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A new generation kinetic model for pyrolytic soot formation



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KEYWORDS: Soot modeling, pyrolysis, shock tube, kinetic mechanism

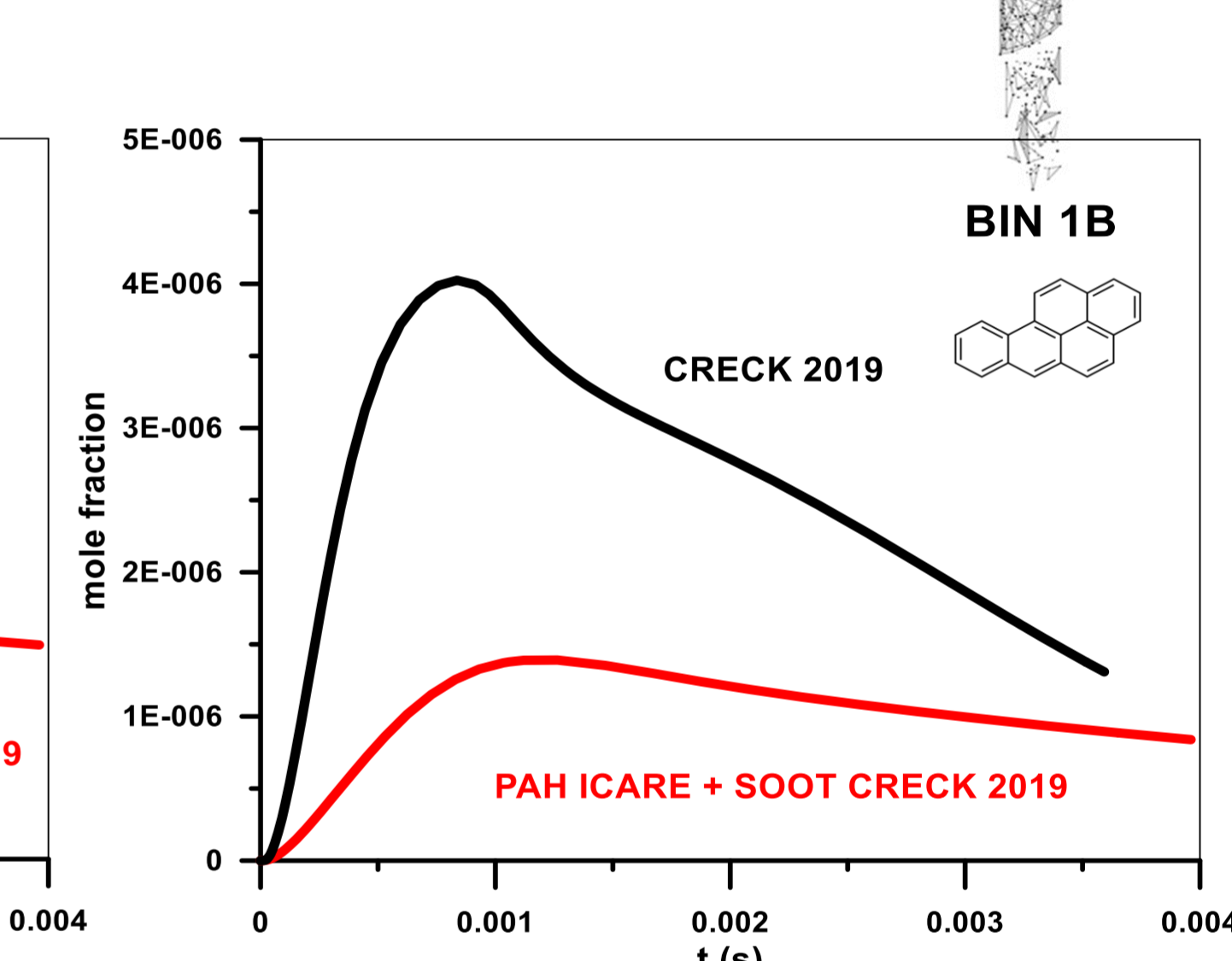
