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Fluid Separation Modelling in the Columns Equipped with Structured Packings using the Hydrodynamic Analogy

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Abstract

A new modelling approach to the description of mass and heat transfer in columns equipped with structured packings is developed based on rigorous equations of continuum mechanics. This approach rests on the analogy between the flow patterns in real structured packings and film flow. The physical model is based on a simplified geometrical representation of the packing. It consists of a bundle of channels with identical cross section. The channel inner surface is wetted by a liquid, whereas the rest of the volume is occupied by a counter-current vapour flow. Both phases are assumed to be laminar and ideally mixed at regular intervals. The mathematical model comprises a set of partial differential equations describing hydrodynamics, heat and mass transfer phenomena. A numerical solution of the whole problem yields velocity profiles as well as concentration and temperature fields throughout the column. The model is verified using experimental data for a binary and a ternary distillation, in a column equipped with Montz-Pak A3-500.

Keywords: Hydrodynamic Analogy, Structured Packing, Laminar Flow

1. Introduction

The general tendency of chemical engineering is to reach increased efficiency and capacity of separation units at possibly minimal size. This has brought about a novel generation of column internals, providing enhanced mass transfer performance and relatively low pressure drop. Among these internals, corrugated packings of the regular type, also referred as structured packings, have gained a wide acceptance (Spiegel & Meier, 2003). However, these packings are quite expensive, and hence, an accurate design of process units is very important for minimisation of investment costs. Such a design cannot be realised without sound and predictive process models.

The modelling accuracy strongly depends on the appropriate description of phase interactions. For the separation processes taking place in geometrically simple flows like films, jets, drops, etc., physical boundaries of the contacting phases can be spatially localised. In this case, the partial differential equations of convective mass and heat transfer offer the most rigorous way to describe the transport phenomena. However, even for the regular geometry provided by corrugated sheet structured packings, the

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exact localisation of phase interfaces represents a difficult problem. Therefore, most often, the modelling of separation processes is accomplished with the traditional stage concept (Taylor & Krishna, 1993), either using the equilibrium-based or rate-based description.

2. State of the Art

2.1 Equilibrium Stage Models

The equilibrium stage models (Sorel, 1893) assume that the streams leaving a stage reach thermodynamic equilibrium. Such an idealisation is usually far from real process conditions, and therefore, process equipment is designed using "the height equivalent to a theoretical plate" (HETP), a gross parameter including the influence of packing type, size and material. The same HETP is assumed for all components in a multicomponent mixture, this value being constant through the packing height. The latter is in contradiction with the experimental evidence and may lead to a severe underdesign (Taylor & Krishna, 1993). Moreover, the equilibrium models are not able to consider explicitly the packing geometry characteristics, which play a key role in mass and heat transfer. Therefore, for kinetically controlled processes, it is very difficult to use these models without significant loss of accuracy.

2.2 Rate-based Stage Models

The so-called rate-based approach presents a different way to the modelling of separation processes, by directly considering actual mass and heat transfer rates (Seader, 1989). In the framework of this approach, the film model (Lewis & Whitman, 1924) is most frequently used due to numerous correlation data available in the literature.

Though widely used, the film theory reveals some problems, when applied to complex processes. A critical analysis shows, that the difficulties are mainly connected with the estimation of the film thickness. First, this model parameter is determined via the mass transfer correlations and therefore directly depends on the diffusion coefficients. This leads to a contradiction, as the film thickness for a multicomponent mixture in not unique. Another difficulty is related to convection, as, by definition, the films are stagnant and hence no mass transport mechanism, except for molecular diffusion in the direction normal to the interface, is possible (Taylor & Krishna, 1993). The film theory, once developed for equimolar binary mass transfer in non-reactive systems (Lewis & Whitman, 1924), was free from contradictions. Nowadays, it is widely applied for much more complicated processes and therefore additional assumptions have to be made. These assumptions are in conflict with physical backgrounds and make the application of the film model problematic (Kenig, 1997).

3. Hydrodynamic Analogy for Structured Packings

An opportunity to employ the rigorous equations of continuum mechanics even for the cases, in which real phase boundaries cannot be exactly localised, is associated with the idea of hydrodynamic analogy between complex and simpler flow phenomena. More precisely, some particular similarities are meant between complex flow patterns encountered in industrial separations and geometrically simple flows like films, jets, drops, etc., as well as their combinations (Kenig, 1997). Hydrodynamic analogies provide a means to process modelling, combining the rigour of exact continuum mechanics equations and rather simple geometric description. In the present work, this general approach is applied to the modelling of separation processes in columns equipped with corrugated sheet structured packings.

