

CO Emission Model for an Integrated Diesel Engine, Emissions, and Exhaust Aftertreatment System Level Model

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ABSTRACT

A kinetic carbon monoxide (CO) emission model is developed to simulate engine out CO emissions for conventional diesel combustion. The model also incorporates physics governing CO emissions for low temperature combustion (LTC). The emission model will be used in an integrated system level model to simulate the operation and interaction of conventional and low temperature diesel combustion with aftertreatment devices. The Integrated System Model consists of component models for the diesel engine, engine-out emissions (such as NO_x and Particulate Matter), and aftertreatment devices (such as DOC and DPF). The addition of CO emissions model will enhance the capability of the Integrated System Model to predict major emission species, especially for low temperature combustion.

In this work a CO emission model is developed based on a two-step global kinetic mechanism [8]. In addition, effect of physical parameters such as start of injection (SOI) and ignition delay are studied and modeled to develop a phenomenological CO emission model. This includes development of a simple spray model to compute amount of fuel missing the bowl in case of PCCI and HCCI type combustion. Results from the spray model are used to simulate the motion of fuel in the cylinder bowl during various stages of combustion. Ignition delay effects are analyzed and modeled to

change the activation temperature of CO oxidation reaction to simulate the affect of increasing peak temperatures with advancing SOI. The results from the CO emission model are compared with experimental data from a multi-cylinder conventional diesel engine as well as a single cylinder version of a low temperature combustion diesel engine. For the LTC engine, the start of injection is advanced using two different injection strategies (single and two-step injection). Overall the results show good agreement of the trends between the experiments and model predictions.

INTRODUCTION

For the development of ultra low emission diesel vehicles, different combustion technologies as well as aftertreatment strategies are being analyzed and developed. A global effort is being made to develop practical low temperature combustion engines which meet the stringent emission norms and operate for all speed-load conditions. Efforts are also being made to develop various aftertreatment devices to have more control on the engine out emissions for different diesel combustion regimes. Steady state and dynamic system level models help the engine manufacturers during early stages of vehicle development. Modeling of entire engine, emission and aftertreatment is necessary to assist in optimization [6].

In previous work a system level model consisting of sub-models for diesel engine, emission and aftertreatment devices was developed [5]. Commercial one dimensional engine simulation tools such as WAVE and GT-Power are used to mainly obtain engine performance and tailpipe exhaust gas pressure and temperature. The emission sub-models developed are for NO_x and PM (particulate matter) predictions. The aftertreatment sub-models used include a diesel oxidation catalyst (DOC) and a diesel particulate filter (DPF). Controllers were developed to allow for transient

simulations, active DPF regeneration via exhaust fuel injection ahead of DOC and intake throttling. The emission models are developed using Matlab, the DPF model is in FORTRAN, the DOC model is in Simulink. Simulink is used to integrate all the sub-models into an overall Integrated System Model [5]. The Integrated System Model is used to simulate the physical processes occurring in real automobiles to save time and cost in vehicle development.

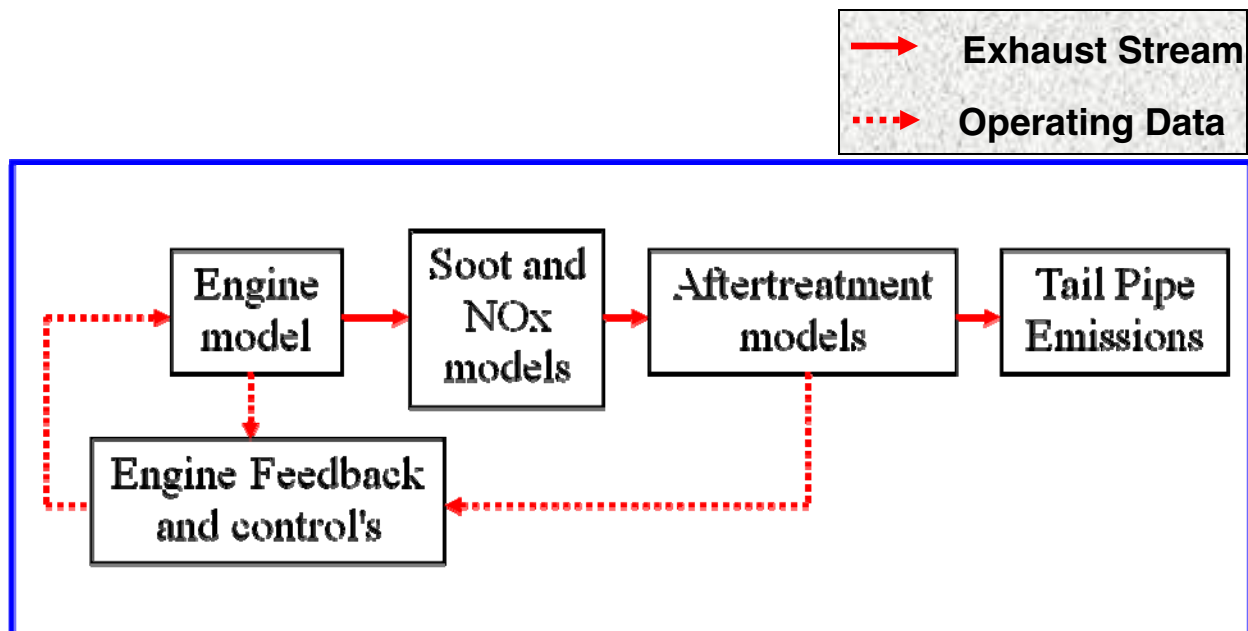


Figure 1: Schematic of Integrated Engine, Soot and NO_x Emission, DOC, and DPF Simulink Model [5, 6].

