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COMPARISON OF THREE SOOT MODELS APPLIED TO MULTI-DIMENSIONAL DIESEL COMBUSTION SIMULATIONS

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In this paper, three soot models previously proposed for diesel combustion and soot formation studies are briefly reviewed and compared. The three models are (1) two-step em- pirical soot model, (2) eight-step phenomenological soot model, and (3) complex-chemistry coupled phenomenological soot model. All three models have been implemented into the KIVA-3V simulation code. For comparison, a heavy-duty DI diesel engine case with fuel injection typical of standard DI diesel operating conditions was studied. Flame structures of a single diesel spray predicted using these three models were compared, and the results offer our perspective on the application of these three models to soot modeling in diesel engines.

Key Words: Soot Model, Diesel Spray, Flame Structure, Multi-Dimensional Simulation

1. Introduction

Multi-dimensional simulation has become an essen- tial analysis tool in modern engine research and develop- ment. Recent practice of integrating multi-dimensional CFD with genetic algorithms (GAs)(1) has made simula- tion a possible design tool for exploring system optimiza- tion and control strategies of diesel engines. In the frame- work of the GA methodology, the merit value of an objec- tive function of performance parameters (i.e., for example, soot, NOx, CO, HC and BSFC, etc.), which are subject to certain physical constraints, is evaluated from the simula- tions. It is therefore crucial to have an accurate prediction of soot formation, as well as other emissions and perfor- mance parameters in the objective function.

Indeed, modeling the soot formation process remains a key topic in studies of diesel engine combustion. Since the early 1970s when Khan et al.(2) first presented a model for the prediction of soot production from diesel engines, a variety of soot models with different levels of complex- ity have been proposed and applied to multi-dimensional simulations. In order to minimize engine-out soot emis- sions, to explore advanced engine operation modes and, in turn, to guide modern engine design and development, it is important that accurate and realistic soot models be used in multi-dimensional diesel simulations in order to

provide reliable predictions of soot formation.

In this paper, we will briefly review soot formation models that have been proposed for studies of diesel en- gine combustion. Using a heavy-duty diesel engine case with fuel injection typical of standard DI diesel operat- ing conditions, we compare three different modeling ap- proaches, ranging in complexity from very simple to rel- atively detailed models. With more detailed models, we can obtain more valuable insights into the soot formation process, including

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information about soot particle size and soot number density distributions.

2. Model Review

2. 1 Two-step empirical soot model

In the invited lecture at the first COMODIA con- ference in Tokyo in 1985, Hiroyasu(3) reviewed the soot models that had been published between 1962 and 1984. Among those, the two-step empirical soot model of Hiroyasu, Kadota and Arai(4) is the most well known. In their two-step model, Hiroyasu et al.(4) considered the soot formation process as involving only two reaction steps:

(1) the formation step, in which soot is linked directly to fuel vapor molecules, and (2) the oxidation step, which describes the destruction of soot particles via the attack of molecular oxygen.

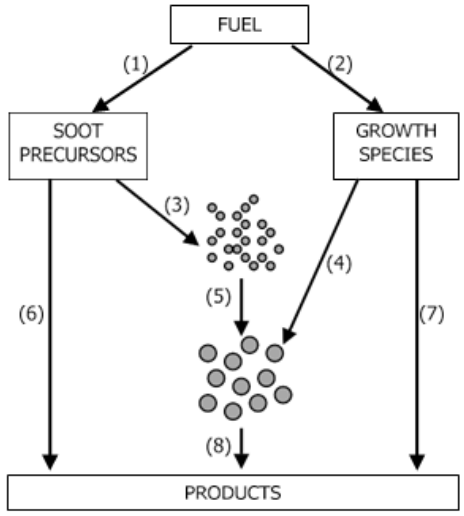

Fig. 1 Schematic of eight-step phenomenological soot model (reproduced from Fusco et al.[8])

