Abstract

This thesis consists of two parts discussing modelling of heterogeneous catalytic reactors.

In the first one, an industrial prototype of a fluidized bed reactor serving as a hydrogen generator based on endothermic decomposition of formic acid is studied. After initial determination of the main reactor characteristics a system of nine constituents is derived and, consequently, reduced to a three phase flow. The solid and bubble particles immersed in a liquid are modelled by the Basset-Boussinesq-Ossen equation. Furthermore, an averaging technique is used to derive a three phase Euler-Euler model. Finally, numerical computations with a verification towards the measurements and a CFD analysis are proceeded.

The second part discusses interfacial transport phenomena between a bulk and catalytic surfaces of a reactor mediated via the boundary conditions. The constitutive relations, that by construction comply with the second law of thermodynamics, follow from the specification of suitable thermodynamic potentials together with an identification of the bulk and surface entropy productions. The derived model is suitable for further analysis providing clear guidelines for the incorporation of the Langmuir-type adsorption model as well as other sorption models.

Keywords: Heterogeneous catalysis, multi-phase flow, Euler-Euler model, fluidized bed reactor, interfacial transport phenomena