)$$

T is the burned zone temperature. The equilibrium oxygen and NO concentrations are given by:

$$[O]_e = \frac{K_{p,O} [O_2]_e^{1/2}}{(\tilde{R}T)^{1/2}} \quad (25)$$

$$[NO]_e = (K_{p,NO} [O_2]_e [N_2]_e)^{1/2} \quad (26)$$

The equilibrium constants are calculated with Arrhenius expressions (parameter values from [5]):

$$K_{p,O} = 3.6 \cdot 10^3 e^{\frac{-31090}{T}} \quad (27)$$

$$K_{p,NO} = 20.3 e^{\frac{-21650}{T}} \quad (28)$$

The equilibrium oxygen and nitrogen concentrations in the burned zone are given by tables:

$$[O_2]_e = f_{O_2}(p, T) \quad (29)$$

$$[N_2]_e = f_{N_2}(p, T) \quad (30)$$

The equilibrium tables are calculated using a Gibbs free energy minimization approach similar to Egnell [1]. The equilibrium approach does have certain limitations compared to a full kinetic approach, as discussed in [7]. Considering its simplicity it is a good choice in this application however.

GAS EXCHANGE MODEL

The gas exchange model used is a “filling and emptying” quasi steady model previously described in [2]. Three control volumes and two restrictions are used to describe the gas flow. All gas compositions are assumed to be constant over time, i.e. the specific heat differentials will be zero. The model is schematically depicted in Figure 5. It uses four states, Table 1.

State	Description
p_{im}	Inlet manifold pressure [bar]
p_{em}	Exhaust manifold pressure [bar]
p_{es}	Exhaust system pressure [bar]
n_{trb}/n_{cmp}	Turbocharger speed [rpm]

Table 1 States of the gas exchange model

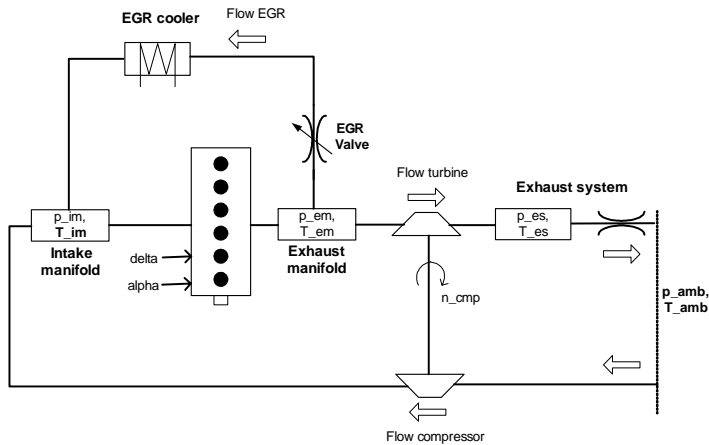


Figure 5 Schematic description, gas exchange model

The intake manifold temperature is not modeled and is used as an input to the model. The reason is that it is difficult to model the charge air and EGR temperatures. Factors such as fouling of the coolers and wind conditions will affect these temperatures in onboard applications. For laboratory use, with controlled ambient conditions, adding a simple intake manifold temperature model would make the model entirely predictive.

The different submodels will be presented following the air/exhaust path through the engine, starting from the intake side.

Compressor

The mass flow and efficiency of the compressor is calculated using look-up tables:

$$W_{cmp} = f_{W_{cmp}} \left(\frac{p_{im}}{p_{amb}}, n_{cmp} \right) \quad (31)$$

$$\eta_{cmp} = f_{\eta_{cmp}} \left(\frac{p_{im}}{p_{amb}}, n_{cmp} \right) \quad (32)$$

The torque is given by:

$$M_{cmp} = \frac{W_{cmp} C_{p,air} T_{amb}}{\eta_{cmp} \omega_{cmp}} \cdot \left(\left(\frac{p_{im}}{p_{amb}} \right)^{\frac{\gamma_{air}-1}{\gamma_{air}}} - 1 \right) \quad (33)$$

T_{amb} and p_{amb} is the ambient temperature and pressure.

