

LOW-DIMENSIONAL MODEL FOR GASOLINE COMBUSTION IN SPARK IGNITED IC ENGINE

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Summary

A low dimensional model for in-cylinder combustion is developed. The gasoline is modeled as 4 lumps involving species from straight chain aliphatic, branched alkanes, cyclic and aromatic compounds. The preliminary results have been shown with gasoline modeled as propane and the results with 4-lumps gasoline will be discussed in full paper. For a given fuel inlet conditions, the model predicts the exhaust composition of regulated gases (total unburned HC's, CO, and NOx) as well as the in-cylinder pressure and temperature. The model is also able to capture the qualitative trends observed with change in fuel composition (gasoline and ethanol blending) and air/fuel ratio. The preliminary results show good qualitative and fair quantitative agreement with the experimental results published in the literature.

Keywords

Novel reactor technologies, Complex reacting flows.

Introduction

The current trend towards simultaneously increasing fuel-to-wheels efficiency while reducing emissions from transportation system powertrains require system level optimization realized through multivariable control. Such an optimization can only be accomplished using fundamentals (first-principles) based models for each of the engine sub-systems, i.e. in-cylinder combustion processes, exhaust after-treatment systems, mechanical and electrical systems (for hybrid vehicles) and sensor systems. Although the after-treatment unit has been extensively studied in chemical engineering literature, the combustion cylinder modeling has mostly been empirical based. But in order to obtain system level optimization the influence of combustion cannot be overlooked. The combustion process can be described by the fundamental conservation laws (species, momentum and energy) of diffusion-convection-reaction type, but such a description (consisting of many partial differential equations and complex chemistry) is extremely demanding computationally and has limited utility for system level optimization studies. For online optimization and real-time control, these physics based models must be low-dimensional, retain the qualitative features of the system, and have sufficient quantitative accuracy. In our view, the bottleneck for attaining real-time onboard system level optimization is the lack of accurate low-dimensional models for the internal combustion (IC) engine. In this work, we develop a low-dimensional model

for IC engine cycle by spatially averaging the 3-dimensional detailed convection-diffusion-reaction model (Bhattacharya et al.¹). The derived model includes relevant physics and chemistry and is reduced to lumped parameter ODE's form so it can be used for real time optimization and control. Another difficulty encountered in modeling combustion occurs because of chemical composition of gasoline. Gasoline is complex chemical mixture of around 500 different hydrocarbons so any single component is insufficient to capture its properties. Thus, in this work we use four lump model to accommodate species from major characteristic groups to characterize gasoline properly. Preliminary result of gasoline modeled as single lump is presented and four lump model will be discussed in full paper.

Mathematical model

The spark ignition (SI) engine cycle consists of 4 consecutive steps: intake, compression, combustion and expansion and exhaust. It is an open system with time dependent control volume (function of crank angle). The combustion in SI engine is initiated by spark which ignites the gas packets around the spark plug leading to flame front propagation. This phenomenon of gas combustion can best be analyzed by considering the reaction kinetics. We employ the global kinetics mechanism given in literature (Westbrook et al.⁵). The modeling approach can

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easily be extended to HCCI, GDI or variable valve engines. The low-dimensional model for IC engine cycle is derived by using the conservation laws (material and energy conservation) and averaging them over the cylinder volume to reduce the spatial degrees of freedom (Bhattacharya et al.¹). The species balance equation in two mode form is given as

$$\frac{d\langle C_j \rangle}{dt} = \frac{1}{V} \left[F_j^{in} - F_j + \sum_{i=1}^{nr} V_{ij} * R_i \langle C \rangle * V - \langle C_j \rangle * \frac{dV}{dt} - F_{cr} \right]$$

Where the flow in crevice region is described by,

$$F_{cr} = a * Q_{cr} * C_{cr} + (1-a) * Q_{cr} * C_{m,j}$$

$$C_{j,m} - \langle C_j \rangle = \frac{1}{\tau_c} (t_{mix,2} C_{j,m}^{in} - t_{mix,1} C_{j,m})$$

The energy balance relation can be derived from the 1st law of thermodynamics.

Results and Discussion

Figures 1 and 2 show the model predicted and experimentally observed trends of exhausts emission with different air/fuel ratio. The model is able to predict the experimentally observed trend of NOx maxima for slightly leaner condition.

