Studying extractive distillation processes using optimization

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ملخص:

في هذا العمل نحن نقدم طريقة للتحقيق في عمليات التقطير المعقدة. استخدمنا نموذج ( MINLP ) الموصوف سابقا كأداة للامثتالية لاختبار أنظمة استخراجية مختلفة. أولا هو استكشاف جدوى المنطقة ثم ندرس كيفية تغيير كل من اقل ارتداد وإجمالي التكاليف السنوية مع عدد الصواني في الأجزاء المختلفة. وأخيرا فإننا حققنا في كيفية التغيير في التكوين الأمثل مع الأوزان المطبقة على عناصر التكلفة.

Abstract

In the present work, we provide a method for investigating complex distillation processes. We use a previously elaborated MINLP model as an optimization tool for examining two different extractive systems. First the feasibility region is explored. Then we examine how the minimum reflux ratio and total annual costs change with the number of trays in different sections. Finally, we investigate how the optimal configuration changes with the weights applied to the cost components.

**Keywords**: extractive distillation, solvent, optimization

* 1. Introduction

Analyzing complex (extractive) [1,2] distillation processes is needed in order to deeply understand these processes from viewpoint of chemical engineering. The analysis is generally performed using process simulators. However, this requires a lot of tests in series, and this may be inconvenient. The analysis can be made simpler by using optimization tools. Optimization tools (MINLP models with required environment) can be used not only for designing economically optimal chemical processes but also for analyzing them both from operational and economical aspects. When determining the minimum reflux ratio for a fixed configuration and specified product purity, the process simulator needs several manual ‘trial and error’ tests, whereas it can be performed in one step with an NLP-model. The boundaries of the feasible region (minimum/maximum number of stages in each section and minimum/maximum reflux ratios).

The data obtained from exploring the feasible region can be used as preliminary data for analyzing the process from economical point of view. Results obtained through these analyses may be essential when deciding on investing to expensive processes. In this paper a methodology is presented developed for using an optimization tool for studying extractive distillation processes from both operational and economical viewpoints.

* 1. Method

An MINLP model developed by Farkas et al. [3] has been applied as optimization tool. The processes contain a large number of stages and, consequently, the problems include a large number of nonlinear equations; this causes difficulty during the solution process. When solving the problem as MINLP, the original outer approximation algorithm has to be modified in order to provide good initial values for the NLP-solver. [4-5]

First the feasibility region of the extractive column is to be explored. This implies finding the minimum number of stages in each column section. Here the reflux ratio is considered as variable. Then, at feasible stage numbers, we calculate the optimum reflux ratio (at minimum total annual cost) at fixed configurations. As the number of stages and, therefore, the binary variables representing them are fixed, the boundaries of feasibility are explored through solving NLP-s.

The results can be used as a help for understanding these processes (e.g. calculating column profiles, etc.). Having obtained the previous results on feasibility, on the other hand, it is possible to determine lower and upper bounds for the variables and a near-optimal configuration which can be used as initial configuration for the MINLP-algorithm.

Finally, by creating an orthogonal matrix containing experiment points as its elements, we explore how the different cost-factors (cost of steam, cost of cooling water, cost of column installation, and payback period) affect the optimal column configuration. An orthonormal matrix containing the set values of the cost factors is designed for this aim, based on the composite design used for multiple regression in the statistical literature [6]. Two basic, reasonably estimated, levels (lower and upper values) are set to each cost factor. The process is optimized at each possible combination of these values; this involves 24 experiments. In order to determine the nonlinear parts in the regression polynomial, an additional experiment is made at the center point of the design and at excessive points (star-points) outside the core of the design; the orthogonal matrix contains 25 experiments altogether.

* 1. Examples

The method has been carried out on two different extractive distillation systems: (1) acetone / methanol separation using water as heavy solvent, and (2) ethanol / water separation using methanol as light solvent.

* + 1. Acetone / methanol system

100 kmol/h acetone/methanol mixture containing 50 mol% acetone is fed to the extractive column. Water is fed to the column above the main feed. Pure acetone is produced at the top. Methanol/water mixture leaves the column at the bottom and is separated in the solvent recovery column. The purity requirement is 98 mol% for each product. The water feed flow rate is limited from above by 100 kmol/h.

The minimum number of stages in each column section for system (1) is displayed in Table 1. The minimum stage numbers strongly depend on the actual stage numbers in the other sections. It is particularly true for the extractive and rectifying sections.

