



Application of a semi-detailed soot modeling approach for conventional and low temperature diesel combustion – Part II: Model sensitivity



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HIGHLIGHTS

- Sensitivity analysis was conducted on soot model reaction chemistry.
- Soot mass predictions were most sensitive to the acetylene and propargyl chemistry.
- Same model constants were satisfactory for an engine operated at various regimes.

ARTICLE INFO

Article history:

Received 8 June 2014

Received in revised form 1 August 2014

Accepted 7 August 2014

Available online 5 September 2014

Keywords:

Soot model

Polycyclic aromatic hydrocarbon (PAH) chemistry

Low temperature combustion

Sensitivity analysis

IC engines

ABSTRACT

In Part-II of the current study, a detailed sensitivity analysis was performed on the soot model that was described in Part-I. The performance of the soot model, which was implemented in the 3-D CFD code KIVA-CHEMKIN, was evaluated by conducting a sensitivity analysis of the soot sub-model formation and oxidation rates and soot precursor chemistry. In terms of soot precursor chemistry, a detailed poly-aromatic hydrocarbon (PAH) chemistry mechanism from the literature was reduced in two stages: (1) using the directed related graph with error propagation (DRGEP) method and (2) using sensitivity analysis, and integrated into primary reference fuel (PRF) chemistry mechanism for simulating different diesel combustion cases. It was seen that the model-predicted soot mass was more sensitive to the acetylene and propargyl chemistry (C_2 – C_3 chemistry) as compared to the aromatic and PAH chemistry. In terms of the soot sub-models, the rates of soot surface growth through acetylene and OH-induced soot oxidation sub-models were modified to understand their effects on the predicted net in-cylinder soot mass, since the net soot mass is understood to be predominantly affected by these sub-models. The pre-exponential rate of the acetylene assisted surface growth rate had to be reduced by a factor of 2.5 (at baseline OH-induced oxidation rate) in order to match the exhaust soot mass of conventional diesel and premixed charge compression ignition (PCCI) experiments at various levels of EGR in a Caterpillar single cylinder oil test heavy-duty diesel engine. Similar results were also obtained when the OH-induced oxidation rate was increased (at baseline soot surface growth rate). It was found that the same sub-model constants were sufficient to yield good exhaust soot mass predictions with respect to the engine experiments operated under varied combustion modes, including single injection conventional diesel combustion at different levels of EGR and multiple injection PCCI experiments at no EGR and high EGR conditions.

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1. Introduction

Modeling soot formation and oxidation for diesel engines has been a long standing challenge. Soot models developed over the past several decades range from simplistic phenomenological to complicated kinetic models. The detailed review of soot models

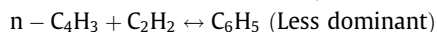
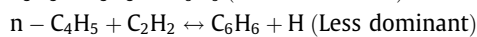
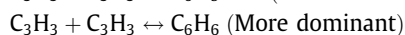
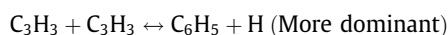
by Kennedy [1] classifies the models as purely empirical correlations, semi-empirical correlations and detailed soot models. Purely empirical correlations are only curve-fits based on experimental data, while semi-empirical models solve rate equations with experimentally obtained model constants. Detailed soot models aim to solve rate equations for soot formation and oxidation and the associated precursor chemistry. Also, the degree of complexity of the semi-empirical and detailed soot models varies in the literature. Also, the choice of precursors for soot formation varies across the literature and type of models. The simplest assumption is to consider the fuel vapor as the precursor since precursors such

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as C_2H_2 and PAHs are generally found in fuel vapor rich regions. The Hiroyasu model [2] used the fuel concentration as the precursor for soot formation. However, with the use of detailed or reduced chemistry mechanisms, C_2H_2 has been widely used as the soot model precursor species, for example, by Leung et al. [3]. In the Leung et al. model, C_2H_2 was considered for both inception and surface growth of soot in laminar non-premixed flames. For relatively detailed models with reduced or detailed chemistry, generally an aromatic or PAH species is considered for the inception step and accordingly, mechanisms for ring formation are incorporated. There is still a lot of debate about whether the first aromatic ring formation (benzene and phenyl) occurs through the odd carbon (C_3) or even carbon (C_4) pathway. Miller and Melius [4] proposed that the first ring formation will be dominated by propargyl (C_3H_3) addition, as compared to originally proposed reactions (Westmoreland et al. [5]) of C_2H_2 with $n-C_4H_3$ and $n-C_4H_5$ that lead to cyclization (e.g., phenyl, benzene, fulvene, etc.), as given below:



More recently Miller, Westmoreland and others have found out that the C_3 pathway is seen to dominate in premixed C_3H_4 isomer (allene/propyne) flames (Hansen et al. [6]), while both the C_3 and C_4 pathways equally contribute in 1-3 Butadiene (C_4H_6) premixed rich flames (Hansen et al. [7]). Hence the subsequent PAH formation chemistry is exposed to higher uncertainties due to uncertainties in the first ring formation itself. A detailed review of the mechanisms of first ring formation is also given by Richter and Howard [8].

