# FROM MACROSCOPIC OBSERVATIONS TO MICRO-KINETIC MODELS OF SURFACE REACTIONS

Ahmed F Ghoniem

Massachusetts Institute of Technology

## EXTENDED ABSTRACT

Surface chemistry, both thermal and electrochemical, is very important in many energy applications including catalysis, fuel cells, membrane reactors, reformers, etc. However, accurate mechanisms describing its kinetics have not been widely developed. *In situ* spectroscopic measurements to determine the reacting species and reaction rates are often rare and incomplete. Frequently one must rely on macroscopic measurements (permeation fluxes) or device performance (I-V curve in fuel cells) in which surface processes play an important role. Models relating the device performance to the surface chemistry are formulated in terms of partial differential equations describing the interaction between different modes of transport and chemistry in both the homogeneous and heterogeneous phases using the mean-field approximation. The source terms are assembled using multistep reaction kinetics (microkinetics) often involving adsorption/desorption, charge transfer, incorporation into bulk and the corresponding species. The choice of the intermediate molecules in the microkinetics mechanism, and the corresponding reaction steps, is often guided by prior knowledge or some *ab initio* calculations. Individual reactions (forward and backward) must satisfy thermodynamic consistency (although this is not always done). Estimating the unknown kinetics parameters is done by matching the solution to the available data over a reasonable range of operating conditions. I will discuss couple of recent examples from our work on solid oxide fuel cell [1,4,5] and ion-transport membranes [2,3].

## REFERENCES

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