CHEMICAL ENGINEERING TRANSACTIONS

VOL. 35, 2013

A publication of AIDIC

The Italian Association of Chemical Engineering
www.aidic.it/cet

Guest Editors: Petar Varbanov, Jiří Klemeš, Panos Seferlis, Athanasios I. Papadopoulos, Spyros Voutetakis

ISBN 978-88-95608-26-6; **ISSN** 1974-9791

DOI: 10.3303/CET1335023

The Use of Reduced Models in the Optimisation of Energy Integrated Processes

Robin Smith*, Lluvia M. Ochoa-Estopier, Megan Jobson

Centre for Process Integration, School of Chemical Engineering and Analytical Science, The University of Manchester, Manchester, UK
robin.smith@manchester.ac.uk

The importance of exploiting degrees of freedom within the process for improving energy performance has been a feature of process integration from the earliest days. Combining process changes with changes to the heat recovery system, leads to far better results compared with changes to the heat recovery system alone. However, in order to obtain the best results, the process models and heat exchanger network models need to be optimized simultaneously. Whilst in principle this is straightforward, there are many difficulties. Methods for the optimization of heat exchanger networks are well developed. It is important that heat exchanger network models are based on the network details for all but grassroot design applications. The process model to be coupled with the heat exchanger network model needs to be simple and robust enough to be included in an optimization model. If process models and heat recovery models can be combined effectively, then there are not just opportunities for design and retrofit, but also operational optimization. One of the big challenges to progress the application of this approach is the effective generation of reduced process models for use in such applications. Shortcut process models can be used, but many other options are available, such as the use of artificial neural networks. This paper reviews the different approaches and highlights the areas of application of the different approaches to producing reduced models. A case study will be presented to demonstrate operational optimization and retrofit for energy and for optimization of heat integrated systems to maximise process profit through manipulation of feeds and products, as well as energy integration.

1. Introduction

Since the early development of thermodynamic approaches to process integration, there has been huge progress in the development of approaches based on optimization. In order to obtain the best results from the optimization of heat integrated processes, degrees of freedom within the process need to be optimized simultaneously with the heat exchanger network. Combining process changes with changes to the heat recovery system, leads to far better results compared with changes to the heat recovery system alone. However, in order to obtain the best results, the process models and heat exchanger network models need to be optimized simultaneously. Whilst in principle this is straightforward, there are many difficulties. Models are needed that allow the designer to simulate, visualize and gain intuition about the process of interest. However, models are never a complete representation of reality, as there will always be factors that cannot be included in the abstraction. A model must include at least the most influential factors involved in the purpose for which the model was initially considered. If the purpose of the model is clearly defined, the characteristics of the model can be identified (e.g. degrees of freedom, type of equations, model generation process, etc.).
The role of modelling for the optimisation of heat integrated processes is of great importance. For example, heat integrated crude oil distillation systems are complex structures with strong interactions between their components. Crude oil distillation systems usually consist of a preheat train, a preflash unit, an atmospheric distillation unit (conformed by a distillation tower with side coolers and strippers) and a vacuum distillation unit. A number of approaches can be developed to obtain models that can represent

Please cite this article as: Smith R., Ochoa-Estopier L.M., Jobson M., 2013, The use of reduced models in the optimization of energy integrated processes, Chemical Engineering Transactions, 35, 139-144 DOI:10.3303/CET1335023

the separation and energy performance of such processes. These approaches can be grouped into three main categories: rigorous models, semi rigorous or simplified models, and statistical models. The selection of which model is most suitable for a certain application (e.g. design, process control) depends on issues such as the amount of information that needs to be provided by the model, the difficulty of generating, implementing and validating the model, and whether the model is to be used to modify the process as well as the heat recovery system. In an optimization scheme, it is crucial to use a model that, in addition to accurately representing the system, can be stable and perform calculations in a short period of time.
The objective of the present work is to discuss the role of reduced models (i.e. simplified and statistical models) in the optimization of energy integrated processes. The benefits and disadvantages of each type of model will be discussed, while indicating the suitability of such models for different optimization purposes. A case study will be used to illustrate the use of reduced models in the optimization of a heat integrated crude oil distillation column, where the goal is to improve net profit and propose retrofit modifications for the associated heat exchanger network.

