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Chapter 8

INTERPLAY OF TRANSPORT AND HETERO-/HOMOGENEOUS CHEMISTRY

John Mantzaras*

Paul Scherrer Institute, Combustion Research, CH-5232 Villigen PSI, Switzerland

Abstract

The coupling of fluid-mechanical interphase transport in laminar or turbulent channel-flows to the heterogeneous (catalytic) and homogeneous (gas-phase) reaction pathways as well as the interplay between the pathways themselves is reviewed under conditions relevant to practical catalytic combustion systems. Analytical formulations and detailed numerical predictions are used in conjunction with in situ non-intrusive measurements of major and minor gas-phase species concentrations over the catalyst boundary layer in order to elucidate this multi-faceted interplay. Starting with laminar transport, analytical heterogeneous and homogeneous ignition criteria based on large activation energy asymptotics are presented, clearly identifying the controlling transport, chemical, flow, and geometrical parameters of the channel-flow configuration. The analytical criteria are further adapted so as to quantitatively reproduce numerically predicted homogeneous ignition characteristics. Detailed simulations are then employed to demonstrate the intrinsic chemical coupling between the two reaction pathways. The impact of diffusionally imbalanced reactants and of chemical non-equilibration on the catalyst temperature is clarified. Investigation of methane/air and hydrogen/air combustion over noble metals exemplifies the importance of reliable low-temperature gas-phase kinetics. It is further shown that the hetero-/homogeneous radical coupling inhibits only mildly the onset of gas-phase ignition. Turbulent transport, an issue of particular interest to power generation systems, is finally addressed. Numerical predictions and experiments indicate that key to the aptness of the turbulence models is their ability to reproduce the strong flow relaminarization induced by the heat transfer from the hot catalytic walls. The regimes of flow relaminarization in channel-flow combustion are delineated in terms of the relevant inflow turbulent properties and the catalyst wall temperature.

* E-mail address: ioannis.mantzaras@psi.ch, Tel: ++41-56-3104046, Fax: ++41-56-3102199