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Advanced prediction of pulsed (packed and sieve plate) extraction columns performance using population balance modelling

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ABSTRACT

A bivariate population balance model (the base of LLECMOD program) for the steady state simulation of liquid extraction columns is extended to simulate pulsed (packed and sieve plate) extraction columns. The model is programmed using visual digital FORTRAN and then integrated into the *LLECMOD* program. As a case study, *LLECMOD* is used to simulate the separation performance of a pulsed extraction column. Two chemical test systems recommended by the EFCE (namely toluene–acetone–water and *n*-butyl acetate–acetone–water) are used in the simulation. Model predictions are successfully validated against steady state experimental data, where good agreements are achieved. The simulated results (holdup, mean droplet diameter and mass transfer profiles) compared to the experimental data show that LLECMOD is a powerful simulation tool, which can efficiently predict the performance of pulsed extraction columns.

Keywords: Pulsed extraction columns; Population balance modelling; Simulation; Hydrodynamics; Mass transfer; LLECMOD

1. Introduction

Liquid–liquid extraction is an important separation processes encountered in many chemical process industries (Lo et al., 1983). Different types of liquid–liquid columns are in use nowadays, which can be classified into two main categories: stirred (RDC and Kühni) and pulsed (packed and sieve plate) columns. The latter are frequently used in liquid–liquid extraction operations due to their high throughput, high separation efficiency and insensitivity towards contamination of the interface. These columns have found wide applications in nuclear fuel reprocessing and chemical industry. They have a clear advantage over other mechanical contactors when processing corrosive or radioactive solutions. The absence of moving mechanical parts in such columns obviates the need for frequent repair and servicing. The internals (packing, sieve plates) reduces axial mixing; increases drop coalescence and breakage rates resulting in increased mass transfer rates, and affect the mean residence time of the dispersed phase. The performance of these columns is markedly dependent on the mechanical pulsation of the continuous phase. This is a result of an increase in shear forces and consequent reduction in size of dispersed droplets so that the interfacial area, and hence the mass transfer rate is increased (Pratt and Stevens, 1992).

To shed more light on the extraction behaviour in pulsed (packed and sieve plate) columns, the hydrodynamics and mass transfer characteristics must be well understood. Our present knowledge of the design and performance of extraction columns is still far from satisfactory. The reason is mainly due to the complex interactions of the hydrodynamics and mass transfer (Luo et al., 1998). It is obvious that the changes of the drop population characteristics (holdup, Sauter diameter, etc.) along the column have to be considered in order to describe conveniently the behaviour of the column. The dispersed phase in the case of liquid–liquid extraction undergoes changes and loses its identity continuously as the drops break and coalesce. Accordingly, detailed modelling on a discrete level is needed using the population balance

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Nomenclature

a	pulsation amplitude, m
A_c	column cross sectional area, m^2
af	pulsation intensity, $m\,s^{-1}$
a_{15}, a_{16}	adjustable parameters
a_{PK}	volumetric surface area of a packing, $m^2\,m^{-3}$
C_i	constant parameter
C_{IP}	interface instability parameter
c_x, c_y	solute concentration (continuous and dispersed phase), $kg\,m^{-3}$
$c_{x,in}$, $c_{y,in}$	inlet solute concentration (continuous and dispersed phase), $kg\,m^{-3}$
ρ_x, ρ_y	axial dispersion coefficient (continuous and dispersed phase), $m^2\,s^{-1}$
d_{col}	column diameters, m
d, d', d_m	droplet diameter, m
d_{100}	characteristic drop diameter due to a breakage probability of 100%, m
d_{stab}	stable droplet diameter, m
f	pulsation frequency, s^{-1}
$f_{d,c_y}\partial d\partial c_y$	number of droplets having concentration c_y and diameter d in the range $[d, d+\partial d]\times[c_y, c_y+\partial c_y]$
H	column and single compartment heights, m
H_{cd}	Hamaker coefficient, Nm
k_v	slowing factor
K_{oy}	overall mass transfer coefficient, $m\,s^{-1}$
N_z	number of daughter drops
$\bar{N}_z$	average number of daughter drops
P_r, P_B	breakage probability
P_C	coalescence probability
Q_{bot}	total flow rate at bottom of the column, $m^3\,s^{-1}$
$Q_{x,in}$, $Q_{y,in}$	inlet flow rate (continuous and dispersed phase), $m^3\,s^{-1}$
Q_{top}	dispersed phase flow rate at top of the column, $m^3\,s^{-1}$
t	time, s
$\bar{u}_x$, $\bar{u}_y$	relative velocity (continuous and dispersed phase), $m\,s^{-1}$
$\bar{u}_r$	relative droplet (slip) velocity, $m\,s^{-1}$
$\bar{u}_t$	terminal droplet velocity, $m\,s^{-1}$
z	spatial coordinate, m
z_d, z_y	dispersed feed inlet, m
z_c, z_x	continuous phase inlet, m

