Phase space structure of complex chemical-kinetic mechanisms: Low-dimensional manifolds for homogeneous chemical kinetics and 1-d premixed flames

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Figure 1 shows a typical result for one-dimensional premixed flames. The mass fractions for several species are plotted vs. the distance from the burner.

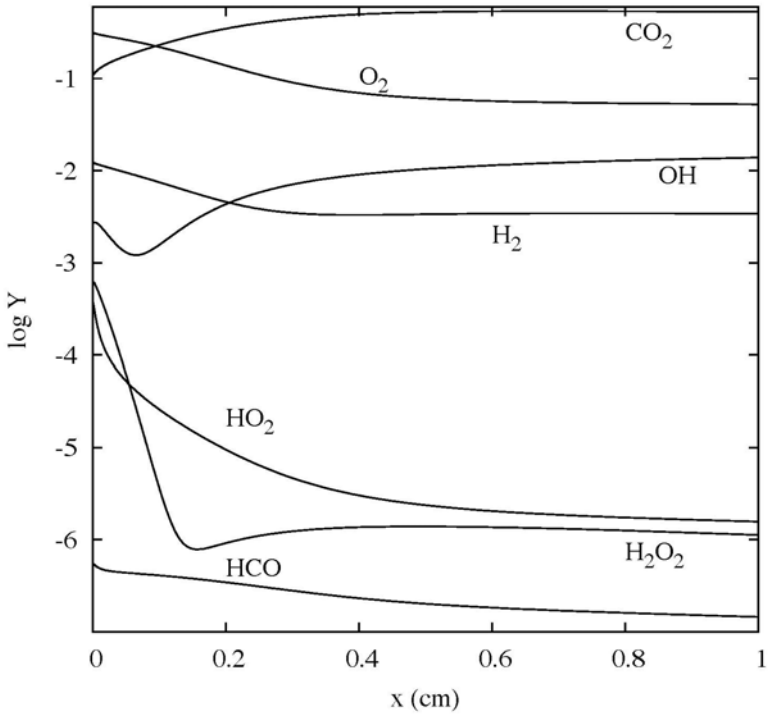
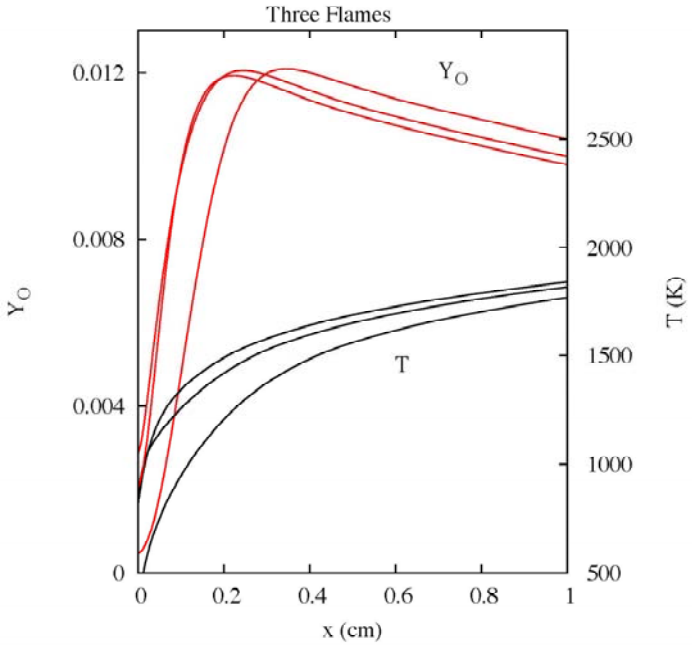


Fig. 1

These results were generated for the formaldehyde/methanol/CO mechanism of Dryer and co-workers. The mixture mole fractions at the burner were: 3/7 CO, 2/7 O_2, and 2/7 H_2, with T = 300 K. This result is extended in Fig. 2 to two additional flames, which have different mixtures at the burner and different initial temperatures in Fig. 2. The additional flames have the following mixtures and temperatures: 1) 1/6 CH_2O, 1/3 CO,

Fig. 2



1/6 H_2, 1/3 O_2, and T = 855 K, 2) 0.08 CH_3OH, 0.42 CO, 0.17 H_2, 0.33 O_2, and T = 809 K.

As Fig. 2 indicates, the behavior of flames can be very similar away from the burner (x > 0.2 cm in the figure), even when the mixtures and temperatures are different at the burner. Figure 3 makes this point more strongly, by plotting projections of these

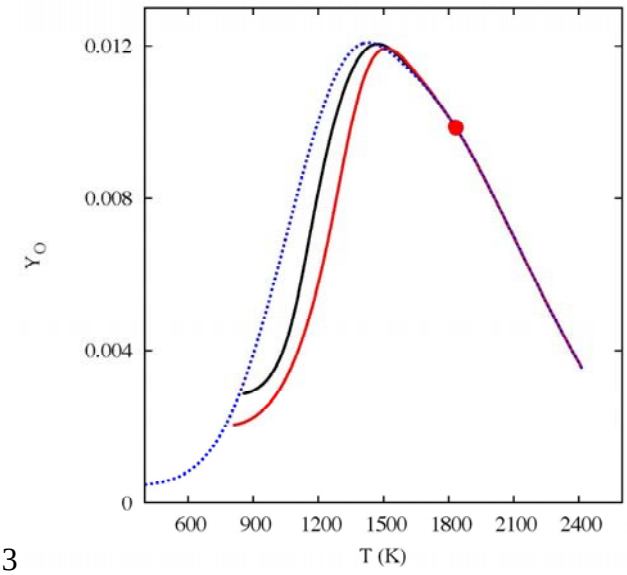


Fig. 3

flames in phase space. This figure makes it clear that the steady flames are approaching a one-dimensional manifold in phase space, although they reach the manifold at different spatial locations (at the dot the spatial locations are 0.98, 1.05, and 1.25 cm).

The purpose of this talk will be to discuss the phenomena observed in the figures in terms of the phase space structure of the system. The talk will also put the behavior in

the broader context of the composite phase space structure of a chemical-kinetic mechanism. Additional topics of the talk will be: 1) how the phase space structure in the flame compares to the phase space structure of the homogeneous chemical kinetics, 2) how the phase space structure changes with stoichiometry, pressure, and enthalpy, and 3) how the phase space structure of this mechanism compares to other hydrocarbon mechanisms. In particular, the latter topic will lead to a comparison of the Princeton methanol mechanism with the C_3 mechanism developed at Galway for the lowest dimensional manifolds.