



Doctoral Thesis

Effects of mass transfer in liquid phase catalytic consecutive hydrogenation of 2,6-dinitrotoluene

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EFFECTS OF MASS TRANSFER IN LIQUID PHASE
CATALYTIC CONSECUTIVE HYDROGENATION OF
2,6-DINITROTOLUENE

A dissertation submitted to the
SWISS FEDERAL INSTITUTE OF TECHNOLOGY
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Presented by
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ABSTRACT

The effects of mass transfer resistances on the selectivity and reaction rates of a consecutive hydrogenation reaction in a stirred tank slurry reactor under constant temperature and pressure were investigated.

As a model reaction the liquid phase consecutive hydrogenation of 2,6-dinitrotoluene in ethanol, over a 0.5% Pt/Al₂O₃ catalyst was studied. The temperature and pressure ranges were between 40-75°C, and 5-100 bar, respectively.

The intrinsic reaction kinetics were described by a Langmuir-Hinshelwood model with the assumption that hydrogen and organic species were adsorbed on different active sites.

In the mass transfer studies, mass transfer processes, the factors affecting them and their effects on observed reaction behavior were first analyzed theoretically in accordance with the intrinsic reaction model and the parameters obtained.

Then the results of mass transfer experiments, which were performed with varying particle sizes, were investigated. The observed reaction behaviour was described quantitatively with a model, which was first order in organic substrates and zero order in hydrogen, and whose rate was limited by pore diffusion and liquid solid mass transfer resistances. The experimental selectivities agreed well with those predicted theoretically from the model.

The results obtained in this work may suggest the use of selectivity as an experimentally observable check of the presence of global diffusion limitations.

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