Intake Manifold

The intake manifold is described as a control volume (an open system of constant volume). The energy balance between the mixed inlet manifold gas and the charge air / EGR is given by:

$$C_{p,air} W_{cmp} T_{cmp} + C_{p,exh} W_{egr} T_{egr} = C_{p,im} W_{im,in} T_{im,in} \quad (34)$$

Note however that the inlet manifold temperature T_{im} is an input to the model; therefore the EGR and charge air temperatures are not needed. By neglecting heat transfer, assuming a constant (slowly varying) temperature in the manifold and differentiating the ideal gas law and internal energies the following expression is achieved:

$$\begin{aligned} \dot{p}_{im} &= \frac{1}{V_{im}} (R_{im} \gamma_{im} W_{im,in} T_{im} - R_{im} \gamma_{im} W_{im,out} T_{im,in}) = \\ &= \frac{R_{im} \gamma_{im} T_{im}}{V_{im}} (W_{im,in} - W_{im,out}) = \\ &= K_{im} \cdot T_{im} (W_{cmp} + W_{egr} - W_{eng,in}) \end{aligned} \quad (35)$$

The constant temperature / adiabatic assumptions have been used in a number of similar models with sufficiently accurate results during both engine testbed and on road conditions [11].

Exhaust manifold

The exhaust manifold is modeled analogously to the intake manifold:

$$\dot{p}_{em} = K_{em} T_{em} (W_{eng,out} - W_{egr} - W_{trb}) \quad (36)$$

EGR system

The EGR flow is modeled using the expression for choked flow through a restriction, described by [5]:

$$W_{egr} = A_{egr} \cdot \frac{p_{em}}{\sqrt{T_{em} R_{exh}}} \cdot \psi \left(\frac{p_{im}}{p_{em}}, \gamma_{exh} \right) \quad (37)$$

where

$$\psi \left(\frac{p_{im}}{p_{em}}, \gamma_{exh} \right) = \begin{cases} \sqrt{\frac{2\gamma_{exh}}{\gamma_{exh} - 1} \left(\left(\frac{p_{im}}{p_{em}} \right)^{\frac{2}{\gamma_{exh}}} - \left(\frac{p_{im}}{p_{em}} \right)^{\frac{\gamma_{exh} + 1}{\gamma_{exh}}} \right)} & \text{if } \frac{p_{im}}{p_{em}} \geq \xi \\ \sqrt{\gamma_{exh} \left(\frac{2}{\gamma_e + 1} \right)^{\frac{\gamma_{exh} + 1}{\gamma_{exh} - 1}}} & \text{if } \frac{p_{im}}{p_{em}} < \xi \end{cases} \quad (38)$$

$$\xi = \left(\frac{2}{\gamma_e + 1} \right)^{\frac{\gamma_{exh}}{\gamma_{exh} - 1}}$$

A_{egr} is the effective flow area of the EGR valve, a function of the valve control signal u_{egr} (f is a look-up table):

$$A_{egr} = f(u_{egr}) \quad (39)$$

Turbine

The turbocharger has a variable geometry turbine, thus the mass flow and efficiency will depend on the VGT control signal u_{vgt} :

$$W_{trb} = f_{W_{trb}} \left(\frac{p_{em}}{p_{es}}, n_{trb}, u_{vgt} \right) \quad (40)$$

$$\eta_{trb} = f_{\eta_{trb}} \left(\frac{p_{em}}{p_{es}}, n_{trb}, u_{vgt} \right) \quad (41)$$

