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Integrating product and process design with optimal control: A case study of solvent recycling

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Abstract

This paper proposes the simultaneous integration of environmentally benign solvent selection (product design), solvent recycling (process design) and optimal control for the separation of azeotropic systems using batch distillation. The previous work performed by Kim et al. (2004. Entrainer selection and solvent recycling in complex batch distillation. Chemical Engineering Communications 191(12), 1606–1633) combines the chemical synthesis and process synthesis under uncertainty. For batch distillation, optimal operation is also important due to the unsteady state nature of the process and high operating costs. Optimal control allows us to optimize the column operating policy by selecting a trajectory for the reflux ratio. However, there are time-dependent uncertainties in thermodynamic models of batch distillation due to the assumption of constant relative volatility. In this paper, the uncertainties in relative volatility were modeled using Ito processes and the stochastic optimal control problem was solved by combined maximum principle and non-linear programming (NLP) techniques. Then the previous work of optimal solvent selection and recycling was coupled with optimal control. As a real world example for this integrated approach, a waste stream containing acetonitrile–water was studied. The optimal design parameters obtained by Kim et al. (2004. Entrainer selection and solvent recycling in complex batch distillation. Chemical Engineering Communications 191(12), 1606–1633), for this separation were used and the optimal control policy is computed first without considering uncertainties by variable transformation technique. The deterministic optimal control policy improves the product yield by 4.0% as compared to the base case, verified using a rigorous simulator for batch distillation. When the stochastic optimal control policy was computed representing the relative volatility as an Ito process, a similar recovery rate was obtained from simulations, but the batch time was reduced significantly, producing the most profitable operation.

Keywords: Batch distillation; Optimal control; Ito process; Middle vessel

1. Introduction

Solvents are widely used in bulk chemical, specialty chemical and pharmaceutical industries. However, waste solvents released from these industries deteriorate the environmental quality and reduce the material economy. In order to recover the solvents from waste streams, separation processes are employed. Batch distillation is one of the separation processes used for solvent recovery in many chemical industries especially those related to the production of high value, low volume specialty chemicals, pharmaceuticals and bio-chemicals. This process offers great flexibility for small-scale production, where there are variations in feed stock and product specifications. On the other hand, the unsteady state nature of this process creates challenging design and operational problems.

One of the most difficult problems is to optimally design and operate batch columns for the separation of systems showing non-ideal mixture behavior. For many industrially important mixtures and some waste solvents, the thermodynamics is complex due to the formation of azeotropes. One way to separate an azeotropic mixture is to use an entrainer to break the azeotrope by changing vapor–liquid equilibrium. The question following this is how to select an effective separating agent or entrainer (chemical synthesis) which complies with environmental regulations and how to synthesize this distillation

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process for solvent separation and recycling. In recent years, researchers have realized the importance of integrating chemical synthesis (i.e., environmentally benign solvent (EBS) selection) with process synthesis (i.e., in-process solvent (IPS) recycling) to ensure improved economic performance and environmental quality. Recently, Kim et al. (2004) derived an innovative batch campaign using the integrated chemical synthesis and process synthesis approach. Furthermore, for batch distillation, we should also consider another important factor: optimal operation. Due to its unsteady state nature, operation is much more difficult and the operating costs are higher for this process. Therefore, optimal operating policies should be found for batch distillation. This results in an optimal control problem where an optimal trajectory for the control variable is found so as to optimize an index of performance. An optimal trajectory would be obtained if the mathematical model accurately captures the dynamics of the batch distillation process. However, for many mixtures the thermodynamic model is not exact and this results in time-dependent uncertainties. Rico-Ramirez et al. (2003) and Ulas et al. (2003) modeled these time-dependent uncertainties by making use of Real Options Theory based on Ito's Lemma (Ito, 1951) and derived the necessary equations for solving stochastic optimal control problems in batch distillation. The usefulness of this approach was demonstrated by case studies with known thermodynamic systems where the optimal reflux profiles obtained resulted in better process yield and product purity.

