Study of soot production in ethylene pyrolysis using a sectional model

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The interest in studying nanoparticle formation from hydrocarbons oxidation and pyrolysis is twofold. On one hand, it is crucial for suppressing undesirable soot emissions that might impact the environment and human health. On the other hand, it is of interest for the developing of more efficient processes for nanoparticle synthesis. Within this context, this work aims at modeling soot production in ethylene pyrolysis using a sectional approach. To that end, the main focus is placed on the assessment of results sensitivity to the gas-phase mechanism, soot precursors and surface growth mechanism.

The consecution of the objective relies on the validation of polycyclic aromatic hydrocarbons (PAH) and major species concentration along with soot predictions. For this validation, two experimental datasets are targeted. The first dataset comprises measurements from experiments conducted in a plug flow reactor (PFR) at atmospheric pressure and low temperature (1223-1423 K) [1]. The second dataset includes time-resolved profiles from the pyrolysis of ethylene in a shock tube (ST) at high pressure (around 0.38 MPa) and high temperature (1961-2179 K) [2]. Cantera is used to solve the chemical kinetics from several gas-phase mechanisms describing ethylene pyrolysis. Implemented within the framework of Cantera, a soot sectional model (SSM) [3] is used to account for soot production. The SSM considers soot particles to be a solid and distinct dispersed phase interacting with the gas-phase through a two-way coupling.

Modeling results evidence large differences in the prediction of PAH mole fraction for the different gas-phase mechanisms evaluated for the PFR cases. These differences, in addition to the choice of soot precursors, are shown to heavily influence soot predictions. Time-resolved soot volume fraction profiles, from the ST cases, allow assessing how the soot onset time is influenced by the soot precursors choice. In relation to the sensitivity of results to the soot surface growth mechanism, both PFR and ST results point out to the importance of the carbon balance between the soot and the gas-phase to the accurate prediction of soot production. In that sense, PFR cases show a clear over-prediction of acetylene mole fraction if soot production is not accounted for.

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