The torque and temperature after the turbine are given by:

$$M_{trb} = \frac{\eta_{trb} W_{trb} c_{p,exh} T_{em}}{\omega_{trb}} \cdot \left(1 - \left(\frac{p_{em}}{p_{es}} \right)^{\frac{1-\gamma_{exh}}{\gamma_{exh}}} \right) \quad (42)$$

$$T_{trb} = \left(1 + \eta_{trb} \left(\left(\frac{p_{em}}{p_{es}} \right)^{\frac{1-\gamma_{exh}}{\gamma_{exh}}} - 1 \right) \right) \cdot T_{em} \quad (43)$$

The turbine speed is calculated using:

$$\dot{n}_{trb} = \frac{60}{2\pi J_{trb}} \cdot (M_{trb} - M_{cmp}) \quad (44)$$

where J_{trb} is the inertia of the turbocharger.

Exhaust system

The exhaust system is modeled using a control volume (analogously to the intake and exhaust manifold):

$$\dot{p}_{es} = K_{es} T_{es} (W_{trb} - W_{es}) \quad (45)$$

A quadratic restriction describes the exhaust mass flow:

$$W_{es}^2 = \frac{p_{es}}{k_{es} R_{exh} T_{trb}} (p_{es} - p_{amb}) \quad (46)$$

where k_{es} is the discharge coefficient and $T_{es} = T_{trb}$.

All the parameters and also the compressor map are optimized to measured (transient) data during the tuning of the model.

THE COMPLETE MODEL

The two models are combined and executed from a common shell. Figure 6 illustrates the inputs and outputs of the complete model. The gas exchange model provides the simulated inlet manifold pressure and EGR rate to the combustion model and the combustion model calculates the exhaust temperature needed in the gas exchange model. External inputs are inlet manifold temperature, speed, EGR valve and VGT actuator signals, injected fuel mass, injection timing and rail pressure (of the common rail injection system). A large number of output signals are possible. Typical outputs are inlet and exhaust manifold pressure, EGR rate, NO concentration, peak cylinder pressure and exhaust temperature.

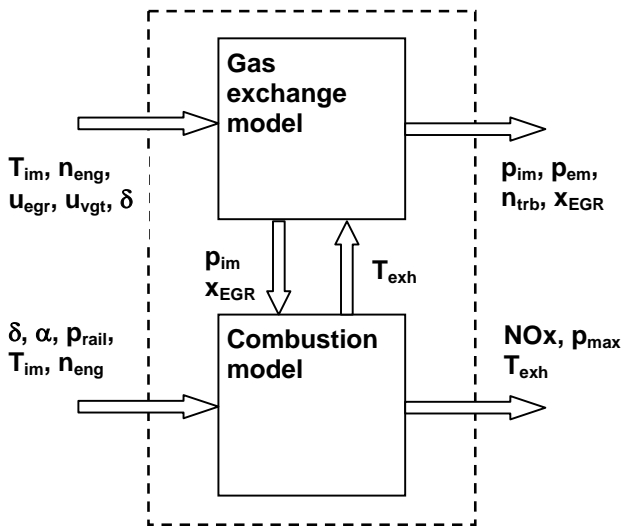


Figure 6 Inputs and outputs of the complete model

The gas exchange model uses a fixed step length of 10ms in order to stay stable in all operating cases. The combustion model is typically executed with a 100ms interval. This will be further discussed in the Computational efficiency section.

RESULTS

The models were validated in two stages, first using steady state data to validate the combustion model, secondly using transient data validating the complete model.

STEADY STATE SIMULATIONS

The combustion model was validated using steady state measurement data collected in an engine test bed, a total of 29 points varying in load from idle to 100% load and in speed from 500 rpm to 2300 rpm.

