

Experimental Validation of Extended NO and Soot Model for Advanced HD Diesel Engine Combustion

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ABSTRACT

A computationally efficient engine model is developed based on an extended NO emission model and state-of-the-art soot model. The model predicts exhaust NO and soot emission for both conventional and advanced, high-EGR (up to 50 %), heavy-duty DI diesel combustion. Modeling activities have aimed at limiting the computational effort while maintaining a sound physical/chemical basis. The main inputs to the model are the fuel injection rate profile, in-cylinder pressure data and trapped in-cylinder conditions together with basic fuel spray information. Obtaining accurate values for these inputs is part of the model validation process which is thoroughly described. Modeling results are compared with single-cylinder as well as multi-cylinder heavy-duty diesel engine data. NO and soot level predictions show good agreement with measurement data for conventional and high-EGR combustion with conventional timing.

INTRODUCTION

The freedom to vary diesel engine settings for a given load and speed requirement has significantly increased over the last decades. This flexibility comes at the cost of a increased complexity of the engine control system annex algorithms. Real-time combustion models that predict heat release rate and emissions would be powerful and valuable tools for controller design, testing and calibration and thus reducing controller development time and costs. Moreover, such models could also be

used as combustion state estimators in model based control strategies.

Preferably, a model should be based on actual physics and chemistry, i.e. phenomenological. This will result in a more generic model. However, to limit computational effort, previous attempts at such models mentioned in literature often had an empirical or semi-empirical character and needed an extensive and expensive set of data for fitting/training of the model, [1],[2],[3].

In the present paper, phenomenological models for both NO and soot formation will be briefly introduced. For more detailed information about the models the reader is referred [4]. The models are developed for both conventional high temperature combustion and for high-EGR low temperature combustion. The models are aimed as an extension to TNO's current mean value engine model library DYNAMO. Focus is on the model validation process and its results. The main steps taken during the validation process are thoroughly described. Modeling results are compared with NO exhaust gas concentrations and soot mass for both a single-cylinder and a multi-cylinder engine.

NO FORMATION MODEL

The present NO formation model was presented more thoroughly in [4]. This section contains a summary of the model. NO formation is only considered for the diffusive combustion phase. With conventional heavy-duty diesel combustion – usually – the majority of the fuel is burned in the diffusion controlled combustion phase.

Furthermore, the equivalence ratio of the premixed burnt mixture is typically too fuel rich for significant NO formation, as experimentally confirmed by Dec [6]. Similarly, local in-cylinder Laser-Induced Fluorescence (LIF) measurements by Verbeizen et al. [7] showed very little NO formation up to the occurrence of the diffusion flame. The NO model follows the approach suggested by Murayama et al. [5] over thirty years ago, but with some differences as listed in [4]. In the used approach the amount of fuel that is burnt at a given crank angle value (within a step of 1 degree crank angle) is determined from a heat release rate analysis. The NO formation rate within the resulting package of combustion products is – at any instant – determined by the combined effect of the evolution of in-cylinder pressure and fresh oxidizer entrainment on package temperature and composition. The success of such approach depends on two important aspects: package initialization and package evolution. The most important characteristics of both aspects are summarized below:

Package initialization

FUEL MASS – The mass of fuel assigned to a new package is derived from a measured heat release rate profile.

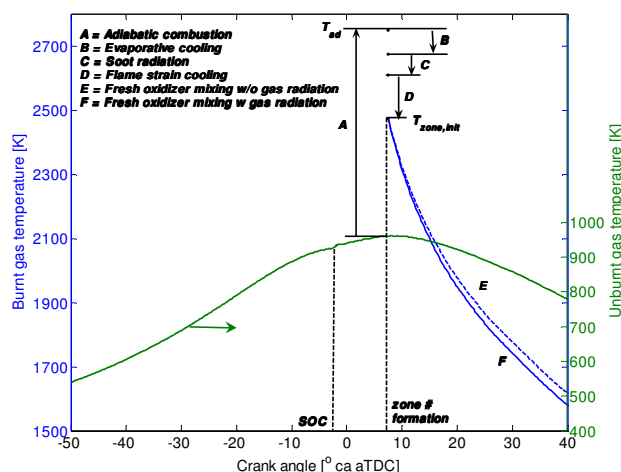


Figure 1 Graphical overview of initial combustion package temperature computation and subsequent evolution. Temperature corrections shown are qualitative; they are not representative for actual values.

