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LLECMOD: A Windows-based program for hydrodynamics simulation of liquid–liquid extraction columns

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Abstract

The simulation of liquid–liquid extraction columns based on a droplet population balance approach provides a useful means for getting more insight into the transient and the steady state behavior of such an extremely important unit operation. This numerical simulation is carried out based on a recently developed algorithm for solving the population balance equation. The algorithm is implemented via a computer program called liquid–liquid extraction column module (LLECMOD). The LLECMOD is designed in a flexible way that allows the user to define the breakage and coalescence frequencies, droplet terminal velocity, and the other internal geometrical details of the column. The user input dialog makes the LLECMOD a user-friendly program that enables the user to select the simulation parameters and functions in an easy way. The program is reinforced by a parameter estimation package for the droplet coalescence models. In this work, a sample of small laboratory and pilot plant simulations as compared to the experimental data is presented as carried out by the LLECMOD.

Keywords: LLECMOD; RDC column; Population balances; Hydrodynamics

1. Introduction

The simulation of chemical engineering processes is now widely used to shed some light on the dynamic or steady state performance as well as equipment scale up of many types of unit operation equipment. This is because in most cases the actual running of the equipment is very expensive or sometimes prohibitive due to safety reasons even at the laboratory scale. An important unit operation in chemical engineering is liquid–liquid extraction that finds many significant applications in mining, petroleum, food and pharmaceutical industries [1]. The hydrodynamics as well as the mass transfer in such unit operations is fundamentally influenced by the behavior of the dispersed phase consisting of populations of distributed rather than lumped characteristics in droplet phase space. Consequently, the natural framework of modelling of such dispersed phase processes is based on the population balance [2–4]. Although such modelling framework is rich in the information it furnishes, it is still expensive from a computational point of view since the full population balance models are normally integral partial differential equations (IPDE) of stretched type [5]. These IPDEs have only a limited number of analytical solutions [6,7] that are in most cases strongly simplified and hence are physically unrealistic. Consequently, for realistic liquid–liquid extraction column (LLEC) simulation based on population balance modelling, it is inevitable to seek numerical solutions. In such cases the need for numerical solutions imposes two levels of difficulties due to the convective, droplet breakage and coalescence events occurring simultaneously. The convective process in dispersed phase systems is actually dominant when compared to the axial dispersion and hence sharp front profiles describing the number or volume concentration distributions are expected to develop along the spatial coordinate

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in the direction of flow. At the same time the evolution of these distributions is governed by the breakage and coalescence mechanisms involving linear integral expressions for breakage and non-linear ones for droplet coalescence. These issues are fully discussed by Attarakih et al. [6] where an efficient numerical algorithm based on the generalized fixed-pivot technique and the central differencing schemes of Kurganov and Tadmor [8] is presented and extensively tested. For user-friendly implementation of such a numerical algorithm we introduce in this work the basics of a Windows-based computer program called liquid–liquid extraction column module (LLECMOD). The basic feature of this program is to provide the simulation of the hydrodynamics of LLECs based on the population balance approach for both transient and steady state through an interactive Windows input dialogue as well as a parameter estimation package for droplet coalescence models based on small scale laboratory devices. The LLECMOD is not restricted to a certain type of liquid–liquid extraction column since it is built in the most general form that allows the user to input the various droplet interaction functions. These functions include droplet terminal velocity taking into account the swarm effect, slowing factor due to column geometry, the breakage frequency and daughter droplet distribution, the coalescence frequency and the axial dispersion coefficients. A sample problem on basis of the performance of a RDC column is given. However, other column types can easily be treated, e.g. Kühni columns, when using adapted correlations [9].

