

Comparative study on nascent soot formation characteristics in laminar premixed acetylene, ethylene, and ethane flames

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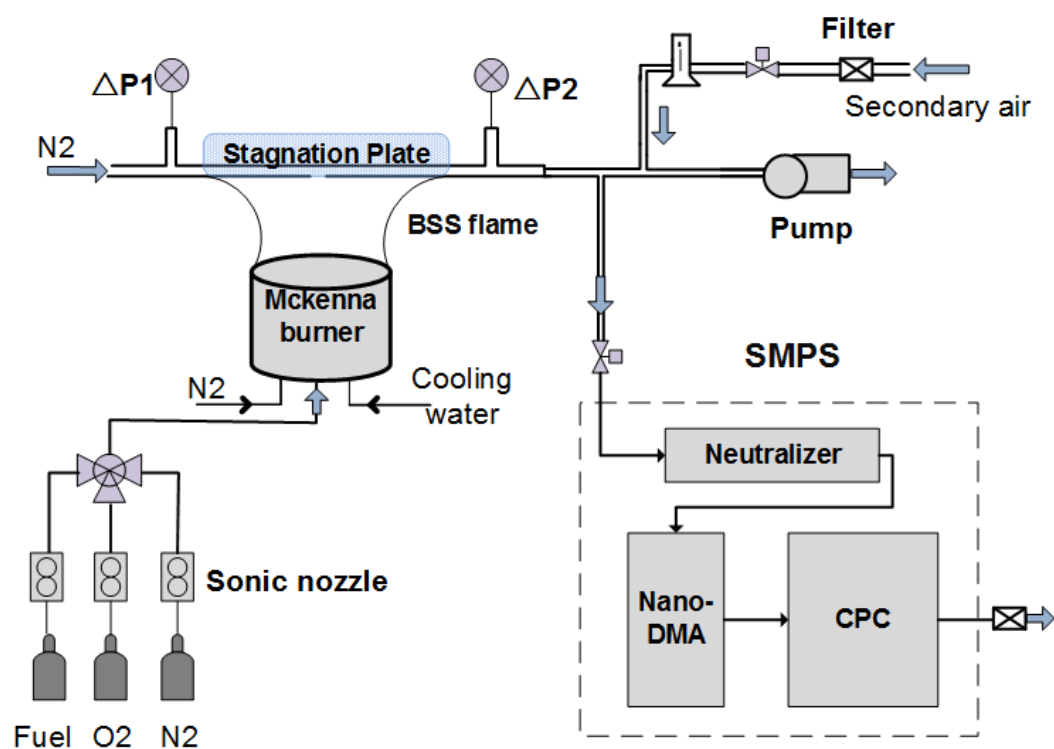


Fig. S1 Experimental setup.

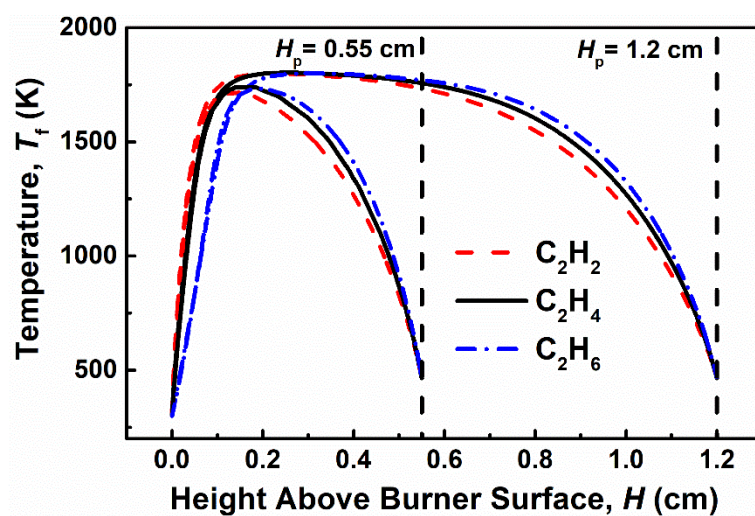


Fig. S2 Comparison of simulated temperature profiles at $H_p = 0.55$ cm and 1.2 cm.

