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Optimal biocompatible solvent design for a two-stage extractive fermentation process with cell recycling

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Abstract

In this study, crisp and fuzzy multiple-goal optimization approaches are respectively introduced to design an optimal biocompatible solvent to a two-stage extractive fermentation with cell recycling for ethanol production. When designing a biocompatible solvent for the extractive fermentation process, many issues, such as extractive efficiency, conversion, amount of solvent utilized and so on, have to be considered. An interactive multiple-goal design procedure is introduced to determine a trade-off result in order to satisfy such contradicted goals. Both approaches could be iterated to solve the interactive multiple-goal design problem in order to yield a trade-off result. However, the crisp optimization design is a tedious task that requires the designer to provide various pairs of the upper bounds for the design problem to obtain the corresponding solution. The fuzzy optimization approach is able to be trade-off several goals simultaneously and to yield the overall satisfactory grade for the product/process design problem.

Keywords: Solvent design; Extractive fermentation; MINLP; CAMD; Fuzzy optimization; Evolutionary computation

1. Introduction

Ethanol derived from crops, which is referred to as bio-ethanol, is a potentially sustainable energy resource that may offer environmental and long-term economic advantages over fossil fuel. Bio-ethanol produced by fermentation results in a solution of ethanol in water. Many steps throughout the ethanol fermentation process may be modified to improve the ethanol productivity, to broaden the substrate utility for microbes, to reduce glucose and ethanol inhibition, and to efficiently separate ethanol from the fermented broth. Most biological researches focus on mutating cell strains and applying recombinant DNA technology in order to enhance ethanol fermentation in batch mode. However, bio-ethanol is a bulk chemical and must carry out continuous fermentation to achieve economic and beneficial production. Continuous fermentation can increase productivity; however, it is unable to be carried out on high cell density culture, resulting in low ethanol concentration and a significant loss of residual substrate. To increase the efficiency of the bio-ethanol fermentation process, various cell culture methods have been investigated (Gil, Jones, & Tornabene, 1991; Kargupta, Datta, & Sanyal, 1998; Nishiwaki & Dunn, 1997, 1998). Cell-recycling bioreactor coupled with membrane filtering modules has gained considerable interest in recent years in order to achieve higher bio-ethanol concentration. However, such a high ethanol concentration may poison viable microorganisms and abrogate the fermentation process. Extractive fermentation is an alternative technique used to reduce the end product inhibition by removing the fermentation product *in situ* (Daugulis, Axford, & McLellan, 1991; Gyamerah & Glover, 1996; Kang, Shukla, & Sirkar, 1990; Kollerup & Daugulis, 1985; Offeman, Stephenson, Robertson, & William, 2005). However, the toxicity of the organic solvent used to remove the end product is always a problem. Few reports have been taken advantage of computer-aided molecular design (CAMD) to design a biocompatible solvent for extractive fermentation process (Papadopoulos & Linke, 2005; Wang & Achenie, 2002b).

CAMD techniques can be further classified in terms of their solution algorithm into heuristic numeration (Brignole, Bottlini, & Gani, 1986; Gani & Brignole, 1983; Hostrup, Harper, & Gani, 1999; Joback & Stephanopoulos, 1989), knowledge-based

