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Introduction

Petroleum is currently the primary raw material for the production of fuels and chemicals. Consequently, our society is highly dependent on fossil non-renewable resources. However, renewable raw materials are recently receiving increasing interest for the production of chemicals and fuels, so a new industrial system based on biomass, an inexpensive, abundant and renewable raw material, is being established with sustainability as the main driving force [1]. The processing facilities for the production of multiple products (including biofuels and chemicals) from biomass are referred as biorefineries [2].

The wide variety and complex nature of components in biorefineries poses a challenge with respect to the synthesis and design of these types of processes. Whereas physical and thermodynamic property data or models for petroleum-based processes are widely available, most data and models for bio-based processes are not. Lipids are present in biorefinery processes: they represent feedstock (vegetable oil, waste cooking oil, microalgal oil), intermediate products (fatty acids, glycerol) and final products in biorefineries, thus the prediction of their properties is of relevance for the synthesis and design of biorefinery networks.

The objective of this work is to show the application of databases of physical and thermodynamic properties of lipid components to the synthesis and design of biorefinery networks.

Problem definition and solution approach

The optimal synthesis of biorefinery networks problem is defined as: given a set of biomass derived feedstock and a set of desired final products and specifications, determine a flexible, sustainable and innovative processing network with the targets of minimum cost and sustainable development taking into account the available technologies, geographical location, future technological developments and global market changes.

The problem of optimal design of biorefinery networks is solved in this work through three different stages: (i) synthesis stage, (ii) design stage, and (iii) innovation stage. At the synthesis stage, the considered alternatives are represented in a superstructure of alternatives, from which a mixed-integer linear or nonlinear programming (MILP or MINLP) problem is derived and solved in order to find the optimal processing network. Next, at the design stage, the selected processing network is simulated and analyzed and targets for improvement are identified. Finally, a more sustainable design is achieved at the innovation stage by generating innovative solutions that satisfy the targets from the design stage. Detailed process models are required in the second stage, the design stage. As part of these process models, property data input or property prediction models (for pure component and mixture properties) are needed.

Databases

The databases used in this work contain both experimental data and model parameters obtained from regression; they were presented by Cunico et al. [3]: CAPEC_Lipids_Database (pure component properties) and CAPEC_Lipids_Mixture_Database (mixture properties). For mixtures, the parameters stored in the database correspond to phase equilibria G^E models (NRTL, UNIQUAC, and original UNIFAC).

Conclusions

The knowledge of physical and thermodynamic data is relevant at the design stage of biorefinery networks since the modelling of processes requires the availability of physical and thermodynamic property data and property prediction models for both pure components and mixtures.

Databases (CAPEC_Lipids_Database and CAPEC_Lipids_Mixture_Database) are used in this work at the design stage of biorefinery processes involving lipids for industrially relevant case studies.

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