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Population balance modelling and laser diagnostic validation of particle evolution in laminar ethylene diffusion flame

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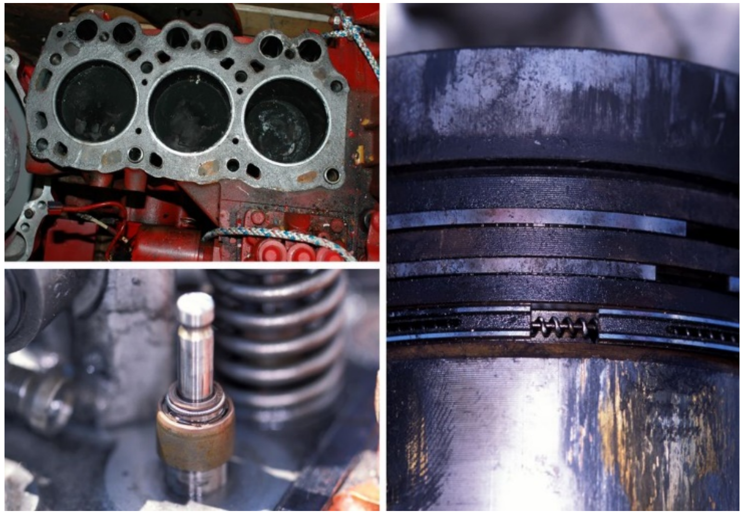
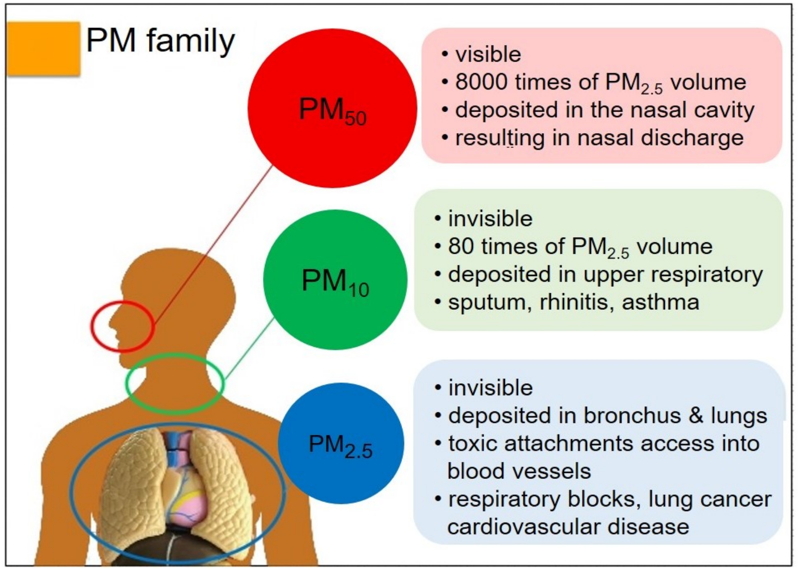
Motivation

- Reacting flows carry a particulate phase in a number of engineering applications – sooting flames；
- Access to the ***Particle Size Distribution (PSD)*** is crucial for engineering and environmental problems.



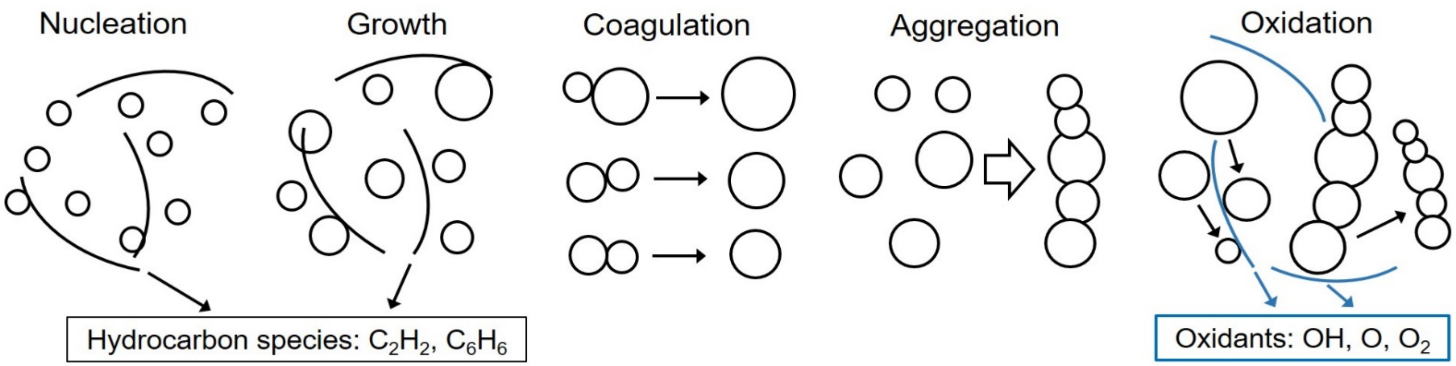
(a) Soot clog in a diesel engine [1]