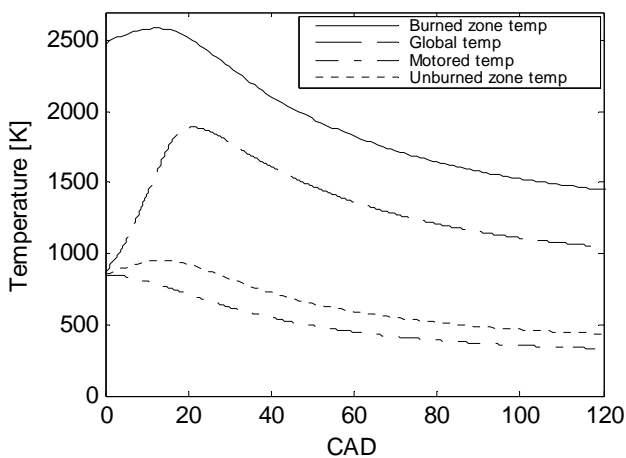


Figure 7 Typical combustion temperatures

Figure 7 shows simulated combustion temperatures at 1000 rpm / 100 % load. The zone temperatures have not been validated on the specific test engine because of a lack of in-cylinder temperature measurements. Based on

previous experience, a peak combustion temperature of 2550K seems reasonable though. An indirect validation can be performed by looking at the NOx formation because of the close correlation to burned zone temperature.

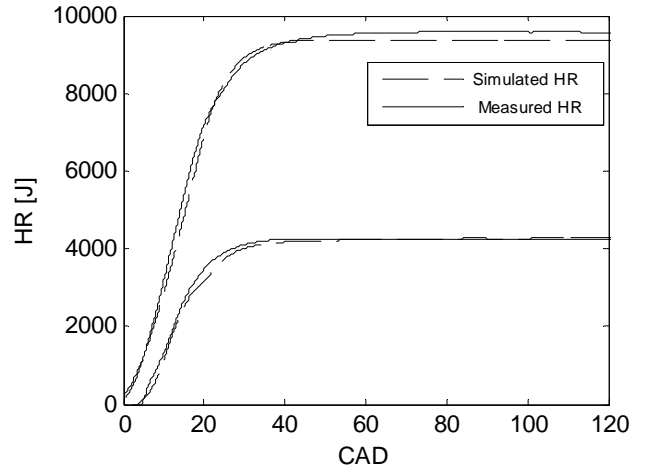


Figure 8 Measured and simulated heat release, two cases

Simulated heat release is a good match to measured quantities. Figure 8 shows the results for two different operating points. The close agreement in released heat at the end of combustion validates the choice of the Woschni expression (and the parameters used) for convective heat losses.

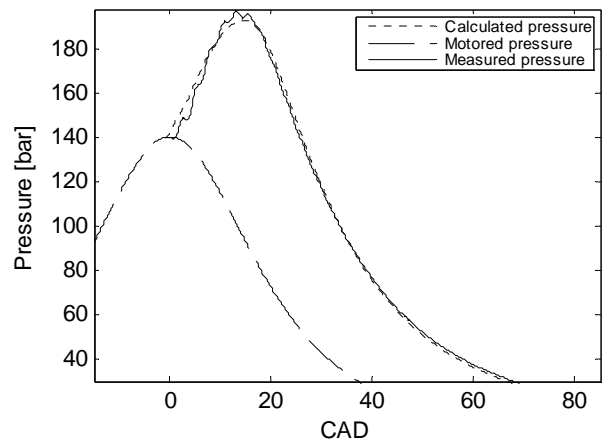


Figure 9 Measured and simulated cylinder pressure

Simulated cylinder pressure is compared with measured pressure in Figure 9 and Figure 10. The agreement is satisfactory in both cases. The pressure oscillations in measured data originate from pulsations in the channels to which the pressure sensors are connected to. Validation would be easier with proper flush mounted pressure sensors. Looking at Figure 10, it seems like the ignition delay is slightly under estimated (although hard to determine the exact figure due to the oscillations). This operating point is unusual though because of the late injection timing (1.4 degrees ATDC). Peak cylinder pressure is predicted with good precision.