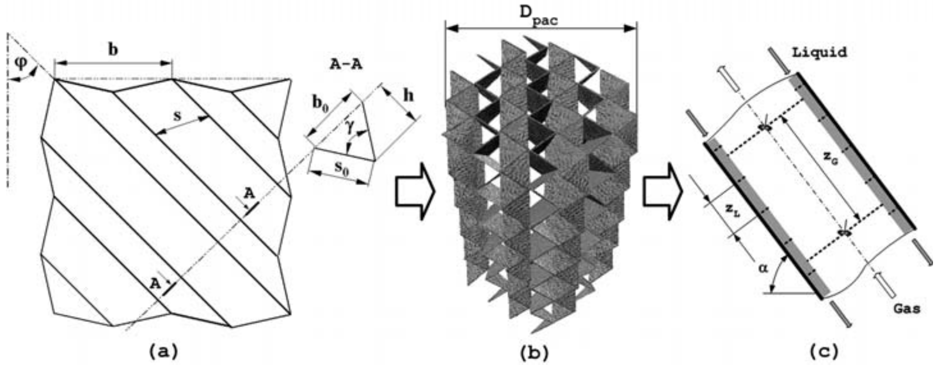

Figure 1. Dimensions of a typical corrugated sheet (a); packing segment (b); physical model (c)

The corrugated sheets are installed counter course in such a way that they form channels, each being formed by the two wall sides s_0 and one open side b_0, which is shared between two neighbouring channels (see Fig. 1, (a)). According to experimental studies (Zogg, 1972), the gas flow interactions in these channels under normal operating conditions are negligible. Hence, the packing segment can be visualised as a channel bundle with identical cross sections and lengths dictated by the channel proximity to the column wall. On the other hand, it has been found experimentally (Stoter, 1992) that liquid generally tends to move in form of laminar, well developed films at the minimal angle with the column axis α.

Using the experimental observations described above, we assume that gas-liquid interactions in a structured packing can be mirrored by a flow through the bundle of inclined cylindrical channels with dimensions derived from the corrugation geometry. The channels inner surface is wetted by a liquid flowing downwards, whereas the rest of the volume is occupied by a counter-current vapour flow. We also assume, that for all channels, the film thickness is the same. Both flows are presumed to be laminar and ideally mixed at regular intervals. The periodical ideal mixing approximation is necessary to account for turbulence caused by the abrupt change in the flow direction. The length of the laminar flow interval for the liquid phase corresponds to the distance between the two neighbouring corrugation ridges, whereas for the gas phase, it is set to be equal to an average channel length. The interval length for each phase represents a model parameter and is estimated from the packing geometry (Shilkin & Kenig, 2004).

4. Governing Equations

4.1 Hydrodynamics

The model hydrodynamics depicted in Figure 2 is described by the system of Navier-Stokes equations in the film flow approximation (Levich, 1962)

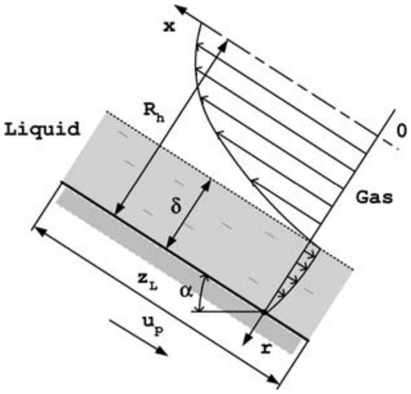

Figure 2. Two-phase laminar counter-current flow in a channel

$$\begin{cases} \mu \cdot \left(\dfrac{\partial^2 u}{\partial r^2} + \dfrac{1}{r} \cdot \dfrac{\partial u}{\partial r} \right) - \dfrac{\partial P}{\partial x} + \rho \cdot g \cdot \sin \alpha = 0 \\ \dfrac{\partial P}{\partial r} = 0 \end{cases} \tag{1}$$

The system Eqs. (1) is written for each phase separately and supplemented by the conjugate boundary conditions (velocity and shear stress continuity) at the interface. The numerical solution of the hydrodynamic equations yields the liquid film thickness δ as well as velocity profiles in each phase. They are used for the description of mass and heat transfer.