2. Classes of models

2.1 Rigorous models

Rigorous models are generally considered as the most acceptable for process optimization. For example in distillation, an accurate distillation model requires detailed information stage-by-stage. Much information is available for analysis of the distillation performance (material and energy balances, physical properties, pressure drops, column hydraulics). However, the detail also creates problems when used in optimization. The equations are highly non-linear and implementation can be problematic. If used in optimization the system of non-linear equations becomes sensitive to initial guesses. Depending on the process, simulation can be slow. However, when used in optimization perhaps the greatest problem is that the models are generally not robust to significant changes from the base case. Frequent failure of simulation during the course of an optimization causes problems for the optimization. But rigorous models remain key in many applications for validating other models.

2.2 Simplified models

In the simplified models, typically a short-cut model is used instead of a rigorous model. For example, if the process is distillation, the Fenske-Underwood-Gilliland (FUG) equations can be used to produce a simplified model. However, the distillation often involves complex features, such as in crude oil distillation. If this is the case, then the complex column needs to be decomposed and the different column sections represented by the Fenske-Underwood-Gilliland equations or some other simplified representation. For example, Suphanit (1999) developed a simplified model for complex crude oil distillation by decomposing it into an indirect sequence of simple columns, then each simple column represented by a combination of modified Fenske-Underwood-Gilliland equations for the rectifier sections of the decomposed columns and multi-stage flash calculations for the stripping sections. Figure 1 illustrates the decomposition of atmospheric and vacuum distillation columns.
Chen (2008) further extended the models developed by Suphanit (1999). The result is that a semi-rigorous model can be developed based on the FUG method but introduces stage-by-stage calculations where appropriate to account for the complexities of the process. The performance is generally in close agreement with rigorous simulation. A significant advantage of this model is its ability to manipulate continuous and discrete features of the design. This allows the designer to implement the model in design strategies that consider, for example, the optimisation of operating conditions (continuous variables) and/or the distillation column structure (discrete variables). Simulation using simplified models is not straightforward, although they have been reported to be accurate, perform calculations in less time and be more robust than rigorous models (Zhang et al., 2013). Simplified models have demonstrated their proficiency over rigorous models for optimisation applied to grassroots and retrofit design of heat integrated distillation systems, as presented in the work of Chen (2008) and Zhang et al. (2013). Chen (2008) presented several case studies, where crude oil distillation systems were revamped to reduce energy demand or improve profit; and proposed new designs that are energy-efficient with minimum capital investment required. Zhang et al. (2013) used simplified models to reduce the energy consumption of a crude oil distillation unit operating in China, achieving significant energy savings and emission reduction.

