Soot Formation Modelling of n-Heptane Spray Combustion Under Diesel Engine Conditions Using the Conditional Moment Closure Approach

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Methodology

In this poster first results of numerical simulations of soot formation of n-heptane spray in a constant-volume vessel under Diesel engine conditions different ambient oxygen molar concentrations (8-21% O₂ range) are presented. Results were validated against high-fidelity measurements from the Sandia constant-volume combustion chamber facility [1, 2], which consists of a cubic shape with 108 mm side length. The experimental temperature and pressure were in all cases 1000 K and approximately 42 bar, respectively. The numerical flow field was solved with the commercial computational fluid dynamics (CFD) solver STAR-CD [3] coupled with an elliptic first order conditional moment closure based combustion model [4, 5] with standard closure modeling approaches for conditional velocity, conditional scalar dissipation rate and conditional turbulent fluxes as proposed in [5]. The high Reynolds number k-ε-RNG turbulence model [3] is used. Fuel spray droplets are treated in an Eulerian-Lagrangian way with STAR-CD built-in primary and secondary breakup models [6, 7]. The reduced n-Heptane chemical mechanism by Liu et al. [8] consisting of 22 species and 18 global reactions is used. Soot formation is modeled with the semi-empirical two-equations model of Leung [9], where simultaneous soot particle inception, surface growth, coagulation and oxidation by O₂ and OH are considered. In the current implementation, particle inception rate is a first order function of acetylene concentration only. Transport equations for soot mass fraction and soot number density were solved with unity Lewis number assumption, neglecting differential diffusion effects of soot particles, whose size distribution was assumed as mono-dispersed. Radiation of soot particles was modeled with an optical-thin formulation after [10] using soot mean absorptivity values from [11].

Results

Ignition delay time was overpredicted for all ambient oxygen concentrations considered. Discrepancy became larger with lower oxygen presence. However, increasing ignition delay times by diminishing oxidizer content was well captured. The same trend for lift-off heights was observed, i.e. increased lift-off heights by reducing ambient oxidizer amount. Simulation trend was fairly predicted. The influence of the ambient oxygen mole fraction on the flame structure is analyzed on the basis of the 21% and 10% O₂ cases. Flame characteristics relevant for soot behavior (mixture fraction, temperature, mass fractions of OH, O₂ and C₂H₂) are illustrated for the two different cases at 5 ms during the quasi steady-state period. The main difference consists in the lower stochiometric mixture fraction for the 10% O₂ case. As a consequence the stochiometric region becomes larger and therefore the entire flame becomes broader. Maximal stochiometric axial distances were approximately 75 mm and 105 mm for 21% and 10% O₂, respectively. With a lower ambient O₂ concentration, as expected, a lower flame temperature
was observed due to the reduced oxidizer availability. All chemical processes are shifted farther downstream from the injector. Mass fractions of C\textsubscript{2}H\textsubscript{2} and OH are roughly one order of magnitude lower compared to the 21% O\textsubscript{2} case.

Soot volume fraction during quasi-steady spray behavior between 3-6 ms was compared with experiment [1] which was performed with laser induced incandescence methodology. Experimental soot distribution was measured until approximately 90 mm axial distance from the injector tip. Soot was observed in the fuel rich zone. In the 21% O\textsubscript{2} case, the entire soot-loaded region was visualized in the experiment, instead for the 10% case peak soot concentration is expected to be out of sight.

Soot volume fraction distribution with the higher oxygen content was well predicted. For the lower oxidizer concentration peak soot volume fraction was overpredicted, although experimental maximal soot concentration was not in the observation region. A lower soot amount and a farther downstream location from the injector with lower oxygen concentration were both predicted correctly. Soot mass fraction an number density distribution and the accordingly source terms are presented in mixture fraction space at the location of peak soot volume fraction.

Soot mass fraction is present only in the fuel rich region and reaches the peak at an equivalence ration of around two for both ambient oxygen concentrations considered. In contrast to the mass fraction, the number density does appear in the fuel lean region because soot particle oxidation is assumed to reduce particle mass but not the particle number. However presence of particles with negligible mass in the fuel lean region do not influence soot volume fraction in space. The relative contribution of oxidation by OH plays an important role only for the 21% O\textsubscript{2} case due to the higher OH/O\textsubscript{2} concentration ratio present in the flame. Molecular diffusion of soot mass fraction towards stoichiometry is mainly balanced with oxidation by OH and O\textsubscript{2}.

First results suggest that the conditional moment closure combustion model approach can be considered a promising framework for soot modeling because of the accurate flame structure description, which is essential for soot predictions.

References

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**Introduction**

Diesel engines offer a very high efficiency and are therefore widely used in power generation and transportation. Soot emissions by Diesel engines are dangerous for the environment and for living organisms. Government legislations for soot emissions are becoming even more stringent, therefore there is the need to better understand the physics of soot formation at those conditions.

In this numerical study, the influence of ambient oxygen concentration on spray flame characteristics and soot formation is investigated. Prediction of precesses e.g., two-phase flow and flame dynamics are a prerequisite for soot modeling.

**Soot model: two-equations model [7]**

Soot model accounts for simultaneous soot particle inception, surface growth, oxidation by O$_2$ and OH and coagulation.

The soot transport equations are given by:

\[
\begin{align*}
\frac{\partial C_s}{\partial t} &+ \mathbf{u} \cdot \nabla C_s = D_s \nabla^2 C_s + S_{inc} + S_{grow} + S_{oxid} + S_{cond} + S_{coag}
\end{align*}
\]

where $C_s$ is the soot mass fraction, $D_s$ the diffusion coefficient, and $S_{inc}$, $S_{grow}$, $S_{oxid}$, $S_{cond}$, and $S_{coag}$ are the source terms for particle inception, surface growth, oxidation, condensation, and coagulation, respectively.

**Experimental setup [1,2]**

**CFD model**

**References**


**Results: Flame structure**

Ignition delay time validation

Lift-off height validation

Influence of ambient O$_2$ concentration with lower O$_2$:

- Higher ignition delay time
- Higher lift-off height
- Lower stoichiometric mixture fraction
- Broader flame
- Lower flame temperature
- Lower C$_{H}_4$/O$_2$ OH concentrations

**Results: Soot formation**

21 % O$_2$ ($\xi_a=0.601$)

10 % O$_2$ ($\xi_a=0.03$)

Volume fraction [ppmv]

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