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Complex Energetic and Process Control Investigations of Distillation Systems

Thesis leaflet

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Introduction

Distillation is a widely applied, well-known, reliable technique. Some industries, like oil refining use distillation on a wide scale. However, the weight of the technique in the world's industry still induces scientific investigation in several fields.

Most of the researches focus on the improvement of distillation process. More efficient use of energy, heat and energy integration, stable operation, and control and design issues are the most frequent topics.

Better energy utilisation can be achieved in two possible ways: more efficient technologies have to be used, or efficiency of operation of existing equipment has to be improved. It is not unusual that existing equipment can be improved by refitting of columns, or by changing column internals. On the other hand the losses not necessarily stem from the equipment or its internals, but the operation mode of the asset.

As the global economic environment challenges refineries in Europe, it has become vital to force changes in the processes. Several oil companies have started to adopt the lean manufacturing philosophy which gives a new framework to their business. Some of these companies apply lean in certain fields, but for example the Hungarian oil & gas company, MOL Group has started full lean transformation of its whole business.

According to the lean philosophy one of the main inhibitors of value flow is inflexibility. It is important to reduce inflexibility in order to shorten lead time, to lower stocks, to quickly react to changes in demand, and to achieve just in time production. This approach also implies Stop & Go operation of plants and devices.

Basically, refineries have not been built flexible neither in terms of stopping and restarting nor considering feedstock. Usually there is only a slight variance in feedstock and products. This fact shows a possible direction for future improvements, thus it is important to concentrate on the design of plants that have better energy efficiency, while they are much more flexible than existing ones.

Apart from the planned operation it is also important to make these plans happen. Process control is an interdisciplinary field that helps the operators to keep the flow of processes in the desired range. Good controls for every equipment, and process is a key to process materials successfully and keep the business profitable.

Literature Review

Several recent papers cover the improvement of heat integrated distillation systems like internally heat integrated distillation column, intensified heat integrated column, and totally heat integrated distillation column.

Complex design including several factors has also been investigated in the last decade, and these methods require large number of simulations, sometimes automatic decisions. This demand induced development of automatic methods to design complex distillation structures.

Exergy analysis

During design engineers have several tools to evaluate and improve distillation structures from energy efficiency point of view. One of the most renowned tools is Exergy Analysis. The idea behind the exergy concept is that the energy content of a material is only valuable until certain parameters reach those of the surrounding environment. This way, exergy content can be found in heat, chemical energy, kinetic energy, potential energy, or any form of energy that differs from the reference environment.

Since the energy related crises, processes were optimised for energy consumption, but usually the quality of the energy was not considered. However, different energy types and even energies of the same type generally have different qualities. The difference can be originated from the conversion of one into the other. Conversion between different forms of energy is not possible without losses.

To summarise the advantages of using exergy analysis: it can handle all types of energies together, it takes irreversibility into consideration and expresses that heat and work are not equivalent. Moreover, it also shows that heat degrades from higher temperatures to lower temperatures.

Another concept became famous in connection with energetic improvements, the total site integration. This concept aims to reach a globally optimal energy integration between plant and processes, and tries to avoid sub-optimal local optimisations. Many tools can aid total site integration, one of them is exergy analysis.

Process Control

Finding the best controlled variable-manipulated variable pairings is the key to proper operation of equipment. Control design usually uses simulations that can be static or dynamic. Dynamic simulations can be carried out in time domain or frequency domain. Dynamic simulations became possible only in the past decades due to the boom in information technology development. Advantages of dynamic simulations are emphasised in many publications.

Process control investigations are carried out both in time domain and frequency domain depending on the preferences of the investigator. Frequency domain simulations are easier to carry out, however the interpretation of results is less obvious, because performance indicators are various and express different types of behaviours. On the other hand time domain simulations deliver more precise results with more work.

In the literature of process control the opinions about investigations in frequency domain are rather ambiguous. Several researchers use frequency domain; however, others warn that the results of time domain load rejection analyses and frequency domain analyses have major differences.

In time domain control quality is usually measured by integral errors, while in frequency domain different control performance indicators are used. These performance indicators often have of common origins, but they describe different behaviours of systems. The three most commonly used indicators are MRI, CN, and RGA-number.

