

Theoretical Analysis of Diesel Engine NO_x and Soot with Heuristic Macro-Parameter-Dependent Approach and Virtual Multi-Zone Real-Time Models

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ABSTRACT

With more stringent emissions regulations, effective emission modeling on NO_x and soot for both on-road and off-road diesel engines becomes increasingly important for diesel engine system design and real-time engine controls. In this paper, a heuristic macro-parameter-dependent approach is proposed by combining theoretical analysis with semi-empirical method. The proposed modeling approach is different from the existing methods, such as empirical modeling, phenomenological modeling, and three-dimensional KIVA modeling. The proposed model uses the macro parameters of engine performance, both cycle-average (e.g., air-to-fuel ratio, EGR rate) and in-cylinder instantaneous data (e.g., cylinder pressure trace) as input. The model computes NO_x and soot as a function of crank angle. A concept of "time-variant virtual space zones (burning, burned, and unburned)" is proposed based on the fraction of fuel burnt. The fundamental theory of soot formation and oxidation processes was applied in the soot model. Soot formation and oxidation was successfully decoupled to make the modeling convenient and effective. A major advantage of the proposed models is that emissions modeling can be conducted by using algebraic equations in real-time. And this makes the approach especially suitable and attractive for engine system design and for real-time emissions-related electronic controls.

1. INTRODUCTION

Diesel engine system design is very important for modern engine development. The system design uses cycle simulation tools to generate engine performance design specifications for each subsystem such as

turbocharging, EGR, cooling, electronic controls, and aftertreatment. The engine system design is conducted for both static (steady state) and dynamic (transient), for various concept configurations, at different engine speed and load, as well as at different ambient temperature and altitude conditions. Real-time engine performance simulation coupled with engine controls is an important part of the system design. Effectively predicting engine-out emissions at both steady state and transient may greatly enhance the quality of the engine system design. The emissions model which is suitable for diesel engine system design needs to possess the following features.

- (1) Firstly, the model needs to be computationally fast in order to enable the large-scale steady-state optimization of the entire system. The model needs to be programmable with algebraic equations (preferable) or ordinary differential equations, rather than partial differential equations. It is desirable to even use the spreadsheet programs (e.g., Microsoft Excel) to conduct the emissions calculations.
- (2) Secondly, it needs to have good predictability based on the fundamental physics and chemistry of engine performance rather than the "black-box" type of empirical approach using surface-fitting. The model needs to be able to capture the characteristics of a given combustion-fuel system. In order to ensure good accuracy in engine-out emissions prediction, the model needs to have a crank-angle resolution with the consideration of the detailed in-cylinder cycle process.
- (3) Thirdly, the model needs to be able to conduct real-time emissions calculation during engine transient

cycles for dynamic optimization in diesel engine system design and advanced controls.

- (4) Lastly, the model must be easy-to-tune with the minimum number of tuning coefficients. Moreover, the coefficients should be tuned by using the easily available engine performance test data in production development.

The role of emissions model in diesel engine system design is illustrated in Figure 1.

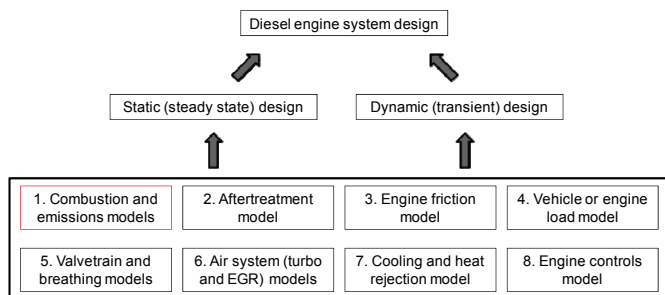


Figure 1. The role of emissions model in diesel engine system design

Cylinder pressure trace and heat release rate are important for emissions models and engine controls. References [1-14] reflect the important progresses in heat release rate analysis. Cylinder-pressure-based real-time combustion control and engine controls were reported in Ref. [15-20]. A review on the modeling for diesel engine controls was provided by Grondin et al. [21]. A real-time crank-angle-resolution simulation technique to predict detailed in-cylinder cycle processes was reported by Pacitti et al. [22]. There is a strong need to develop real-time emissions models of NO_x and soot for diesel engines based on crank-angle-resolution in-cylinder pressure information.

In the combustion and emissions modeling areas, there exists a vast body of literature on the theoretical and numerical simulations of diesel engine NO_x and soot. The models can be classified into four categories to date: (1) empirical model; (2) zero-dimensional model; (3) phenomenological model; and (4) three-dimensional (3D) model. A brief description is given below for the four categories.