(b) Impacts of particle size on respiratory system

Population Balance

- ***Population Balance Equation (PBE or PBM)*** is a rigorous way to solve the full ***PSD,*** modelling all processes of the soot formation



(a) Soot formation history

$$\frac{\partial N(v;x_j,t)}{\partial t}+\underbrace{\frac{\partial}{\partial x_j}(u_j\cdot N(v;x_j,t))}_{\text{convection}}=\underbrace{\frac{\partial}{\partial x_j}\left(D_p\frac{\partial N(v;x_j,t)}{\partial x_j}\right)}_{\text{diffusion}}+\underbrace{\dot{B}_0(Y_a)\delta(v-v_0)}_{\text{nucleation}}-\underbrace{\frac{\partial}{\partial v}\left[G(v,Y_a)\cdot N(v;x_j,t)\right]}_{\text{growth \& oxidation}}$$

$$+\underbrace{\frac{1}{2}\int_0^v \beta(v-v',v')N(v-v';x_j,t)N(v';x_j,t)\mathrm{d}v'}_{\text{coagulation birth}}\underbrace{-N(v;x_j,t)\int_0^\infty \beta(v-v',v')N(v';x_j,t)\mathrm{d}v'}_{\text{coagulation death}}$$

(b) Continuous population balance equation

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Challenges

- The *PBE,* essentially a 1D partial differential equation (PDE), needs to be discretized and incorporated with the CFD codes, representing the two phases will be bilaterally affected. Stiffness of the combined PBE-CFD solver may happen.

- Each process during the soot formation requires accurate models.

- The predicted PSD needs to be validated by experiment. Most laser experiments for the laminar diffusion flames offer the lumped or integrated parameters. Connection between the PSD and the lumped result should be established.

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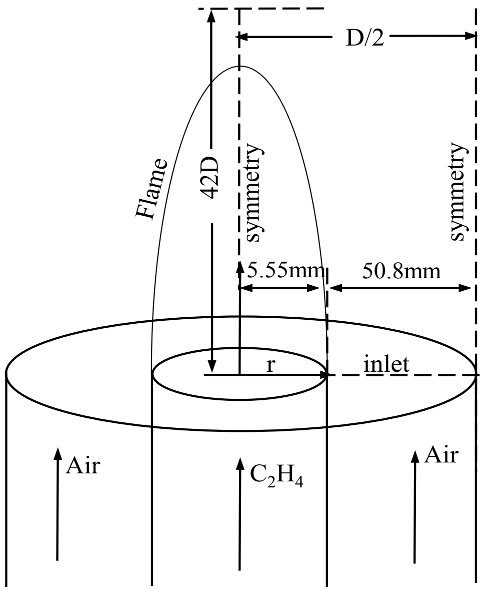
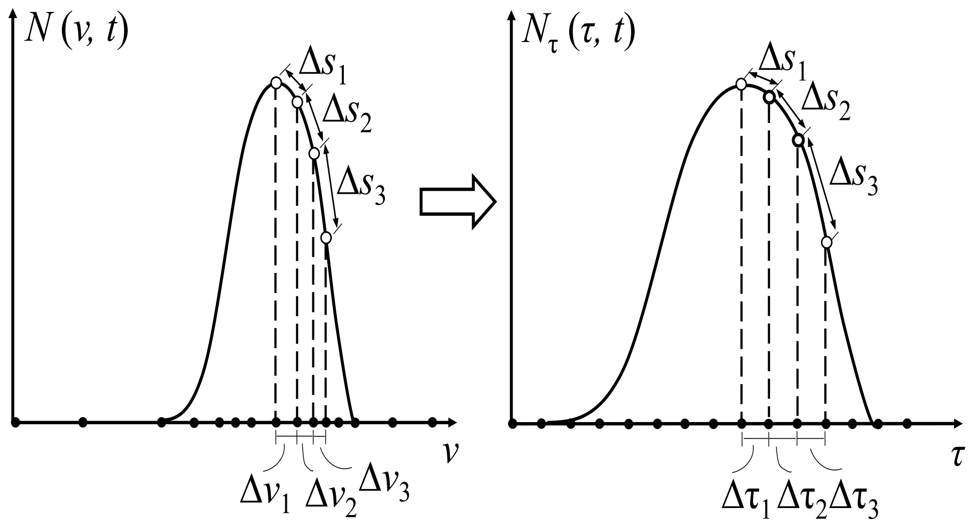
Numerical Approach

