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Eprints ID: 4890

To cite this document:

Arias-Barreto, Alien and Rodriguez-Donis, Ivonne and Gerbaud, Vincent *Multi-objective optimization of three-phase batch extractive distillation*. (2011) In: 21th European Symposium on Computer-Aided Process Engineering (ESCAPE 21), 29 may - 01 June 2011, Chalkidiki, Grece

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Multi-objective optimization of three-phase batch extractive distillation

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Abstract

A multi-objective genetic algorithm with constraints is used to obtain the Pareto front of heterogeneous extractive batch distillation (HEBD). Genetic algorithm (NSGA-II) real-coded in MATLAB is coupled to a commercial simulator ProSim Batch to consider optimization variables related to the energy consumption of the process. Illustration is done by the separation of chloroform – methanol mixture with water considering both a constant and a two piecewise constant policy for all optimization variables.

Keywords: batch extractive distillation, heterogeneous entrainer, genetic algorithm

1. Introduction

Optimal operation of batch distillation column is a daily concern in industry. Extractive distillation is a common technology and the use of a heterogeneous entrainer has increased the number of feasible distillation alternatives. Continuous feeding of heterogeneous entrainer at the top of the batch distillation column allows the substitution of the unstable ternary azeotrope by the saddle binary heteroazeotrope at the column top [1] as is the case for the separation of the azeotropic chloroform – methanol mixture with water [2]. Heterogeneous extractive batch distillation (HEBD) tasks are: (T1) steady-state startup at infinite reflux with non entrainer feeding; (T2) continuous entrainer feeding (F_E) at total reflux until the unstable ternary azeotrope is replaced by the saddle binary heterogeneous azeotrope chloroform – water; (T3) distillation of chloroform at a given R_{T3} together with the F_E ; (T4) off-cut distillate product at constant reflux ratio and (5) separation of methanol – water at (R_{T5}) with $F_E=0$. Key differences arise between homogeneous and heterogeneous distillation. In the latter, distillate composition is the heterogeneous key component – rich phase and is different from the reflux composition that is made from the whole entrainer-rich phase along with a portion “ α ” of the distillate phase, so as to obtain high recovery and purity of the distillate product. Definition of “ α ” is not straightforward because it has a controversial influence over the economical and environmental optimization of HEBD.

Previous optimization of HEBD was done by using the short-cut modeling [3]. In the present paper, we couple rigorous simulation with optimization tools to handle variables related to energy consumption such as the entrainer temperature (T_{FE}). The others manipulated variables are (F_E) and the reflux ratios R_{T3} and R_{T5} . Multi-objective genetic algorithm (NSGA-II) real-coded in MATLAB [5] was coupled with energy balances, (BatchColumn® simulator [4]) and the optimization problem deals with maximizing the economical profit EP while minimizing the environmental impact Env_{imp} . The set of optimal operating conditions is displayed by means of a Pareto front.

2. Formulation of the optimization problem

The optimization problem deals with maximizing the economical profit EP while minimizing the environmental impact Env_{imp} . EP is the positive balance between the incomes of the product per batch (\$/mole) and the pay-off giving by the solvent consumption cost (\$/mole) and the total operating cost (\$/time). Env_{imp} includes CO_2 emission related to the total heat duty and the hazardous properties of the liquid waste generated by HEBD (aqueous phase from the decanter (task T3) and the off-cut product (task T3). Manipulation of chemicals in a particular unit operation has a most important influence on the human health. This effect is commonly measured by using single indices, such as human toxicity potential by ingestion (HTPI) and by dermal exposure (HTPE). They are evaluated by means of LD_{50} and TLV factors, respectively [6]. The classical formulation of multi-objective optimization with typical constraints is:

$$\text{Min } \begin{cases} EP(x) \\ \sum_{i=1}^2 n_i * price_i - n_{EntrainH_2O} * price_{H_2O} - \text{Operation Cost} \end{cases} \quad \text{Eq.1}$$

$$\text{Min } Env_{imp}(x) = \sum_j n_{j(moles)} \sum_k x_i^j I_i^k + Q_{tot}(KW) \times \frac{n_{CO_2}}{KW}$$