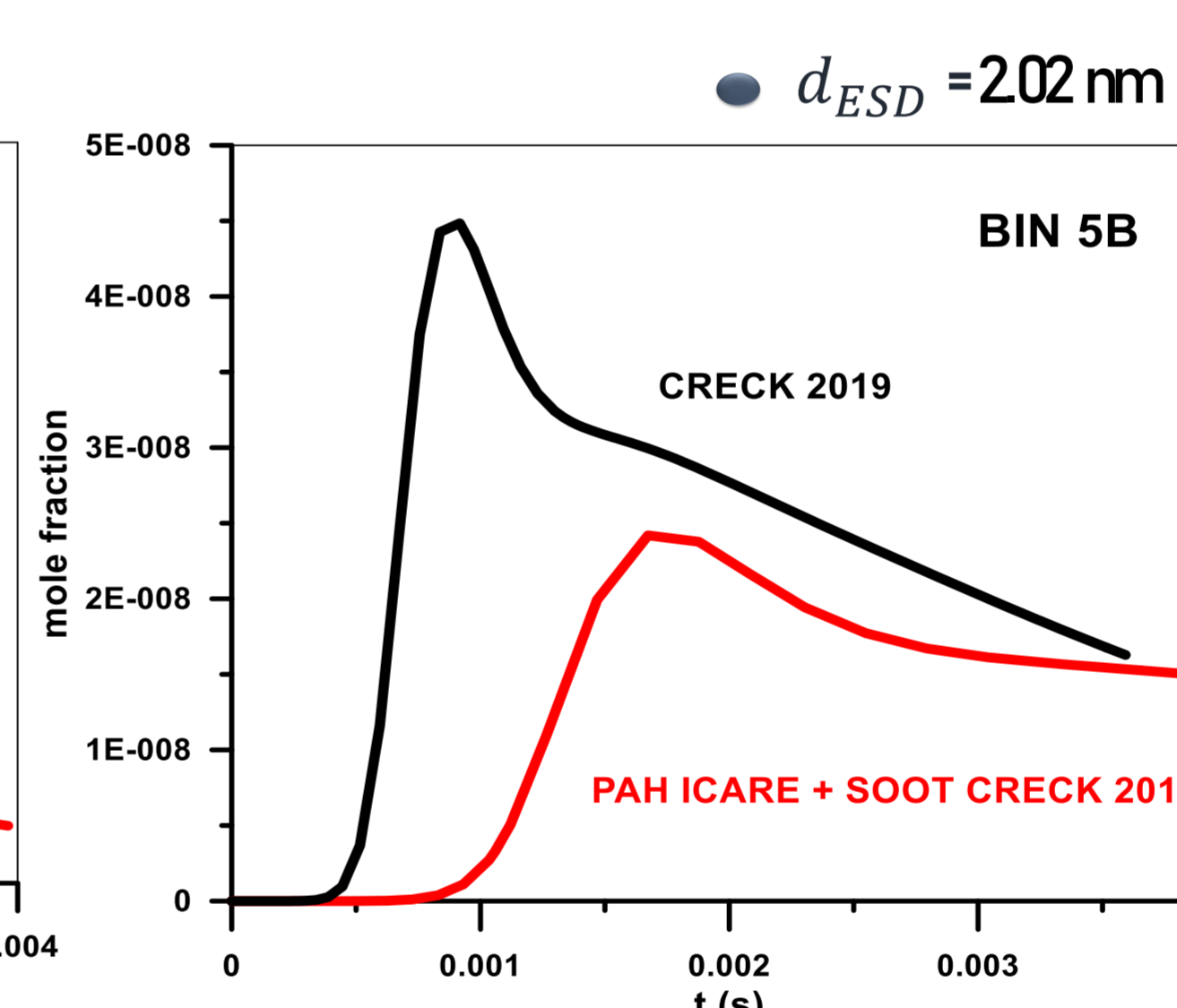
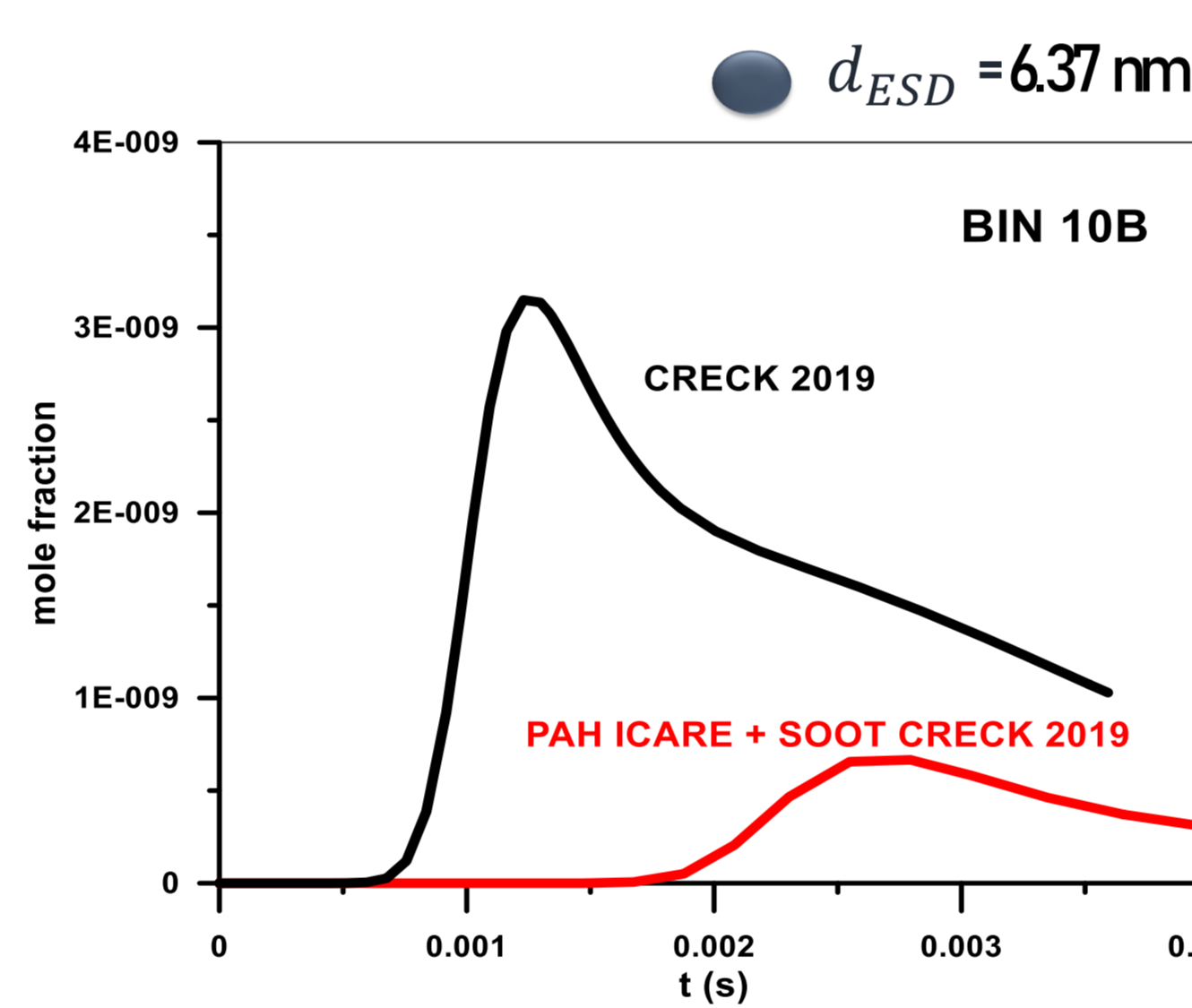
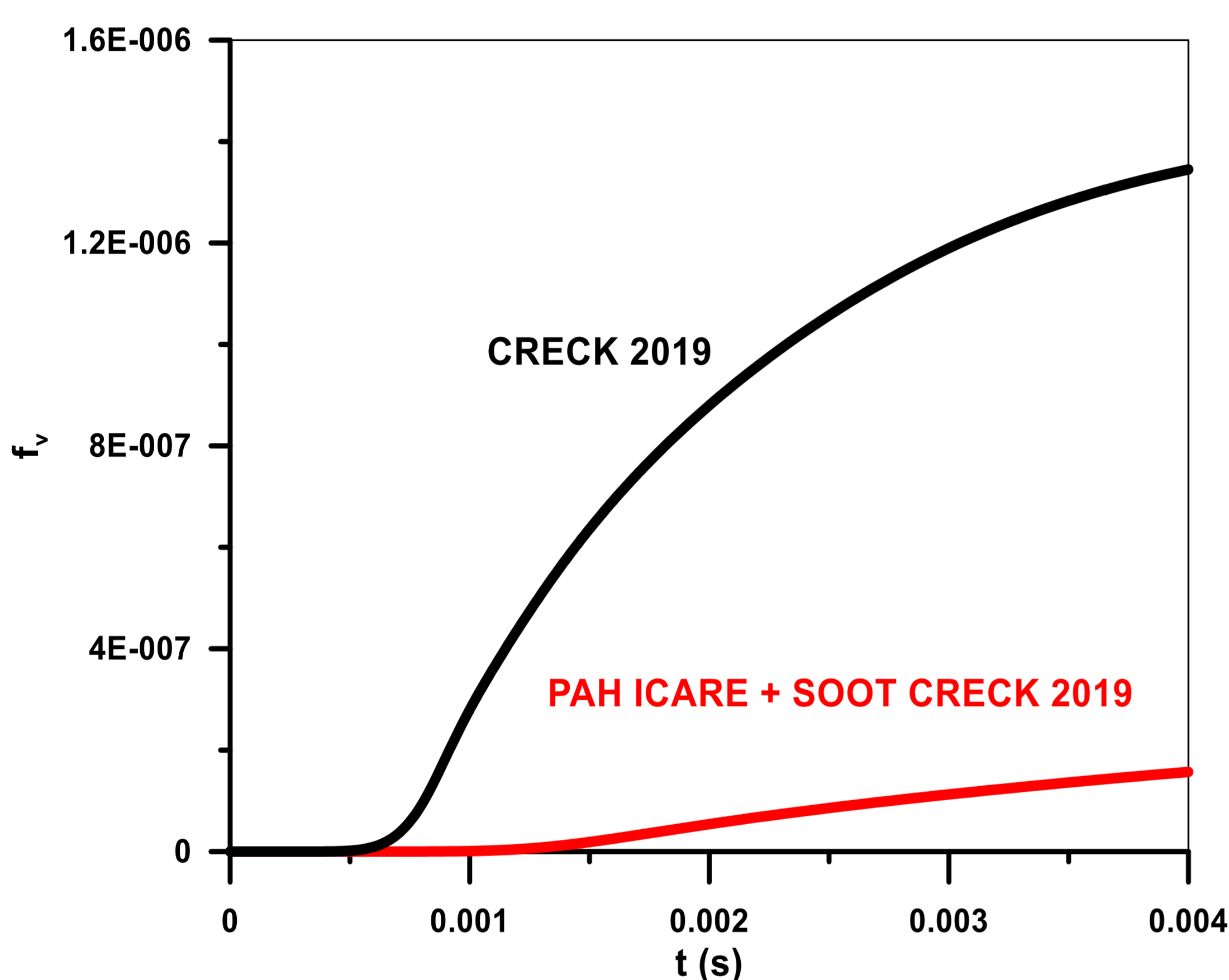
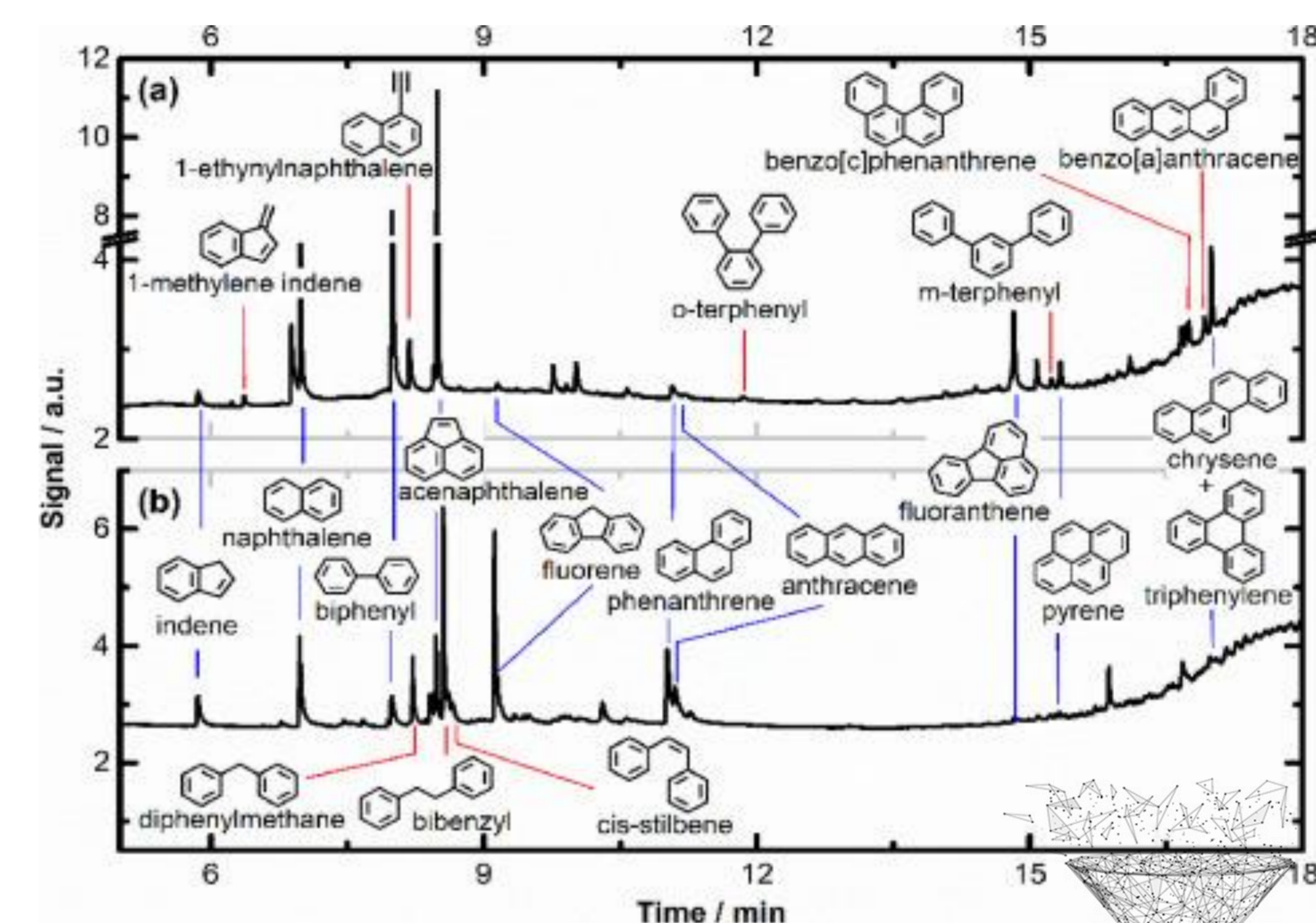
Despite decades of investigations, soot chemistry still represents a challenge for experimentalists and theoreticians, mainly due to the complexity of the processes involved. The goal of this work is to develop a comprehensive and semi-detailed kinetic model for soot prediction based on an up-to-date PAHs chemistry growth model developed in our serial works on the pyrolysis of a large number of fuels and fuel mixtures using single-pulse shock tube technique at ICARE. The solid-phase sub-model, generated by a Python code, will be based on the sectional method, using pseudo lumped carbon species, called BINs, able to approximate the soot particle distribution by discrete sections of C and H atoms. All the main classes of the soot chemistry will be considered: HACA, inception, growth, coalescence, dehydrogenation and aggregation. The kinetic parameters will be chosen based on reaction classes. The mechanism validation will be done against shock tube laser-based experiments.

