Mechanistic Modelling of a Fatty Acid Distillation Plant: Iterative Approach for Component Lumping and Industrial Validation

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Although the oleochemical industry is mature, the use of modelling and simulation within this industry is limited because of (i) the complexity of vegetable oils and fats, (ii) the lack of predictive models for the physical properties of lipid compounds and (iii) the lack of specific unit operation models.[1] A specific challenge in fatty acid production is the pronounced feedstock variability. Operating a continuous process with a variable feed composition and quality poses significant challenges for process control to ensure high yields, low utility costs and excellent product quality.[2] In the petrochemical industry, crude oil feedstocks are successfully modelled as a mixture of pseudocomponents (lumps), where each pseudocomponent is associated with a boiling point range, molecular weight or C-number distribution.[3] This motivates the development of a lumping approach to simplify the composition of oleochemical feedstocks. Lipid components can be divided into two groups, major and minor components, depending on the amount in which they are present. Major components are the fatty acids, with carbon chain lengths between 4 to 26, and the glycerol esters of these fatty acids (mono-, di- and triglycerides). Minor components are non-glyceridic materials such as sterols, tocopherols, phosphatides, terpenes and volatile hydrocarbons like alcohols, ketones and aldehydes.[1, 4] In fatty acid distillation, a crude fatty acid mixture is purified by separation into a top fraction containing low boiling impurities, a side fraction containing the purified fatty acids and a bottom fraction containing glyceridic components and high boiling impurities

In this study, a model of an industrial fatty acid distillation plant, operated by Oleon NV in Belgium, is developed in the commercial process simulator Aspen Plus®. First, a thermodynamic property method was selected to predict the missing properties of pure components and mixtures.[5] In this study, existing property methods were validated using vapour-liquid equilibrium data of fatty acid mixtures. Secondly, an iterative approach for lumping components was developed and used to determine an optimal set of key components to simplify the feedstock composition. In the first iteration, a simplified composition having only one key component per lump of components is used. In the case of fatty acid distillation, these lumps are fatty acids, glyceridic components and impurities. After simulation, the composition of the acquired product streams are validated with industrial data using Theil's inequality coefficient (TIC). In case the model does not properly simulate the behaviour of all components in one lump, this lump will be split into a new set of lumps, each represented by a different key component. This methodology will be repeated until the TIC value drops below a pre-set threshold, or increases again due to overfitting. This way, the complexity of the required characterization is gradually increased in order to find the characterization with lowest complexity that still delivers an acceptable prediction. The availability of physical property data for pure components and mixtures should be taken into account when selecting key components to represent each group. Finally, a sensitivity analysis followed by an optimization using Response Surface Methodology (RSM) was performed to investigate the effect of independent model parameters, such us reflux ratio, on the yield, product quality and utility cost of fatty acid production.

The results of the property method validation showed that UNIQ-HOC resulted in the best estimation of fatty acid VLE. Using the iterative lumping approach, a total of 10 key components were selected to represent the feedstock, acquiring a TIC below 0.05. Based on the results of the sensitivity analysis, the most important process parameters and their effect on yield, product quality and utility cost were identified.

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