1.1 Empirical approach

An empirical approach widely used in the engine industry to predict emissions is to build empirical parametric correlations between “factors” and “responses” from engine performance test data by using curve fitting or response surface method (RSM). The factors can be any parameter of engine design hardware (e.g., turbine effective area), calibration parameter (e.g., EGR valve opening or fuel injection timing), or engine performance parameter (e.g., intake manifold boost

pressure). The responses are emissions data (unburned hydrocarbon, NO_x, soot, or particulate matter). Such an empirical modeling approach bypasses the difficulties of modeling the complex in-cylinder physical and chemical processes involved in combustion and emission formation. The model can be built directly based on a large amount of engine test data to allow a quick estimate on emissions (for example, Jiang and Gerpen [23], Ramamurthy et al. [24]). However, such an empirical model has limited predictability, especially during transient, due to lacking the physics of the emission formation process. Its predictability is also limited by the given engine hardware, availability of test data and the experimental factor range. Usually, a prediction by extrapolating the model outside the factor range of the test data is not reliable. Neural network has been used to build transient emissions models for diesel engines (e.g., Traver et al. [25]). Its real-time predictability and the applications in advanced intelligent engine controls are limited by the quality of the neural network adopted and the availability of test data.

1.2 Zero-dimensional approach

In the zero-dimensional models, the in-cylinder volume is treated as a single zone or divided to burned and unburned zones without modeling the details of fuel spray and turbulent air entrainment, etc. (Zhang [26], Lafossas et al. [27])

1.3 Phenomenological approach

The phenomenological combustion and emissions models are usually referred to the diesel jet models or the fuel-drop evaporation/combustion models (e.g., Ref. [28-42]). In the diesel jet model, the fuel spray is assumed as a gas jet. The model simulates the mixing rate of the fuel spray and air, and calculates the local temperature, air-to-fuel ratio and combustion in each zone of the spray. The computed in-cylinder gas properties vary with both space and time. The fuel-drop model simulates the evolution of the fuel spray from the start of injection to the end of combustion. The physical and chemical processes of spray atomization, penetration, air entrainment, fuel evaporation, ignition delay, premixed and diffusion combustion (including heat release rate and cylinder pressure) and emissions are simulated as output. The model consists of analytical and semi-empirical sub-models for each of the above-mentioned phenomena. The phenomenological models may reflect certain physical and chemical mechanisms in the combustion processes. Through proper calibration the model can have limited predictability on heat release rate and NO_x. The phenomenological emissions models have several disadvantages. First of all, they are very computationally intensive. At the current computer speed it is impossible to use them for real-time emissions prediction or advanced engine controls. Secondly, the models contain many simplified assumptions on spray penetration, turbulence, swirl,

heat transfer, vapor concentration distribution, wall impingement, flame propagation, combustion, and emissions formation. There are many model tuning parameters as a result of many detailed sub-models. Usually, there is a practical difficulty in engine development to obtain the in-cylinder experimental data of combustion and emissions in order to justify or calibrate each sub-model.

1.4 Three-dimensional CFD-KIVA modeling

The 3D CFD-KIVA is a very complex multi-zone combustion model built based on partial differential equations of viscous fluid dynamics, turbulence, chemical reaction, boundary layer, heat transfer, etc. (e.g., Chikahisa et al. [43], Klingbeil et al. [44], Liu et al. [45]). Although it has demonstrated potential and practicality to be used as a design tool to predict emissions for combustion system design, at present time it is not possible to use it for diesel engine system design and real-time simulation due to its complexity and long computing time.

A different approach of diesel engine emissions modeling is proposed in this study for engine system design and advanced electronic controls. The approach is defined as a heuristic macro-parameter-dependent method. It lies between the zero-dimensional and phenomenological approaches.

Heuristics are the doctrine of obtaining new insights and universally valid design and calculation methods with the law of similarity or partially empirical simplification. Heuristic method is typically used to rapidly come to a solution that is reasonably close to the best possible answer, or optimal solution. The “macro” means the measurable engine performance parameters, either as a cycle-average or instantaneous at crank-angle resolution. The examples of the macro parameters include the following three types: (1) apparent cycle-average parameters such as air-to-fuel ratio, total EGR rate, intake manifold boost pressure, exhaust manifold pressure, intake and exhaust manifold gas temperature; (2) apparent instantaneous zero-dimensional in-cylinder bulk gas pressure, temperature, heat release rate, and burned fuel fraction (used as input in order to predict emissions); and (3) theoretical parameters in fundamental emissions research such as homogenous air-to-fuel ratio and adiabatic flame temperature. The heat release rate or burn rate can be obtained from either engine measurement or combustion models. The idea of “macro-parameter-dependent” is especially important for the soot modeling.

