

General Considerations for Process Modelling on a Thermochemical Basis

T. Ginsberg, M. Modigell

RWTH Aachen, AVT.MVT, Germany

Abstract

Computational thermochemistry is frequently and successfully applied to model high temperature chemical processes. Since thermochemical data is available for a large number of phases and compounds it is possible to consider very large and complicated chemical systems including minor and trace components.

However, there are some processes which are on the one hand characterized by very complex chemical conditions, but assuming homogeneous mixing or negligible chemical kinetics due to high temperatures is not quite justified. Since apparently no other method than thermochemistry is available to treat chemically complex systems, kinetic inhibitions and inhomogeneous mixing must be somehow accounted for when setting up a process model. For example, in order to account for incomplete conversion, certain portions of reactands must be excluded from a thermochemical equilibrium calculation.

Thus, beyond pure thermodynamic description of a chemical reaction system, thermochemical process modelling also comprises the analysis of transport and temperature conditions in the considered processes and derivation of a certain model structure from that. By means of modelling examples it is shown that agreement between simulation results and measurement data is significantly improved already by accounting for transport conditions and inhomogeneous mixing in a quite simple yet plausible way.