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Evaluation of Models for Heterogeneous Catalysis

John Mantzaras

7.1
Introduction

The progress in many industrial devices employing heterogeneous catalysis, such as chemical synthesis, exhaust gas cleanup, and heat/power generation plants, crucially depends on key advances in multidimensional modeling necessary for reactor design. The numerical models should entail detailed description of the heterogeneous (catalytic) and low-temperature homogeneous (gas-phase) kinetics, as well as of the underlying interphase and intraphase fluid transport. There is currently a pressing need for hetero-/homogeneous chemical reaction schemes valid over broad ranges of operating conditions, which for the heat/power generation systems alone encompass pressures from 1 bar in industrial boilers and household burners [1] to 5 bar in microreactors [2] and to 20 bar in large stationary gas turbines [3]. Moreover, the temperatures in industrial catalytic applications range from a few hundred degrees up to 1400 K.

Recent developments in surface science measuring techniques, as briefly discussed in Section 7.2, have assisted the construction of detailed catalytic reaction mechanisms by probing key elementary reaction pathways and identifying pertinent surface species. As most of the surface science data refer to ultrahigh vacuum (UHV) and to single-crystal surfaces, the extension of the resulting reaction mechanisms to realistic pressures and technical catalysts (polycrystalline surfaces) is not warranted. This necessitates additional validation tools, which are mainly based on measurements of gas-phase thermoscalars, either average or spatially resolved, in suitable laboratory-scale reactors.

In an effort to bridge the pressure and materials gap between surface science and technical heterogeneous catalysis, *in situ* spatially resolved measurements of major and minor gas-phase species concentrations over the catalyst boundary layer using spontaneous Raman and laser-induced fluorescence (LIF), respectively, have fostered fundamental hetero/homogeneous kinetic studies at elevated pressures and temperatures, realistic reactant compositions, and technical catalyst surfaces [4–7]. It is demonstrated in the forthcoming sections that the combination of *in situ*

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