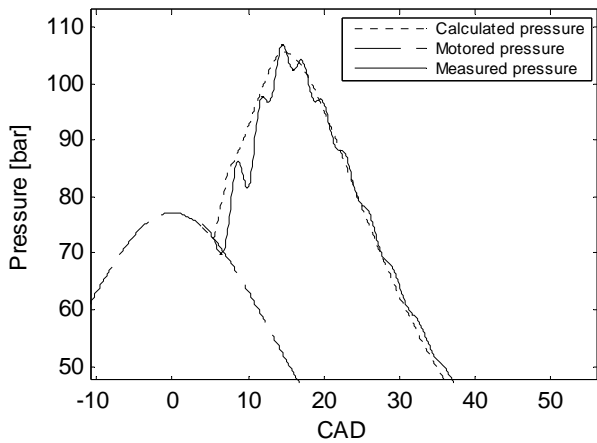


Figure 10 Measured and simulated cylinder pressure

Figure 11 shows measured and simulated NO_x for the steady state points studied. The agreement is quite good except for point 1. Point 1 is 500 rpm / 0% load (idle) which results in extremely low cylinder pressure and temperature. Under these conditions other NO_x formation mechanisms than the Zeldovich are dominating, therefore this deviation is expected. In [3] the author applies a black box compensation for low load operating conditions with good results. Disregarding from point 1, the mean relative error is 9.0%.

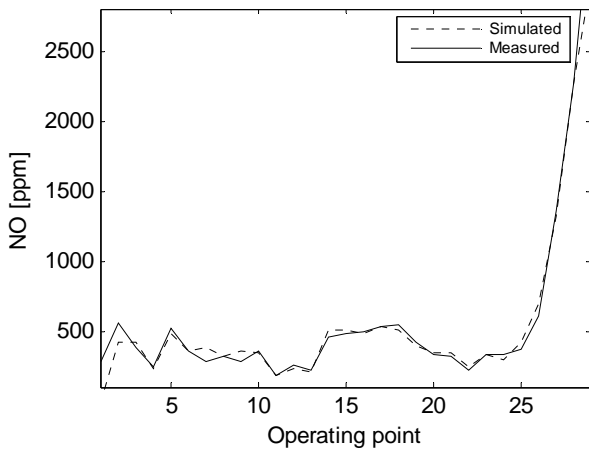


Figure 11 Measured and simulated NO_x steady state

TRANSIENT SIMULATIONS

The complete model was validated using the European Transient test Cycle (ETC). Figure 12 shows measured and simulated inlet manifold pressure from a sequence of the ETC. This figure is representative of the overall results. The mean relative error is 5.9%.

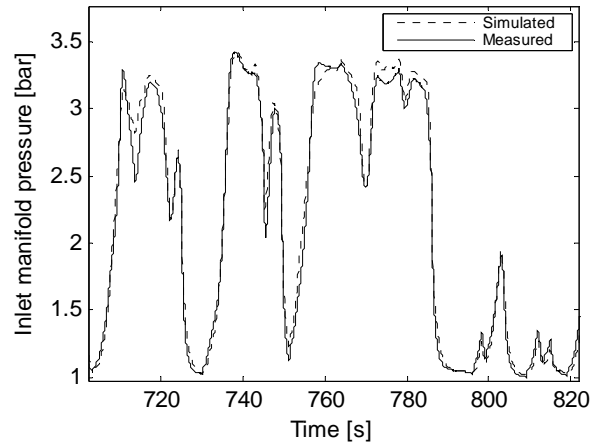


Figure 12 Measured and simulated inlet manifold pressure

NO_x was measured using a 1Hz sample rate (time averaged values) and compared with simulated results. Figure 13 and Figure 14 shows two sequences of the ETC where the agreement is quite good. The measurements do not have fast enough dynamics to make a proper validation. This is clear during the highly transient parts between 135s and 165s in Figure 13 and 220s to 230s in Figure 14. The measured values are obviously smoothed because of mixing in the pipes leading to the gas analyzer. Comparing instantaneous mean relative errors is therefore not relevant. The accumulated specific NO_x emissions have a mean relative error of 7.14% using parameters optimized to the previously described steady state data.