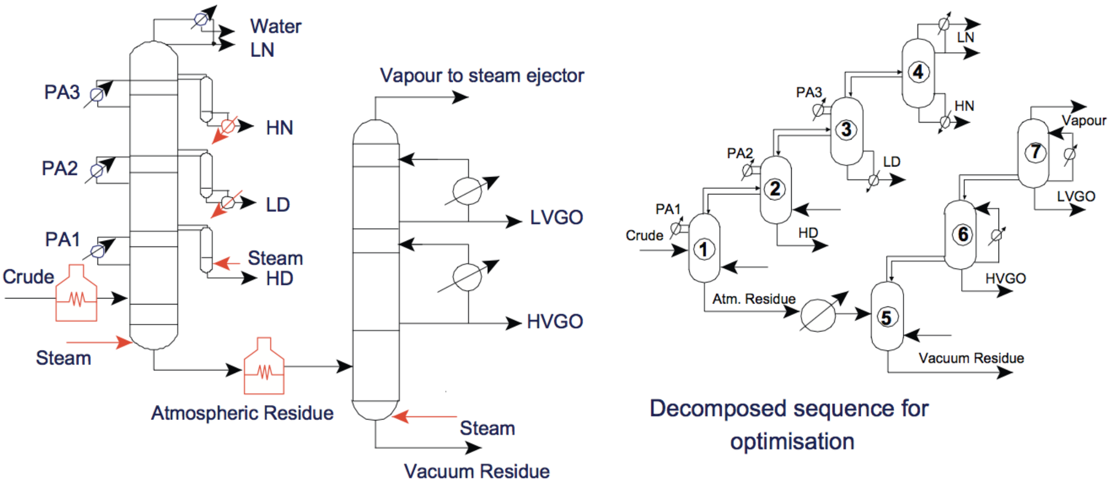

Figure 1: Decomposition of complex distillation systems. Figure taken from Zhang et al. (2013).

2.3 Statistical models

In general, statistical models represent relationships between variables in a simplistic manner, using a set of samples to find the approximation function that best describes the process of interest. Statistical models are employed as an alternative to deterministic, complex models, such as rigorous and simplified models. The use of statistical models is typically preferred in circumstances where computation time is important, when phenomena or properties affecting the process are not fully known, or when the scope of application does not require extensive deterministic models (Hartmann, 2001).

Much work has been published on statistical modelling for many applications. The general framework consists mainly of three stages: data gathering, regression and validation. In the data gathering stage, the designer needs to identify the degrees of freedom that are relevant to the purpose for which the model is built. Additionally, the method to obtain such data needs to be established, since the model depends on the quality of the data employed. The identification of degrees of freedom frequently relies on the experience of the designer, although sometimes sensitivity analysis techniques are employed (Saltelli et al., 2008). As for the method of data gathering, the selection is based on the scope of the model and on whether real measurements are available. For example, for the purpose of optimisation of heat-integrated distillation columns, using models regressed with real measurements may be unsound, as scenarios that differ from the current and past operation of the distillation column need to be evaluated to find an improved design. As a consequence, Ochoa-Estopier et al. (2013) and López and Mahecha (2009) proposed the use of rigorous models to generate samples that are used to regress the reduced distillation model. The choice of degrees of freedom and method of data gathering is not trivial, and constitutes one of the main drawbacks of this type of model.

Regression is the second stage of the statistical modelling framework. During this stage, an optimisation algorithm calculates the parameters of the regression function that minimize the error between model predictions and data. An appropriate selection of the regression function (e.g. lineal, polynomial, non-linear) and method of regression is necessary. The third stage of the statistical modelling strategy is model validation. In this stage, the regressed model is tested to evaluate the consistency of its predictions. In general, obtaining regressed models requires nontrivial statistical expertise. Hence, the use of statistical models needs to be justified by the reasons mentioned at the beginning of this section.

The simplest application of statistical models that can be used are simple regression models. The approach starts with the development of a rigorous simulation model for the process. The main operating parameters of the model are then varied across reasonable ranges and the performance correlated by simple empirical equations. For example, suppose the heat integration of a simple distillation column is to be explored. The performance for the main energy parameters can be represented by simple equations of the form:

$$Q_{REB} = a_1 q^{\,2} + a_2 q_i + a_3 P^2 + a_4 P + a_5$$

$$T_{REB} = b_1 q_i + b_2 P^2 + b_3 P + b_4$$

where Q_{REB} is the reboiler duty, T_{REB} is the reboiler temperature, q_i is the quality of feed, P the column pressure, and a_i and b_i are regression parameters fitted to the rigorous model. Such equations are readily coupled with a model of the heat exchanger network to optimize for energy performance. The approach is readily extended to deal with multiple feeds, interreboilers and intercondensers. However, this approach is limited in accuracy and limited by the complexity of the process arrangement that can be represented by such simple models. Much more general, flexible and robust are models based on Artificial Neural Networks (ANN).