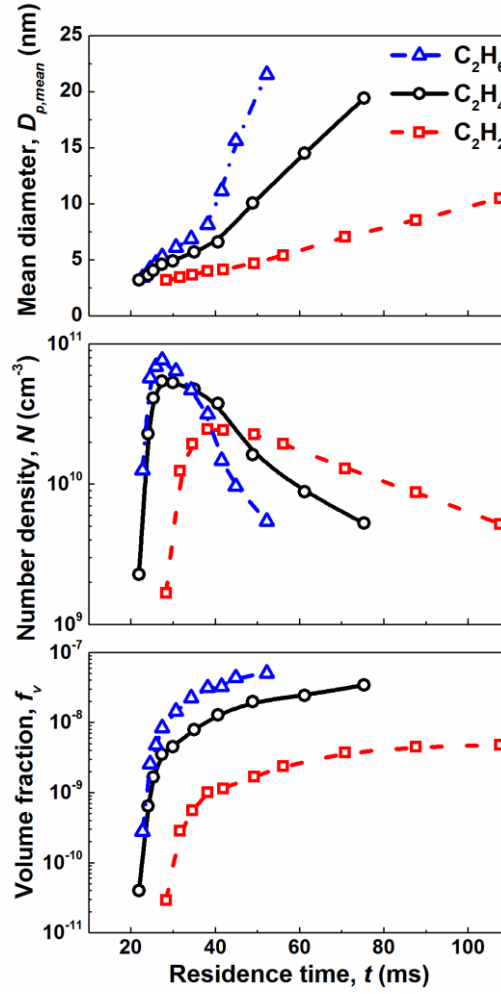


Fig. S3 Particle mean diameter, absolute number density and volume fraction measured as a function of residence time. Symbols are the experimental data. Lines are fits to data.

The residence time is defined as the time interval of particles travelling from the maximum flame temperature position to the burner-to-stagnation separation surface, which is expressed as Eq. (1).

$$t' = \int_{x_{T_m}}^{H_p} \frac{dx}{v(x)} \quad (1)$$

where x_{T_m} is the distance from the position of peak temperature to the burner surface, $v(x)$ is the particle velocity that equals to convection velocity $v_c(x)$ plus thermophoretic velocity, $v_t(x)$.

According to previous studies [1], the soot samples are obtained from an average of a gas volume adjacent to the orifice, which can be represented by shifting the probe position by 1 mm upstream [2]. Therefore, the actual particle residence time used in this work is expressed as Eq. (2).

$$t = \int_{x_{T_m}}^{x_s} \frac{dx}{v_c(x) + v_t(x)} \quad (2)$$

where $x_s = H_p - 0.1$ cm, $v_c(x)$ is obtained directly from the simulation results using Chemkin-Pro package [3] and $v_t(x)$ can be calculated using Eq. (3) from Ref. [4].

$$v_t(x) = \frac{\lambda}{5(1+\pi\phi/8)Nk_B T} \frac{dT}{dx} \quad (3)$$

In the above equation, λ is the thermal conductivity coefficient, N the number of gas molecules,

φ the momentum accommodation factor, which is 0.9 [2], and k_B Boltzmann constant. The gas properties, φ and N , are calculated using a modified OPPDIF code [4] with a detailed mechanism of USC Mech II [5].

