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Chapter 1

TRANSIENT MODELING IN HETEROGENEOUS COMBUSTION

John Mantzaras*
Paul Scherrer Institute, Combustion Research, Villigen PSI, Switzerland

ABSTRACT

The dynamic behavior of catalytic combustion systems involves complex interactions between heterogeneous kinetics, interphase and intraphase transport, heat conduction in the solid substrate and, in many cases, of homogeneous (gas-phase) kinetics. Numerical models describing the dynamic behavior of catalytic systems at the reactor scale are presented, with emphasis on multidimensional CFD simulations with detailed heterogeneous mean-field chemical description, elementary homogeneous (gas-phase) reactions, and detailed transport. In terms of the temporal treatment, models encompassing quasisteady approaches for the flow and chemistry, to full direct numerical simulation (DNS) are introduced. Dynamic response due to reactor changing operating conditions is presented in catalytic ignition (light-off) applications of fuel-lean and fuel-rich methane/air mixtures over noble metals. The impact of solid material properties, catalytic reactivity, gas-phase chemistry and in-channel heat transfer mechanisms on the light-off behavior is illustrated and the advantages of spatially multidimensional models are exemplified. Dynamic behavior driven by interactions between homogeneous chemistry and catalytic walls is then addressed using full direct numerical simulation (DNS). It is shown that although catalytic reactions restrain homogeneous-kinetics-driven instabilities, depending on the catalytic reactivity and operating conditions, flame dynamics can still persist in the form of oscillatory or chaotic combustion modes. The impact of turbulent temporal fluctuations of flow and thermoscalars on the coupling between hetero-/homogeneous chemistry and transport is outlined. The origin of heterogeneous-kinetics-driven dynamic oscillations is finally addressed using low-dimensionality reactive/diffusive systems. Advanced multidimensional CFD models can be used to gain insight on catalytically-driven dynamics, their potential coupling with homogeneous-kinetics-driven dynamics, and their response to time-varying reactor operating conditions (ignition, load change etc.).