Calculation Method

Exergy Analysis

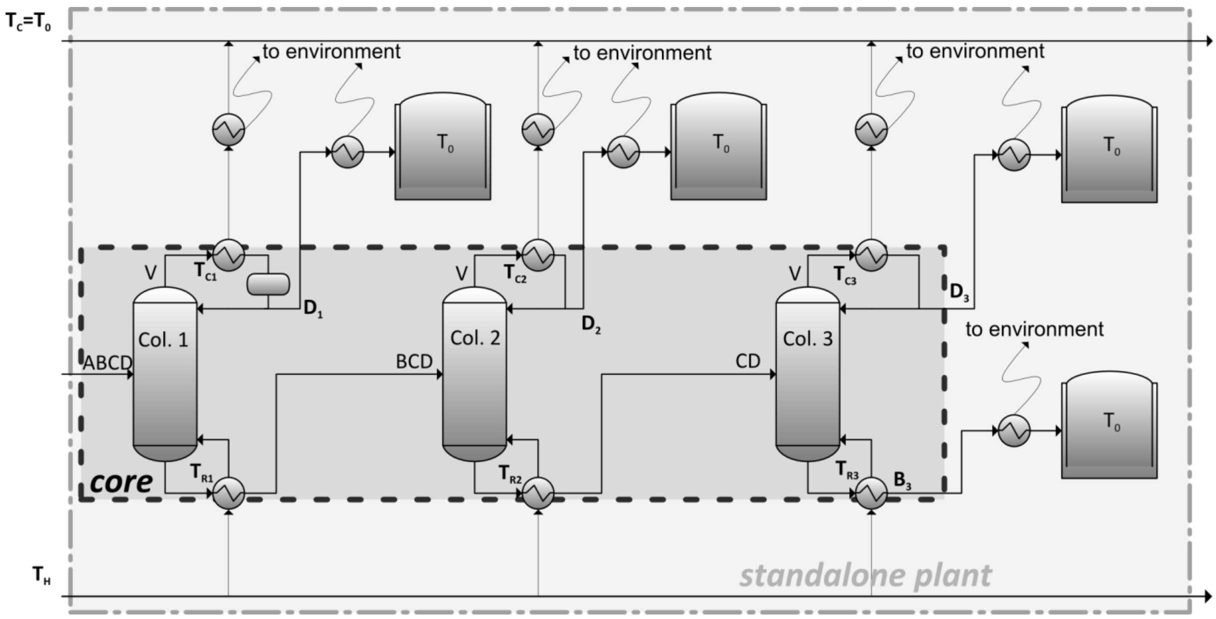
A new idea is used in the investigations that can be used in ordinary and future optimisation concepts, like flexibility improvements according to lean philosophy. A necessary expression has to be introduced: the ideal background heat cascade. This heat cascade can source and sink any amount of heat at any temperatures. Optimal integration to this heat cascade has the lowest destroyed exergy that can be achieved by the application of the investigated system. Any feasible integration with existing sites will make the investigated system thermally less efficient.

The method of exergy analysis has to be improved accordingly: dual analysis has to be carried out with two kinds of boundaries, in most cases one being the core process that represents the system that was optimally integrated to the ideal heat cascade.

The difference between the results with two boundaries can quantify potential exergy savings and gives an insight into the flexibility of the system's thermal efficiency.

For exergy analysis a simple method is used that requires only the material, heat, etc. streams passing the boundary for the calculations. First the irreversible entropy loss needs to be calculated. Having the entropy loss calculated and knowing the temperature of the heat reservoir, it is possible to calculate the exergy loss. Exergy loss (lost work/anergy) can also be calculated directly from the availability (exergy) balance. The work of separation is also needed; that is, the difference of the exergy flowing in and flowing out with material streams. Finally, the efficiency is calculated by dividing the minimal useful work by the overall energy input.

Two mixtures are used, and two cases of purities are examined with two boundaries. Different boundaries are representing the same system working as a separate system, and one that is optimally heat integrated with an ideal background heat. Five distillation schemes are examined.



