Extension of tabulation technique to soot formation simulation

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Soot emission from combustion devices represents a serious concern because of negative effects on human health and environment. In this context, numerical simulations of formation and evolution of soot particles in flames is gaining importance as a tool to support the design of existing and new combustion. One of the most important challenges for numerical simulations is the description of the complex chemical and physical phenomena governing the production of gaseous PAHs (Polycyclic aromatic hydrocarbons) and soot particles.
A kinetic scheme combining a detailed gas-phase mechanism (DGM) and a discrete sectional model (DSM) for soot have been developed by the CRECK team of the Politecnico di Milano. It provides a detailed insight of PAHs and soot production and it accounts for ~300 species and ~17000 reactions. The use of such a detailed description for the simulation of turbulent sooting flames is computationally not yet affordable. The development of affordable models, allowing an accurate description of soot production in realistic configurations is needed.
On one side, species and reaction number reduction technique can be used. The Species-Targeted Sensitivity Analysis (STSA) [1] have been already applied to the DGM+DSM model, producing an accurate reduced description. However, this mechanism is still to expensive from a CPU point of view. On the other side, tabulation techniques [2-4] are often used to introduce detailed chemical description into simulation of turbulent flames. These models have been originally developed for purely gaseous flames based on the flamelet assumption of Peters [5]. The turbulent flame front is seen as an ensemble of laminar mono-dimensional flamelets that can be pre-calculated and stored into look-up tables. This assumption is valid until the flame structure is not strongly modified by the turbulent flow. However, due to the long characteristic time scales [6] of soot production strong interaction with the turbulence is expected as shown at a flame-vortex interaction by Rodrigues et. al [7].
The aim of this work is to propose a reduced description of the DGM+DSM model based on a combination of tabulated and reduction techniques, by identifying the indispensable soot species to be transported and, consequently reducing the kinetic scheme describing their evolution. This optimization will lead to the definition of an accurate but computationally effective description of PAHs and soot in turbulent flames.

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