The proposed model has “multiple virtual space zones” at multiple time steps. Such a feature is different from the simple single-zone or two-zone approach used in the zero-dimensional models. Moreover, the zones in the proposed model are virtual zones instead of the physical space zones which have simulated physical boundaries

in the phenomenological approach. Furthermore, as real-time in-cylinder pressure measurement has become available for engine controls and advanced combustion control, a real-time engine-out emissions model is desirable to improve the capability of engine controls. The heuristic macro-parameter-dependent model developed in this paper has real-time fast computing speed. And it satisfies the four requirements mentioned earlier for diesel engine system design and advanced engine controls. This study is the first attempt to develop such a new approach for NO_x and soot modeling.

2. DESCRIPTION OF THE HEURISTIC MACRO-PARAMETER-DEPENDENT MODEL

The outline of the heuristic NO_x and soot emissions models is illustrated in Figure 2. The input to the model include the following: fuel composition, engine speed, fuel rate, global air-to-fuel ratio, total EGR rate (external EGR plus internal residue fraction), and in-cylinder thermodynamic bulk quantities as a function of crank angle (gas pressure, temperature and burned fuel fraction), etc. The in-cylinder cycle process parameters can be obtained from either experimental data or numerical simulation such as GT-POWER. The details of the model structure are presented as below.

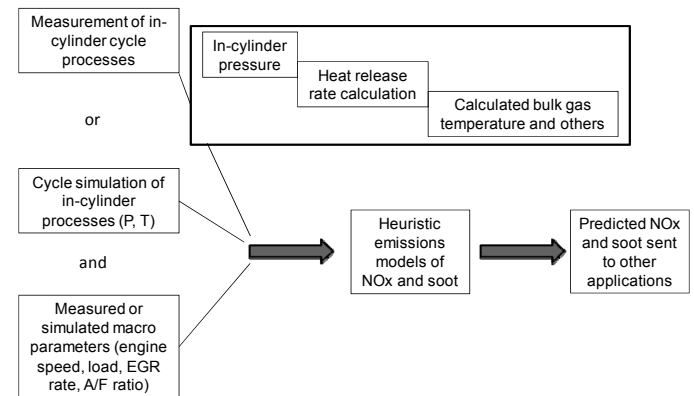


Figure 2. Outline of the heuristic emissions model

2.1 Time step

In the emissions calculations in this paper, the global oxygen concentration, nitrogen concentration and gas temperature in the engine cylinder refer to the bulk zero-dimensional quantities. The local quantities refer to the values in different virtual space zones. Emission formation has strong time dependency during the cycle process. Therefore, it is important to discretize the in-cylinder cycle process into different time steps (or equivalently crank angle steps), as shown in Figure 3. The time steps start from the start of combustion (SOC) timing and last to the exhaust valve opening timing. The calculations of concentration, pressure, temperature and emissions were usually conducted at the middle point within each time step. Fifteen time steps were chosen in

this study, although a much finer resolution (e.g., one degree crank angle) may be selected as well. The more time steps, the more accurate the simulation results but the longer the computing time. The number of time steps should be selected to ensure sufficient resolution along the burn rate curve and to balance the trade-off between accuracy and computing time.

2.2 Virtual space zones

As shown in Figure 3, within each time step, several space zones are defined in the entire cylinder. The space zones are “virtual” zones with volumes defined based on certain criteria (to be detailed below) but without the need to define their clear physical boundaries, unlike the physical zones used in the phenomenological models. Within the first time step, there are two virtual space zones, namely burning zone and unburned zone. The fuel burned fraction during the first time step is a known value from heat release rate. Stoichiometric combustion was assumed for the burning zone. Moreover, it was defined that the oxygen is completely consumed (i.e., the oxygen concentration becoming zero) at the end of a given time step within the virtual burning zone. In real combustion, the physical burning zones are distributed to many local flame kernels in an extremely complicated manner. It is very difficult to simulate the moving boundaries of the physical flame kernels. Therefore, in the heuristic model, the physical burning zones were artificially “lumped” into one virtual burning zone on the mass basis, as shown in Figure 4. In the following time steps, the virtual burning zone in the previous time step becomes a virtual burned zone. In each space zone, at any moment of time, the physical and chemical properties of the gas mixture (e.g., temperature, concentration) are assumed to be spatially homogeneous within that zone. At any moment of time, the gas pressure is uniform everywhere in the entire cylinder. Given the pressure, temperature and the mass in a virtual space zone, its volume can be determined by ideal gas law. At the end of the final time step, the entire cylinder has only one virtual burned space zone where all the gas properties become homogeneous.