1. Figure: Boundaries of investigations

Process Control

A simple distillation column and its variables are examined in order to find the best controllable controlled variable-manipulated variable pairing. I compared the successful pairings' list to find out if time domain and frequency domain simulations are able to deliver the same rank.

MRI, CN, and RGA performance indicators are calculated in frequency domain, and Integral Absolute Error is calculated in time domain to evaluate different controlled and manipulated variable pairings.

The frequency domain performance indicators quantify different properties of investigated control structures, and they are aggregated in order to reflect all of these properties in one number with the help of the desirability function.

Results

Exergy Analysis

In the case of the core distillation process the most simple direct sequence (DS) prove to be the most efficient in all cases. The first thing to mention is the higher efficiency of lower pressure systems. At higher pressures vaporisation of liquids requires molecules with higher energy and, thus, the boiling point rises. In terms of exergy higher temperature heat is of higher quality; therefore, a more valuable energy is used for the same work of separation, which means that efficiency is lower at higher pressures.

The most interesting result is the difference between the results of DS and direct sequence with backwards heat integration (DS-BHI) configurations. Heat integration is a popular way to achieve lower energy consumption. In spite of the fact that heat consumption can be significantly reduced, these results show that despite sparing a lot of heat, this kind of heat integration is not necessarily the best solution. The reasons for the worse performance of the heat integrated scheme have been mentioned before: firstly, this kind of integration needs elevated pressures, which requires more exergy; secondly, heat transfer is better distributed without heat integration. On the one hand, DS scheme uses more energy; on the other hand it also provides more energy for other processes, and these energies are of higher quality when they pass the boundary.

One more thing deserves our attention: single column (SC) scheme has even better efficiency than DS-BHI in sloppy cases, when reflux rate is low. This shows that this kind of integration is be better, because it does not need any pressure elevation.

In the other case of boundary where standalone operation of the system is assumed. In this case the results are very similar to those of the enthalpy analysis's. The very limited number of heat exchanging temperatures results that exergy analysis does not give more useful information; thus, the system that consumes less enthalpy will be the most efficient. That system is the direct sequence with backwards heat integration.

The sensitivity investigation regarding the effects of the change in ambient temperature show that in the case of the core process ambient temperature does not play a significant role, however in the case of standalone mode it has an influence.

Process Control

After the estimation of time constants of the open loop dynamic load rejection for an individual process, critical frequencies are found to be in the range of $7.29*10^{-4}$ and $5.85*10^{-3}$ rad/s in the frequency domain. All indices are constant in this range, thus the corresponding indices are easy to read. High MRI, low CN and low RGAno values are better.

In frequency domain MRI values show the same situation for all mixtures: DQ structure has the highest value; all other structures have their MRI values close to each other, significantly lower than in the case of DQ structure. CN values generally are all acceptable, showing good controllability. LQ is the only structure, the value of which exceeds 10, but only in one case being significantly higher than 10. For all mixtures DQ structure has the lowest values and LQ has the highest. RGAno-s also present results showing similar properties. For all mixtures RB structure has the lowest value, while LQ the highest. This one is the only index predicting worse controllability of DQ than most of the other structures, because DQ structure has relatively high RGAno values.

It is clear, that the three controllability indices deliver results that do not support each other unquestionably. These facts encourage us to make an attempt to aggregate the different indices with the desirability function. The results speak for themselves: for all three mixtures the rank is the same. The best controllable structure with the highest D-fct values is DQ. It is followed by LB, RB, RQ in this order, and finally the worst controllable pairing is LQ.

For comparison, time domain simulations are also carried out for both feed flow rate load rejection and feed composition load rejection. In every case RQ earns first place in all cases with the lowest IAE values meanwhile DQ is the worst with IAE an order of magnitude bigger than that of the better controllers.

LQ is the worst controller structure according to the frequency domain results, however, in time domain; in many cases it has one of the lowest values. IAE values of LQ structure are lower in all cases than that of the DQ's.

In our case the DQ structure — which is the best controllable according to frequency-domain results — proves to be almost useless in time domain simulations. Meanwhile LQ is at the end of the rank list in the frequency domain, however, in many cases in time domain it is one of the best performing structures. RQ structure is undoubtedly the best control structure in time domain, but in the frequency domain this excellent behaviour is not predicted. Consequently it can now be declared that frequency domain examinations, even with the application of the overall desirability function, are not able to replace time domain simulations when used for control structure design of a single distillation scheme.