Figure 1 is the schematic of the Integrated System Model implemented in Simulink [5, 6]. The Integrated System Model currently lacks CO and UHC emission models. CO is an important emission species for new low temperature combustion strategies being studied. Homogeneous Charge Compression Ignition (HCCI) and Premixed Charge Compression Ignition (PCCI) are the two prominent low temperature combustion strategies being studied which have low NO_x and particulate matter emission along with high diesel like efficiencies. The disadvantages of these strategies are high CO/UHC emissions and high peak pressures. While HCCI requires very advanced injection for a complete homogeneous mixture before combustion starts, PCCI requires less advanced fuel injection. Advanced fuel injection created issues such as wall wetting and high UHC/CO emissions due to incomplete combustion.

In the current work a simplified kinetic CO emission model is developed based on a two-step global kinetic mechanism. The in-cylinder average pressure, temperature and species concentration inputs to the kinetic mechanism are obtained from the engine which is modeled using commercially available 1-D engine simulation software. Different temperatures are used for the CO generation and oxidation reaction after studying the physics governing in-cylinder CO formation and oxidation. The effect of physical parameters such as start of injection (SOI) and ignition delay for LTC are incorporated into the model. A simple spray model is developed to be used for capturing the effect of advancing SOI. The spray model computes the amount of fuel missing the bowl for advanced fuel injection.

Two independent data sets from a conventional and a low temperature diesel engine were used to validate the

model CO predictions. The spray model results are also validated with the GENSPRAY model [17] results for varying SOI. The data set from the conventional engine is for different speed-load operating conditions. The operating data range from low load low speed (idling) to high load high speed conditions with varying EGR. The second data set is from a single cylinder version of a LTC engine with high EGR ($\approx 67\%$) and advanced SOI.

KINETIC MODEL

The Integrated System Model does not have an emission model to predict engine out CO. The commercial 1-D engine simulation codes provide only equilibrium values for CO. However CO is kinetically governed and this is especially important for LTC applications. For the Integrated System Model to predict the correct emission species concentration for conventional as well as low temperature diesel combustion, a CO emission model is developed and implemented. Chemical kinetics and physical laws governing CO formation and oxidation were studied and modeled for diesel combustion.

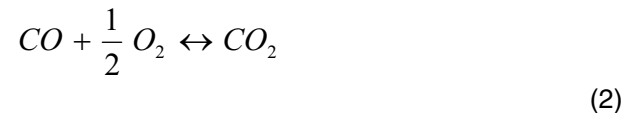
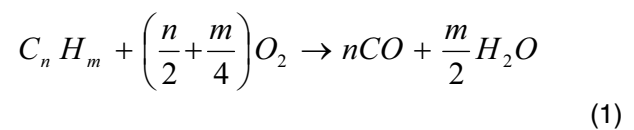
CO emissions are the result of incomplete combustion of fuel. CO is an intermediate species which is formed before complete combustion when fuel reacts with the oxidizer. The rate of CO oxidation is slow compared to many hydrocarbon species. Thus, CO can lag behind in oxidation even with the presence of enough oxygen. Oxidation of CO with the help of hydroxyl (OH) radicals is the final step in complete combustion of fuel. CO oxidation is a highly exothermic reaction and an important heat releasing step in combustion of hydrocarbon fuels.

There are two main sources of CO emission from diesel engines: over mixing and under mixing of fuel with air. The case of over mixing of fuel is associated with lean combustion during the ignition delay period [7]. The low temperatures associated with lean combustion fail to oxidize CO completely within the engine time scale even though there is enough oxygen present. In the case of under mixing of fuel, CO is the product of rich premixed combustion. This type of situation arises in low temperature combustion where the fuel is not mixed properly with air [14]. The CO formed fails to mix with the available oxygen to complete combustion.

The primary reaction for CO oxidation involves hydroxyl (OH) radicals that are formed as a result of chain branching reactions involving oxygen [22, 23]. These reactions occur at high temperature and are very temperature sensitive. Thus the oxidation of CO involving OH radicals requires both; the correct amount of oxygen concentration and sustained high temperatures. Conventional diesel combustion is lean

and takes place at high in-cylinder temperatures, thus CO is not a prominent emission species for conventional diesel combustion. Low combustion temperatures due to high EGR produces significant CO emission for LTC. Mixing plays an important role in distribution of oxygen in the cylinder, thus oxidation of CO is also greatly impacted by mixing in the case of low temperature diesel combustion where high amount of EGR is present.

