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Numerical Modeling of Soot Emissions in n-Heptane Spray Using Multistep Soot Model with Detailed PAH Chemistry

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Clean Energy Technologies

Introduction

The present day oil crisis and need for more fuel economy has driven the demand for diesel powered automobiles. Diesel soot is one of the primary emissions of diesel combustion and accurate modeling of soot formation is a challenging area for combustion researchers. The soot formation in diesel engine combustion has been previously modeled using a two-step phenomenological model which includes the inception of soot from a precursor species and oxidation of soot [1]. More complex soot models have been developed in the recent past [2],[4],&[7]. The multi-step soot model has gained interest due to its ability to predict the soot much more accurately in EGR systems [7].

In this current study, a multi-step soot model is implemented with a detailed PAH mechanism in the CFD solver KIVA-3 and it is used to study the soot emission characteristics in diesel combustion.

Soot Modeling

The traditional soot model uses a two-step model which considers two competing reactions of soot formation and soot oxidation. Acetylene is typically used as the inception species of soot formation [3]. Recently conducted studies has shown that using a PAH species as the soot inception species can improve the soot characteristics predictions [8]. The multi-step soot model uses a PAH mechanism to predict the evolution of soot precursor species during combustion. The different steps in the soot evolutions are inception of soot from the PAH species, soot surface growth, soot coagulation, PAH condensation, soot oxidation by oxygen and soot oxidation by OH.

Reaction Mechanism

The diesel combustion is modeled using an n-heptane mechanism. The mechanism consists of a basic n-heptane combustion mechanism [5] and a PAH chemistry mechanism [4]. The new mechanism contains 68 species and 145 reactions. The PAH mechanism is a part of a detailed n-heptane mechanism, NICE mechanism and it has been previously used to model the soot formation in combustion systems [4]. However, the NICE mechanism uses 210 species and approximately 2000 reaction steps, which makes it difficult to use in CFD modeling of practical applications.

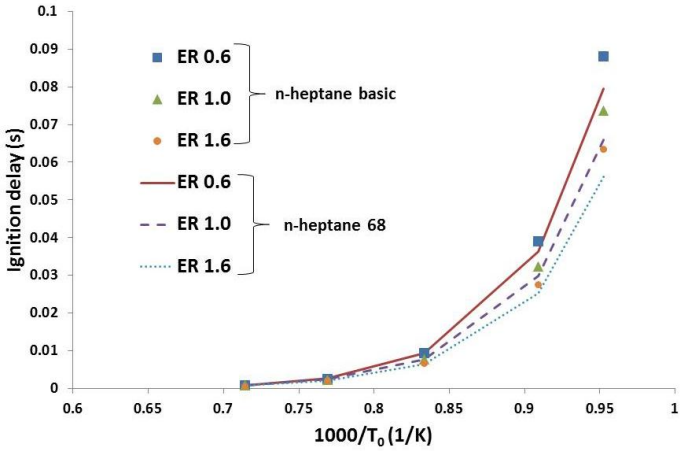

Figure 1. Ignition delay of new mechanism compared with the n-heptane basic mechanism

The new mechanism, n-heptane68 is validated against the basic n-heptane mechanism for ignition delay and flame speed. Figure 1 compares the ignition delay results using basic n-heptane mechanism and the 68 species

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n-heptane mechanism. The ignition delay results agree reasonably well with the 35 species n-heptane mechanism. However, the new mechanism initiates a faster ignition than the basic n-heptane mechanism at lower temperatures. Flame speed of both mechanisms also shows a very good agreement.

In order to enable the new mechanism to produce soot similar to that of NICE mechanism, some of the soot formation parameters had to be tuned. It was observed that the soot surface growth and soot coagulation parameters are the ones most sensitive to soot evolution. The rates of these parameters were modified to predict similar results corresponding to the NICE mechanism at different EGR conditions. The soot mass fraction comparison using the NICE mechanism and n-heptane68 mechanism are shown in Figure 2.

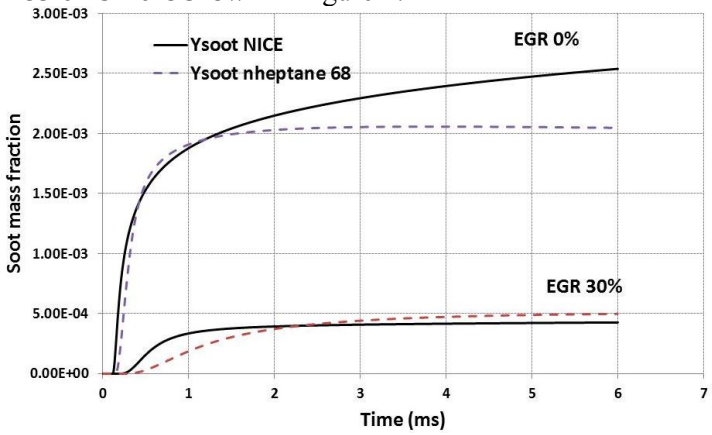

Figure 2. Soot mass fractions using NICE mechanism and n-heptate68 mechanism at 0% EGR and 30% EGR.

Modeling Details

The new mechanism and tuned soot model is further used to simulate the soot formation in n-heptane spray experiments under EGR like conditions [6]. In order to model the experiment using CFD, a computational domain of 15cmX12cm was used. For simplifications, the model is assumed to be 2-dimensional and symmetric about the injector axis. KH-RT breakup model was used for the spray and the chemical reactions were modeled with the help of CHEMKIN subroutine implemented in KIVA-3.

Results

The soot distribution from the experiments and simulations are shown in Figure 3. The model was able to capture the soot formation regions well. The magnitude of soot formed however differed in the experiment and simulation. Further research has to be conducted in order to improve the predictions by the new mechanism.

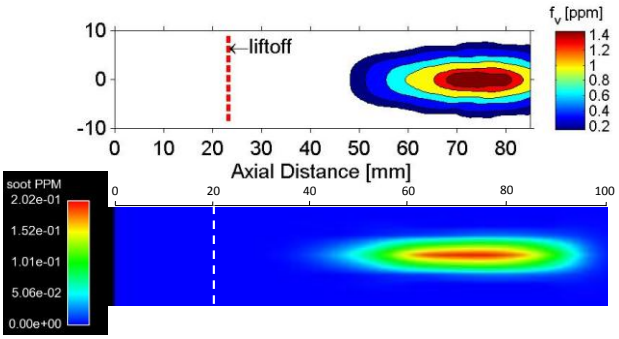

Figure 3. Soot PPM contours from experiment [7](top) and simulation.

Conclusion

The multi-step soot model was implemented in KIVA-3. A new soot mechanism was developed and the soot model rates were tuned to enable the mechanism to perform well in high EGR conditions. The mechanism is well validated against the traditional n-heptane mechanism and NICE mechanism. The soot model and mechanism was further used to model an n-heptane spray combustion experiment. Good qualitative agreement was obtained using this mechanism under low density conditions.

Acknowledgements

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