Theses

Thesis 1 [4]

I elaborated a method in which exergy analysis of a system should be carried out with dual boundaries for the sake of the determination of the maximal exergy saving potential that can be achieved by better integration to other processes. I also proved that this method, the dual exergy analysis, gives an insight into the thermodynamic flexibility of separation systems.

Thesis 2 [4]

I elaborated the concept of the ideal background heat cascade that can source and sink any amount of heat at any temperature. I proved that the optimal integration of the investigated process to this cascade defines the core process that involves only the necessary exergy losses.

Thesis 3 [4]

I proved that the exergy analysis of the core process is not sensitive to changes in ambient temperatures, but in other cases difference in ambient temperatures can causes change in thermodynamic efficiency ranks.

Thesis 4 [2,3,4]

I proved that sensitivity of thermodynamic efficiency to product purity prescriptions is different in case of different distillation schemes.

Thesis 5 [3,4]

I proved that backwards heat integration of distillation columns decreases thermal efficiency, compared to cases when the heat integration can be solved outside of the distillation system without increasing pressures.

Thesis 6 [1]

I proved that frequency domain controllability indices (CN, MRI, RGAno) cannot be used for the design of the best control structure of an individual rectification system, neither individually, nor in an aggregated form; therefore, load rejection investigations in the time domain should be applied to complete such a design task.

Fields of application

The possible fields of application of the dual exergy analysis are design and energetic improvement of existing processes. The number of connections between plants of sites is growing in order to improve energy efficiency. In these cases a tool might be useful to highlight plants or processes with the highest saving potentials by better integration. The advantage of exergy analysis over enthalpy analysis is that in such cases the lowering of enthalpy usage can be less efficient than inter-process integration.

In the past two decades huge fluctuations could be seen in the demand for products and services; thus, lean thinking has been applied in growing number of fields. One of the elements of lean thinking is flexibility that also has huge advantages in hydrocarbon processing.

However, the above mentioned flexibility and inter-process integration together can be problematic. If a plant stops, integration becomes impossible. In that case the process without integration will have worse efficiency; and depending on the stopped time of the to-be-integrated process the chosen process can perform worse than another flexible but basically less efficient process. To overcome this problem the most adequate plant can be chosen based on dual exergy analysis and different economic scenarios.

Process control is an evergreen topic in all fields of life; and its first field of application – distillation – is not an exception. The development of IT and software the possibilities in modelling and simulation have been multiplied. Present computational capacities have obsoleted some methods that were famous for their simplicity. It seems that investigations in frequency domain will go out of fashion due to their inaccuracy compared to the precise time domain simulations. Especially if those simulations can be automated and carried out fast as it is already possible with certain software

Publications

Journal Articles

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[3] Haragovics, Máté and Péter Mizsey (2012). “Ranking of rectification structures separating quaternary mixtures with exergy analysis”. Periodica Polytechnica: Chemical Engineering 56.1. (**IF=0.217**), pp. 31–35. doi: 10.3311/pp.ch.2012-1.04.

[4] Haragovics, Máté and Péter Mizsey (2014). “A novel application of Exergy Analysis: lean manufacturing tool to improve energy efficiency and flexibility of hydrocarbon processing”. In: Energy. *Accepted*, **(IF=4.159)**.

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[6] Haragovics, Máté, Hajnalka Kencse, and Péter Mizsey (2010). “Frekvenciavizsgálatok alkalmazhatósága desztillációs oszlopok szabályozhatóságának megállapítására”. Oláh György Doktori Iskola konferenciája 2010. Budapest, HU.

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[11] Haragovics, Máté and Péter Mizsey (2011). “Applicability of desirability function for control structure design in frequency domain”. Interfaces ’11. Sopron, HU.

[12] Haragovics, Máté and Péter Mizsey (2012). “Exergy analysis of distillation structures separating quaternary mixtures”. Műszaki Kémiai Napok ’12. Veszprém, HU: Pannon Egyetemi Kiadó, p. 86.