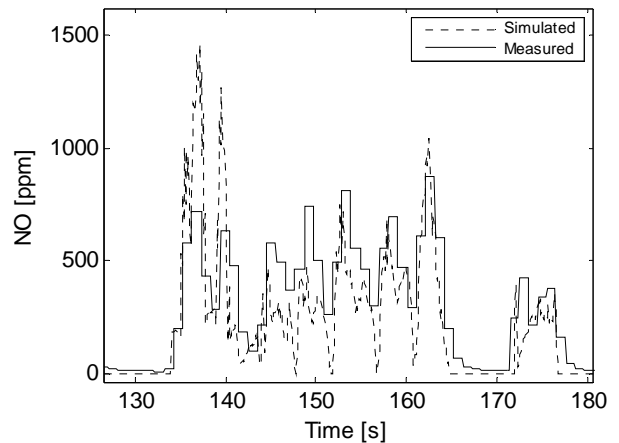


Figure 13 Measured and simulated NO_x , ETC part 1

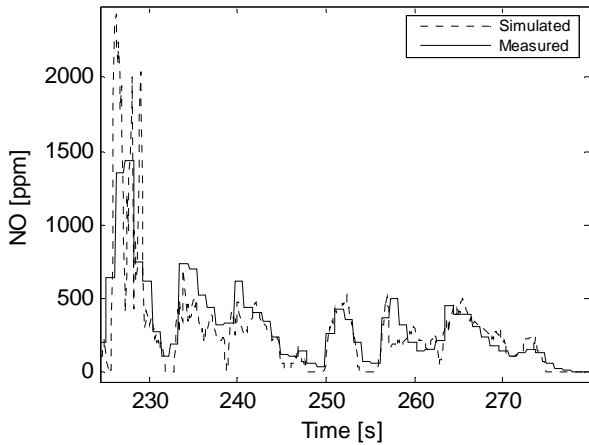


Figure 14 Measured and simulated NOx, ETC part 2

In Figure 15 the agreement between measured and simulated data is not as satisfactory as in the earlier plots. During a fairly steady state sequence (425s-450s) the model overestimates NO by approximately 100%. This is possibly related to an error in the EGR rate estimation in the gas exchange model. Experience from the engine lab has shown that the effective flow area of the EGR valve used is dependent on not only actuator position but also on temperature history. This will be apparent mainly during transient operation.

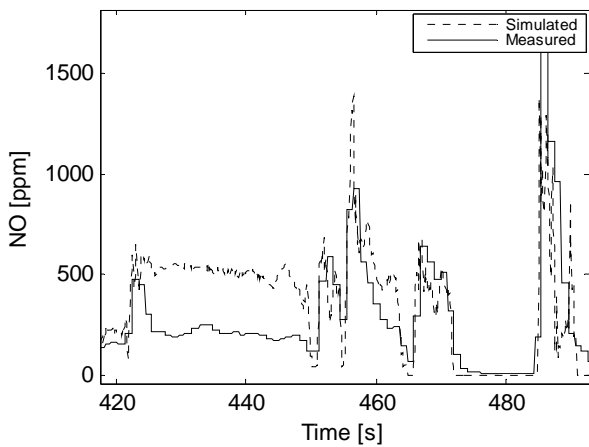


Figure 15 Measured and simulated NOx, ETC part 3

COMPUTATIONAL EFFICIENCY

One of the main goals for the model is computational efficiency. In this section the computational power requirements and what can be done to improve it is discussed.

The combustion model uses a 0.1 CAD step length for the pressure and heat release calculations in the reference case. The burned zone temperature and NO concentration are calculated with a 1 CAD interval. Using non-compiled Matlab code on a 1.6 GHz laptop computer, the average speed is 0.25 seconds per

complete calculation (mean value for the 29 steady state points). The obvious choice to improve performance is to increase the step length. Table 2 shows the influence of some different step length combinations on calculation time and mean relative error. The conclusion is that the NO / burned zone temperature calculation is the critical part. Increasing this step length does make the model substantially faster, although at the expense of a higher mean relative error. Increasing the heat release step length offers slightly faster performance in some cases.