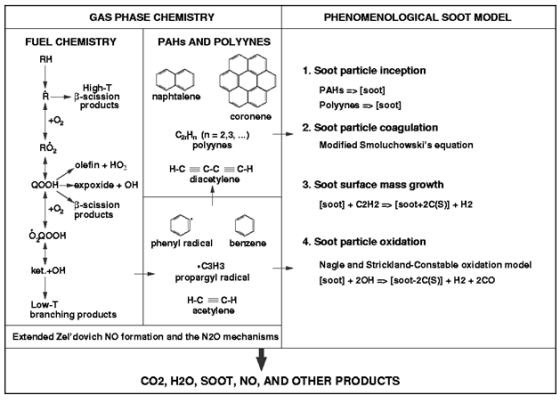

Fig. 2 Modular structure of the chemical mechanism coupling the phenomenological soot model with detailed gas-phase chemistry (reproduced from Tao et al.[19])

Table 1 Engine specification and operating conditions

Engine	Caterpillar 3401E SCOTE
Bore	137.2 mm
Stroke	165.1 mm
Compression ratio	16.1:1
Displacement	2.44 Liters
Connecting rod length	261.6 mm
Squish height	1.57 mm
Combustion chamber geometry	In-Piston Mexican Hat with Sharp Edged Crater
Piston	Articulated
Charge Mixture Motion	Quiescent
Maximum Injection Pressure	190 Mpa
Injector type	A production style Caterpillar electronic unit injector (EUI)
Number of Nozzle holes	6
Nozzle Hole Diameter	0.214 mm
Injector position from the head	2.05 mm
Speed	821 rpm
Load	25%
SOI	-10 degree ATDC
EGR	7.79

The modular structure of the mechanism(18) is illus- trated in Fig. 2. The idea of constructing this mechanism followed the same reasoning as for the eight-step phe- nomenological model of Fusco et al.(8) and Kazakov et al.(15) Instead of using global reaction steps for acetylene and precursor formation, the mechanism includes detailed chemical reactions for the formation of poly aromatic hy- drocarbons (PAHs) and polyyne formation, both of which were considered to be possible precursors leading to soot particles. The PAH formation mechanism of Wang and Frenklach(21) was used to construct the formation reac- tions of higher, linear hydrocarbons (up to C6 species), and the formation of benzene and further reactions lead- ing to naphthalene.

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The soot formation model includes the following important steps: particle inception, in which naphtalene (A2) and diacetylene (C4H2) grow irreversibly to form soot; surface growth via the addition of acetylene (C2H2); surface oxidation via OH and O2 attack. This soot formation mechanism is combined with n-heptane ig- nition chemistry and small hydrocarbon oxidation chem- istry, forming the main body of the mechanism. The full listing of the mechanism is provided elsewhere(20).

3. Engine Experiments

A series of experiments on a Caterpillar 3401E sin- gle cylinder oil test engine have been performed at En- gine Research Center (ERC), University of Wisconsin – Madison. The engine specifications and operating con- ditions are listed in Table 1. Kong et al.(22) have carried out numerical simulations to validate many test cases, and thus we do not repeat the same validation work in this paper. We choose one of the cases (Case B2 in Table 3 of Ref. (22)) and compare the predicted results using dif- ferent soot modeling approaches.

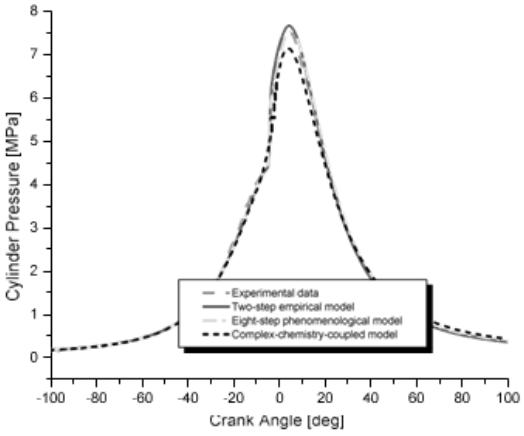

Fig. 3 Comparison of in-cylinder pressure traces between the measured data and the predicted results using three di□erent soot modeling approaches

4.Results and Discussion

4. 1 Experimental background

In the following comparisons, we illustrate the pre- dicted spatial distributions of combustion and soot using three different soot modeling approaches and discuss the differences. However, as there were no direct imaging measurements from the experiments of Caterpillar 3401E engine, Dec's diesel conceptual model(23) is referred to as a guideline.

