SENSITIVITY ANALYSIS ON SOOT FORMATION AND PSDFs

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Many large scale uses of combustion, including transportation, power generation and waste incineration are major sources of airborne species, such as soot and polyaromatic hydrocarbons (PAHs), which are not only pollutant, but also of significant health concerns.
Soot particles can also reduce the efficiency of some combustion equipment, such as diesel engines.
It has been found that airborne particulate is responsible for various diseases as lung cancer and cardiopulmonary diseases on the long term, but also cardiovascular and respiratory diseases on the short term and soot is the second most important individual climate-warming agent after carbon dioxide.
The deepening of the knowledge of the chemical processes involved in hydrocarbon oxidation, formation and depletion of PAH and soot would allow to achieve a better design of the combustion systems with improved energy efficiency and a simultaneous reduction of particulate emissions.
This work aims to present a mechanism of soot nucleation, growth and oxidation.
The kinetic model is based on a sectional approach: the investigated range of particles has been divided in classes of pseudo-species with similar reactivity (BINs). Each of the classes is defined by the average molecular mass and a given number of carbon and hydrogen atoms. Classes with same mass and different hydrogenation are considered to follow better the chemical evolution of the system.
Particle kinetic can this way be defined in analogy with the gas phase chemistry, the two phases are coupled and both written in the common form A + B → C + D, with the usual Arrhenius form to describe the formation and growth rates.
Different classes of reactions are considered to describe soot evolution in the flame and they include nucleation, metathesis, unimolecular decomposition with hydrogen production, dehydrogenation, demethylation, surface growth, oxidation and coagulation.
In this work, a sensitivity analysis is conducted to show the influence of the different reaction classes on soot formation and on the particle size distributions.

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