# A new generation kinetic model for pyrolytic soot formation

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## Abstract for Work-In-Progress presentation

Despite decades of investigations, soot chemistry still represents a challenge for experimentalists and theoreticians, mainly due to the complexity of the processes involved. Long-standing questions still remain unsolved, especially concerning the chemistry of the particle precursors, the so-called polycyclic aromatic hydrocarbons (PAHs), and the nucleation process which leads to the appearance of the first solid structures. The aim of this work is the development of a new kinetic mechanism for soot formation under pyrolytic conditions validated against shock tube experiments.

The kinetic model contains an up-to-date kinetic mechanism for PAH growth which has been developed in our serial works on the pyrolysis of a large number of fuels and fuel mixtures using single-pulse shock tube techniques. Such comprehensive model is essential to guarantee the accuracy in the prediction of the particle precursors and for the validation of the solid-phase chemistry, including nucleation and particle growth. The soot model, generated using a Python code, is based on the sectional method, thus on the definition of pseudo lumped carbon species, called BINs, capable to approximate the particle distribution in terms of discrete sections characterized by a certain number of C and H atoms. The kinetic parameters are chosen based on reaction classes.

The preliminary validation of the pyrolytic mechanisms for particle appearance and growth will be carried out based on laser-based experimental data (induction delay time and soot volume fraction time-history profiles) in the heated shock tube present at ICARE - CNRS Orléans. Numerical comparison will be made with other kinetic mechanisms available in the literature to test the performance and effectiveness of the developed model.

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