A global mechanism for oxidation of different hydrocarbon fuels has been developed using a numerical laminar flame method [8]. In the current work a two step mechanism is used for the oxidation of diesel fuel. The first step in the mechanism is the oxidation of fuel or generation of CO (Eq. 1), and the second step is the oxidation of CO through a reversible reaction (Eq. 2).



The rate expressions for the two step mechanism used to develop the kinetic CO emission model are shown in Eqs. 3-5.

$$\frac{dCO_g}{dt} = P_g Y_{fuel}^{0.25} Y_{O_2}^{1.5} e^{\frac{-E_g}{RT}} \quad (3)$$

$$\frac{dCO_{of}}{dt} = P_{of} Y_{CO} Y_{O_2}^{0.25} Y_{H_2O}^{0.5} e^{\frac{-E_{of}}{RT}} \quad (4)$$

$$\frac{dCO_{ob}}{dt} = P_{ob} Y_{CO_2} e^{\frac{-E_{ob}}{RT}} \quad (5)$$

Eq. 3 is the rate of molar concentration of CO generation or rate of molar concentration of fuel oxidation. Eq. 4 and 5 are the forward and reverse rate of CO oxidation respectively. These equations are modeled using Matlab.

The temperature (T) used in the rate equations is the crank angle resolved bulk mean temperature of the cylinder. Y_{O_2} , Y_{H_2O} and Y_{CO_2} are the crank angle

resolved equilibrium in-cylinder oxygen, water and carbon dioxide molar concentration. These parameters are obtained from sensors on cylinder in the engine model. The net rate of change of CO concentration is defined by Eq. 6 as follows:

$$\frac{dCO}{dt} = \frac{dCO_g}{dt} - \frac{dCO_{of}}{dt} + \frac{dCO_{ob}}{dt} \quad (6)$$

Engine out CO concentration is computed after integrating the above rate equation as shown in Eq. 7 below:

$$CO_{engine\ out} = \int_0^{t_{cycle}} \frac{dCO}{dt} dt \quad (7)$$

The Matlab ODE solver is used to integrate the non-linear stiff differential equations (Eqs. 3-5). This is only a temporal integration as spatial variation within the cylinder is not considered.

Initially, the modeled kinetic CO emission results did not compare well with the experimental data. The emission model over-predicted the engine out CO concentration by an order of magnitude when compared with experimental data for all the eight operating modes. This is due to the fact that the mechanism was developed using a laminar premixed flame model whereas diesel combustion takes place as a turbulent diffusion flame. Similar observations were made by Aceves et al. [9] who studied HCCI combustion and emission using a similar two step mechanism for gasoline combustion. Aceves et al. [9] modified the pre exponential constants to get good prediction for combustion characteristics but over-predicted CO predictions.

CO oxidation is dominated by $CO + OH \rightarrow CO_2 + H$ reaction. Formation of OH radicals ceases after a certain temperature ($\approx 1400-1500$ K) [13] and thus it freezes the CO oxidation when the local in-cylinder temperatures fall below 1400K. An approximate average temperature of 1500 K is required for OH radical formation and thus complete oxidation of CO [19]. This chain reaction of oxidation of CO is combined into a global oxidation reaction in the two step mechanism, which was modeled to compute the engine out CO concentration. Using the correct temperature for the formation and oxidation reaction is critical to obtain meaningful result from the two step mechanism for diesel emission applications.

Since soot and CO are oxidized simultaneously in the rich combustion regimes of the diffusion flame [19] the soot model was used to obtain temperatures for the CO model. The soot model was previously implemented into the Integrated System Model [1, 2]. Neural network weights were added to the model to build a predictive soot emission model that incorporates physical laws as well as information derived from experimental data [3, 4]. The soot model consists of sub-models to compute local equivalence ratio, soot formation and oxidation and has been validated extensively.

The soot oxidation model calculates the post reaction temperature by an enthalpy balance of reactants and products at the rich initial reaction zone. Since this is a post reaction temperature, it is used in the CO kinetic model for CO oxidation. An average of bulk mean temperature and post reaction temperature from the soot model is used as the input temperature for the CO oxidation reaction. This temperature will be referred to as T_o for the rest of this paper. CO is formed during the main combustion event which is represented well by bulk mean temperature. Thus, two different temperatures are used in the emission model. The bulk mean temperature is used for the CO formation rate and T_o is used for the CO oxidation rate.

CONVENTIONAL DIESEL COMBUSTION RESULTS

The model results are compared with the experimental dataset from a conventional diesel engine. The dataset has eight data points corresponding to eight-mode engine operating conditions for varying speed/load with EGR. The dataset is from a light duty 4.9L diesel engine with EGR, boost and pilot injection [5]. A summary of the eight mode experimental data is shown in Table 1 in the appendix

Figure 2 shows the comparison of the CO emission model results with CO from correlated engine model using WAVE and the experimental eight mode data. The CO emission results from the correlated engine model in WAVE are using the built in kinetic CO emission model [25]. The comparison for operating mode 7 is not included in the figure as there was uncertainty in collecting the experimental data for this mode.