In the conceptual model (see Fig. 4), Dec summarized the work carried out by his research group using a variety of laser diagnostic methodologies on the combustion of a diesel fuel jet in a quiescent heavy-duty diesel engine, and depicted an idealized schematic of a reacting diesel fuel jet during the quasi-steady period, i.e. the period af- ter the initial premixed burn until the wall impingement of the reacting jet. Dec characterized the structure of the free reacting jet as consisting of a very rich premixed re- action zone, which leads to the initial soot formation, fol- lowed by a soot-filled central region that is surrounded by a diffusion flame. The diffusion flame is lifted a certain distance downstream from the nozzle tip. The fuel vapor does not penetrate too far to form the rich premixed zone. As long as the diffusion flame remains intact, the soot par- ticles travel down the jet along with the other rich products and burn out at the near-stoichiometric diffusion flame.

4. 2 Two-step empirical soot model

The modified version of two-step soot model pro- posed by Patterson et al.(5) was used for the present simu- lations. The model has been implemented into the stan-

dard ERC KIVA-3V code, which features the "Shell"

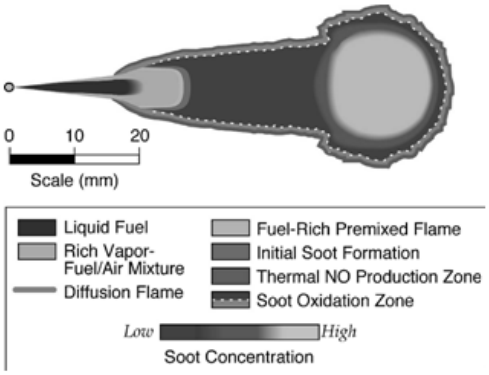

Fig. 4 Schematic of Dec's conceptual diesel model, showing the main features of a reacting diesel fuel jet during the quasi-steady portion of combustion (reproduced from Dec[23])

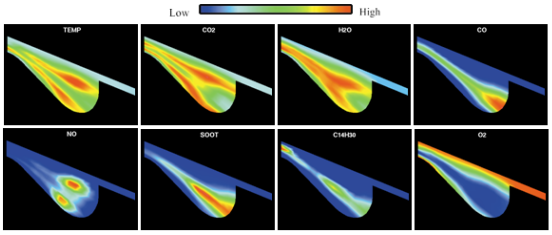

Fig. 5 Spatial distributions of temperature, carbon dioxide (CO_2), water (H_2O), carbon monoxide (CO), NO, soot mass, fuel vapor, and molecular oxygen (O_2) at the end of injection. The blue color indicates the low end of the legend and the red color for the high end of the legend: temperature (500 – 2 500 K), CO_2 (0 – 1 200 g/m^3), H_2O (0 – 700 g/m^3), CO (0 – 3 200 g/m^3), NO (0 – 10 g/m^3), soot (0 – 12 g/m^3), $C_{14}H_{30}$ (0 – 3 000 g/m^3), and O_2 (0 – 5 300 g/m^3)

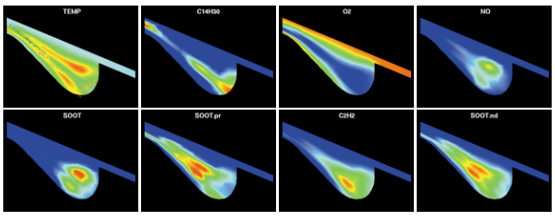

Fig. 6 Spatial distributions of temperature, fuel vapor, molecular oxygen (O_2), NO, soot mass, soot precursor, soot growth species (acetylene C_2H_2) and soot number density at the end of injection. The blue color indicates the low end of the legend and the red color for the high end of the legend: temperature (500 – 2 500 K), $C_{14}H_{30}$ (0 – 3 000 g/m^3), O_2 (0 – 5 300 g/m^3), NO (0 – 10 g/m^3), soot (0 – 12 g/m^3), soot precursor (0 – 0.015 g/m^3), C_2H_2 (0 – 80 g/m^3), and soot number density (0 – 6 × 10^{16} particles/m^3)