2. The mathematical model

The population balance equation (PBE) based on the number concentration distribution along the column can be formulated as follows [4]:

$$\frac{\partial n}{\partial t} + \frac{\partial F}{\partial z} = \frac{\partial}{\partial z}\left(D_\mathrm{d}\frac{\partial n}{\partial z}\right) + \frac{Q_\mathrm{d}}{A_\mathrm{c}}\left(\frac{n^\mathrm{feed}}{v_\mathrm{f}}\right)\delta(z - z_\mathrm{d}) + \rho\{n, v\} \quad (1)$$

where $n(v; z, t)\delta v = N(t, z)f(v)\delta v$ is the average number concentration associated with droplets having a volume between $v \pm \delta v$ at the time instant t and column height z, $N(t, z)$ is the total number concentration and $f(v)$ is the droplets number density. The convective flux of these droplets along the column of a constant cross-sectional area, A_c, is represented by $A_\mathbf{c}F\delta v = A_\mathrm{c}U_\mathrm{d}n\delta v$, where U_d is the velocity of the dispersed phase relative to the column walls. The first term on the right-hand side of Eq. (1) represents the axial dispersion of the dispersed phase due to the non-ideal flow in which a random movement of the fluid on the microscopic level is superimposed on the main flow [10]. This is assumed to follow Fick's law with a dispersion coefficient, D_d, and is distinguished from the forward mixing effect due to the droplet velocity distribution that is taken into account by the convective term [11]. The second term on the right-hand side represents a number concentration rate of droplets entering as a feed of volumetric flow rate, Q_d, at the level z_d of the column. The positive direction of flow coincides with the dispersed phase flow from z_d to the top of the column. Note that the feed distribution is represented mathematically by a point source through the use of the Dirac delta function [12]. The last term on the right-hand side of Eq. (1) represents the net rate of the number of droplets generated by breakage and coalescence events per unit volume and is reported in detail by Attarakih et al. [6].

The boundary conditions are greatly simplified since the dispersed and the continuous phases are included in the mathematical model given by Eq. (1) as point sources. Accordingly, the Danckwert's boundary conditions based on the discussion of Wilburn [13] could be written by considering the LLEC to behave like a closed vessel between 0^+ and column height H:

$$0 = \max(F, 0) - D_\mathrm{d}\frac{\partial n}{\partial z} \quad \text{at } z = 0 \quad (2)$$

$$0 = -\min(F, 0) + D_\mathrm{d}\frac{\partial n}{\partial z} \quad \text{at } z = H \quad (3)$$

$$n(v; z, t) = n_0(v; z) \quad \forall z \in [0, H] \quad (4)$$

The first step in the numerical solution of these equations is to project the infinite system (with respect to droplet volume or diameter) of IPDEs given by Eq. (1) onto a finite system of partial differential equations (PDE) using the generalized fixed pivot technique. The idea in this technique is to divide the internal droplet coordinate (volume) into contiguous finite subdomains covering the range of this internal coordinate. In each subdomain, the total volume concentration is obtained by integrating the volume concentration distribution with respect to volume (diameter) over the boundaries of this subdomain. This local volume concentration is then concentrated at a single point in this subdomain called the fixed-pivot, x_i, and is given by

$$\varphi_i(z, t) = \int_{v_{i-1/2}}^{v_{i+1/2}} v(v)n(v; z, t)\,\mathrm{d}v = v(x_i)N_i(z, t), \quad i = 1, 2, \ldots, M_x \quad (5)$$

This replaces the IPDE given by Eq. (1) by M_x finite number of PDEs that are non-linearly coupled through the convective and the source terms. These PDEs are then discretized based on upwind and central differencing schemes resulting in the following semi-discrete formulation:

$$\frac{\mathrm{d}\varphi_{i,l}}{\mathrm{d}t} + \frac{F_{i,l+1/2} - F_{i,l-1/2}}{\Delta z_l} = \frac{D_\mathrm{d}\partial\varphi_i/\partial z|_{l+1/2} - D_\mathrm{d}\partial\varphi_i/\partial z|_{l-1/2}}{\Delta z_l} + \frac{Q_\mathrm{d}}{A_\mathrm{c}}\frac{\varphi_i^\mathrm{feed}}{v_\mathrm{f}}\frac{\delta_{l,l_\mathrm{d}}}{\Delta z_l} + \rho(\boldsymbol{\varphi}_l, \boldsymbol{d}), \quad i = 1, 2, \ldots, M_x, \quad l = 1, 2, \ldots, L \quad (6)$$