Within each time step, it was assumed that there are mass transfer and heat transfer among the virtual burning zone, burned zone and unburned zone. At the end of the final time step the in-cylinder temperature and the concentrations of all species become uniform through mixing. Based on that assumption, the mass and heat transfer coefficients can be tuned in the heuristic model.

The above discussions show that the definitions of the space zone and time step are inter-related. The number of space zones is usually not less than the number of time steps. The heuristic model can be used for any diesel engines with a known heat release rate (for example, with multiple fuel injections).

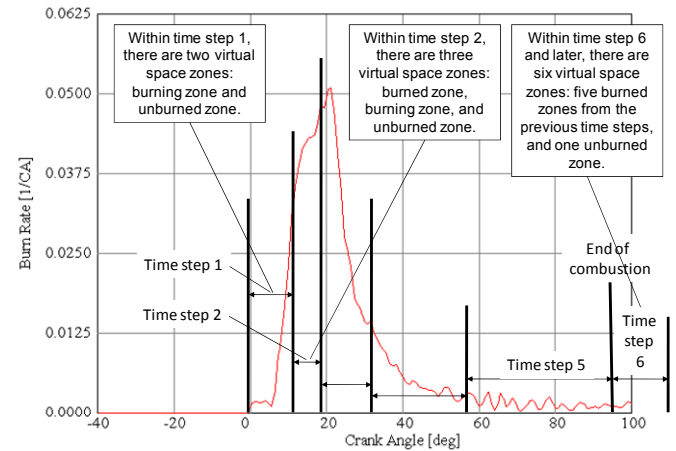


Figure 3. Illustration of time steps and space zones

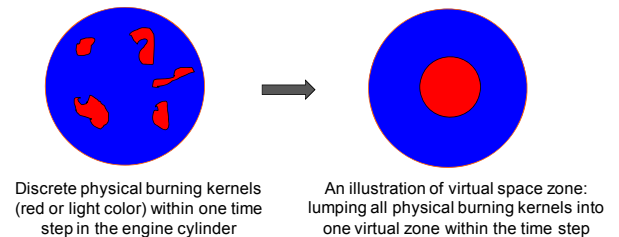


Figure 4. Definition of virtual burning space zone

2.3 The mass fraction of in-cylinder species prior to combustion

Provided a known combustion efficiency (100% here), fuel rate and air-to-fuel ratio, the gas compositions in the residue gases and EGR at the end of the combustion event can be determined. The oxygen mass fraction in the total cylinder charge prior to combustion is

$$O_{2,frac} = \frac{M_{O_2}}{M_{air} + M_{EGR_i} + M_{CxHy}} \quad [1]$$

Equation [1] is derived in details in the Appendix. Since NO_x and soot emissions are small in magnitude compared to other main combustion products, it was assumed that the amount of O₂ consumed during NO_x formation and soot oxidation is negligible, especially for the low NO_x engines under the EPA off-highway Tier 4 and 2010 on-highway emissions regulations. The mass fractions of CO₂, H₂O and N₂ were determined similarly.

2.4 The mass concentration and temperature during combustion in the burning and burned space zones

Since the oxygen mass concentration was supposed to be zero at the end of combustion in a burning space

zone, and the fuel in the burning zone was assumed fully consumed, all the combustion products were determined based on their atomic balances from Heywood [46].

Because the local gas temperature in each space zone (burning, burned and unburned) is critical for NOx and soot emissions, using a zero-dimensional homogenous bulk temperature in the entire cylinder would produce large errors. In the burning zone, its local maximum temperature at the end of the time step mainly depends on the following four factors: (1) the gas temperature in the unburned zone at the end of the last time step; (2) the heat released in the burning zone at the end of the current time step; (3) the gas mass in the burning zone; and (4) constant pressure specific heat. The calculation of the local maximum temperature was conducted similar to the adiabatic flame temperature at constant pressure condition, as shown in equation [2]

$$T_{LocalMax} = T_{unburned} + C_1 \cdot \frac{H}{m_t \cdot c_p} \quad [2]$$

where the constant-pressure specific heat c_p was modeled as $c_p = 0.952 + 0.00027 \cdot T_{LocalMax}$, in the unit of kJ/(kg.K). $T_{LocalMax}$ is in the unit of Kelvin. H is the heat released from fuel in the unit of kJ. The m_t is the total mass in the burning zone in the unit of kg. C_1 is a dimensionless heat transfer coefficient with a maximum value of 1. In the burned zone, $H=0$.

