MULTI-DIMENSIONAL MODELING OF SOOT FORMATION IN DISI ENGINES BASED ON DETAILED PAH KINETICS AND PARTICLE DYNAMIC FRAMEWORK

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ABSTRACT

In this study, in-cylinder soot formation in direct-injection spark-ignition engines was modelled based on the combined framework of detailed polycyclic aromatics hydrocarbon (PAH) chemical kinetics and particle dynamics. The turbulent flame propagation in partially premixed condition was described by G-Equation, while the burned gas compositions behind of the flame front were determined by flamelet library which incorporates the PAHs kinetics. The post flame particle dynamics includes further growth of PAHs and particle inception, surface growth, coagulation and oxidation, and it is modelled by method of moments. In order to improve the model prediction through whole mixing and combustion process, the droplet distribution of spray injection was tuned by measuring sauter mean diameter (SMD) from rig test, and the laminar flame speed was calculated using mixing rule. The numerical simulation was validated with the single-cylinder research engine experiments under cold start, catalyst heating conditions. The developed model were able to represent the basic physics of soot formation and bridge the gap between operating parameters and engine-out soot emissions with enhanced interpretation capability.

MODELING OF LAMINAR FLAME SPEED OF GASOLINE FUEL BY MIXING RULE

The laminar flame speed of gasoline fuel was modelled by mixing rule based on the Le-Chatelier's rule by energy fraction in this study. For gasoline fuel, the toluene reference fuel (TRF), composed of iso-octane, n-heptane and toluene, was selected for its surrogate component. The calculation were done with Premixed Laminar Flame-Speed module of CHEMKIN-PRO 15131 and proper chemical kinetic models from literature. It is efficient to formulate an algebraic equation for the laminar flame speed calculation instead of the database concept, so the fitting of the results were carried out. To determine the overall shape of the flame speed along the equivalence ratio, its range from 0.5 to 2 were chosen. Similarly, the temperature and pressure dependency were also evaluated under 600 to 900 K and 5 to 25 bars, respectively. The base form of the model equation is a function of temperature, pressure and equivalence ratio reads

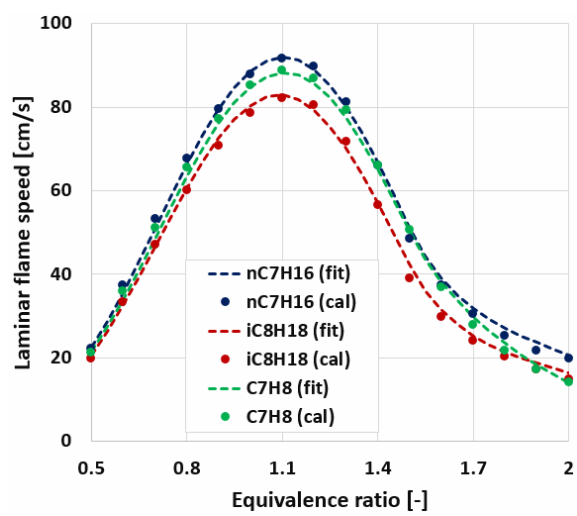

Figure 1 Database fitted with algebraic equation for each surrogate component

$$s_L\left(T_u, P, \phi\right) = s_{L,0}\left(\phi\right)\left(\frac{T_u}{T_0}\right)^{\alpha(\phi)}\left(\frac{P}{P_0}\right)^{\beta(\phi)} \qquad [1]$$

where subscript 0 indicates the reference value in calculation. The overall shape was fitted by exponential form, whereas the temperature and pressure dependency were by polynomial fitting,

respectively. Figure 1 shows the laminar flame speed of each surrogate component along the equivalence ratio; the peak value occurs at slightly rich mixture and it is decreased for both lean and rich side.

FLAMELET LIBRARY FOR BURNED GAS COMPOSITION INCLUDING PAH SPECIES

The G-Equation defines the geometrical shape and location of the flame front, while the chemical structure of the flame should be additionally provided. Because the G-Equation based on the flamelet assumption, in which the turbulent flames can be regarded as an ensemble of the thin-reactive diffusive layers embedded within the flow field, so that the separation of the scale between turbulence and chemical reaction. Thus, the finite rate of the chemical kinetics can be introduced and the details of the flame structure include the inner layer can be resolved by the flamelet equation. In order to obtain the PAH species behind of the flame front, the gas-phase chemistry developed by Raj et al. was adopted in this study. This model is a semi-detailed mechanism containing 226 species and 2121 reactions (counting forward and backward reaction separately). It consists of a high temperature oxidation of gasoline surrogate and a detailed description of large PAHs formation up to coronene ($C_{24}H_{12}$). The flamelet calculation was conducted with Laminar Flame Speed-Calculation module in CHEMKIN-PRO 15131. The propagating flame may encounter wide range of temperature, pressure and equivalence ratio in DISI engines, hence thermodynamic conditions of 600 to 800 K, 5 to 30 bar, and chemical composition of 0.5 to 3.5 were selected, respectively. The mass fraction of burned species and burned gas temperature profile were re-distributed in the domain of distance apart from the flame inner layer. Tabulated flamelet library contains major species of combustion products, intermediate species such as radicals, and PAHs related species.

OVERVIEW OF SIMULATION MODEL

The Figure 2 shows the conceptual diagram of the combustion process in partially premixed turbulent combustion; the primary premixed flame propagates through the air-fuel mixture while the secondary diffusion flame develops by the partially oxidized fuel and redundant air which diffused from rich and lean region, respectively. The burnt composition were determined by the flamelet library and the formation of pollutants was modelled by post-flame reaction.

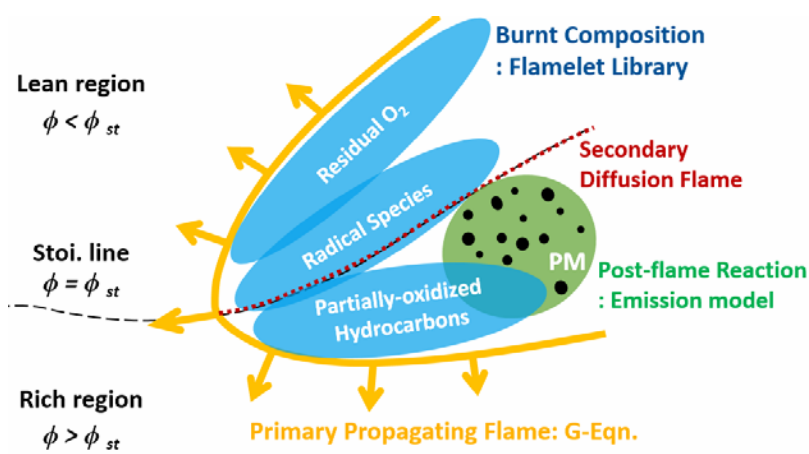

Figure 2 Conceptual diagram of partially premixed turbulent combustion and emission in DISI engines