CFD Simulation of Pilot HDS Trickle-Bed Reactor

Tukač, V.

2012

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V. Tukač, A. Prokešová, J. Hanika, [1]M. Zbuzek, [1]D. Kubička
Institute of Chemical Technology, Prague, Dep. Organic Technology, Technická 5, 166 28 Prague, CZ; E-mail: *vratislav.tukac@vscht.cz*; [1]VÚAnCh, a.s., Revoluční 84, 400 01 Ústí n. Labem, CZ.

Introduction

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 the bed of industry scale catalyst particles by fine grain inerts 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 is to compare experimental measurement obtained by RTD method with result of computational model. The goal of this work is to evaluate influence of dilution extent on operation of pilot test reactor and to forecast interaction between intrinsic reaction kinetic, hydrodynamics and mass transfer.

Experimental

Hydrodynamic model of pilot test reactor was made from Plexiglas tube of 30 mm I.D. equipped by three conductivity electrodes with joint ground, which was represented by temperature probe located in axis of tube. The reactor bed consists from three section of different porosity. From top to bottom, a 765 mm calming section of 1-2 mm grain inert which was followed by two section (110 and 172 mm) of industrial shaped catalyst diluted by different amount of inert. Catalyst particles in form of trilobe alumina extrudes of 1.3 mm O.D. and 6 mm mean length, silicon carbide of grain diameter 0.1 and 0.2 were used as inert.

Responses to impulse injection of dissolved potassium chloride were measured by three conduct-meters connected with fast multichannel data acquisition system. Air ($7.10^{-4} - 42.10^{-4}$ kg m^{-2} s^{-1}) and water ($0.02 - 0.12$ kg m^{-2} s^{-1}) feed rate was controlled by mass flow meters on the same values of mass superficial velocities as in the case when diesel fuel and hydrogen are applied. Hydrodynamic parameters (residence time, liquid holdup and Peclet number of axial dispersion) were obtained by moment method of response curves.

CFD model

Hydrodynamic CFD model of pilot reactor was formulated 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.

Results and discussion

Solution of CFD model of concentration field and fluid velocity profile of tested trickle bed reaction zone are presented in the Fig. 1. An evaluation of an influence of resulting parabolic velocity profile on sulphur compound concentration is possible. Decreased porosity of diluted catalytic reactor bed exhibits more flat velocity profile than the undiluted one. Also more even reactants concentration profile on bed cross-section was found.

Fig. 1. Axisymmetric CFD model of pilot reactor, color maps sulphur content concentration field and arrows are proportional to fluid velocity.

Left boundary represents axis and right wall of the reactor.

Conclusion

Effect of different inert diluent grain size on performance of pilot scale HDS catalytic reactor was successfully evaluated by CFD model. Both experimental RTD method and CFD results were used to evaluate catalyst bed parameters.

Acknowledgement

Grant no. FR-TI3/084 of Ministry of Industry and Trade, Czech Republic is acknowledged.