- s.t: overall operating time (minutes): $t_{ov} - 480 \leq 0$
 chloroform and methanol product recovery (%): $90 - \eta_i \leq 0$
 boiler maximal capacity (mole): $U - 3U_{initial} \leq 0$

x is the vector of the continuous variables of HEBD. n_j is the molar amount of pollutant j (aqueous phase and off-cut product), x_i is the molar fraction of component i (chloroform and methanol) in n_j , I_i^k is the environmental impact index (EI_{ik}) for the factor k , LD_{50} or TLV , for each component i . As LD_{50} and TLV units and meanings are not similar, I_{ik} is an average contribution of the pollutant mixture chloroform – methanol computed as:

$$I_i^k = \sum_{k=1}^2 100 * \beta_i^k * \frac{EI_i^k}{EI_{CHCl_3}^k + EI_{CH_4O}^k} \quad \text{Eq. 2}$$

β_i represents the relative weight of impact factor k for each component. β_i^k is identical to ensure comparable results. The decision variables in HEDB process are i) the entrainer flowrate F_E/V and (ii) the entrainer temperature T_{FE} for tasks T2 and T3; (iii) the portion α of distillate phase refluxed to the column during task T3; (iv) the reflux R_{T5} for task T5. Bounds are set based on practical operation conditions [2]: $25^\circ C \leq (T_{FE}) \leq 100^\circ C$, $1.4 \leq (F_E/V) \leq 2$, $0.4 \leq \alpha \leq 0.9$ and $1 \leq R_{T5} \leq 10$. The multi-objective algorithm NSGA-II uses controlled elitist to favors both individuals with better fitness value and the diversity of the population, the crossover and mutation fraction is 0.80 and 0.05, respectively. Both objective functions Env_{imp} and EP are evaluated with results of the rigorous simulation software that gets in return new operating variables values for each individual. For non converging simulation, the genetic algorithm allocates an infinite heat duty.

3. Separation of chloroform – methanol with water by HEBD

The ternary residue curve map is shown in Figure 1. Calculations were done with Simulis®Thermodynamics property server in Microsoft Excel [4] using NRTL. Binary coefficients were published elsewhere [2]. Because water is fed continuously at the column top, the saddle heteroazeotrope chloroform – water is obtained in the overhead vapor and condensed in two liquid – liquid phases [2]. The fraction $(1-\alpha)$ of the

chloroform-rich phase (x'') is withdrawn as distillate and the portion α is refluxed to the column with the whole water-rich phase (x'). Characteristics of the real batch distillation column are given elsewhere [2]. Matching a real mixture, the initial conditions are [2]: initial charge (20 mol), composition charge ($x_1=0.2704/x_2=0.6714/x_3=0.0582$), decanter holdup (1 mol), vapor flow (0.016 kmol/hr), at atmospheric pressure.

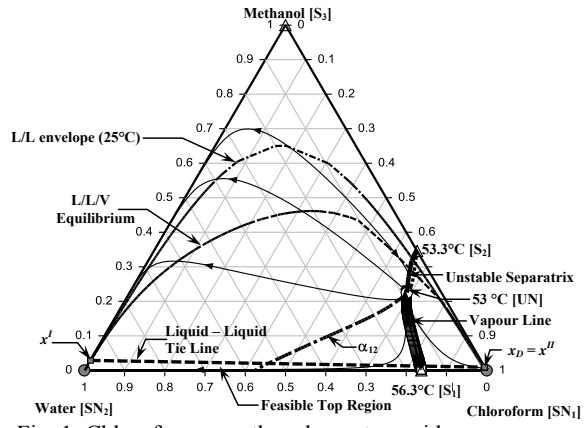


Fig. 1. Chloroform – methanol – water residue curve map

4. Results and discussion

Optimization of HEBD is performed considering a constant F_E/V and T_{FE} and following two piece-wise constant policy for α and R_{T5} . They correspond to reflux policies commonly used in industrial practice. Case I keeps constant all optimization variables T_{FE} , F_E , α_{T3} , R_{T5} . Case II uses a two piece wise reflux policy ($R_{1,T5}$ and $R_{2,T5}$) for task T5. Case III uses a two piece wise reflux policy ($\alpha_{1,T3}$ and $\alpha_{2,T3}$) for task T3. Case IV combines case II and case III with a two piece wise reflux policy ($\alpha_{1,T3}$ and $\alpha_{2,T3}$) and ($R_{1,T5}$ and $R_{2,T5}$). Figure 2 shows the front of Pareto for all studied cases.