State of the work at present

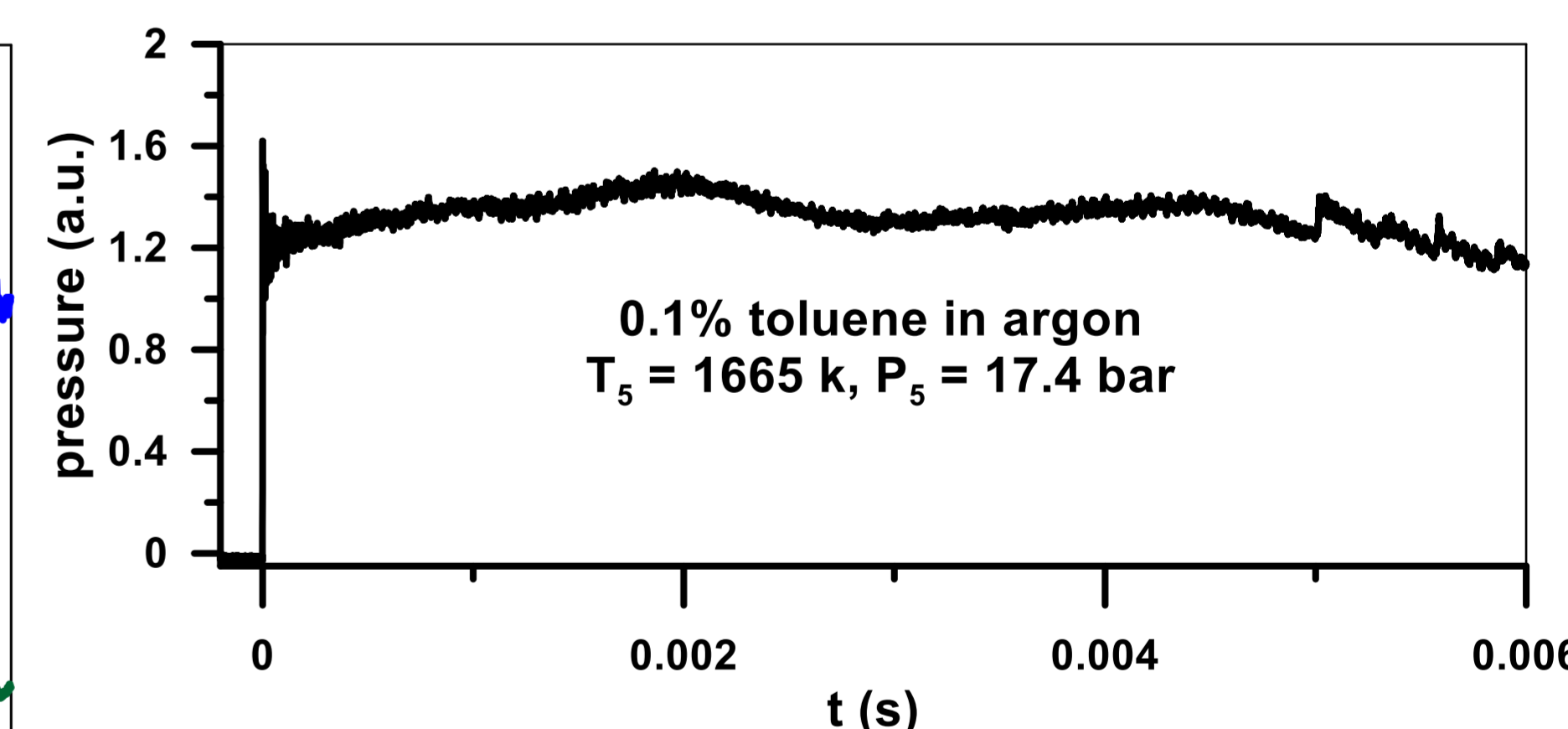
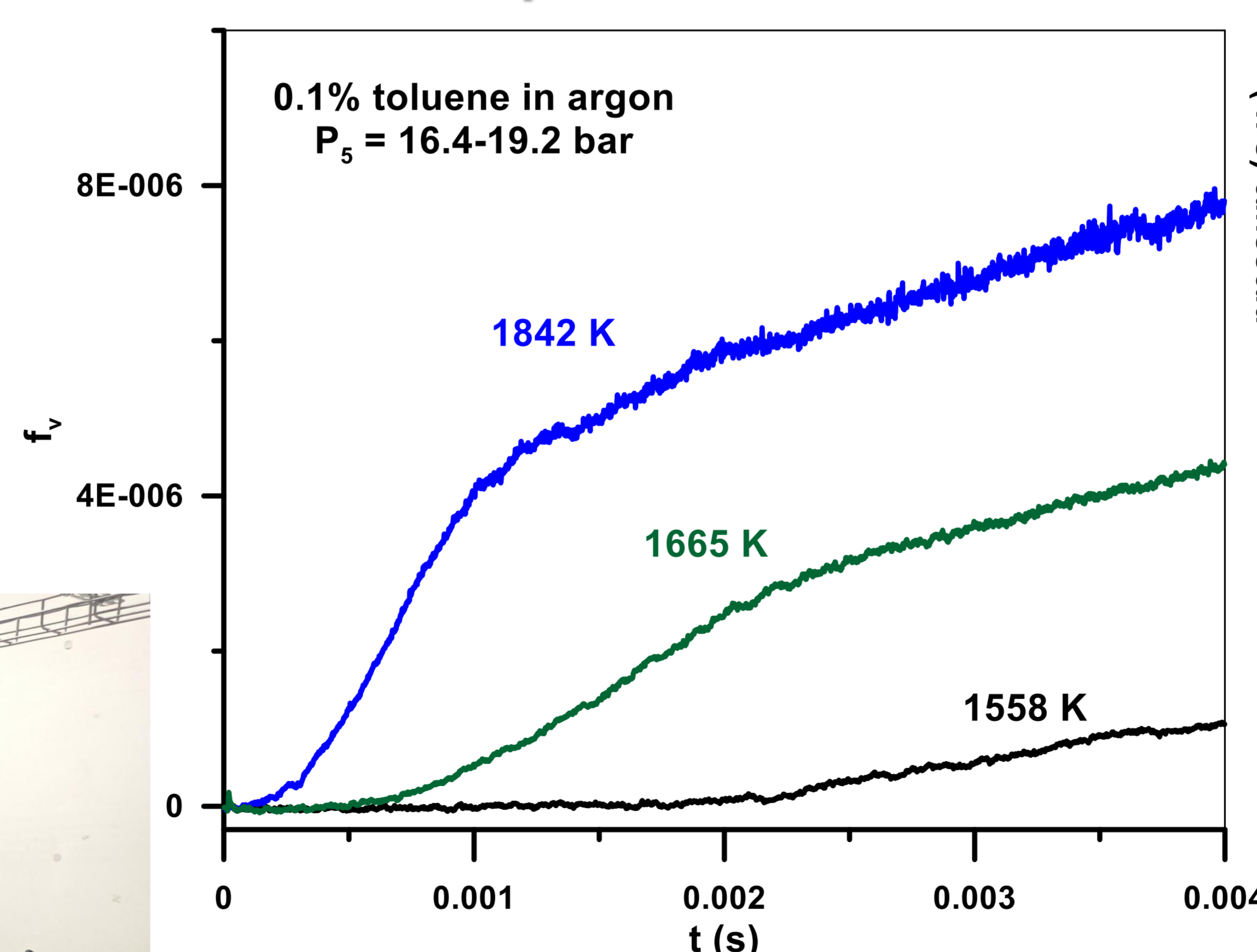
- ✓ Gas phase C1 up to C18 [1]
- ✓ Soot model based on CRECK model from Politecnico di Milano [2]
- ✓ Discrete sectional method with pseudo lumped species BINs
- ✓ Creation of the **Soot Mechanism Automated Generator SMAuG** framework in Python;
