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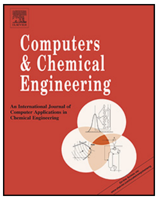

Cyclic operation as optimal control reflux policy of binary mixture batch distillation

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ABSTRACT

We revisit the maximum distillate optimal control problem of batch distillation of non-ideal binary zeotropic mixtures. The direct method with full discretization is used. The problem formulation is based on full column dynamics and the distillate flow rate is used as control variable instead of the reflux. The purity constraint is handled as a new state variable, the purity deviation. Literature simulations showed that the cyclic reflux policy (bang-bang type control) performs better than variable reflux (singular type control) or constant reflux policy for small amount of light product in the load. For the first time, a cyclic reflux policy is found as the optimal control solution. The results are confirmed by rigorous simulation of the batch distillation, as the cyclic policy improves by 13% the product recovery over the variable reflux policy. Influence of the relative volatility, vapour flow rate, plate hold-up and initial load is discussed.

Nomenclature

$u(t)$	Distillate flow rate (control variable) [mol/h]
V	Vapour flowrate (constant) [mol/h]
$L(t)$	Liquid flow rate [mol/h]
$x(t)$	Mole fraction of the light component in the liquid phase
$y(t)$	Mole fraction of the light component in the vapour phase
N	Total number of plates
$U_0(t)$	Tank liquid hold-up [mol]
U_i, $i = 1, \ldots, N-1$	Liquid hold-up on the plates (constant) [mol]
$U_N(t)$	Reboiler liquid hold-up [mol]
$R(t)$	Reflux ratio [mol/h]
$x_{D,spec}$	Desired purity specification
$p(t)$	Purity deviation
$\sigma_{sepdiff}$	Degree of separation difficulty
t_f	Overall time of the process [h]
n_{cycle}	Total number of cycles

1. Introduction

Our study is motivated by the problem of industrial solvents regeneration. For example, in France, the solvent regeneration has a strong potential: according to a 2011 French national environmental agency ADEME, only 18% of waste solvent is partially regenerated, while 82% is incinerated (Gerbaud and Rodriguez-Donis, 2010). Typically, the concerned binary mixtures are non-ideal, and suitable processes (such as azeotropic or extractive distillation) are required (Van Dongen and Doherty, 1985; Bernot et al., 1991; Rodriguez-Donis et al., 2001; Kim et al., 2001; Gerbaud et al., 2006). In the solvent regeneration industry, the batch operation mode gives the flexibility enabling to handle various solvent lots over the year. In practice, batch operation reflux and heating policies are mostly set based on a valuable know-how which might not be optimal though.

Over a century, many works have focused on operating strategies for the conventional batch column configuration. Kim and Diwekar (2001) reviewed the three operating modes for a batch rectifier, namely constant reflux rate with variable distillate composition, variable reflux rate with constant distillate composition, and finally optimal reflux rate with optimal reflux composition. They defined the last operating mode as the one leading to the most profitable operation. Compared with other operating modes, their optimal reflux rate was also a policy of increasing reflux policy and it led to the shortest batch time. Sorensen (1999) and earlier Jorgensen and Toftegard (1987) discussed the cyclic operation and its practical implementation in batch distillation. It consists in

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an alternation of three tasks: a reflux drum filling situated below the condenser, total distillate removal into a tank and total reflux from the reflux drum with varying hold-up. Bai et al. (2010) applied Sorensen's strategy by focusing on the influence of the reflux drum hold-up and of the plate hold-up dynamics on operation time. They showed by simulation and experiments how these hold-up dynamics impact the optimal product yield for a given number of cycles. Earlier, Sorensen and Skogestad (1994) proposed an optimal reflux policy based on cycles, and noticed that the number of cycles increases as the batch time decrease. Sorensen (1999) developed a heuristic equation using gPROMS tool for finding the total number of cycles in order to study the cyclic operating policy for a batch distillation column configuration. She found that a cyclic operating policy could significantly reduce the total operating time for mixtures with a low amount of light key component. But clearer guidelines for other mixtures were difficult to formulate, because they depend on the mixture, on the column number of plates and on the product purity and recovery specifications. Jiang and Bai (2012) simulated the cyclic total reflux batch distillation without reflux drum and demonstrated its higher performance compared to constant reflux operation when the initial load contains a low amount of product. Hasebe et al. (1999) and Noda et al. (2001) studied the optimal operating policy, which minimizes the energy consumption in a total reflux column assuming negligible hold-up and constant vapour flow rate. They showed that a higher performance was achieved by optimizing the reflux flow rate, thereby adjusting reboiler and reflux drum hold-up's with time. Finally Bildea et al. (2015) published a review on cyclic distillation technology, where they noted that cyclic operation can be easily implemented in old distillation columns by changing internals.