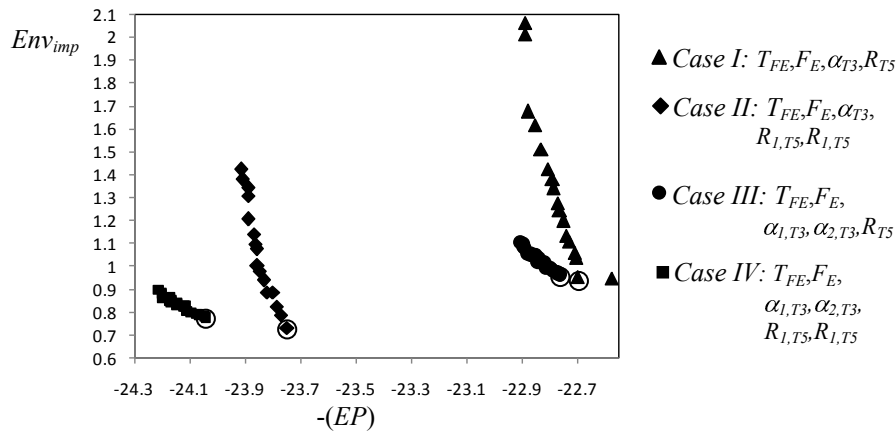


Fig. 2. Pareto optimal front in terms of environmental impact vs economical profit

Every optimal operating condition of the Pareto Front satisfies all problem constraints. Economical profit improves as the environmental impact increases. Hence, the highest profit implicates the most pollutant alternative. Comparing to the simplest operating case I, the use of two values for R_{T5} in case II improves significantly both objective functions. However, two piece wise policy for α_{T3} (case III) is an intermediate alternative between case I and case II giving a much better improvement for Env_{imp} than EP . In general, the application of two piece-wise policy for α_{T3} or/and R_{T5} improves both objective functions and, therefore, case IV is the best option. However, implementation of two piece-wise policy for α_{T3} increases EP very slightly. Indeed, the

variation range (*v.r.*) of the optimum of EP is less than 3 % taking into account all cases. Nevertheless, Env_{imp} exhibits a wider variation range but depending on constant α ($\approx 20\%$) or two piece wise α ($\approx 4\%$). This behaviour can be used as a practical criterion for selecting the values of the operating variables linked to the minimal value of Env_{imp} together with the easier manoeuvring and control of the variables in industrial practice. Variation of R_{T5} is worthier than variation of α_{T3} . Figure 3 displays the optimal value for all operating variables T_{FE} , F_E , α_{T3} , R_{T5} of each point of the Pareto Front for all studied cases. Optimal values of F_E , α_{T3} , R_{T5} are almost constant in each case, exhibiting a *v.r.* lower than 3%, 1% and 2%, respectively. T_{FE} exhibits the greatest *v.r.* around 20% along the Pareto Front. However, T_{FE} remains below 60°C, rather far from the typical usage of feeding a saturated liquid entrainer (100°C for water). That shows the significant inclusion of T_{FE} as optimization variable.