- The *PBE,* essentially a 1D partial differential equation (PDE), needs to be discretized and incorporated with the CFD codes, representing the two phases will be bilaterally affected. Stiffness of the combined PBE-CFD solver may happen.

- PBE-BOFFIN in-house code
  → laminar diffusion sooting flame



- Moment–conserved coagulation discretization
- Adaptive Grid approach [2]



Numerical Approach

- Each process during the soot formation requires accurate models

Ethylene diffusion flame [3]

Gas phase: ABF mechanism (101 species), to pyrene (A4)

Nucleation: $C_2H_2 \rightarrow 2C_2 + H_2$ $\quad B_0 = 2N_A k_N [C_2H_2]/C_{min}$

Growth [4]: $C_2H_2 + nC_S \rightarrow (n+2)C + H_2$ $\quad G(C_2H_2) = k_G [C_2H_2] A_S / \rho_S$

$A_i + nC_S \rightarrow (n+6i)C + H_2$ $\quad G(\mathrm{PAH}) = 2.2 \sum_{i=1}^{4} \sqrt{\frac{R_J MW_{A_i}}{2\pi}} [A_i] C_E(A_i)$

Oxidation: $C_S + 0.5O_2 \rightarrow CO$ $\quad G_{O_2} = \frac{120 A_S}{\rho_S} \left[\frac{k_A X_{O_2} \chi_1}{1 + k_Z X_{O_2}} + k_B X_{O_2} (1 - \chi_1) \right]$

$C_S + OH \rightarrow CO + H$ $\quad G_{OH} = 167 X_{OH} A_S / \rho_S \sqrt{T}$

Coagulation: size-dependent kernel [5]

$$\left.\begin{aligned} \beta^{\mathrm{fm}}(v_i, v_j) &= 2.2 \sqrt{\frac{\pi k_B T}{\rho_s (v_i + v_j)}} (d(v_i) + d(v_j))^2 \\ \beta^{\mathrm{c}}(v_i, v_j) &= \frac{2k_B T}{3\eta} \left(\frac{C(v_i)}{d(v_i)} + \frac{C(v_j)}{d(v_j)} \right) (d(v_i) + d(v_j)) \end{aligned}\right\} \Rightarrow \beta^{\mathrm{tr}}(v_i, v_j) = \frac{\beta^{\mathrm{fm}}(v_i, v_j) \beta^{\mathrm{c}}(v_i, v_j)}{\beta^{\mathrm{fm}}(v_i, v_j) + \beta^{\mathrm{c}}(v_i, v_j)}$$

$$\begin{cases} v < v_p, & \text{Spherical primaires} \\ v > v_p, & \text{Fractal aggregates} \end{cases}$$