INITIAL STATE – Initial combustion product temperature is based on the adiabatic flame temperature, including the effect of dissociation, computed using a chemical equilibrium solver based on minimizing Gibbs free energy. This temperature is corrected for the occurrence of several phenomena, as is graphically shown in Figure 1:

- *Evaporative cooling*: fuel evaporation extracts heat from the surroundings. By including the latent heat of evaporation into the computation of the adiabatic flame temperature, the flame temperature is corrected for this.
- *Hot soot particles radiative cooling*: Part of the wall heat transfer results from soot radiation. The radiative energy transferred during the crank angle of zone formation is used to correct the flame temperature.

- *Turbulence*: Turbulence results in so-called flame straining. At high levels of turbulence, physical time scales associated with the flow influence the chemical time scales. Equilibrium species concentration values are not reached which results in lower flame temperatures. One-dimensional diffusion flame computations with detailed chemistry have been used to quantify this temperature decrease. The inclusion of the influence of flame strain on NO formation is an extension to the model presented in [4].

Package evolution

After package formation, the combustion products are entrained with fresh oxidizer. It is well known that in modern DI diesel engines the fuel injection is the primary energy source driving the mixing process. In this study the mixing process is therefore linked to the fuel injection process: it is assumed that mixing of oxidizer into the combustion product packages is analogous to mixing of oxidizer into the fuel spray.

AIR ENTRAINMENT – The mixing process is described on the basis of the one-dimensional model for a free, fully developed, quasi-steady fuel spray as presented by Naber and Siebers [8]. This model gives the cross-sectional averaged equivalence ratio as a function of axial position along the spray axis:

$$\phi(\tilde{x}) = \frac{AFR_{st}}{\dot{m}_{ox}(\tilde{x})/\dot{m}_f} = \frac{2 \cdot AFR_{st}}{\sqrt{1 + 16 \cdot \tilde{x}^2} - 1} \quad (1)$$

where AFR_{st} is the stoichiometric “air”-fuel ratio and $\tilde{x}$ is the normalized axial position in the spray. According to Siebers [9] the oxidizer entrainment into a diesel spray follows the relation:

$$\dot{m}_{ox}(x) \propto \sqrt{\rho_{ox} \cdot \rho_f} \cdot d_f \cdot x \cdot U_f \cdot \tan[\theta_{spray}/2] \quad (2)$$

where ρ_{ox} and ρ_f are respectively the ambient oxidizer and fuel density, d_f is the diameter of the fuel stream at the injector nozzle hole exit, x is the axial position along the spray axis, U_f is the fuel exit velocity at the nozzle hole and θ_{spray} is the fuel spray cone angle.

As mentioned before, combustion products are assumed to be formed at the stoichiometric location. The model assumes that the equivalence ratio of a package continues to follow the relation described by equation (1) from this point onwards. In Figure 2 a graphical representation of this process is shown. Through this, every package is given a spatial position and can therefore also be referred to as a zone. The resulting temperature in the zones follows from solving the energy conservation equation.

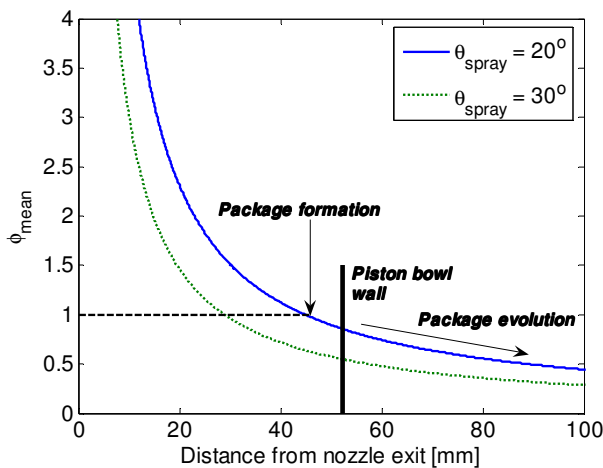
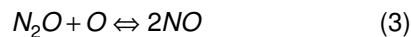


Figure 2 Evolution of 1-D quasi-steady spray according to model assumptions. $\bar{\rho}_{ox} = 30 \text{ kg/m}^3$, $d_{noz} = 0.178 \text{ mm}$. Conditions as given in Table 2 for sweep D (14.0 bar IMEP at 1500 rpm) and SOA of -10°ca aTDC .

TEMPERATURE CORRECTION – Hot species of CO , CO_2 and H_2O radiate to the environment. This results in a cooling of the hot combustion gases as is also graphically shown in Figure 1.