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Nomenclature

b_i bleed ratio for ith extractive fermentor
C_{ij}^{E} concentration of component j for extractive phase at the ith extractive fermentor (g/L)
C_{ij}^{R} concentration of component j for raffinate phase at the ith extractive fermentor (g/L)
$\mathrm{Conv_{ov}}$ overall substrate conversion (%)
D_1, D_1^{R} dilution rate based on influent and effluent aqueous flow rate at the first extractive fermentor, respectively (h^{-1})
D_2, D_2^{R} dilution rate based on influent and effluent aqueous flow rate at the second extractive fermentor, respectively (h^{-1})
D_{1v}, D_1^{E} dilution rate based on influent and effluent solvent flow rate at the first extractive fermentor, respectively (h^{-1})
D_{2v}, D_2^{E} dilution rate based on influent and effluent solvent flow rate at the second extractive fermentor, respectively (h^{-1})
$\mathrm{EE_{ov}}$ overall extraction efficiency (%)
k_{ij} distribution coefficient for component j between extract and raffinate phase at the ith extractive fermentor (w/w)
k_j overall distribution coefficient for component j between extract and raffinate phase (w/w)
K_s saturation coefficient for cell growth on glucose
K_{sI} inhibition coefficient for cell growth on glucose
K_p saturation coefficient for cell growth on ethanol
K_{pI} inhibition coefficient for cell growth on ethanol
L_{C50} the lethal concentration causing 50% mortality in fathead minnow (mol/L)
M_{W_j} molecular weight for j component
N_l number of group l in the compound
P_1^{R}, P_2^{R} effluent ethanol concentration in raffinate phase at the first and second fermentor (g/L)
P_1^{E}, P_2^{E} effluent ethanol concentration in extractive phase at the first and second fermentor (g/L)
S_{f_1}, S_{f_2} influent substrate concentration at first and second stage (g/L)
$\sum_{1v}$, $\sum_{2v}$ influent solvent concentration at the first and second fermentor (g/L)
V_i the volume for the ith extractive fermentor (L)
W_1^{R}, W_2^{R} water concentration in raffinate phase at the first and second stages (g/L)
W_1^{E}, W_2^{E} water concentration in extractive phase at the first and second stages (g/L)
x_{ij}^{E} mole fraction of component j in extractive phase for the ith extractive fermentor
x_{ij}^{R} mole fraction of component j in raffinate phase for the ith extractive fermentor
X_{10}, X_1 influent and effluent cell concentration in raffinate phase at the first stage (g/L)
X_{20}, X_2 influent and effluent cell concentration in raffinate phase at the second stage (g/L)

Greek letters
μ_i specific growth rate for ith extractive fermentor (h^{-1})
μ_{max} maximum specific growth rate (h^{-1})
α fermentor volume ratio
δ_l contribution of group l in group contribution-based model for L_{C50}
β_i flow rate ratio for the ith extractive fermentor
η the overall solvent selectivity (w/w)
γ_{ij}^{E} activity coefficient of component j in extractive phase for the ith extractive fermentor
γ_{ij}^{R} activity coefficient of component j in raffinate phase for the ith extractive fermentor
ν_l valence of group l
π_v overall mass flow rate of fresh solvent (g/hL)

approaches (Bolis, Pace, & Fabrocini, 1991; Gani, Nielsen, & Fredenslund, 1991) and optimization-based methods. The heuristic numeration and knowledge-based approaches are based on the formation of all possible molecular structures from a specified set of building groups and the screening of the generated molecules according to molecular design feasibility rules and pre-selected target physical property values. In optimization approaches, CAMD problems are formulated as mixed-integer nonlinear programming problems. A number of deterministic optimization methods have been proposed to solve CAMD problems, such as local optimization approaches (Karunanithi, Achenie, & Gani, 2006; Macchietto, Odele, & Omatsone, 1990; Odele & Macchietto, 1993; Pistikopoulos & Stefanis, 1998), global optimization approaches (Sinha, Achenie, & Ostrovsky, 1999; Wang & Achenie, 2002b), hybrid method (Harper, Gani, Kolar, & Ishikawa, 1999), branch and bound approach (Ostrovsky, Achenie, & Sinha, 2002), outer approximation approaches (Wang & Achenie, 2002a), interval analysis (Achenie & Sinha, 2003), mixed-integer dynamic optimization (Giovanoglou, Barlatier, Adjiman, Pistikopoulos, & Cordiner, 2003), decomposition method (Karunanithi, Achenie, & Gani, 2005), and Tabu search (Lin, Chavali, Camarda, & Miller, 2005). Such deterministic optimization methods have applied to many areas, such as extraction solvents (Gani & Brignole, 1983; Giovanoglou et al., 2003; Hostrup et al., 1999; Marcoulaki & Kokossis, 2002; Pretel, Lopez, Bottini, & Brignole, 1994), polymer designs (Camarda & Maranas, 1999; Peter, Harper, Kolar, & Ishikawa, 1999; Vaidyanathan & El-Halwagi, 1996; Venkatasubramanian, Chan, & Caruthers, 1995), absorption solvents (Eden, Jørgensen, Gani, & El-Halwagi, 2004; Odele & Macchietto, 1993; Pistikopoulos & Stefanis, 1998), refrigerant design (Churi & Achenie, 1996; Duvedi & Achenie, 1996), distillation solvents (Chen, Lei, Li, & Li, 2005; Van Dyk and Nieuwoudt, 2000), reaction solvents (Gani, Jiménez-González, & Constable, 2005), catalysts (Chavali, Lin, Miller, & Camarda, 2004), value added products (Camarda & Sunderesan, 2005) and crystallization solvent (Karunanithi et al., 2006). As an alternative philosophy, stochastic optimization technology has