It is generally well accepted in the literature that C_2H_2 leads to predominant soot mass addition in the post-inception phase by surface growth processes. The pioneering work of Harris and Weiner [9] proposed that the dominant contributor to surface growth was C_2H_2 in premixed flames, but later on Weiner and Harris [10] performed line-of-sight absorption measurements at a suite of laser wavelengths (488–1100 nm) on a laminar premixed $C_2H_4/O_2/Ar$ flat flame and found out that there may be a possibility of surface growth through PAHs. They observed that, subsequent to the post-inception region, the surface growth profiles follow closely the higher PAH concentrations, which consequently reduce after the growth regime.

Benish et al. [11] proposed that the contribution of C_2H_2 to surface-growth is marginal, while the PAHs contribute around 95% of the growth in C_2H_4 -air flames. The authors measured PAH profiles in the Harris and Weiner flames and argued that PAHs contributed significantly to surface growth since the collision efficiencies of PAH-soot interaction are 5000 times more than those of soot- C_2H_2 . However, this was later contradicted through a brief communication by Kazakov and Frenklach [12], who concluded that it was purely the data reduction technique that was responsible for significant over-prediction of PAH-soot surface growth rates. In fact, Kazakov and Frenklach [12] applied the Hydrogen Abstraction Carbon Addition (HACA) model, which neglects PAH induced soot growth, and obtained similar results as Benish et al. One of the inconsistencies pointed-out by Kazakov and Frenklach in the work of Benish et al. was the assumption of identical collision efficiencies between C_2H_2 -soot and C_2H_2 -PAH. However, Kazakov and Frenklach pointed-out that the C_2H_2 -PAH collision efficiency will be relatively much smaller due to reaction reversibility. It has to be mentioned that Frenklach and Wang [13] were one of the earlier proponents of PAH-assisted surface growth and later went on to challenge the validity of this theory.

Based on the above discussion, it is seen that there are numerous uncertainties in the soot formation process involving aromatic and PAH chemistry and the soot surface growth process involving both C_2H_2 and PAH and their relative contributions. In the current study the soot mass prediction sensitivity to the PAH chemistry mechanism, including the C_4 pathway of aromatic formation, was tested along with the sensitivity to the soot surface growth model with C_2H_2 as the surface growth species. The relative contributions to soot mass by different soot surface growth species (C_2H_2 and C_6H_6) were already established in Part-I. In addition, the soot mass sensitivity to the OH-induced soot oxidation sub-model was also tested.

2. Model framework and implementation

2.1. Sensitivity to PAH chemistry mechanisms

In the current study, two reduced PAH chemistry mechanisms were tested for studying the sensitivity of soot model predictions to aromatic and PAH chemistry. The first PAH chemistry mechanism is the PAH-1 mechanism that was used in the Part-I of the paper, comprising 21 species and 52 reactions.

The second PAH chemistry mechanism that was used in the current study was reduced based on the work of Appel et al. [14]. Since PAH-1 considers benzene formation only through propargyl radicals and since the size of the reduced PAH-1 mechanism is small, it may lack essential pathways of higher PAH formation (e.g., C_4 pathway of A_1 formation). In order to assess the sensitivity of these pathways and in general, to evaluate the sensitivity of the soot model to the PAH mechanism, a second approach was taken to reduce a fairly detailed PAH chemistry mechanism. The Appel-Bockhorn-Frenklach (ABF) mechanism (Appel et al. [14]), comprising 101 species and 1037 reactions, was found suitable for PAH predictions up to A_4 in C_2H_6 , C_2H_4 , and C_2H_2 laminar premixed flames and was therefore used for the reduction. The reduction was done in two-stages as follows:

2.1.1. First stage reduction

The directed relation graph with error propagation (DRGEP) technique was used for first-stage reduction of the chemistry mechanism (Lu and Law [15], Pepiot-Desjardins and Pitsch [16], and Shi et al. [17]). This method requires a set of search initiating species (e.g., fuel, CO, etc.) for driving the mechanism reduction, and species are eliminated if their contribution to the initial species is less than a user-specified error tolerance. The searching can be done using tree algorithms. In the present case, the breadth-first search algorithm was used [17]. Since the ABF mechanism was devised for CH_4 , C_2H_2 , and C_2H_4 combustion and not for diesel combustion, the DRGEP method was used for C_2H_4 combustion at $\Phi = 2$ for a single cell constant volume reactor calculation using SENKIN (Lutz et al. [18]). C_2H_4 and A_4 were taken as the search initiating species. The first-step reduction yielded a chemistry mechanism comprising 63 species and 565 reactions. Although the mechanism was obtained for $\Phi = 2$ it was also tested at other conditions e.g. $\Phi = 4$, initial temperature of 1100 K and initial pressure of 75 atm. and $\Phi = 4$, initial temperature of 1200 K and initial pressure of 50 atm. for validating satisfactory PAH predictions.

2.1.2. Second stage reduction

For the second stage reduction, a sensitivity analysis of the first stage reduction species, mainly aromatics and PAH, was done to eliminate the less dominant ones. For each species that was eliminated, the time evolution profiles of C_2H_2 and A_4 were compared with the detailed mechanism predictions. The analysis was done for C_2H_4 combustion at a condition of $\Phi = 4$, initial temperature

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