NO-FORMATION – The NO formation is computed as a post processing on the derived zone conditions. At any instant the species relevant for NO formation in a zone are assumed to be in chemical equilibrium as computed by the equilibrium solver. NO formation is computed according to the extended Zeldovich mechanism [10]. It is well-known that this mechanism can only account for NO formation at high temperatures ($> 1800 \text{ K}$) [10]. In an attempt to capture NO formation for low temperature combustion, e.g. when high levels of EGR are applied, the main NO formation reaction of the N_2O -intermediate route is added:



SOOT FORMATION MODEL

The soot formation model is strongly based on the zero dimensional soot model presented by Bayer and Foster [11]. Here, only a short summary of the model will be presented.

The soot model of Bayer and Foster is chosen because it describes soot formation in a burning diesel spray that follows the current conceptual view of diesel spray combustion as presented by Dec [12]. Besides this, through the used zero-dimensional approach, the model is also computationally efficient. This makes the model very suitable as a simulation tool in the controller development process.

The soot model is of the so-called two-step type as first suggested by Hiroyasu and Kadota [13]. The net soot production rate is the net effect of a soot formation and a soot oxidation contribution:

$$\frac{dm_s}{dt} = \frac{dm_{s,f}}{dt} - \frac{dm_{s,ox}}{dt} \quad (4)$$

Commonly, this two-step mechanism is applied in a multi-dimensional environment, where soot production is computed for local conditions. Bayer and Foster have applied the mechanism on a macroscopic level. The soot formation and oxidation rates are computed for characteristic regions of temperature and equivalence ratio of the burning fuel spray.

Figure 3 shows a schematic and simplified representation of a lifted, steady, burning fuel spray. The injected fuel is vaporized by the entrainment of hot oxidizer. Initial fuel pyrolysis occurs at the rich initial premix reaction zone present just downstream of the liquid length LL . The spray interior is fed with the fuel-rich products of this initial reaction. In this region, conditions are ideal for soot formation: temperatures are high and oxygen concentration is low. In the spray interior, soot particles are formed which grow as they are transported through the spray. Finally, the particles are oxidized in the vicinity of the diffusion flame formed around the periphery of the spray plume where the soot particles are exposed to high temperatures and oxygen.

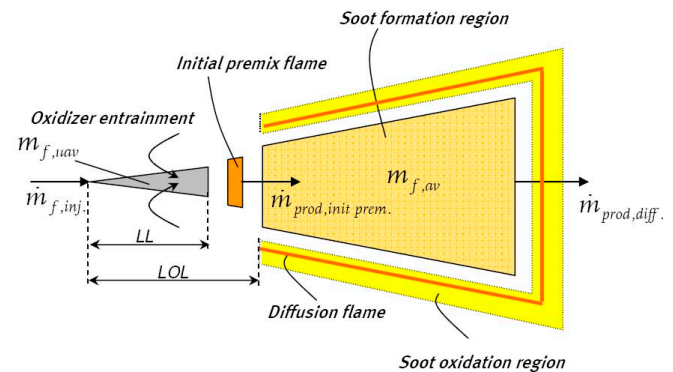


Figure 3 Schematic representation of a burning fuel spray with main regions of soot production process.

SOOT FORMATION – Following Bayer and Foster, the soot formation rate in equation (4) is given by the following expression:

$$\frac{dm_{s,f}}{dt} = C_{s,f} \cdot \bar{\phi}_{prem} \cdot m_{f,av} \cdot p^{0.5} \cdot e^{-\frac{E_{s,f}}{RT_{s,f}}} \quad (5)$$

The pre-exponential factors include a soot-formation constant $C_{s,f}$, the mean equivalence ratio of the rich initial reaction $\bar{\phi}_{prem}$, the available fuel mass for soot formation $m_{f,av}$ and the pressure p . The soot formation constant is used to tune the model to a specific fuel type and engine. The soot formation temperature $T_{s,f}$ is equal to the combustion product temperature of the rich initial reaction at the equivalence ratio $\bar{\phi}_{prem}$. The temperature is computed using the chemical equilibrium solver. The

fuel mass available for soot formation follows from a mass balance between the injected fuel and the already burned fuel following from the rate of heat release.

In contrast to the soot formation equation of Hiroyasu and Kadota [13], equation (5) includes the mean equivalence ratio of the rich initial reaction $\bar{\phi}_{prem}$. This equivalence ratio is included by Bayer and Foster following the observations of Chomiak et al. [14]. They observed that the absolute mass of soot formed during a combustion cycle is linearly dependent on the equivalence ratio of the initial combustion. The probability of the available mass of fuel to actually transform into soot increases when $\bar{\phi}_{prem}$ is increased.

Values of $\bar{\phi}_{prem}$ are typically in the range of 2 – 7 [14],[15].

