

Comparing Mechanistic and Thermochemical Modelling of Reaction Rate-Controlled Multiphase Systems: Simulation of the Titanium(IV)Chloride Oxidiser

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While Gibbs Free energy minimisation is conventionally used for calculation of global equilibria and for producing stability diagrams, the Constrained Gibbs Free energy (CFE) technique provides a computation method for such chemical and phase changes that are restricted e.g. by chemical reaction kinetics. CFE then allows for the thermochemical modelling of non-equilibrium chemical reactors with competing reactions, including phase transformations. A recent case study that compares the constrained Gibbs energy minimisation technique with a conventional Detailed Kinetic Mechanism calculation will be outlined with examples of CFE uses in thermochemical reactor simulation.