Hetero-/homogeneous combustion of low hydrocarbons, syngas and hydrogen, from the fundamentals to power generation applications

Ioannis Mantzaras

Paul Scherrer Institute, Switzerland

Abstract

Multidimensional numerical modeling and in situ spatially-resolved measurements of gas-phase thermoscalars over the catalyst boundary layer have fostered fundamental investigation of the heterogeneous and homogeneous chemical reaction pathways and their coupling at realistic operating conditions. The methodology for validating catalytic and gas-phase reaction mechanisms is firstly outlined for industrially-relevant fuels. Combination of advanced modeling and in situ near-wall species and velocity measurements is then used to address the intricate interplay between interphase fluid transport (laminar or turbulent) and hetero-/homogeneous kinetics. Controlling parameters of this interplay are the homogeneous ignition chemistry, flame propagation characteristics, competition between the catalytic and gaseous pathways for fuel consumption, diffusional imbalance of the limiting reactant, flow laminarization due to heat transfer from the hot catalytic walls, and fuel leakage through the gaseous reaction zone. Dynamic reactor operation and intrinsic flame dynamics driven by interactions between homogeneous kinetics and catalytic walls are outlined using detailed transient simulation. It is shown that the presence of catalytic reactions moderates flame instabilities. Future directions for transient modeling and for temporally-resolved in situ near-wall measurements are finally summarized.