Oxidizer can only be entrained into that part of the spray not sheathed by the diffusion flame. As a result, the equivalence ratio of the initial reaction is dependent on the so-called flame lift-off length *LOL*, see Figure 3: the distance between the nozzle and the most upstream location of combustion as found by Siebers and Higgins [15]. The *LOL* is determined using a semi-empirical correlation [11]. The equivalence ratio of the rich initial reaction is taken equal to the spray cross sectional averaged equivalence at the position of the *LOL* as follows from the one-dimensional spray model, see equation (1).

SOOT OXIDATION – Soot oxidation is assumed to occur in the vicinity of the stoichiometric diffusion flame. The soot oxidation rate is again given by an Arrhenius-type expression:

$$\frac{dm_{s,ox}}{dt} = C_{ox} \cdot m_s \cdot X_{O_2,st}^{C_{O_2}} \cdot p^{1.8} e^{-\frac{E_{s,ox}}{RT_{s,ox}}} \quad (6)$$

The pre-exponential factors include a tuning constant $C_{s,ox}$, the mass of soot m_s , the molar fraction of oxygen at the stoichiometric diffusion flame $X_{O_2,st}$ and the pressure p . The exponent C_{O_2} is equal to one in the model of Bayer and Foster. The momentary soot oxidation temperature $T_{s,ox}$ used in equation (6) is taken equal to the adiabatic flame temperature, computed by the equilibrium solver, of the stoichiometric diffusion flame. A single step reaction from pure fuel to complete combustion products is assumed to compute this temperature.

ADAPTATIONS TO ORIGINAL MODEL – The zero-dimensional approach used by Bayer and Foster results in a computationally efficient model. However, this comes at the cost of some crude approximations. In an attempt to overcome some of these shortcomings, several adaptations are made to the original model.

Fuel mass available – In the original model the fuel mass available for soot formation is given by the balance between the total amount of fuel injected and the cumulative amount of fuel already burnt as derived from the heat release rate. By doing so, the injected amount of fuel present upstream of the initial premixed reaction zone $m_{f,uav}$, see Figure 3, also contributes to the soot formation during the fuel injection period. In reality, this amount of fuel only becomes available at the end of fuel injection. The mass of fuel upstream of the initial reaction zone is therefore subtracted from the momentary fuel injection rate. The corresponding mass of fuel is consumed at the end of injection following a constant rate over the period of time it takes an injected fuel element to reach the initial reaction zone. The available fuel mass is computed from:

$$m_{f,av} = \int_{t_{SOI}}^t \dot{m}_{f,inj} dt - m_{f,uav} - \int_{t_{SOC}}^t \frac{ROHR_{diff}}{LHV} dt \quad (7)$$

where *LHV* is the lower heating value of the fuel.

In contrast to Bayer and Foster only the diffusive combustion phase is considered. It is postulated that the fuel that burns as premixed does not lead to significant soot formation. Therefore, only the diffusive part of the heat release rate is used in equation (7). The fuel mass associated with the premixed burn is subtracted from the instantaneous fuel injection rate.

Soot oxidation temperature – In the soot model presented by Bayer and Foster, the soot oxidation temperature changes instantaneously to the mean bulk gas temperature at the end of combustion. In doing so, it is implicitly assumed that soot oxidation continues to occur at the stoichiometric diffusion flame, with corresponding high temperatures, until the end of combustion. In reality, the steady combusting fuel spray, as assumed in the model, gradually breaks up into smaller soot formation clouds before the end of combustion. As a result of this break up, a steady combusting spray is no longer present and soot particles can avoid oxidation at the diffusive reaction layer. These soot particles are (partially) oxidized at lower temperatures and off-stoichiometric conditions. In an attempt to obtain a more realistic description of the oxidation process during the final stages of the combustion process, a more gradual decrease of the oxidation temperature from the adiabatic flame temperature to the bulk gas temperature is used by introducing a mixing time scale τ_{EOSS} :

$$T_{s,ox}(t) = T_{ad,EOSS} - (T_{ad,EOSS} - T_{bulk}(t)) \cdot \left(1 - e^{\frac{t-t_{EOSS}}{\tau_{EOSS}}} \right) \quad (8)$$

where $T_{ad,EOSS}$ is the adiabatic flame temperature at the assumed End Of Steady-State (EOSS) combustion.