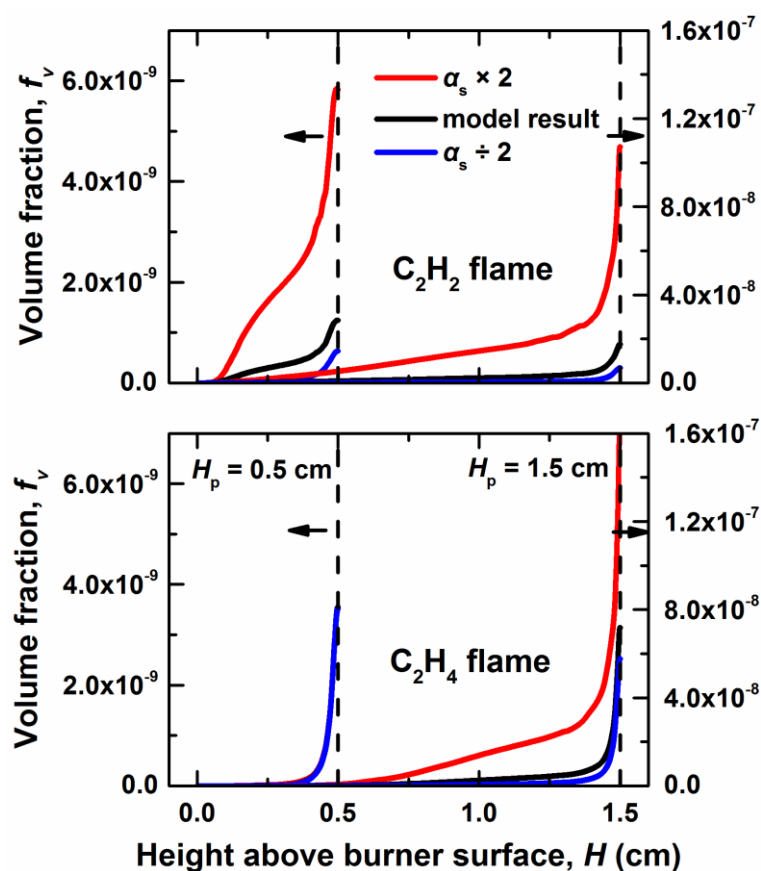


Fig. S4 Soot volume fractions at $H_p = 0.5$ and 1.5 cm for C_2H_2 and C_2H_4 flames when the surface reaction rate, α_s , is changed by a factor of 2 or 0.5.

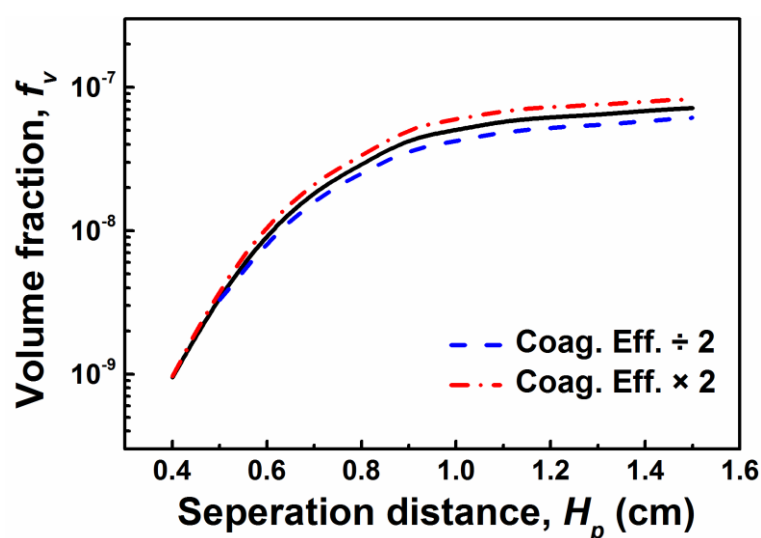


Fig. S5 Sensitivity of the soot volume fraction to coagulation efficiency.

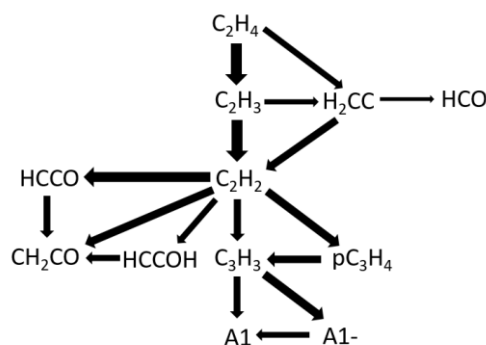


Fig. S6 Rate-of-production analysis at the height where the production of benzene reaches the maximum for $H_p = 1.0$ cm in the ethylene flame. The thickness of the line indicates the relative significance of the reaction pathway.

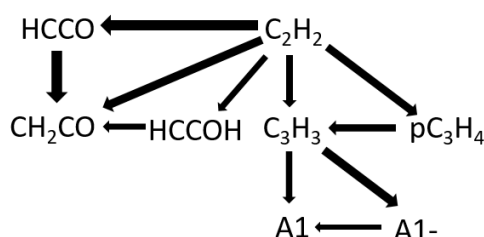


Fig. S7 Rate-of-production analysis at the height where the production of benzene reaches the maximum for $H_p = 1.0$ cm in the acetylene flame. The thickness of the line indicates the relative significance of the reaction pathway.

Reference

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