Greek symbols

β_n	daughter droplet distribution based on droplet number, m^{-1}
Γ	droplet breakage frequency, s^{-1}
Δt	time interval
ε	energy dissipation, $m^2\,s^{-3}$
ζ	time and space vector
λ	coalescence efficiency
μ_x, μ_y	viscosity (continuous and dispersed phase), $kg\,m^{-1}\,s^{-1}$
ρ_x, ρ_y	density (continuous and dispersed phase), $kg\,m^{-3}$
σ	interfacial tension, $N\,m^{-1}$
ξ_i	parameter
ϕ_x, ϕ_y	hold up (continuous and dispersed phase)
ϕ_p	packing void fraction, $m^3\,m^{-3}$
$\vartheta(d')$	mean number of daughter droplets from mother droplet of diameter d'
Υ	source term
φ_{st}	relative free cross-sectional area of a sieve tray plate, $m^2\,m^{-2}$
ω	coalescence frequency, $m^3\,s^{-1}$

Dimensionless numbers

π_{af}	pulsation intensity
π_{ap}	volumetric surface area of a packing
π_d	drop diameter
π_{hp}	height of a packing
π_σ	interfacial tension

equation as a mathematical framework. The multivariate non-equilibrium population balance models have emerged as an effective tool for the study of the complex coupled hydrodynamics and mass transfer in liquid–liquid extraction columns.

The simulation of modern industrial chemical processes is becoming extremely important as an economical tool in the integration of steady state and dynamic design as well as the simulation of the existing plants. The development of computational tools to model industrial processes has increased in the last decades. However; to the best of the authors' knowledge, there are no comprehensive non-equilibrium population balance models to describe in sufficient detail the behaviour of pulsed extraction columns. One of the recent approaches in modelling liquid–liquid extraction columns is by adequately describing the complex behaviour of the dispersed phase using the population balances equation (PBE). However, the numerical solution of the resulting system of PBEs is still not efficiently developed, particularly when coupled hydrodynamics and mass transfer take place simultaneously.

The main objective of this work is to develop a model that is capable of describing the dynamic and steady state behaviour of pulsed (packed and sieve plate) extraction columns. The models of both columns are integrated into the existing program: *LLECMOD* (Attarakih et al., 2008), which can also simulate stirred extraction columns (RDC and Kühni). *LLECMOD* can simulate the steady state and dynamic behaviour of extraction columns taking into account the effect of dispersed phase inlet (light or heavy phase is dispersed) and the direction of mass transfer (from continuous to dispersed phase and vice versa). So, scale-up and simulation of agitated and pulsed extraction columns based on population balance modelling can now be carried out successfully (Attarakih et al., 2008; Jaradat et al., 2010).

2. Mathematical modelling

The modelling of extraction columns still demands improvement. Simulating liquid–liquid extraction columns is a challenging task due to the discrete character of the dispersed phase. This results from random breakage and coalescence of droplets, which are highly coupled to the mass transport of solutes between the two existing phases. Modelling of such extremely important and complex transport phenomena is resolved by using a multivariate population balance