Advanced Prediction of Pulsed Extraction Column Performance using LLECMOD

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Abstract— A bivariate population balance model (the base of LLECMOD program) for the dynamic simulation of liquid extraction columns is extended to simulate pulsed and sieve extraction columns. The model is programmed using visual digital FORTRAN and then integrated into the *LLECMOD* program. In addition pulsed and sieve tray columns, *LLECMOD* simulates stirred two types of agitated columns (RDC & Kühni). As a case study, *LLECMOD* is used to simulate the steady state performance of a pulsed extraction column. Two chemical test systems recommended by the EFCE are used in the simulation. Model predictions are successfully validated against steady state and dynamic experimental data, where good agreements with the experimental data are achieved.

I. INTRODUCTION

Liquid-liquid extraction is an important separation processes encountered in many chemical process industries [2]. Different types of liquid-liquid columns are in use nowadays, which can be classified into two main categories: agitated (RDC & Kühni) and pulsed (packed & 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 [3].

To shed more light on the extraction behaviour in pulsed (packed & 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 [4]. It is obvious that the changes in the characteristics (holdup, Sauter diameter, etc.) of the drop population 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 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 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 equations (PBE). However, even 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 & sieve plate) extraction columns. The models of both columns are integrated into the existing program: *LLECMOD* [1], which can also simulate agitated extraction columns (RDC & 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 [1, 5].

II. MATHEMATICAL MODELLING

The modelling of extraction columns still demands improvement. Simulating liquid-liquid extraction columns is a

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