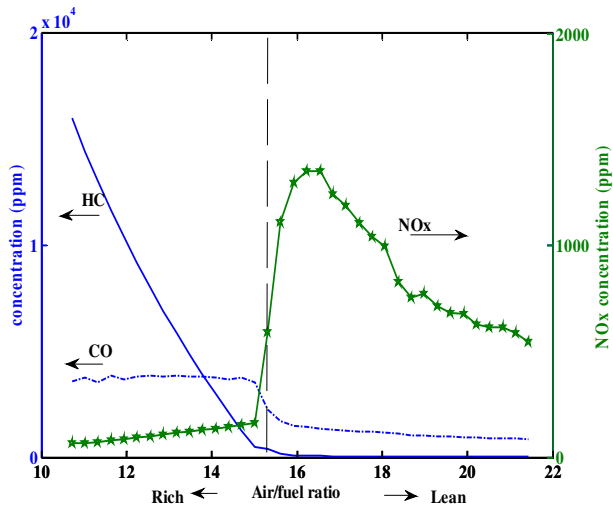


Figure 1: Variation of engine exhaust with air/fuel ratio

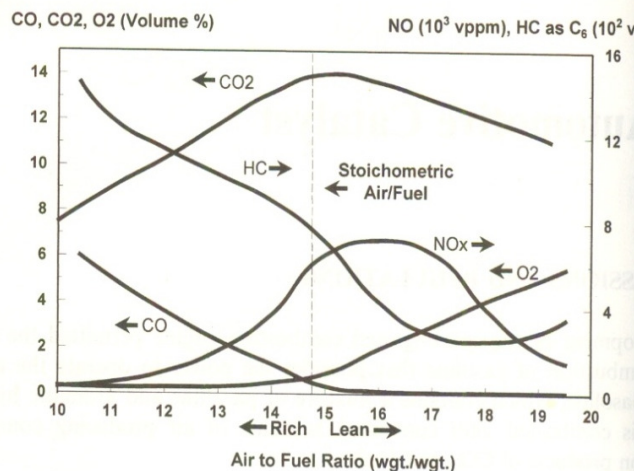


Figure 2: Experimentally observed total hydrocarbon and NOx emission with ethanol blending (Ronald et al.⁴)

The model was also simulated with blended fuel condition. The simulation result shows good agreement with experimentally observed trend. CO and unburned hydrocarbon decreases with blending, while the NOx emission will decrease if the fuel is changed from pure gasoline to gasoline blended with ethanol maintaining the constant relative air to fuel ratio (λ). While if the air and fuel flow rate is left constant and the fuel is changed from pure gasoline to ethanol blended, then one will observe an initial rise in NOx concentration (fig. 3). This happens as the mixture becomes leaner because of lower oxygen requirement by ethanol ((8.9 kg air)/(kg of ethanol)) as compared to gasoline ((14.6 kg air)/(kg of gasoline)) for complete combustion.

Thus to summarize, we apply the reaction engineering principle to model combustion as an open system with time dependent control volume and the results shows that the model is able to capture the relevant experimental trends correctly. Improvements and extensions to the model are discussed.

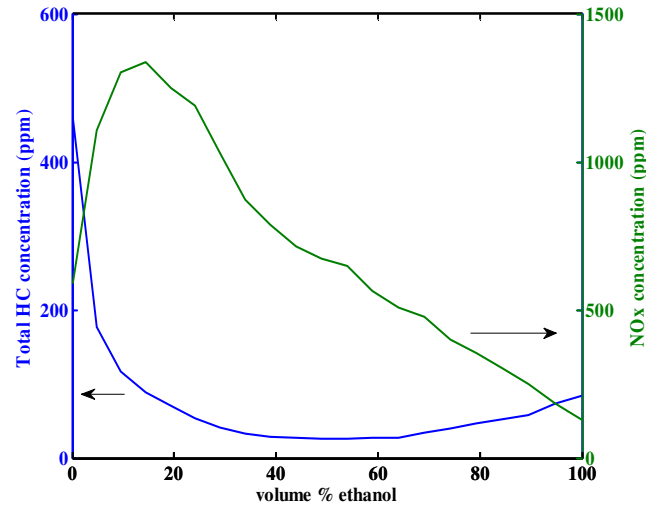


Figure 3: Effect of blending on emission at constant air and fuel flow rate

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