Phase space structure for reaction mechanisms of hydrocarbon combustion

Michael Davis
Argonne National Laboratory, Argonne, Illinois, US

Modern reaction mechanisms for hydrocarbon combustion are very large, with hundreds or thousands of species and even a greater number of reactions, so it is useful to have ways to understand and reduce these systems. In this talk, the composite phase space structure is considered for such mechanisms. The composite consists of the low-dimensional manifolds of a series of systems that span the constants of the mechanisms. For example, chemical-kinetic mechanisms for hydrocarbon combustion in pure oxygen run under adiabatic/isobaric conditions consist of the elements H/C/O and constant pressure and enthalpy. Together with an equation of state these conditions lead to a composite phase space structure that consists of a 4-dimensional surface for the equilibrium states, a five-dimensional surface for the one-dimensional manifolds, etc. This structure is studied for two mechanisms, a methanol mechanism that describes the behavior of 18 species and a propane mechanism with over 100 species. It is shown how the study of the phase space structure can lead to insights about what reactions are important in the mechanism, changes that occur with pressure and enthalpy, and the ways in which different mechanisms can be compared. Results for steady flames are also presented.