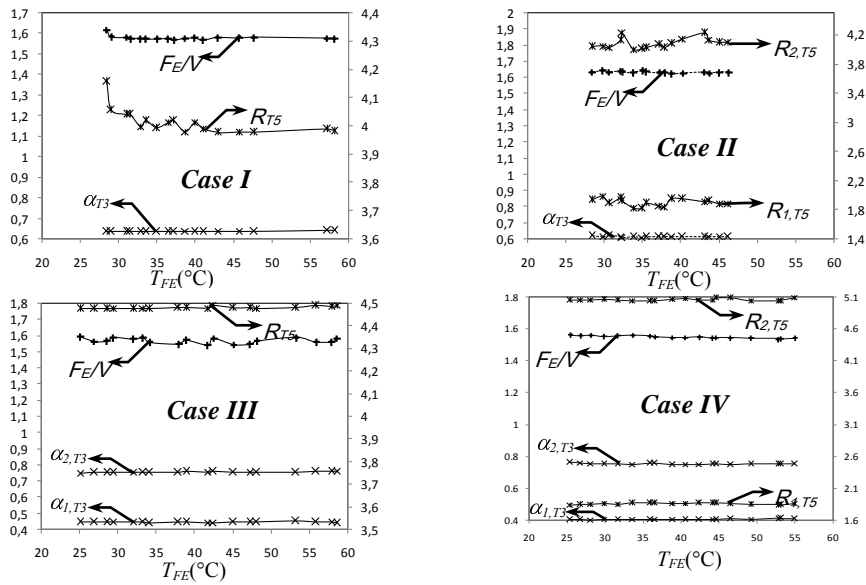


Fig. 3. Evolution of optimization variables in the multi-objective optimization of HEBD

Table 1 displays the simulation results with ProSim Batch for the optimal conditions marked (circle) in Figure 2 giving suitable EP and excellent Env_{imp} . Operating conditions are: case I: $T_{FE}=29^{\circ}\text{C}$, $F_E/V=1.58$, $\alpha_{T3}=0.636$, $R_{T5}=4.06$; case II: $T_{FE}=28.4^{\circ}\text{C}$, $F_E/V=1.63$, $\alpha_{T3}=0.636$, $R_{1,T5}=1.94$; $R_{2,T5}=4.04$; case III: $T_{FE}=28.4^{\circ}\text{C}$, $F_E/V=1.63$, $\alpha_{1,T3}=0.44$, $\alpha_{2,T3}=0.751$, $R_{T5}=4.04$; case IV: $T_{FE}=25.4^{\circ}\text{C}$, $F_E/V=1.56$, $\alpha_{1,T3}=0.405$, $\alpha_{2,T3}=0.763$, $R_{1,T5}=1.84$, $R_{2,T5}=5.05$. General remarks linked to Table 1 arises: (1) The operating time for Task 2 is almost identical for all cases; (2) Off-cut operation (task 4) is not required because the recovery yield of chloroform is almost 100%; (3) methanol recovery is always close to the limit value; (4) the economical profit and the environmental impact of the HEBD is mainly determined by decreasing the operating time and, consequently, a reduction in energy consumption; (5) two piece wise policy for α_{T3} becomes only important when it is combined with varying R_{T5} resulting in the most attractive alternative, case IV. But, case III is similar to case IV.

Table 1. Rigorous simulation of HEBD for optimal operation conditions of each case.

	Case I	Case II	Case III	Case IV
Task T2				
t₂ (min)	34.3	33.0	34.1	34.9
Task T3				
t₃ total time(min)	62.4	60.4	49.7	46.5
t₃ switch time(min)	-	-	41.1	37.8
Tank I (mol)	5.44	5.44	5.45	5.45
x_{Dist,TankI} CHCl₃	0.9930	0.9930	0.9900	0.9900
CH₃OH	0.0030	0.0030	0.0048	0.0050
H₂O	0.0040	0.0040	0.0052	0.0050
CHCl₃ recovery (%)	99.97	99.99	99.92	99.97
aqueous phase(mol)	0.169	0.169	0.367	0.360
entrainer amount(mol)	152.9	152.2	133.2	127.0
Q average (Kcal)	232.9	197.3	201.3	186.1
final still (mol)	56.72	56.46	50.81	49.22
Task T5				
t₅ total time (min)	209.6	147.2	229.3	159.8
t₅ switch time (min)	-	86.8	-	86.9
Tank II (mol)	12.19	12.20	12.28	12.48
x_{Dist,TankII} CH₃OH	0.9900	0.9900	0.9900	0.9900
H₂O	0.0100	0.0100	0.0100	0.0100
CH₃OH recovery(%)	90.06	90.07	90.72	92.19
final still (mol)	44.49	44.22	39.49	36.7
x_{H2O} still	0.9710	0.9710	0.9760	0.9800
Q average (Kcal)	514.3	361.3	562.5	391.1
Total time (min)	306.3	240.6	313.1	241.2

5. Conclusions

Genetic algorithm (NSGA-II) real-coded in MATLAB was coupled to ProSim Batch simulator. The approach maximizes the economical profit together with minimization of environmental impact of HEBD. Non pollutant HEBD process required the entrainer feeding around 30°C avoiding the typical entrainer heating. Combination of two piecewise reflux policy for the product withdrawals is the most attractive alternative.

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