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General design methodology for reactive liquid–liquid extraction: Application to dicarboxylic acid recovery in fermentation broth

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ABSTRACT

A general design methodology for reactive liquid–liquid extraction is introduced in this paper. It is composed of three different steps: feasibility analysis, pre-design determination and simulation validation. This paper is focused on the first and the second step. This methodology leads to the design specifications of the units from the information concerning the physico-chemical behaviour of the studied system, exploiting the equilibrium and material balance equations. The results of this methodology are a good starting point for an optimization study or for an investment calculation process. This methodology has been applied to different case studies: two different strategies of extraction and several solvents to recover succinic acid in fermentation broth.

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1. Introduction

The reactive separation involves the combination of reaction and separation in a same unit. Esterification is mainly chosen as case study in the literature. The transformation of the molecule in its esterified form confers better physico-chemical and equilibrium characteristics which can be used for an easier separation. Furthermore, merging reaction and separation in a single apparatus can lead to energy integration and process intensification.

The efficiency of reactive separation strategies (especially reactive distillation) has already been proved [13]. The advantages of reactive distillation are multiple: increased conversion, increased selectivity and energy integration or production quality can be cited. But distillation is energy consuming to maintain boiling and will be an expensive solution in the case of a very diluted system (especially in water). For this type of diluted system, a cost effective way to recover valuable products especially from fermentation, such as acids or alcohols, is reactive liquid–liquid extraction.

The work of Samant and Ng [11] proposes a calculation procedure for determining the design of a reactive liquid–liquid extraction column. They apply this procedure to a general pattern four reactive compounds at the maximum with an inert as an extracting agent.

The objective of this study is to adapt this procedure for real systems, and transcribe it in a design approach similar to the one introduced by Tuchlenski [14] for reactive distillation. A design methodology consists in determining the key structural parameters of an operation unit. This study proposes a design methodology for reactive liquid–liquid reaction.

The design approach developed here is based on thermodynamic equilibrium calculation to determine the design of the reactive extraction process. The aim is to obtain the operating parameters such as possible raffinate and extract composition, solvent rate and number of theoretical stages. The design approach includes three parts: the feasibility analysis, the pre-design and the validation step. This article is focused on the first and second step of the approach

In the first part, the general design methodology for reactive liquid extraction is presented with the reactive liquid–liquid diagram. It shows the location of the compositions of the organic phase and the aqueous phase, which respect both chemical and phase equilibrium. The second step of the methodology is also

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Nomenclature

| | |
|----------------------|--|
| E | Molar organic phase flow (mol.s ⁻¹) |
| F | Molar feed flow (mol.s ⁻¹) |
| H | Liquid retention of the one stage extraction process (mol) |
| K_{eq} | Chemical equilibrium constant |
| M | Mixture of F and S flow or R _N and E ₁ flow (mol.s ⁻¹) |
| m | Variable for RECM defined in the variable change |
| N_T^0 | Initial total amount of mole for reactive liquid diagram (mol) |
| Nc | Number of compound |
| Nr | number of reactions |
| Q | fractional conversion |
| R | Molar aqueous phase flow (mol.s ⁻¹) |
| S | Molar solvent feed flow |
| (S/F) | Solvent rate |
| (S/F) _{min} | Minimum solvent rate |
| t | Time (s) |
| V | Variance |
| w | Molar composition of the liquid retention H |
| X | Reactive molar composition of phase |
| x | Molar composition of phase |
| z | Molar composition of feed flow F |
| Z | Reactive molar composition of feed flow F |
| γ | Activity coefficient |
| β | Fraction of phase I in the mixture |
| ξ | Chemical extent: mol |
| τ | Dimensionless time |
| ϑ | Stoichiometric coefficient |
| ϕ | Matrix of the reference compounds' stoichiometric coefficient |
| Exponents | |
| I | Aqueous phase |
| II | Organic phase |
| Subscript | |
| i | Component |
| j | Stage |
| L | Limit |
| N | Last stage |
| r | Reaction |
| ref | Reference |
| Acronym | |
| DMS | Di-Methyl succinate |
| DOS | Di-octyl succinate |
| MeOH | Methanol |
| MMS | Mono-Methyl succinate |
| MOS | Mono-Octyl succinate |
| NTS | Number of theoretical stage |
| OcOH | Octanol |
| P-X | Para-Xylene |
| RECM | Reactive extraction curves map |
| rLLD | Reactive liquid-Liquid diagram |
| rLLE | Reactive liquid-Liquid extraction |
| SMILES | Simplified molecular input line entry specification |
| SA | Succinic acid |

are explained and a graphical illustration of the method is proposed using the reactive liquid–liquid diagram.

In the second part of this article, the design methodology is applied to succinic acid recovery. The production of succinic acid by fermentation of biomass presents a viable alternative [19,20]. The recovery of succinic acid in the fermentation medium is quite complicated because of the presence of a large amount of water. Several separation techniques have been studied such as crystallization [3–5], electrodialysis [2,16] or reactive extraction with tertiary amines [1]. However, all these methods have a high operation cost and this is a serious brake to the development of alternative ways of production. Several reactive liquid–liquid extraction strategies will be considered, including the number of reactive or not reactive compounds.

2. General design methodology for reactive liquid–liquid extraction

2.1. Strategy

Fig. 1 presents the principle of the design methodology that we proposed, based on the analogy with reactive distillation. It is composed of three steps [13]. This method allows us to determine the design parameters of the extraction column with the introduction of more complexity along the method and from known data:

- Thermodynamic property of the system (thermodynamic models parameters, chemical reaction constant);
- The chemical data (stoichiometric coefficient for each reaction);
- The product purity, rate recovery or conversion rate, objectives to achieve.

Step 1: Feasibility analysis

The feasibility analysis allows to verify that the separation specifications are thermodynamically feasible. If applicable, the maximum attainable compositions of the organic and aqueous phase respecting the separation specifications are determined. If these are not feasible separation objectives are revised. In the feasibility step, two tools have been identified: the reactive liquid–liquid diagram (rLLD) and the reactive extractive curve map (RECM). These tools allow to determine the thermodynamically feasible composition useful for the next step of the methodology. The last part of the article on the application of the method shows that in some cases, the application of the reactive liquid–liquid diagram is sufficient and that in more complex cases, RECM are needed to determine thermodynamically feasible compositions. That's why the two tools are identified.

The cited tools are respectively based on the work of [10] and [15]. The feasibility analysis involved some simplified assumptions on infinite solvent rate, infinite intern organic and aqueous phase flow. They allow to identify the feasible composition for the organic and the aqueous phase from a thermodynamic point of view and independently of material balances consideration.

Step 2: Pre-design

In the pre-design step, the studied physical-chemical phenomena are more complex, and this step allows the determination of a column configuration required to achieve the separation goals by using data from the previous step. For the pre-design step the structural parameters of the column are determined. To begin with, the minimum and maximum solvent rates are calculated. Then, the aqueous and organic phase compositions of the process are determined. To complete this step, the design of the column is made (number of theoretical stages, composition and flow profile). The boundary value design method introduced by Wuithier and Giraud book, [17,18] for simple extraction process and expanded to

detailed; it is the pre-design method. It allows to evaluate the minimum solvent flow rate and the number of theoretical stages based on this reactive liquid–liquid diagram. The model equations

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