

Modeling of Soot Formation in Internal Combustion Engines

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Soot formation is a complex process, which incorporates many chemical and physical steps [1–4]: (1) homogeneous inception of large molecular precursors, (2) surface growth in the reactions with the gas-phase active species, (3) coalescent coagulation to form larger particles, and, finally, (4) agglomeration of the primary particles to form chain-like aggregates.

For modeling soot formation in internal combustion engines using CFD software there is a need in simple and efficient soot models predicting satisfactorily the soot yield under different operation conditions. The detailed kinetic models of soot formation incorporating all the processes mentioned above can be used for validating such models.

The objective of this study was to develop a computationally efficient overall soot model based on the detailed soot formation model. The approach has been developed based on the implications obtained from the analysis of the detailed mechanism. These implications are listed below:

- (1) In order to avoid soot yields exceeding 1.0 it is necessary to take into account fuel depletion in the soot formation reaction.
- (2) In order to correctly simulate soot oxidation in fuel-rich mixtures, it is necessary to take into account soot oxidation by both oxygen and water.
- (3) The reaction steps dealing with hydrogen and carbon monoxide formation and oxidation in the course of fuel oxidation can

be assumed infinitely fast. Therefore fuel can be assumed to oxidize to CO_2 and H_2O rather than to CO and H_2O .

(4) It can be roughly assumed that oxygen and water are not consumed in the soot oxidation reactions as it is done in the majority of available overall soot oxidation mechanisms.

In view of the implications (1) to (4), the new overall mechanism of soot formation can be represented as follows:

Reaction of soot formation: $\text{C}_{cn}\text{H}_{hm} + \text{C}_{cn}\text{H}_{hm} = 2(cn)\text{C} + \text{Product}$,

Reaction of soot oxidation by oxygen: $\text{C} + \text{C} + \text{O}_2 = \text{Product}$,

Reaction of soot oxidation by water: $\text{C} + \text{H}_2\text{O} = \text{Product}$

where "Soot" is represented by the C atom. Since water participates in the soot oxidation reaction, the "Product" is worth to be attributed to either CO_2 or N_2 in order to keep minimal the number of reactive species.

The engine used for the validation study was a single-cylinder research engine with electro-hydraulic valve actuation, three intake ports with swirl flaps, and omega-shaped piston bowl. The overall model was validated for one operating point with conventional Diesel oil combustion. For this point, a significant number of combustion system variations have been applied by simultaneously changing the start of injection, residual gas amount, swirl level, and injection pressure. For the entire set of operating parameters, test-bed measurements have been made for the investigated speed/load points. The measured in-cylinder pressure traces and engine out emission data for NO, soot, CO and unburned hydrocarbons were then used for the assessment of the performance of the combustion/emissions model adopted in the CFD calculations. The 3D calculations using AVL FIRE code with the new overall soot formation model described above have been performed and compared with the measurements. Excellent agreement of predicted and measured results was obtained (Fig. 1).

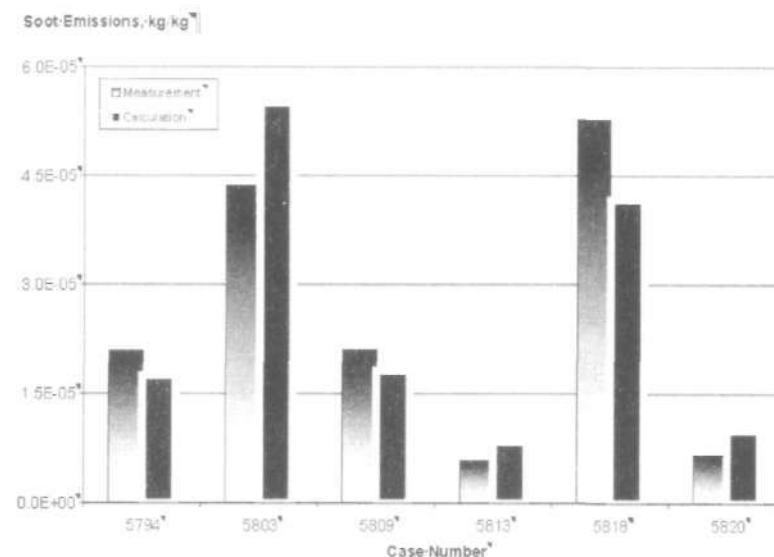


Fig. 1. Comparison of predicted and measured soot emission indices

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