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Numerical Modelling and Performance Studies of the original and advanced TEMKIN Reactor in Laboratory Scale Testing of Industrial Egg Shell Catalysts for the Selective Hydrogenation of Acetylene

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Abstract

Strong interactions between reaction kinetics and transport phenomena force the use of specialised reactors for catalysis experiments. Our working group developed an advanced version of the so called TEMKIN reactor by Temkin and Kul'kova (Temkin and Kulkova, 1969), intended for the direct testing of industrial catalysts, e.g. egg shell catalysts used for the selective hydrogenation of acetylene. This work is dealing with modelling of the complex mass and heat transport to investigate and evaluate the influence on the reaction kinetics. Modelling was done using the commercial modelling software COMSOL Multiphysics® and was successfully validated by pulse tagging as well as catalysis experiments. Due to the flexible coupling possibilities in COMSOL, modelling distinguishes between the free gas phase, catalytically active porous shell and inert porous core of the catalyst pellets, ab initio depicting inner as well as outer mass transport limitations. Simulations confirmed good isothermal conditions in both reactor versions, but point out significant transport limitations in the original TEMKIN reactor due to dead zones near the catalyst pellets. Although direct numerical modelling is still challenging due to high computational demands, this work was able to show up its potential in studying laboratory scale reactor designs and catalytic systems.

Keywords

selective acetylene hydrogenation, catalyst testing, temkin reactor, reactor modelling, finite element method

1 Introduction

Many industrial, especially heterogeneously catalysed processes are characterized by a strong interaction between reaction kinetics and transport phenomena. As a result of this, the optimization of such processes requires to account for both of these aspects and therefore plays an important role in the field of catalytic reaction engineering (Berty, 1999). However, laboratory scale experiments using heterogeneous, in particular industrial catalysts can be difficult and cost-intensive.

Simple reactor designs like the plug-flow-reactor (PFR) require relatively large amounts of catalyst and feed-streams to ensure a consistent flow field through the catalyst bed (Berger et al., 2002; Calis and Sie, 2005; Temkin and Kulkova, 1969). Moreover, the thermal conditions are difficult to control so that the occurrence of