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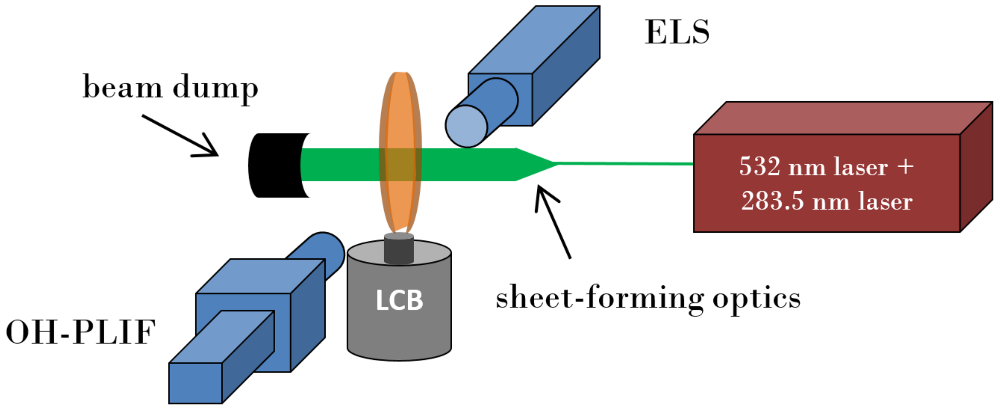
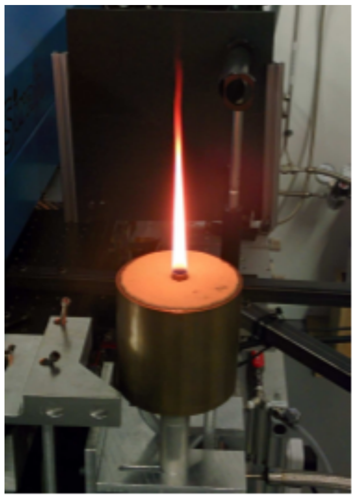
Experimental Approach

➢ The predicted PSD needs to be validated by experiment. Most laser experiments offer the lumped or integrated parameters. Connection between the PSD and the lumped result should be established.

- OH-PLIF (Planar laser-induced fluorescence) → key gas-phase species
- ELS (Elastic Light Scattering) → PSD of soot
- Light Extinction → Integrated soot volume fraction





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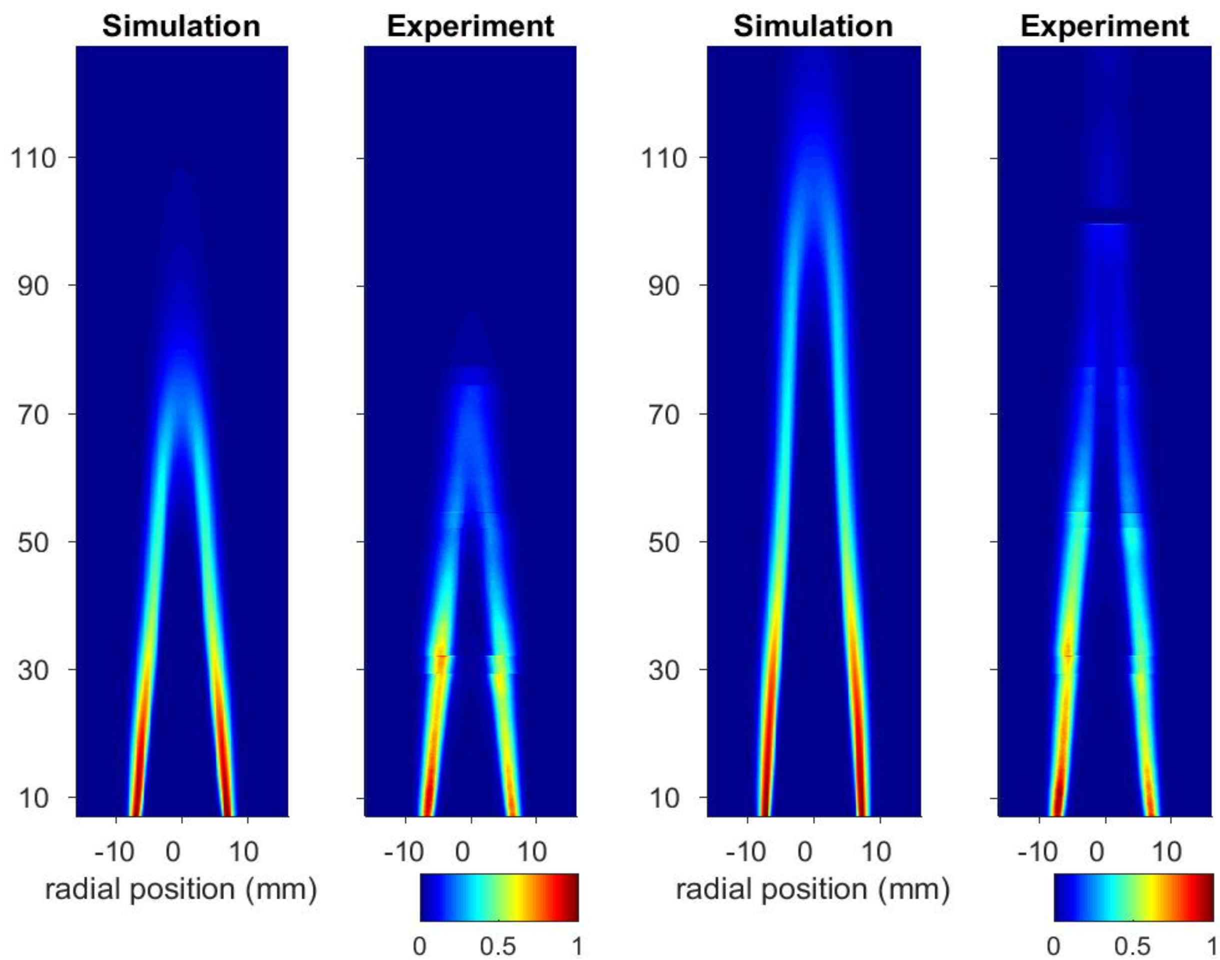
Results: Normalized OH-PLIF

