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Computers and Chemical Engineering 29 (2005) 1369–1378
Computers & Chemical Engineering
www.elsevier.com/locate/compchemeng

Development of a software for simulation analysis of the phenomenon of phase change of three-phase catalytic slurry reactor

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Available online 18 April 2005

Abstract

The principal aim of this work was the development of a software capable to simulate, via deterministic modelling, the phenomenon of phase change observed in three-phase catalytic slurry reactors, that occurs in the reacting medium and in the refrigerant fluid. Intending to achieve a realistic representation of the system, a detailed dynamic model was formulated. The model was applied to describe the reactor dynamic behaviour during the hydrogenation of *o*-cresol on Ni/SiO_2 catalyst. However, other reactions can easily be incorporated to the software due to the generality adopted during the development of the model. The model allowed to reproduce the main dynamic characteristics of the reactor, in face of several changes in operational parameters of the reactor, and the developed software allows the user to simulate different possibilities introduced in the model, with the aim of a better reproduction of chemical plant data.

Keywords: Slurry reactor; Three-phase reactor; Dynamic modelling; Phase change; Software

1. Introduction

A three-phase slurry catalytic reactor is a system in which a gaseous and a liquid phase are connected with a catalyst in the solid phase; thus, three phases are present. In many applications, the reaction occurs between the dissolved gas and the reagent in the liquid phase, in presence of the solid catalyst. In other cases, the liquid acts as an inert medium, and the reaction is carried out in the surface of the catalyst between the dissolved gases (Ramachandran & Chaudhari, 1983).

Three-phase catalytic reactors are present in numerous industrial processes, such as hydrogenation and oxidation processes. The applications of these reactors are very diversified and they are found in petroleum, petrochemical, chemical, pharmaceutical and food industries. Due to the spread use of the three-phase reactors and the economic advantages resulted from an optimum operation, the modelling of these reactors plays an important role in the continuous improvement of the multiphase technology.

The development of an efficient and reliable model of three-phase catalytic reactors is still a difficult task, because it involves many aspects including hydrogenation, gas–liquid and liquid–solid mass transfers, heat transfer, pore diffusion, reaction kinetics and deactivation (Bergault, Rajashekharam, Chaudhari, Schweich, & Delmas, 1997). Model assessment has mostly been reported for a single reaction, or reactions obeying simplified kinetic laws, under isothermal conditions. Nevertheless, exothermic reactions undergoing a multistep reaction scheme and complex kinetics are industrially of interest and rigorous comparison of the performances of several multiphase reactors, for such reactions, has hardly ever been published (Vasco de Toledo, Santana, Wolf Maciel, & Maciel Filho, 2001). Therefore, despite the large amount of effort put into the modelling of three-phase catalytic reactors, many issues still remain to be solved, for instance, the phenomenon of phase change in both reacting medium and refrigerant fluid, which occurs, frequently, in three-phase reactors. The impact of the phase change in the dynamic behaviour of the reactor can be very intensive, compromising seriously the efficiency

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doi:10.1016/j.compchemeng.2005.02.011

Nomenclature

a	interfacial area (m^{-1})
C_A	concentration of the component A (kmol/m^3)
C_B	concentration of the component B (kmol/m^3)
C_p	heat capacity (kJ/(kg K))
D_e	effective diffusivity (m^2/s)
D_t	reactor intern diameter (m)
D_{te}	reactor extern diameter (m)
D_{ts}	diameter of the jacket tube (m)
E	activity energy (J/mol)
F_A	molar flow of the component A (kmol/s)
F_B	molar flow of the component B (kmol/s)
F_C	molar flow of the component C (kmol/s)
h_e	external convective heat-transfer coefficient (kJ/(m^2 s K))
h_i	internal convective heat-transfer coefficient (kJ/(m^2 s K))
ΔH_R	heat of reaction (kJ/(k mol))
k	kinetic constant (kmol/(kg cat s))
K	mass-transfer coefficients (cm/s)
K_A and K_B	constants of adsorption to components A and B, respectively (m^3/(k mol))
L	reactor length (m)
Q_{flash}	heat of phase change of the reacting medium (kJ/s)
Q_l	liquid feed volumetric flow (m^3/s)
r_p	dimensionless particle radial position
R	universal gas constant (J/(mol K))
R_p	radius particle (m)
R_W	rate of hydrogenation of *o*-cresol (k mol/(kg cat s))
T	temperature (K)
t	time (s)
u	linear velocity (m/s)
U	global heat-transfer coefficient (kJ/(m^2 s K))
w	catalyst concentration ((kg cat)/m^3)
z	dimensionless reactor axial position

Greek letters

λ	thermal conductivity (kJ/(m s K))
ν	stoichiometric coefficient
ρ	density (kg/m^3)
ε_g	gas phase hold-up
ε_l	liquid phase hold-up
ε_s	solid porosity
τ	tortuosity

Subscripts

g	gas phase
fo	feeding
l	liquid phase
i	initial value (reactor inlet)
p	particle
r	refrigerant fluid
s	solid

Superscript

s	catalyst surface

of the controllers in order to maintain a stable reactor operation. The previous knowledge, obtained through simulations, of the operating conditions at which this phenomenon can occur is very important. Thus, the aim of the developed software presented in this work is to allow the user to simulate different aspects involving the phase change in a tubular reactor.

2. Description of the dynamic model used in the software

A dynamic model was formulated aiming to incorporate the main phenomena present in three-phase reactors. The model consists of mass and energy balance equations, and also an equation for the refrigerant fluid. This non-isothermal heterogeneous model includes: the resistances to mass and heat transfers at the gas–liquid and liquid–solid interfaces, as well as for the catalyst particle; the heat exchange with the refrigerant fluid; and the consideration of the variation of physicochemical properties and of the mass and heat-transfer coefficients that are calculated through correlations available in the literature. Also, the model includes a multicomponent flash to evaluate the effect of phase change of the reacting medium, and an appropriate procedure of correction of the heat-transfer global coefficient to incorporate the effect of phase change of the refrigerant fluid. As mentioned before, the formulation was made focusing on hydrogenation reactions that are important reactions of industrial processes. This work considers the hydrogenation of *o*-cresol on Ni/SiO_2 catalyst (Hichri, Armand, & Andrieu, 1991). However, as there are many other hydrogenation reactions of industrial interest, the software can easily incorporate other reactions due to the generality adopted during the development of the model. The scheme utilized to represent the tubular reactor is displayed in Fig. 1.

The hypotheses adopted during the development of the dynamic model of the tubular reactor are (Vasco de Toledo et al., 2001):

1. A pseudo-homogeneous media is assumed for the liquid and the solid with respect to solid movement. This means that there is no velocity difference between solid and liquid.
2. Negligible pressure variations.