Sensitivity analysis of chemical kinetic systems
with large time scale separation

J. Zador, I.Gy. Zsely, T. Turanyi

ABSTRACT:

Local sensitivity functions of many chemical kinetic models
exhibit three types of similarity:

(i) ratio of the sensitivities of two variables with respect to the
same parameter is equal for any parameter;

(ii) this ratio is equal to the ratio of the gradients of the
corresponding variables with respect to the independent variable;

(iii) ratio of the sensitivities of any variable with respect to any
two parameters is equal at any value of the independent variable.

These types of similarity are called here local similarity, scaling
relation, and global similarity, respectively. Similarity of
sensitivity functions is investigated in homogeneous explosions,
freely propagating and burner-stabilized laminar flames of hydrogen
and methane, at several fuel-to-air ratios, with and without
constrained temperature profile. Several new visualization tools are
used for the study of similarity relations, including a dissimilarity
function, cobweb and correlation plots. Previously, scaling relation
was assumed to be the consequence of the presence of a single dominant
variable in the kinetic system and diffusion was considered to be the
reason for global similarity. It is shown that the existence of low
dimensional manifolds in chemical kinetic systems cause scaling
relations and it is confirmed that global similarity emerges if the
sensitivity functions are pseudo-homogeneous and if there is a single
dominant variable in the system. However, diffusion usually decreases
the level of global similarity. Practical consequences of the
similarity of sensitivity functions are discussed, including parameter
estimation in chemical kinetic systems, testing of complex reaction
mechanisms and utilization of flame velocity sensitivities.