The aim of this work is to combine the previous work of computer-aided EBS selection and in-process recycling with optimal control in one platform considering the uncertainties at each stage. This complete integrated approach enables us to optimally design and operate batch distillation processes for azeotropic systems under uncertainty.

2. Integrated framework for waste solvent reduction

As mentioned above, the integrated framework consists of three stages:

(1) Environmentally benign solvent selection (EBS).
(2) In-process solvent recycling (IPS).
(3) Optimal control and operation.

2.1. Solvent selection—product design

The first stage of this integrated framework is product design which is an approach to generate candidate solvent molecules that have desirable physical, chemical, and environmental properties. Computer-aided molecular design (CAMD) is one commonly used method. Based on the reverse use of group contribution methods, CAMD can automatically generate promising solvent molecules from their fundamental building blocks or groups (Kim and Diwekar, 2002a). Solvent selection model includes properties such as (a) distribution coefficient, (b) solvent selectivity, (c) physical properties like boiling point, ash point, density, and viscosity, (d) toxicology, (e) environmental properties like LC_{50} (lethal concentration at 50% mortality), LD_{50} (lethal dose at 50% mortality), BCF (bio-concentration factor), and persistence, and (f) cost. The basic diagram of CAMD is given in Fig. 1. This method can generate a list of candidate solvents with reasonable accuracy within a moderate time scale. However, CAMD is limited by the availability and reliability of property estimation methods and there are uncertainties in the prediction of environmental properties. These uncertainties will be mentioned in Section 3.

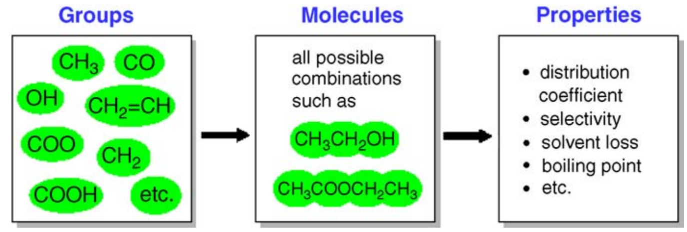

Fig. 1. Basic diagram of CAMD based on group contribution methods (Kim and Diwekar, 2002a).

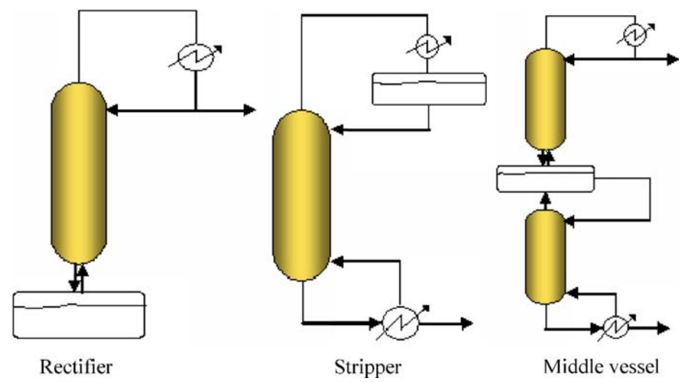

Fig. 2. Batch column configurations.

2.2. Solvent recycling—process design

At this stage the EBS selection and IPS recycling models are simultaneously integrated. Three competing batch column configurations: the rectifier, the stripper, and the middle vessel column are considered which are given in Fig. 2. Heuristics and optimization are used to find the best possible column configuration. A multi-objective optimization framework with possible objectives: maximum product recovery, maximum column feasibility and minimum heat duty provide the various trade-offs necessary for a smooth and robust operation. Kim et al. (2004) applied this framework to an industrial case study involving acetonitrile (ACN) and water and derived two innovative batch campaigns. In this paper, to further improve waste reduction, optimal operation is also considered as well as product and process design, which is described in the following subsection. The same case study will be used to see the effect of optimal operation on process recovery in Section 4.

2.3. Optimal control—optimal process operation

The final stage of this integrated framework is to apply optimal operation strategies to achieve maximum product yield