CFD Model of HDS Catalyst Tests in Trickle-Bed Reactor

Tukač, V.
2014
Dostupný z http://www.nusl.cz/ntk/nusl-175020

CFD model of HDS catalyst tests in trickle-bed reactor

V. Tukač, A. Prokešová, J. Hanika, [1]M. Zbuzek, [1]D. Kubička_
Institute of Chemical Technology, Prague, Dep. Organic Technology, Technická 5, CZ-16628 Prague, Czech Rebublic, e-mail: vratislav.tukac@vscht.cz, [1] Research and education centre UniCRE Litvínov, Chempark Záluží 1, CZ-43670 Litvínov, Czech Rebublic

Sustainable deep hydrodesulphurization of engine fuels is dominantly carried out in catalytic trickle bed reactors. Also testing of catalysts life cycle needs long time experimentation in pilot scale reactors to evaluate catalyst decay and activity loses. To avoid occurrence of temperature gradients, poor catalyst wetting and fluid maldistribution a dilution of bed of industry scale catalyst particles by fine inert grains is used. In contradiction to full scale reactors this dilution changes interfacial area in the bed and affects namely external mass transfer of hydrogen. Also hydrodynamics, pressure drop, gas and liquid holdups and fluid axial dispersion seems to be quite different.

The goal of this study was to evaluate hydrodynamic influence on experimental HDS catalyst activity measurement carried out in pilot scale trickle-bed reactor. Hydrodynamic data were evaluated by RTD method in laboratory glass model of pilot reactor. Mathematical models of the process were formulated both like 1D pseudohomogeneou and 3D heterogeneous ones. The aim of this work was to forecast interaction between intrinsic reaction kinetic, hydrodynamics and mass transfer.

Catalyst activity tests were carried out in high pressure trickle-bed reactor of 30 mm I.D and 887 mm lenght. Reactor bed consists of three section of different porosity, from the top to the bottom: a) calming section of 2 mm grain inert SiC, b) followed by two section of industrial scale 1.3 mm trilobe alumina extrudes of catalyst diluted by 0.1 mm SiC fines. Middle distillates – atmospheric gas oil (AGO) and light cycle oil (LCO) were chosen for catalyst hydrodesulfurization (HDS) activity tests.

Psudohomogeneous plug flow 1D model in Aspen Plus™ was used to evaluate kinetic parameters of HDS from the pilot tests.

CFD 3D model of hydrodynamics in pilot reactor was made in Comsol Multiphysics FEM solver. The developed model incorporates of Navier-Stokes momentum balance of fluid flow with Brinkman extension for porous reactor bed. Both chemical kinetic, mass transfer of reactants and heat convention and conduction are taking into account.

In the CFD model solution of concentration field and fluid velocity profile of tested trickle bed reaction zone are presented. To evaluate an influence of resulting parabolic velocity profile on sulphur compound concentration is possible. Decreased porosity of diluted catalytic reactor bed exhibit more flat velocity profile, so as more even reactants concentration on bed cross-section. Kinetic equation of hydrodesulfuration of different compounds, e.g. dibenzothiophene, was incorporated into model to simulate real reactor behavior.

Both experimental RTD method and CFD results were used to evaluate catalyst bed parameters. Effect of different inert diluent grain size on performance of pilot scale HDS catalytic reactor was successfully evaluated by CFD model. Time dependent kinetic description of catalyst activity decay in combination with steady state flow velocity was used to compare with experimental measurements.

This publication is a result of the project no. FR-TI3/084 MPO which is being carried out in the UniCRE centre and financial support from Specific University Research (MSMT no. 20/2013) Czech Republic.