HR step length [CAD]	NO step length [CAD]	Average speed [s]	NOx mean relative error [%]
0.1	1.0	0.25	9.0
0.1	2.0	0.20	10.2
0.1	4.0	0.17	19.3
0.2	2.0	0.19	10.3
0.2	4.0	0.13	16.2

Table 2 Influence of step lengths, combustion model

Another option to increase the calculation speed was explored; terminating the heat release / NOx calculations when the NOx rate has been stabilized. Once the burned zone temperature reaches below a certain level (typically 1800K) the NOx formation according to Zeldovich is essentially zero. In the model, this point is typically around 25-35 deg ATDC. The results using this "fast mode" with a fixed termination point of 30 deg ATDC are shown in Table 3.

HR step length [CAD]	NO step length [CAD]	Average speed [s]	NOx mean relative error [%]
0.1	1.0	0.10	9.0
0.1	2.0	0.07	10.3
0.2	2.0	0.05	10.4
0.2	4.0	0.04	16.2

Table 3 Influence of step lengths, fast mode, combustion model

The best choice is to choose a 0.2 degree step length for the heat release loop and a 2.0 degree step length for the NOx calculations. The resulting average speed of 0.05 seconds corresponds to real time performance up to 2400rpm which should cover all operating conditions of a heavy duty engine. By rewriting the code in a more efficient programming environment using compilation the performance could probably be improved even further.

The gas exchange model has been implemented in two versions, one in Matlab code with a 10 ms fixed step length using the Euler method to solve the differential equations and one in Simulink using either the ODE45 solver with variable step length or Euler with fixed step length. The Matlab version typically needs 40 ms per step which means that it is not quite real time. The Simulink version is considerably faster. Using automatically generated C-code from this version results in a code which is real time executable on computers of similar performance to the current engine control units. More work is needed to explain this difference in performance. The computationally heavy part of the gas exchange model are the interpolations. Possibly these are performed more efficiently in Simulink. Increasing the fixed step length beyond 10 ms results in instabilities, the mean relative error increases from 5.9% to over 50%. Increased step length in the gas exchange model is thus not a solution for improved performance.

When combining the two models, a fixed time scale is used. The combustion model is executed 10 times per second and the gas exchange model is run continually. Using the "fast mode" combustion model with the Simulink version of the gas exchange model, the result is a simulation time of less than 15 minutes for a complete ETC (2X real time performance). The combustion model could be executed more sparsely, saving valuable computational power. Considering that the NO_x measurements in the data set used has a 1 Hz sampling rate, it would be sufficient for validation purposes to execute the combustion model one time per second (using time averaged inputs), saving 90% computing time.

For the purpose of simulating engine plus exhaust aftertreatment systems (where the dynamics typically range in seconds) a 1Hz execution rate would be more than sufficient. For engine control purposes, a higher resolution would be useful though.

The currently used engine control units are too slow to run this model in its current form. Using more powerful CPU:s and by using compiled code, real time performance is within reach.

CONCLUSION

A two zone zero dimensional combustion and NO_x model is presented. The model is predictive, heat release rate is simulated using fuel flow data. Simplified methods of calculating burned zone temperature and NO formation according to Zeldovich is implemented resulting in an unusually fast model. On a 1.6 GHz PC using uncompiled Matlab code, the computational time is only 0.05 seconds per time step compared with several minutes with the previous models. Yet the accuracy is quite good, a 10.4% mean relative error is noted over 29 steady state operating points. Maximum combustion pressure is simulated with reasonable accuracy.

The gas exchange model presented is of the filling and emptying quasi steady type. Flow and efficiency maps are used to calculate compressor and turbine flows. The mean relative error in simulated inlet manifold pressure is 5.9% over the ETC.