Table 1 Minimum number of stages in sections of the extractive column for acetone / methanol system

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| NS | NE | NR,min |  | NS | NR | NE,min |  | NE | NR | NS,min |
| 31 | 31 | 10 |  | 31 | 31 | 15 |  | 31 | 31 | 2 |
| 31 | 16 | 20 |  | 31 | 11 | 24 |  | 31 | 11 | 6 |
| 6 | 31 | 10 |  | 6 | 31 | 16 |  | 16 | 31 | 6 |
| 6 | 16 | 25 |  | 6 | 11 | 25 |  | 16 | 21 | 9 |

After exploring the minimum number of stages in sections, the relationship between the minimum and maximum reflux ratio and the number of trays in different sections is determined. The optimal reflux ratio as a function of the number of trays in different sections for system (1) is shown in Figures 1a-c. It can be seen that the gap between the upper and the lower limits (the feasible interval) of the reflux ratio becomes smaller toward smaller stage numbers, and the increase of the gap in increasing stage number is smaller at higher stage numbers. The figures have similar shapes, i.e. interactions are hardly experienced.



Figure 1a Relationship between the minimum and maximum reflux ratios and number of stages in the rectifying section for acetone / methanol system



Figure 1b Relationship between the minimum and maximum reflux ratios and number of stages in the extractive section for acetone / methanol system



Figure 1c Relationship between the minimum and maximum reflux ratios and number of stages in the stripping section for acetone / methanol system

Using the above results for initializing the structure, the 25 experiences described in Section 2 were performed. It has been found that none of the studied cost factors have significant effect on the optimal column configuration. This is due to the fact that in the case of extractive distillation an increase in the number of stages does not cause decrease in the minimum reflux ratio, and vica versa. The optimal total number of stages as function of cost factors is shown in Figures 2a-c.





Figure 2a. Optimal total number of trays as function of cost factors

* + 1. Ethanol / water system

100 kmol/h ethanol/water mixture containing 80 mol% ethanol is fed to the extractive column. Methanol is fed to the column below the main feed. Pure water is produced at the bottom. Methanol/ethanol mixture leaves the column at the top and is separated in the solvent recovery column. The purity requirement is 98 mol% for each product. The methanol feed flow rate is limited from above by 300 kmol/h.

Table 2 Minimum number of stages in sections of the extractive column for ethanol / water system

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| NS | NE | NR,min |  | NS | NR | NE,min |  | NE | NR | NS,min |
| 31 | 31 | 9 |  | 31 | 31 | 0 |  | 31 | 31 | 0 |
| 31 | 0 | 11 |  | 31 | 11 | 0 |  | 31 | 11 | 0 |
| 0 | 31 | 11 |  | 0 | 31 | 0 |  | 0 | 31 | 0 |
| 0 | 0 | 25 |  | 0 | 11 | 19 |  | 0 | 11 | 13 |

As it can be seen in Figures 3a-c, the minimum reflux ratio does not decrease with increasing stage numbers in the extractive and stripping sections if they are above their minimums and, therefore, there is no need and it is not economical to use more stages than the minimum. The interactions between sections are somewhat stronger that in the case of the acetone / methanol system as the shapes of curves are more dissimilar.



Figure 3a Relationship between the minimum and maximum reflux ratios and number of stages in the rectifying section for ethanol / water system



Figure 3b Relationship between the minimum and maximum reflux ratios and number of stages in the rectifying section for ethanol / water system



Figure 3c Relationship between the minimum and maximum reflux ratios and number of stages in the stripping section for ethanol / water system

Using the above results for initializing the structure, the 25 experiences described in Section 2 were performed. Similarly to the acetone / methanol system, it has been found that none of the studied cost factors have significant effect on the optimal column configuration. The curves are similar to those in Figures 2a-c.

* 1. Conclusion

An effective method for analyzing complex (extractive) distillation systems has been developed. Optimization tools are used for performing the analysis, and this is more convenient than the use of process simulators. Behavior of extractive distillation systems may be different of conventional systems. As a conclusion of investigating the effect of cost factors, we conclude that an uncertainty in estimating the future price will not cause serious error in determining the optimal configuration. Additionally, investors have no reason to be afraid of investing in extractive distillation plants.

**Notations**

N number of trays Ns number of trays in stripping section

NE number of trays in extractive section NR number of trays in rectifying section

*bpay* payback period [yr]

*Cs* unit price of steam [$/kJ]

*Cw*unit price of cooling water [$/kJ]

*UF* update factor of the price of column installation

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