As mentioned earlier, it was assumed that there are mass transfer and heat transfer among the space zones caused by the differences in specie concentration and temperature. In real combustion processes, the mass and heat transfer is very complex. In this study, the heat transfer was handled globally by considering the temperature difference between a given space zone and the in-cylinder thermodynamic bulk temperature at a given time step. A time-varying coefficient β was used to modify the temperature difference. The mass transfer was handled similarly. In Figure 5, the β in the “monotonically increasing” model was defined as the ratio between the time step and the time duration from the beginning of the time step to the exhaust valve opening timing. Note that based on this definition, at the final time step, the β is equal to 1. Such an assumption of β implies an increasing coefficient vs. time to modify the driving differential for heat or mass transfer. At the beginning of the combustion, the β must be much lower than 1 in order to avoid unrealistically large heat transfer from a small burned zone to a large unburned zone. At the end of the combustion event, the β should not be larger than 1. Therefore, the β should generally increase with time. The nonlinearity behavior of the β versus time depends on the number of time steps assumed, as shown in Figure 5. Another model of a non-monotonically increasing β can be adopted (as shown in Figure 5) to simulate the impact of in-cylinder processes

(e.g., turbulence) on heat transfer or mass transfer when piston speed varies during the stroke. These assumptions on the β may be improved in the future.

At any time step, the in-cylinder pressure was either measured or computed as a known input. In the burning zone, its mass was determined as defined in Section 2.3. Its temperature was calculated based on equation [2]. Therefore, its virtual volume was calculated by

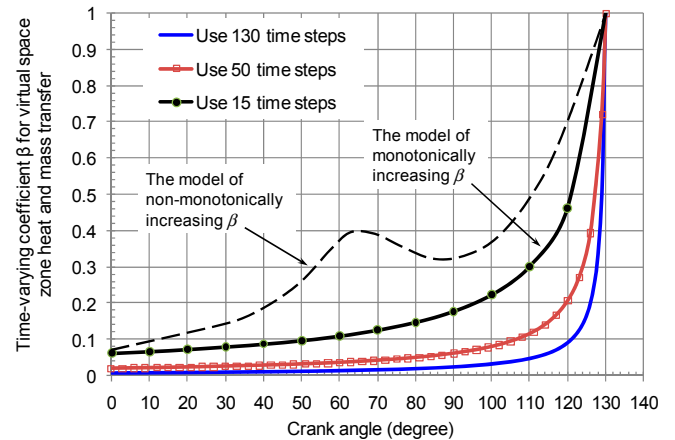


Figure 5. The characteristics of the coefficient β

using the ideal gas law. It should be noted, for example, if there is 5% of fuel burnt at a given time step, it is assumed that eventually at exhaust valve opening there should be 5% of nitrogen out of the total nitrogen amount in the cylinder “globally matching” that burning event through mass transfer.

In the burned zone, its initial temperature at the beginning of the time step was taken from the previous zone (burning or burned) at the end of the last time step. Its mass transfer and heat transfer were determined based on the coefficient β . Its final gas temperature (or mass) at the end of the time step was calculated based on the initial temperature (or mass) and the heat (or mass) transfer. Again, its virtual volume was calculated by using the ideal gas law. Particularly, the mass transfer calculation was handled as follows. For example, the required mass of nitrogen which participated in combustion at the beginning of the time step was determined by stoichiometric combustion requirements. This stoichiometric mass is apparently lower than the “globally matching” mass of nitrogen mentioned above. The difference is the driving factor for mass transfer. The difference becomes smaller and smaller with time, and eventually at exhaust valve opening it becomes zero. An overall coefficient β is used to account for the mass transfer of nitrogen for burned and unburned zones. There is no need to use any diffusivity coefficients. The mass transfer of all other species was handled similarly. Moreover, the heat transfer calculation was conducted in the following way. The burned zone temperature at the beginning of the time step is equal to the burning zone temperature at the