$$S^{\text{OH-LIF}} \propto I_{\text{inc}} n_{\text{OH}} \sigma_{\text{A}} Q_{\text{Y}}$$

$$\boxed{S^{\text{OH-LIF}} \propto [\text{OH}] \frac{f_{v,J}(T)}{w(T)}}$$



(a) Non-smoking flame (b) Smoking flame

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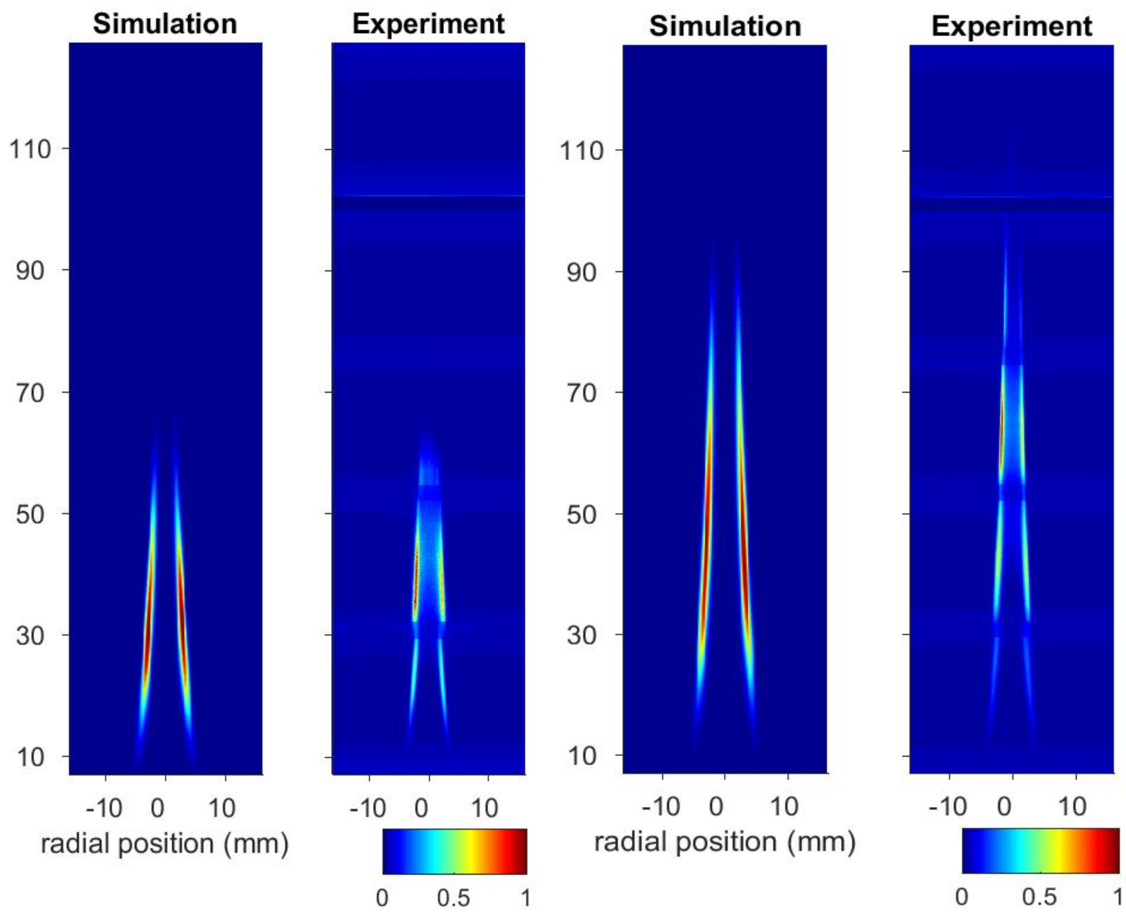
Results: Normalized ELS [6]

