SYNTHESIS AND DESIGN OF MULTIPHASE CHEMICAL AND BIOCHEMICAL REACTORS

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ABSTRACT

The ultimate aim of chemical process design is to synthesize a process that enables the production of desired fuels and chemicals in the most cost effective and environmentally benign manner. This is also the goal of the emerging biorefinery design. For the fractionation of biomass and its conversion to products, new chemistries are recently developed or are still under research. The design of the biochemical reactors is mainly based on experience and heuristics developed for conventional reactors. Biochemical reactors are mainly heterogeneous systems, strongly non-ideal consisted of two or more phase, whose thermodynamic correlations are difficult to extract. Heterogeneous reaction systems imply the necessity for the determination of supplementary factors, which are introduced into the corresponding mathematical models. In contrast with the homogeneous case, in the heterogeneous schemes, apart from the kinetics and the heat transfer effects, the mass transfer and the general hydrodynamic behaviour of the system has to be determined. The overall reaction rate depends on kinetics and on the system's ability to exchange mass between different phases. Consequently, the need for determination of the necessary mass transfer and hydrodynamic coefficients cannot be avoided. This work presents a superstructure based simulated annealing approach to the synthesis of reactor networks in an equation-oriented environment. The problem under consideration entails the optimization of a superstructure representation of ideal reactor units involving CSTRs and PFRs with feed distribution options as proposed by Kokossis and Floudas (1990) for the full conceptual design of multiphase chemical and biochemical reactors. The objective of this study is two developed a systematic superstructure framework for the synthesis and design of biorefineries process. Hydrodynamic and mass transfer correlations are introduced into the mathematical model of the optimization problem for different real reactor designs, investigating the impact of these correlations to the final design decision of biochemistries recently developed for their implementation in biorefineries. The appreciation of different, competitive equations and their final selection is dominated by their operability, as far as the optimization process and the corresponding mathematical programming are concerned. The importance of the proposed correlations, not only of the objective function itself, but also in other parameters, such as the reactor type and volume will be based on the final results obtained from the optimization model. Finally the aim is to automatize this systematic complete optimisation framework to be applied for the design and optimisation of almost any chemical and biorefinery processes.

Keywords: Superstructure, Multiphase Reactor, Optimization, Simulated Annealing

REFERENCE

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