Wide scope combustion reaction mechanism coarse graining

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Combustion science and technology need reaction mechanisms that are both valid within wide parameter range and very reduced in size. This demands the development of coarse-grained phenological mechanisms. This talk introduces our latest progresses on mechanism coarse-graining method based on community states and milestone community states identification as well as wide parameter statistic with the help of bifurcation analysis that get the ignition and extinction conditions.

Case study in CH4 combustion system described by the GRI-3.0 mechanism demonstrates that the evolution process represented by the coarse-grained states not only can distinctively separate the pyrolysis from oxidation processes but is also capable of effectively identifying commonalities of the states over a wide range of parameters. Milestone states defined by the community classification of species with high rank of betweenness further clarify the boundary and distribution of the states on the P-T bifurcation diagram. In addition, analysis of the stable community indicates that the hydrogen sub-mechanism and the methane oxidation (formaldehyde, methanol, carbon monoxide) parts of the mechanism are the core for methane ignition. By analyzing the difference of the community states near the critical bifurcation condition, the most influential reactions for the ignition process are also identified, which agrees well with previous related reports.