$$\sigma_s = k_f \begin{cases} k^4 F(m)\left(\dfrac{d(v)}{2}\right)^6 & \text{Primaries} \\ k^4 F(m) S(q) N_{\mathrm{p}}(v)^2 \left(\dfrac{d_{\mathrm{p,a}}(v)}{2}\right)^6 & \text{Aggregates} \end{cases}$$

$$S(q) \propto \begin{cases} 1 & \text{if } qR_{\mathrm{g}} < 0.1 \\ 1 - \dfrac{\left(qR_{\mathrm{g}}\right)^2}{3} & \text{if } 0.1 \le qR_{\mathrm{g}} \le 0.1 \\ \left(qR_{\mathrm{g}}\right)^{-D_f} & \text{otherwise} \end{cases}$$

$$\boxed{S^{\mathrm{ELS}} \propto \int_0^{\infty} N(v)\sigma_{\mathrm{s}}(v)\mathrm{d}v}$$



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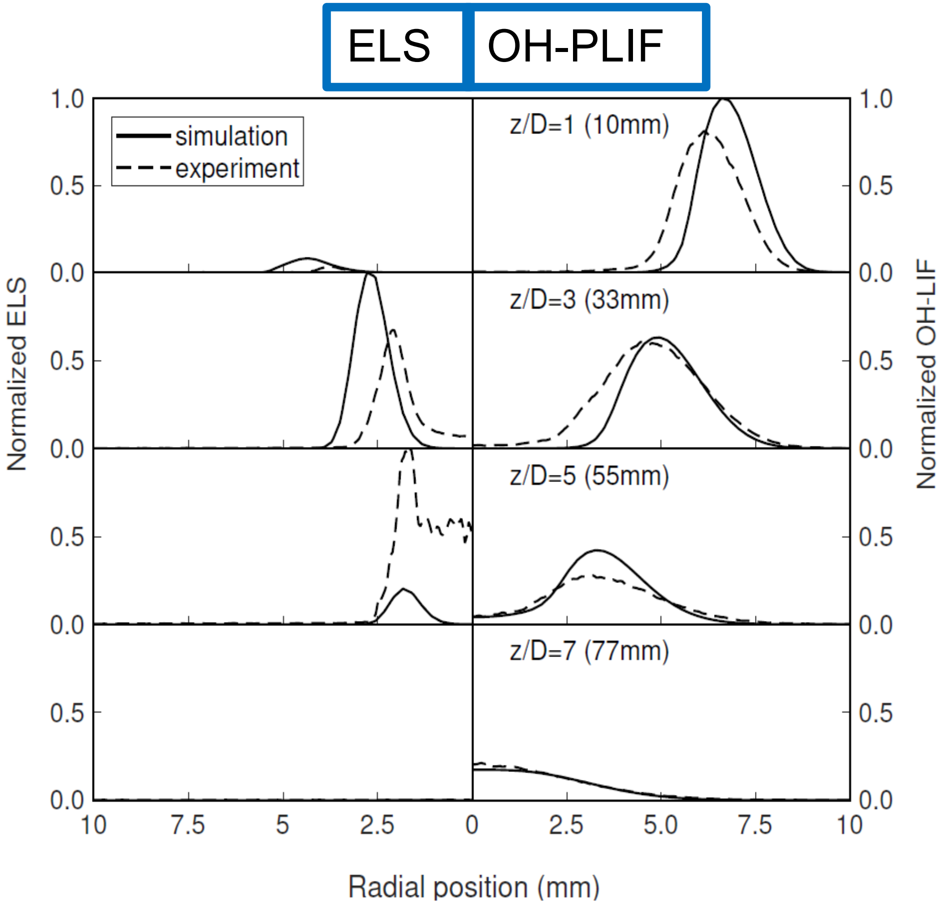
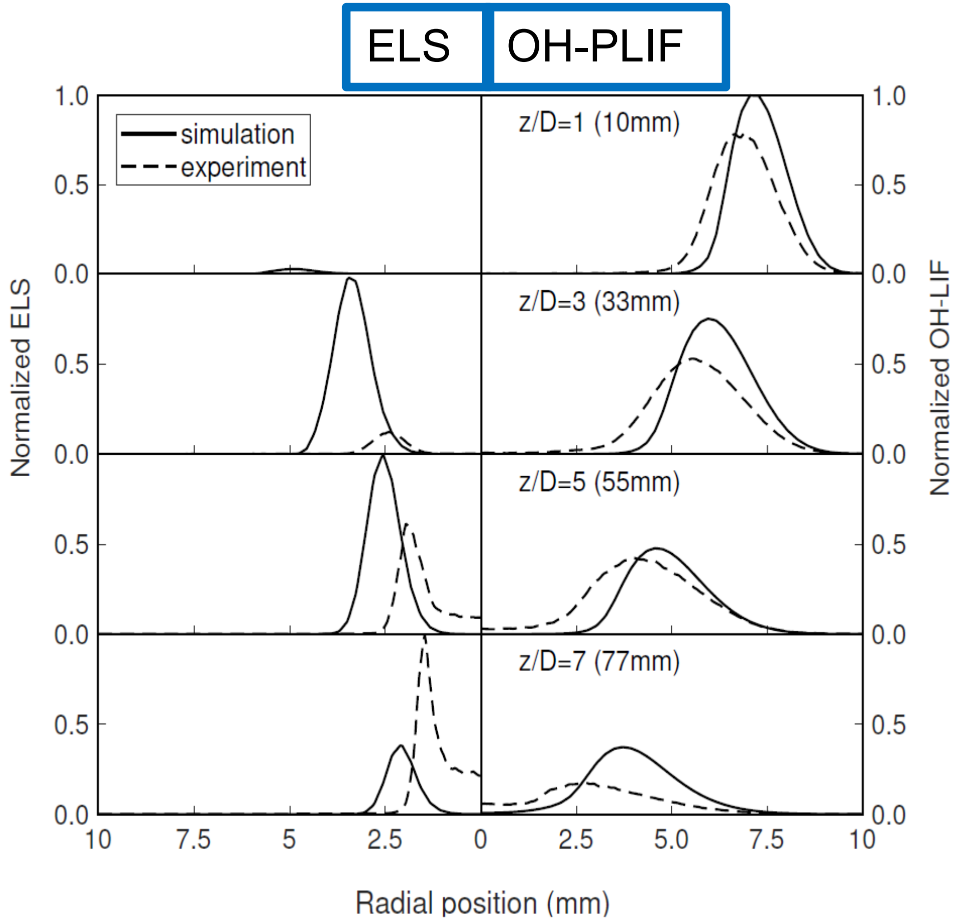
Results: Radial profiles



