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Globally optimal reactor network synthesis via the combination of linear programming and stochastic optimization approach

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ABSTRACT

Reactor network synthesis based on superstructure optimization is often a complex non-linear programming problem (NLP), which is very difficult to solve by means of the traditional optimization approaches. To solve this problem, a double-level new optimization method which combines linear programming and stochastic optimization approach is proposed in this paper. In addition, a superstructure network that includes continuous stirred-tank reactor (CSTR) and plug flow reactor (PFR) which is approximated as a series of CSTRs is constructed. By the proposed method and the superstructure network, the NLP is divided into a linear programming in flow rate and reactor volume space, and a stochastic optimization problem in concentration space. We solve two cases to illustrate the feasibility of the proposed method. The results show that this new optimization method can reduce the scales and difficulties of the problem and give more suitable structure of the reactor network, as well as better reactor size than those reported in the literature.

Keywords: Reactor network; Process synthesis; Double-level optimization; Global optimization

1. Introduction

Under the conditions of known reaction kinetics and feed concentration, the task of reactor network synthesis (RNS) is to find suitable reactor types, process structures and key design parameters, which will optimize a specific objective function. Two significant mathematical programming strategies for reactor networks synthesis are superstructure optimization (Achenie and Biegler, 1990; Chitra and Govind, 1985) and targeting (Balakrishna and Biegler, 1992; Feinberg, 2002; Hildebrandt and Glasser, 1990). Other efficient methods such as heuristic method (Douglas, 1992), attainable region method Glasser (Glasser et al., 1987; Benjamin et al., 2008) have also been used to synthesize reactor networks. Superstructure optimization is a class of methods in which a network structure is initially proposed and an optimal sub-network that optimizes a desired variable is derived from the initial network. The advantages of superstructure optimization are that constraints can directly be added and objective function can be modified conveniently, and the optimal objective function value and the reactor network can also be obtained simultaneously. However, mathematical model of superstructure network is often a complex non-linear programming problem (Schweiger and Floudas, 1999), which is very difficult to solve by means of the traditional optimization approaches. Many researchers proposed different superstructure methods to reduce the complexity of this problem. A brief review of superstructure optimization is given in the next section.

Superstructure optimization evolved as a method starting in the 1960s. Jackson (1968) studied a reactor network composed of plug flow reactors (PFR) connected by sidestreams. A great many different superstructure models were studied and a variety of solution methodologies for the resulting optimization problems were proposed from then on. Chitra (Chitra and Govind, 1981) performed work in 1981 on the determination of optimal reactor types and configurations using superstructure approach. Kokossis (Kokossis and Floudas, 1990) proposed a superstructure network that is interconnected

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