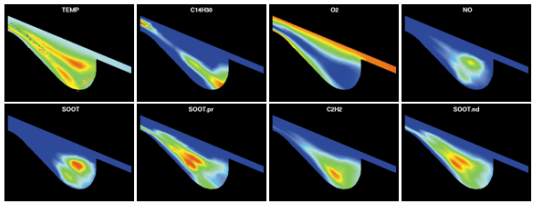

Fig. 6 Spatial distributions of temperature, fuel vapor, molecular oxygen (O_2), NO, soot mass, soot precursor, soot growth species (acetylene C_2H_2) and soot number density at the end of injection. The blue color indicates the low end of the legend and the red color for the high end of the legend: temperature (500 – 2 500 K), $C_{14}H_{30}$ (0 – 3 000 g/m^3), O_2 (0 – 5 300 g/m^3), NO (0 – 10 g/m^3), soot (0 – 12 g/m^3), soot precursor (0 – 0.015 g/m^3), C_2H_2 (0 – 80 g/m^3), and soot number density (0 – 6 × 10^{16} particles/m^3)

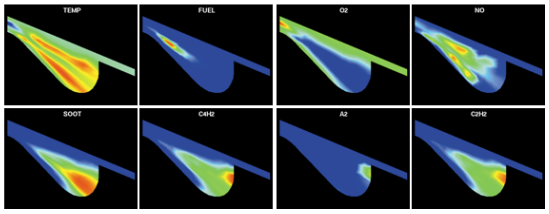

Fig. 7 Spatial distributions of temperature, fuel vapor, molecular oxygen, NO, soot mass, soot precursors (C_4H_2 and A_2), soot growth species (acetylene C_2H_2) at the end of injection. The blue color indicates the low end of the legend and the red color for the high end of the legend: temperature (500 – 2 000 K), Fuel (0 – 3 000 g/m^3), O_2 (0 – 5 300 g/m^3), NO (0 – 10 g/m^3), soot (0 – 12 g/m^3), soot precursor (0 – 0.015 g/m^3), C_2H_2 (0 – 80 g/m^3), and soot number density (0 – 6 × 10^{16} particles/m^3)

5. Conclusion

In this paper, three soot models that have been pro- posed for multi-dimensional diesel engine simulations are reviewed. By applying these three different models to the same test case of a heavy-duty diesel engine with fuel injection typical of standard DI diesel operating condi- tions, important differences between the predictions are revealed.

(1) The two-step empirical soot model is ease to be implemented into CFD codes and to be adjusted for matching the predictions with measurements. The sim- ulation can capture the main features of flame and soot distributions of diesel sprays in engines, but the present results show that the predicted flame in the near-nozzle re- gion does not agree well with the diesel flame structure of Dec(23). The detailed information of soot formation cannot be obtained using this modeling approach.

(2) The eight-step soot phenomenological model shares similar advantages to the two-step model and, be- sides, it is very computationally efficient. The simulations using the eight-step model can predict the same flame structure of diesel sprays as that of using the two-step soot model. The prediction of soot distribution is improved and, additionally, the simulations provide

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more useful in- formation such as soot precursor, acetylene, soot number density as well as soot particle size. Compared to the pre- vious model, the eight-step model offers better description of physics of soot formation. However, the parameters of the rate constants leading to soot precursor, soot particles and soot surface growth require a little more tuning work. Recently, further improvement of the phenomenological soot model was pursued and its application to high-speed direct injection (HSDI) diesel engines(24), (25) leads to some new insights in low-temperature diesel combustion.

(3) The implementation of complex-chemistry and phenomenological soot model into multi-dimensional CFD codes offer many advantages for the prediction of the diesel flame structure over the previous two models. The prediction shows that the flame of diesel sprays injected at standard DI operating conditions is lifted from nozzle tip, allowing substantial oxygen to be entrained into the core region of the spray jet. This predicted flame structure, as well as the predicted fuel vapor penetration, soot and NO distributions, agrees well with that of Dec(23). The sim- ulations provide also very detailed information of many other species such as naphthalene and diacetylene, all of which are important agents in the soot formation proc- ess. However, the complexity of the chemical mechanism introduces many uncertainties and increases significantly computational times.

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