(a) Non-smoking flame



(b) Smoking flame

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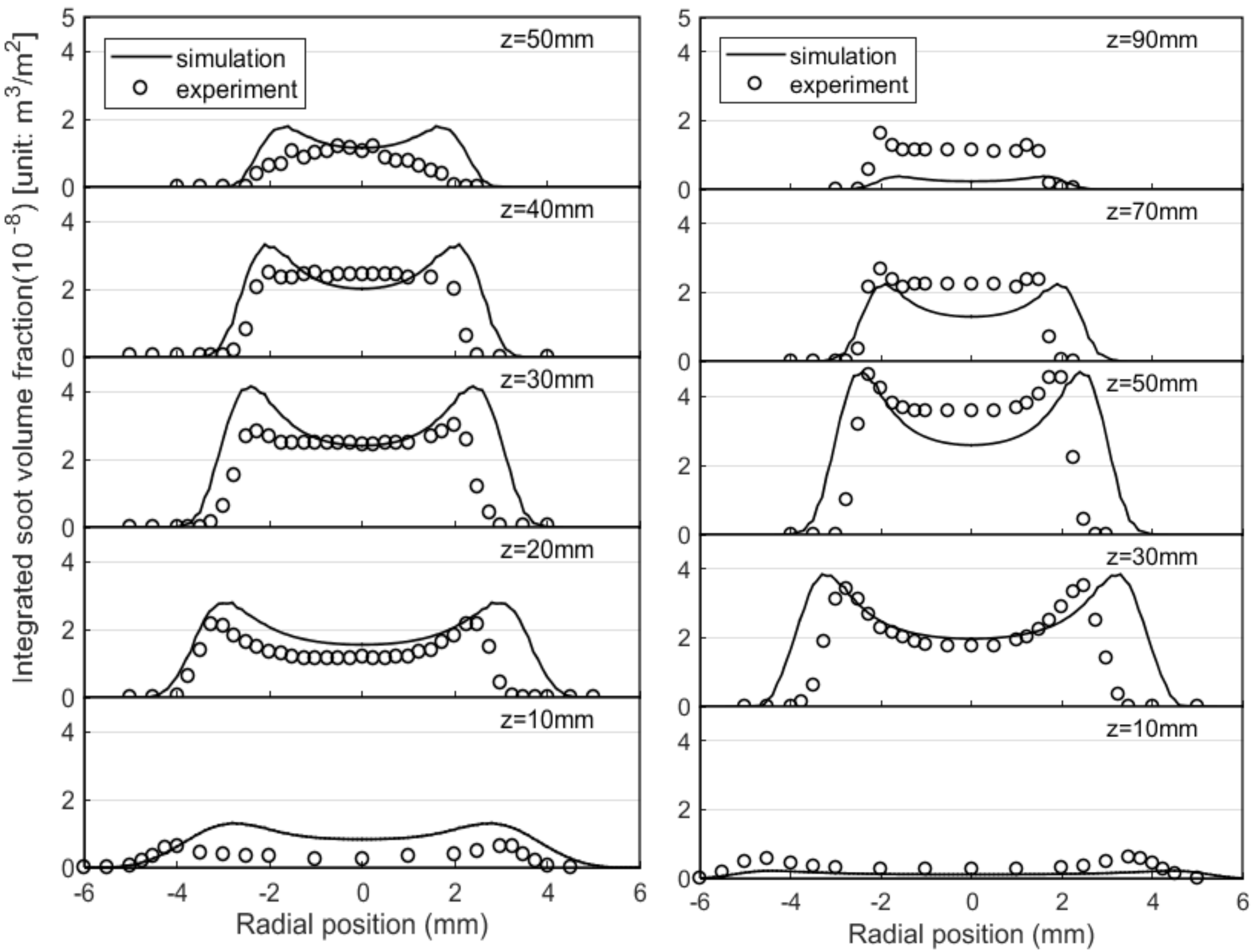
Results: ISVF

Integrated Soot Volume Fraction along a line

$$\int_0^L f_v(s)\mathrm{d}s = -\frac{\lambda}{6\pi \,\mathrm{Im}\left\{\frac{m^2+1}{m^2-1}\right\}} \ln\left(\frac{I}{I_0}\right)$$



(a) Non-smoking flame (b) Smoking flame

Summary

In this work, we presented a combined ***laser diagnostic experimental*** and ***population balance modelling*** investigation to characterize chemistry and soot formation in a laminar diffusion flame. The population balance equation governing the soot particle size distribution is incorporated into a reactive flow solver for multicomponent gases.

- The experimental laser diagnostic signals are indirectly but well predicted by the numerical solutions;
- The particle size distribution (PSD) is captured by our physical model and validated by ELS experimental data;
- For the smoking flame the discrepancies in the ISVF and the OH-PLIF signal may be due to a mismatch between the nominal fuel flow rate and the true experimental value;
- Soot kinetics needs improvement.

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Thank you