4.2 Simultaneous mass and heat transfer

Mass and heat transfer in each phase is described by the following convective diffusion and convective heat conduction equations

$$\begin{aligned} u(r)\frac{\partial C_i}{\partial x} &= D_i \left(\frac{\partial^2 C_i}{\partial r^2} + \frac{1}{r}\frac{\partial C_i}{\partial r} \right) \\ u(r)\frac{\partial T}{\partial x} &= \kappa \left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} \right) \end{aligned} \tag{2}$$

Similar to the hydrodynamic part of the problem, these equations are supplemented by the conjugate boundary conditions at the phase interface (thermodynamic equilibrium, heat and mass flux continuity). The Eqs. (2) are solved numerically using the TriDiagonal-Matrix Algorithm (Patankar, 1980). The solution gives temperature and concentration fields throughout the channel.

4.3 Model Parameters

The main model parameters (see Figure 2) are calculated as follows:

- the total number of the channels is a function of wetted packing surface a_w and packing diameter D_{pac}

$$n_k = \frac{a_w \cdot \sin\alpha \cdot D_{pac}^2}{4 \cdot d_h} \tag{3}$$

- the minimal angle with the column axis α (Zogg, 1972)

$$\alpha = \arctan\left(\frac{\cot\varphi}{\sin(\arctan(\cos\varphi \cot(\gamma/2)))} \right) \tag{4}$$

- the channel diameter d_h is assumed to be equal to the hydraulic diameter of the corresponding triangular channels (see Figure 1)

$$d_h = \frac{b_0 \cdot h}{s_0} \tag{5}$$

5. Model Verification

The proposed modelling approach has been verified using the total reflux distillation data for the binary mixture chlorobenzene/ethylbenzene (CB/EB) and ternary mixture methanol/acetonitrile/water (MEOH/ACN/WATER), obtained at the University of Dortmund (Pelkonen, 1997). The experiments were carried out in a column of 100 mm diameter, equipped with Montz-Pak A3-500 structured packing. The measured concentrations, temperature and flow rates at the condenser outlet were used as input parameters.

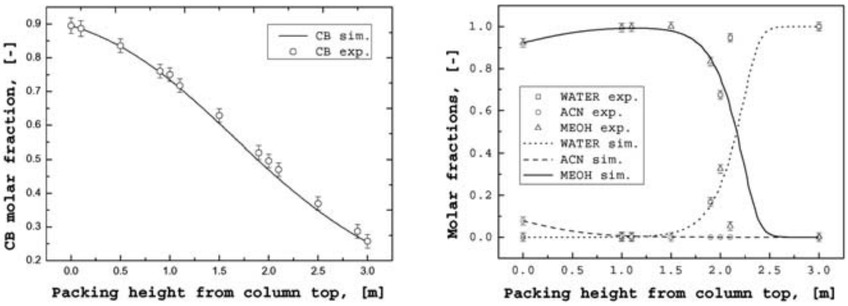

Figure 3. Comparison of simulated and experimentally obtained concentration profiles

The averaged concentration profiles were obtained based on the calculated local concentration fields. Figure 3 shows a good agreement between the simulated and experimentally measured concentration profiles.

6. Conclusions

A new approach to rigorous modelling of separation processes has been applied to modelling of columns equipped with corrugated sheet structured packings. This approach is based on the hydrodynamic analogy between real complex hydrodynamics dominating most industrial separations and geometrically simpler flow patterns.

The physical model gives a simplified geometric representation of the packing. It consists of a bundle of channels with identical triangular cross section. The inner surface of these channels is wetted by a liquid flowing downwards, whereas the rest of the volume is occupied by a counter-current vapour flow. Both flows are presumed to be laminar and fully developed within intervals of a certain length, being totally mixed between them. The interval lengths for each phase represent the packing specific model parameters and are derived from the packing geometry. This simplified hydrodynamic picture allows an exact localisation of the phase boundaries, which permits a direct application of continuum mechanics equations.

The mathematical model comprises a set of partial differential equations of convective diffusion and heat conduction as well as the Navier-Stokes equations written for each phase separately. These equations are supplemented by the conjugate boundary conditions at the phase interface. The solution yields local concentration and temperature fields, which are used for calculation of the concentration and temperature profiles along the column.

The proposed model has been verified using the total reflux distillation data in the column, equipped with the Montz-Pak A3-500 structured packing. A very good agreement between the calculated and experimentally obtained concentration profiles is reported.

The suggested approach appears advantageous as compared to widely used simpler rate-based models (film, penetration, surface renewal), since it is free from assumptions which may cause difficulties when applied to complex separations processes.

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