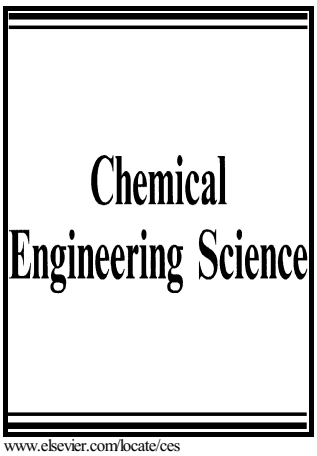
Modelling of a Simulated Moving Bed in case of non-ideal hydrodynamics

L. Fangueiro Gomes, F. Augier, D. Leinekugel-le-Cocq, I. Vinkovic, S. Simoëns



www.elsevier.com/locate/ces

PII: S0009-2509(16)30401-8
DOI: http://dx.doi.org/10.1016/j.ces.2016.07.027
Reference: CES13076

To appear in: *Chemical Engineering Science*

Received date: 1 February 2016
Revised date: 19 July 2016
Accepted date: 21 July 2016

Cite this article as: L. Fangueiro Gomes, F. Augier, D. Leinekugel-le-Cocq, I Vinkovic and S. Simoëns, Modelling of a Simulated Moving Bed in case of non ideal hydrodynamics, *Chemical Engineering Science* http://dx.doi.org/10.1016/j.ces.2016.07.027

Modelling of a Simulated Moving Bed in case of non-ideal hydrodynamics

L. Fangueiro Gomes[1,2], F. Augier[1*], D. Leinekugel-le-Cocq[1], I. Vinkovic[2], S. Simoëns[2]
[1]IFP Energies nouvelles, Rond-point de l'échangeur de Solaize, BP3, 69360 Solaize, France
[2]LMFA, UMR CNRS 5509, Ecole Centrale de Lyon, Université de Lyon 1, INSA Lyon, 69131, Ecully Cedex, France
[*]Corresponding author. frederic.augier@ifpen.fr

Abstract

The one-dimensional hydrodynamic model proposed by Gomes et al. (2015) is coupled with adsorption and validated by comparing the concentration profiles of the one-dimensional model with those given by the CFD model of one adsorption column including obstacles as distribution network and beams. This one-dimensional model is capable of predicting the CFD results for different mass transfer rates, while the traditional dispersed plug flow (DPF) model is relevant for slow mass transfer rates only. The model proposed by Gomes et al. (2015) is capable of reproducing the adsorber Residence Time Distribution (RTD) while dissociating the selective zones from the non-selective ones. It is based on the CFD techniques developed by Liu and Tilton (2010) and Liu (2012) that transport the moments of the fluid age distribution and consequently calculate the degree of mixing (Danckwerts, 1958 and Zwietering, 1959). Then, this new model is integrated in a cyclic solver in order to perform Simulated Moving Bed (SMB) studies. The new model provides a detailed hydrodynamic description, which appears to be mandatory especially when mass transfer exchanges are fast, without undergoing the prohibitive simulation times of CFD models.

Keywords: Adsorption, CFD, Simulated Moving Bed, 1D modelling

NOTATIONS

b_i	adsorbent coefficient of affinity for the component i (m^{-3} kg^{-1})
C_i	concentration of the component i in the bulk phase (kg m^{-3})
$C_{m,i}$	concentration of the component i in the macro-porous liquid phase (kg m^{-3})
D_M	molecular diffusion coefficient (m^2 s^{-1})
D_P	mechanical dispersion coefficient (m^2 s^{-1})
d_p	particle diameter (m)
D_T	turbulent diffusivity coefficient (m^2 s^{-1})
J	degree of mixing (dimensionless)
K	bed permeability (m^2)
k_1	fluid film mass transfer coefficient (s^{-1})
k_2	internal mass transfer coefficient (s^{-1})
m_n	raw moment of order n (s^n)
N	number of equivalent CSTR (dimensionless)
N_i^{ε}	mass flux between the bulk phase and the macro-porous phase (mol m^3 s^{-1})