- ✓ Cantera for **tests and comparisons** -in progress

Simulation @ T=1770K, P=18 bar, C7H8 0.1% in Ar

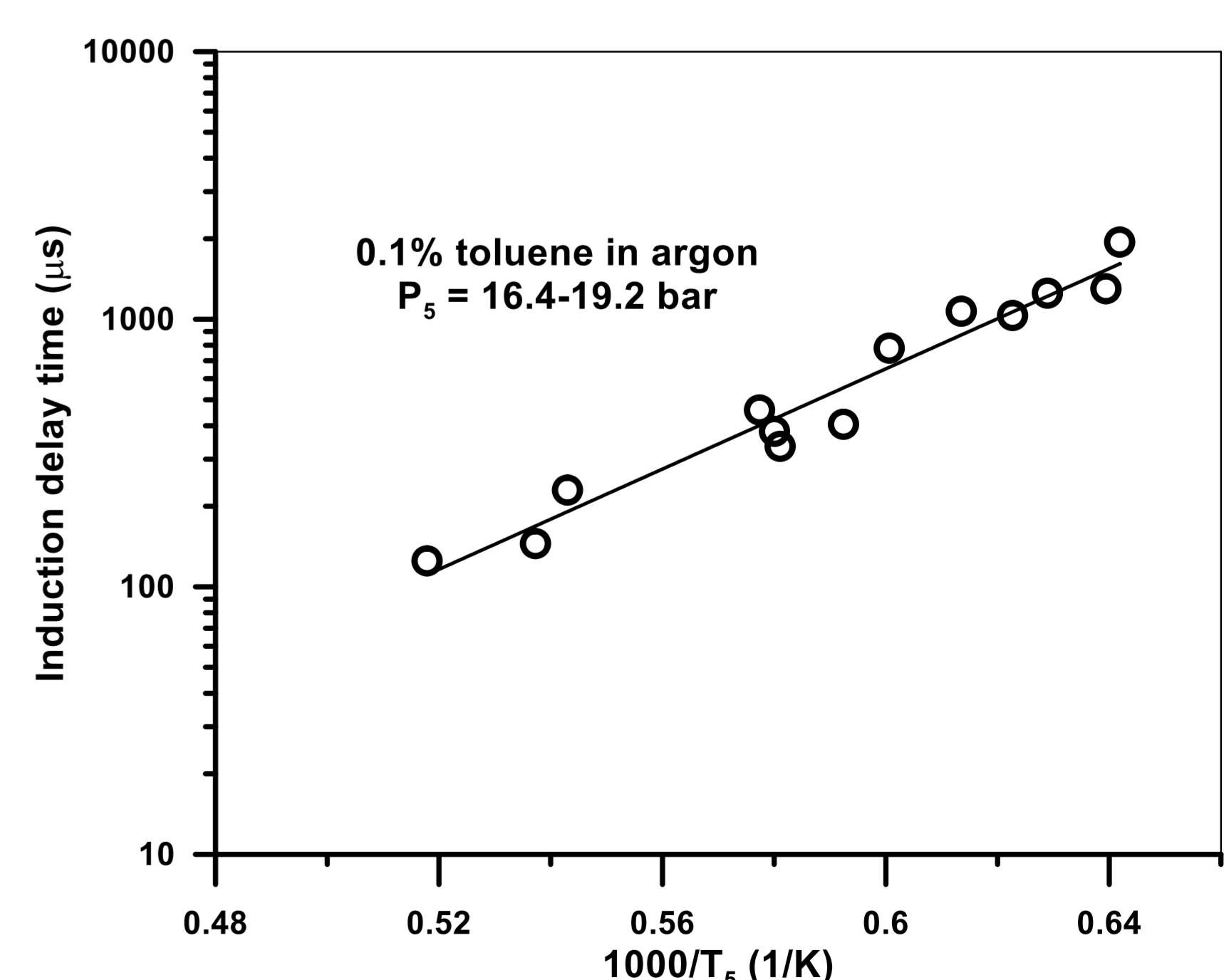
d_{ESD} = equivalent spherical diameter



Detailed profiles



Example of global parameters



$$f_v = \frac{\lambda}{6\pi l \operatorname{Im} \left(\frac{m^2 - 1}{m^2 + 1} \right)} \ln \frac{I}{I_0}$$

m = complex refractive index of soot particles
 l = length crossed by the incident ray
 λ = wavelength of the incident ray
 I = intensity of the transmitted ray
 I_0 = intensity of the incident ray
 $\operatorname{Im} \text{value} = 0.19$

References

- [1] Hamadi A et al. 2022, *Combustion and Flame* 237, 111858
 [2] Polimi Pejpichestakul, W et al. 2018 *Fuel*, 234, 199-206

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