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Steady state modeling of perforated plate extraction columns

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Abstract

A linear steady state model is developed for perforated plate liquid–liquid extractors conducting a slow pseudo first order reaction in the extract phase. The model assumes complete mixing of the continuous phase on each individual stage and plug flow of the uniformly sized dispersed phase droplets. An analytical relationship is developed to relate the achievable purification within a given number of actual plates in terms of three dimensionless parameters which are the extraction factor, a mass transfer rate factor, and a reaction rate enhancement factor. The developed model enabled the expression of the effect of the mass transfer and extraction factors on the overall cascade efficiency in the case of physical extraction and to demonstrate the qualitative and quantitative implications of the enhancing chemical reaction. It is also applicable in the analysis of the steady state control of the extract and raffinate product compositions in an existing column. In this case, the operating range constraints arising from the non-linear hydrodynamics relating the above three dimensionless parameters to the phase flow rates have to be considered. © 2006 Elsevier B.V. All rights reserved.

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1. Introduction

Modeling of heterogeneous fluid reactors involves the consideration of the fluid mixing patterns in formulating the conservation equations for each phase along with their appropriate boundary conditions, and the simultaneous application of physical equilibrium relations, inter-phase mass transfer rate expressions, and kinetic equations reflecting the mechanism and stoichiometry of the reaction. In continuous contact equipment, such as packed and spray columns, the contacting efficiency depends on the hydrodynamics and mixing characteristics within the phases. Plug flow and axial dispersion models have been used to study the steady-state [1], dynamic behaviour [2] and control [3] of continuous counter-current extractive reactors of various kinetics ranging between infinitely fast, pseudo first order, and second order reactions. Slow first order reactions conducted in mixer-settlers have been also studied assuming perfect mixing for the mixer, while various extents of mixing have been allowed with respect to both phases in the settler [4].

In equipment featuring complicated flow patterns such as pulsed and agitated extractors, cell models with inter-stage backflow have been proposed in order to consider the effect of the dispersed phase droplets size distribution, coalescence, and redispersion on the mass transfer efficiency. Models involving forward mixing led by drop size distribution and axial mixing of the continuous phase have been also suggested [5]. Recent models of extractive stirred column reactors are based on the droplet population balance model [6]. The bivariate droplet population balance model [7] uses computational fluid dynamics for describing the complex flows associated with droplet interactions such as breakage and coalescence, and axial transport [8,9] as well as the effects of inter phase mass transfer on viscosity, density, and interfacial tension [10]. A new approach to the application of population balance models relies on relatively straight forward single droplet experiments for incorporating the hydrodynamic characteristics into the model [11].

Un-agitated perforated plate extraction columns are of simple construction and suitable for conducting extractive reactions. These columns are appropriate for systems which are characterized by low interfacial tension and thus do not require mechanical agitation for good dispersion. They are effective both with respect to liquid handling capacity and extraction efficiency. This is because mixing within the continuous phase is confined to the holdup between individual trays, it does not spread through-

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out the tower from stage to stage, and because the tendency to establish concentration gradients within the droplets is avoided as the dispersed phase droplets coalesce and are reformed at each tray. Unlike pulsed and agitated column contactors, the hydrodynamic characteristics of perforated columns are relatively simple and fairly predictable by a number of existing correlations. This makes them amenable to a straightforward modeling approach.

The purpose of the present paper is to develop a steady state analysis of perforated plate extractive reactors modeled as a hybrid between staged and continuous contact equipment. The continuous phase on each plate is assumed to be well mixed and traversed by the dispersed phase droplets assumed in plug flow. Although pilot testing maybe required for finalizing design details of extraction equipment, a simple model would be useful in preliminary process analysis because the effects of the basic design and operating conditions are not overshadowed by system complexity. The developed model enables the expression of the column behaviour in terms of meaningful dimensionless parameters. It is applicable in the evaluation of alternative design configurations as well as in the analysis of the steady state response of existing perforated plate extractors subject to feed flow and/or composition disturbances.

2. The model system

A counter current un-agitated perforated plate extractive reactor is considered. The solute is transferred to the dispersed solvent phase where it undergoes a slow pseudo first order reaction with either the solvent itself or another dissolved reactant present in excess.

2.1. Assumptions

The following assumptions have been applied in the subsequent derivation:

1. The reacting solute is the only species transferred between the two immiscible phases. The transfer is according to a linear equilibrium relation:

$$y_n^* = m x_n \tag{1}$$

- 2. The reaction is confined to the solvent phase while heat and volume effects associated with the solute transfer and chemical reaction are negligible so that the interfacial tension, densities, and viscosities of the phases remain constant. Thus for given fixed values of the phase flow rates, the fractional holdup and overall solute mass transfer coefficient are the same for all plates.
- 3. Continuous phase liquid on a plate is perfectly mixed while the dispersed phase is in plug flow over the distance (h)between the plate and the coalesced layer of thickness (h_c) beneath the plate above.
- 4. The dispersed phase drops behave as spheres of uniform diameter, and no mass transfer takes place between the continuous phase and the coalesced solvent layer.

2.2. Model equations

Referring to Fig. 1, the solute undergoes a slow extractive reaction with the excess dispersed phase reactant which is insoluble in the continuous phase. The concentration (u) of this reactant remains therefore approximately constant throughout the column. Thus the reaction rate will be proportional to the concentration of the solute in the dispersed phase (y). Considering a plate (n) with effective contact height (h), a steady state material balance on the solute in an increment of height (dz) gives:

$$Vy + Ka'(y^* - y)A_a\phi_D \,dz = V(y + dy) + kyA_a\phi_D \,dz$$
(2)

Substituting from Eq. (1) and integrating between z=0 and z=h gives,

$$\int_{n-1}^{n} \frac{dy}{Ka'mx_n - (Ka' + k)y} = \int_{0}^{h} \frac{A_a \phi_D \, dz}{V}$$
(3)

Which integrates to:

$$x_n = \frac{(1+\gamma)y_n - (1+\gamma)y_{n-1}e^{-\beta(1+\gamma)}}{m(1-e^{-\beta(1+\gamma)})}$$
(4)

where:

$$\beta = \frac{Ka'A_{a}\phi_{D}h}{V}$$
 and $\gamma = \frac{k}{Ka'}$



Fig. 1. Concentrations of excess dispersed phase reactant (u) and solute (x and y) across the interface at plate (n).

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