Mujtaba (2004) reviewed the optimal control problem definition for batch distillation, dividing all problems to belong to one of the three following groups: time minimization, distillate maximization, and profit maximization. He found that the inequality constraint for all groups must be relative to the distillate purity, with the exception of the time minimization problem where one have to add the amount of distillate. Further, he stressed that the control variable chosen should always be the reflux ratio with linear bounds imposed on it, with the exception of the time minimization problem where the final time is to be added to the list of the controlled variables.

Optimal control of batch distillation is challenging in practice compared to 'classical control' due to 1) strong control loop interactions; 2) large measurement delay in composition analyzers (>10 min); 3) frequent occurrence of disturbances. There were many attempts to solve the batch distillation optimal control problem with simplified models (Diwekar et al., 1987; Jorgensen and Toftegard, 1987). Nearly 30 more papers addressing the maximum distillate problem, the minimum time problem or the maximum profit problem have been discussed in the review by Kim and Diwekar (2001). Among them, Coward (1967a, 1967b) applied Pontryagin's maximum principle to the minimum time problem in binary batch distillation with a constant boilup rate to achieve a fixed quantity and purity in terms of minimum batch time. Hold-up on the column internal plates was neglected by Coward. Indeed, the optimal control problem of batch distillation can be written in a standard optimal control form and solved by using Pontryagin's Maximum Principle (PMP). The associated Hamiltonian H is affine with respect to the control variable, u; $H = H_0 + u.H_1$ and u is bounded between a lower and an upper bound. According to PMP, along the optimal solution the Hamiltonian takes its maximal value among all possible values of the control function. One has to distinguish between two possibilities: either the maximal value of H is reached in interior part of the control interval or on the bounds. In the first case the optimal control is called singular, it can be computed from the extremality condition $dH/du = 0$, which in the affine case reads $H_1 = 0$. Otherwise, the corresponding control is said to be of bang type (Bonnard and Chyba, 2003). A detailed analysis of the batch distillation optimal control problem is found in Stojkovic et al. (2017) where it was verified that the Hamiltonian found has the right properties.

Confirmed later by others (Robinson, 1970), the optimal reflux policy found by Coward was an increasing reflux policy to maintain a constant purity operation. In any case, it performed much better than a constant and unique value reflux policy. The increasing reflux policy will be later observed in the optimal control policy pattern and be called a singular arc in reference to the optimal control framework explained above. Aside from that preference for a variable optimal reflux policy regarding the minimum time problem, Hansen and Jorgensen (1986) found that an optimal control policy of the boilup rate performed better than an optimal reflux policy. Solving the maximum distillate problem under fixed purity, Farhat et al. (1991) found that a stepwise constant reflux policy achieved a better recovery in a shorter time than a reflux increase policy for the distillate withdrawal periods, followed by a large reflux policy for the off-cuts periods. Regarding the problem of maximizing the total profit, Low and Sorensen (2004) proposed for a multiproduct batch distillation, an optimal operation that consisted in sequences of constant reflux for each product distillation task. Other optimization variables were the number of plates, each task period and the constant boilup vapour flow rate. But other authors recommended earlier to use a variable reflux policy for that problem type (Logsdon and Biegler, 1993).

Then Diwekar (1992) solved the optimal control problem of batch distillation by using a short-cut method based on a quasi-steady-state model for each of the three problem categories listed by Mutjaba. They used this model in an algorithm combining Pontryagin's Maximum Principle and non-linear problem techniques. This formulation reduced the dimensionality of the problem and the computational effort, and it allowed to set bounds on variables such as the reflux ratio. Comparing the optimisation results with those obtained in open literature, Diwekar reached the same conclusions about the optimal operation, namely that an increasing reflux policy is the optimal one. Raducan et al. (2005) took a step further in defining the optimal control problem as they studied the free time optimal control problem. They were the first to describe the reflux ratio optimal control to be of 'bang-bang' type. But they did not refer to a cyclic zero reflux—total reflux policy that was studied by Sorensen, but to a 'bang-bang' shape around an optimal increasing reflux function due to piecewise step approximation. Their simplified mathematical model consisted in a one-plate distillation process. A zero reflux—total reflux policy shall occur in the optimal control patterns and it will be called through the paper a bang type optimal control policy, in accordance with standard optimal control analysis (Bonnard and Chyba, 2003).

In the present paper, we investigate the optimal control problem in order to find the optimal reflux policy for a maximum distillate problem. Although it is a fifty years old problem solved in many ways in the literature, new contributions are added in several other aspects:

- Our study is limited to binary mixtures of various relative volatilities with a single distillation task under constant average product. Behind the simplicity of such a separation, compared to literature works dealing with the distillation of multicomponent mixtures to product multiple product, it requires extensive computational effort because the distillation column model includes the full column dynamics, unlike most literature work that used simplified models.
- A new optimal control formulation is proposed in two ways. First, the optimal design problem is formulated with respect to a 'desired purity deviation', defined not as an inequality constraint