Oxygen dependency – Preliminary simulations, using the original soot model, showed that the model was not able to correctly describe the increase in soot mass for increased EGR rates. To overcome this shortcoming, an additional tuning parameter C_{O_2} is introduced on the molar oxygen concentration in the soot oxidation rate expression, see equation (6). Because the equivalence ratio of the premixed initial reaction is unaffected by the residual gas fraction [15], the source of found deviation is believed to be in the soot oxidation. The soot oxidation process is primarily a particle surface oxidation process. The actual ambient oxygen concentration is therefore likely to have a great influence. By introducing the parameter C_{O_2} , the influence of EGR, which lowers the ambient oxygen concentration, on soot oxidation is increased. A value of 2.5 is found as a best fit.

MODEL VALIDATION

Figure 4 shows an overview of the different chronological steps taken to validate the emission formation model. The result of this process is an emission model for which the modeling concept has been validated, but which is not yet optimized regarding computational effort. This will be the main focus of planned future research to obtain a real-time emission model. The different steps taken during the validation process will be described in more detail in the following sections.

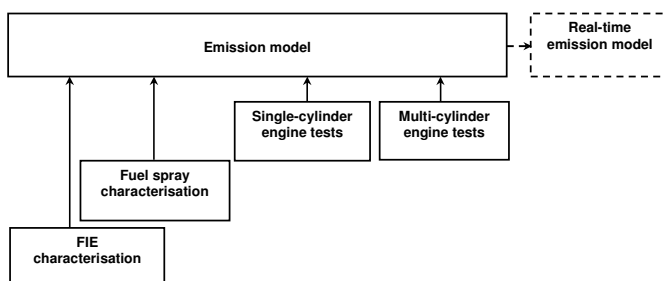


Figure 4 Overview of model validation process

FIE CHARACTERISATION - The first step in the validation process is the characterization of the Fuel Injection Equipment (FIE), which is of the Common Rail type. Both the NO and soot model are very dependent on inputs associated with the fuel injection process: the fuel mass flow rate and fuel exit velocity as is clear from equations (2) and (7) for example. Through the characterization of the FIE equivalent injection profiles, for the injection parameters set during a given engine test, can be reconstructed. The fuel injection rate is

reconstructed as a top-hat profile with finite opening and closing times.

For the reconstruction of both the fuel injection rate and corresponding fuel exit velocity, the flow through the injector nozzle needs to be characterized by determining two specific flow coefficients: the discharge coefficient C_d and the velocity coefficient C_v . These coefficients quantify the influence of cavitation on respectively the mass flow rate and fuel exit velocity. At the Combustion Technology group of the Eindhoven University of Technology full characterization of the nozzle flow is achieved by performing both mass flow rate and momentum flow rate measurements using dedicated experimental set-ups. Mass flow rates are measured using the method suggested by Zeuch [16]. More details on these measurements can be found in [17],[18]. The momentum flow rate is directly measured by impinging a fuel spray onto a force sensor. The required coefficients can be determined by combining both types of measurements considering that:

$$\dot{m}_f = A_{noz} \cdot \rho_f \cdot U_f = C_d \cdot A_{noz} \cdot \rho_f \cdot \sqrt{2\Delta p / \rho_f} \quad (9)$$

$$\dot{M}_f = \dot{m}_f \cdot U_f = \dot{m}_f \cdot C_v \cdot \sqrt{2\Delta p / \rho_f} \quad (10)$$

where ρ_f the fuel density, A_{noz} the geometrical nozzle flow area, Δp the pressure differential across the nozzle holes. Frequently, two additional flow coefficients are used. The area contraction coefficient C_a , which is defined as the ratio of the discharge coefficient to the velocity coefficient describes the loss in flow area by cavitation. Subsequently, the product $C_a \cdot C_v^2$ is referred to as the momentum coefficient C_M . Besides for the nozzle flow characterization, the mass flow rate measurements are also used to quantify the dynamics of the fuel injection process regarding the injection timing and the rise and fall rates of the mass flow rate during opening and closing of the injector. This is required to obtain accurate values for the actual start of injection as a function of rail pressure and injector start of actuation.

FUEL SPRAY CHARACTERISATION – The next step in the model validation process is the characterization of the fuel spray. In both the NO formation model and the soot formation model characteristic spray parameters are required: the spray cone angle, spray penetration distance, liquid length and flame lift-off length.

At the Eindhoven University of Technology extensive spray (combustion) analysis is performed in the Eindhoven High Pressure Cell (EHPC) using several optical techniques. Spray penetration and spray cone angle are determined using the Shadowgraphy and Schlieren method. Mie-scattering is used for liquid length determination. Flame lift-off lengths are determined using line of sight laser extinction techniques to measure soot incandescence. For more information regarding these measurements and results please refer to one of the following papers [18], [19],[20].