By combining the combustion and gas exchange models the result is a low complexity complete engine model. The agreement between measured and simulated NO_x is satisfactory, simulated specific NO_x emissions (accumulated) has a mean relative error of 7.14%. During certain parts of the test cycle larger than acceptable errors occur though. This is possibly related to an error in the EGR rate estimation.

Compared to earlier models, the presented model is considerably faster. The computational time can be improved using longer step lengths in the NO calculation and likely further by using more efficient and compiled code. Real time performance in the engine control unit should be possible in the near future using CPU:s with higher performance.

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DEFINITIONS, ACRONYMS, ABBREVIATIONS

VGT		Variable geometry turbocharger
SCR		Selective catalytic reduction
EGR		Exhaust gas recirculation
CAD		Crank angle degree
α_{SOI}	[deg]	Start of injection
$\alpha_{SOC}, \alpha_{SODC}$	[deg]	Start of combustion / diffusion combustion
θ	[deg]	Crank angle degree
$Q_{fuel,inj}$	[J]	Injected fuel energy
Q_g, Q_n	[J]	Gross / Net heat released
$Q_{ht,conv}, Q_{ht,rad}$	[J]	Convective / radiative heat loss
δ	[kg/stroke]	Injected fuel mass
W_{fuel}	[kg/s]	Fuel mass flow
m_{burn}	[kg]	Burned zone mass
n_{eng}	[rpm]	Engine speed
λ, λ_{local}	[1]	Global / local air fuel equivalence ratio
x_{egr}	[%]	EGR rate
w	[m/s]	Av. Gas cylinder velocity
h_c	[J/m ² K]	Convective heat transfer coefficient
p_{rail}	[bar]	Common rail pressure
p	[bar]	Cylinder pressure
p_{im}, p_{em}	[bar]	Intake / exhaust manifold pressure
p_{amb}	[bar]	Ambient pressure

p_{es}	[bar]	Exhaust system pressure
T	[K]	Cylinder gas temperature
T_{wall}	[K]	Wall temperature
T_{im}, T_{em}	[K]	Intake / exhaust manifold temperature
T_{egr}	[K]	EGR temperature
T_{es}	[K]	Exhaust system temperature
T_{amb}	[K]	Ambient temperature
T_{flame}	[K]	Flame temperature
$T_{burn,perf}, T_{burn}$	[K]	Burned zone temp before / after compensation
T_{exp}	[K]	Expanded burned zone temp
n_{trb}, n_{cmp}	[rpm]	Turbine/compressor speed
$\omega_{trb}, \omega_{cmp}$	[rad/s]	Turbine/compressor angular speed
W_{trb}, W_{cmp}	[kg/s]	Turbine / compressor mass flow
η_{trb}, η_{cmp}	[rpm]	Turbine/compressor efficiency
M_{trb}, M_{cmp}	[kg/s]	Turbine / compressor torque
$W_{eng,in}, W_{eng,out}$	[kg/s]	Engine mass flow in / out
W_{im}	[kg/s]	Intake manifold mass flow
W_{egr}	[kg/s]	EGR mass flow
W_{es}	[kg/s]	Exhaust system mass flow
A_{egr}	[m ²]	EGR valve active flow area
u_{egr}	[V]	EGR valve actuator control signal
u_{vgt}	[V]	VGT actuator control signal
K_p	[1]	Equilibrium constant
$[X]$	[mol/m ³]	Concentration of species X
$[X]_e$	[mol/m ³]	Equilibrium concentration of species X
B	[m]	Cylinder bore
J_{trb}	[Nm/s ²]	Turbocharger inertia
R	[J/kgK]	General gas constant
γ	[1]	Specific heat value ratio
Q_{LHV}	[J]	Lower heating value
C_p	[J/kgK]	Specific heat value
A	[m ²]	Cylinder wall area
V	[m ³]	Cylinder volume