Successful applications of statistical modelling, particularly artificial neural networks and metamodelling, for optimisation of heat integrated distillation columns can be found in Ochoa-Estopier et al. (2013) and López and Mahecha (2009). Ochoa-Estopier et al. (2013) presented a systematic approach to optimise the operating conditions of an atmospheric crude oil tower while proposing retrofit modifications to the associated heat exchanger network (HEN). In this case, the distillation tower was modelled using ANNs. López and Maheca (2009) developed a methodology to perform operational optimisation of several crude oil distillation units. Metamodels were employed to represent the distillation operation. Additional work using ANN for the optimisation of crude oil distillation columns without considering details on the heat exchanger network can be found in Liau et al. (2004) and Motlaghi et al. (2008). Liau et al. (2004) developed an ANN model regressed from plant measurements to optimise the operating conditions of the distillation column. Motlaghi et al. (2008) also employed production data to obtain the distillation model. The ANN model was used to optimise product yields using a genetic algorithm method.

3. Choosing the appropriate type of model

3.1 Problems Common to All Models

Problems common to all models are:

(i) Defining the degrees of freedom relevant to the purpose of the model (degrees of freedom for operational optimisation are different for grassroots design, and so on).

(ii) Validation and reconciliation: even though rigorous models are regarded as the most accurate and accepted model, they still need to be validated with reality. For statistical models, they need to be validated first with data prior to use with "reality".

(iii) The process model needs to be coupled with a model of the heat recovery network that includes all of the network details. Although thermodynamic targets can be used in some grassroot optimisation applications, retrofit and operational optimisation demand network models that include all network details.

3.2 Effort Required

The effort required to create different classes of models is significant. For rigorous models, commercial software is most often available to set up the model, making this straightforward for most cases. Simplified models are available to a lesser extent commercially, but when available, require significantly less effort than rigorous models. One of the major problems for simplified models is the decomposition of complex problems, which is often not straightforward. Statistical models require each model to be tailor made. Time is required to define how the model will be structured, and also time needs to be invested in gathering/building the data for regression. In contrast with rigorous and simplified models, this is the most computationally demanding step for this type of model. Most effort is spent in the creation of the model rather than in the simulation of the model.

3.3 Suitability for Use in Optimisation

Rigorous models tend to be complex and time consuming for computation. Rigorous models have been used commercially for operational optimisation, but tend not to be robust to significant changes from the base case operation. For optimisation, the system of non-linear equations presents a problem. Simplified models are more robust, and computationally less time consuming. By contrast, statistical models are more straightforward to implement, are faster than the former two types, and extremely robust. Statistical models are mainly used for continuous variables but can also be applied to integer variables.

3.4 Design Changes

If the optimisation is required to make changes to the design configuration, then both rigorous and statistical models are not well suited. For example, in distillation it might be desirable to change the number of stages in column sections, change the location of a pumparound, and so on. Both rigorous and statistical models are not well suited to make such changes. On the other hand, simplified models tend to be better suited. This does not necessarily prevent design changes to the heat exchanger network model, as this can be a separate model linked to the process model.

3.5 Operational Optimisation

For operational optimisation, computation time is a major issue. For most operational optimisation only continuous variables are needed. The model is most often not required to manipulate process structural modifications. More practical constraints tend to be required compared with grassroots and retrofit design. So, the space of search (upper and lower bounds of optimisation variables) is smaller than for grassroots and retrofit. The model needs to be validated with the existing process and expected to appropriately represent the modified process with more confidence than for retrofit design.

3.6 Summary of Suitability

Considering the characteristics of the different types of models and the requirements for each purpose of optimisation discussed above, the most suitable model for each application can be generally classified as:

- Grassroots: simplified models preferred that allow process design changes.
- Retrofit with process configuration changes: simplified models preferred.
- Retrofit with no process configuration changes: statistical models preferred but simplified models can also be used.
- Operational optimisation: statistical models preferred. Simplified models can also be used and rigorous models in cases where there are no significant changes to conditions from the optimisation.

4. Case study

In this work, the benefits of using reduced models are demonstrated in two case studies for the optimisation of heat-integrated distillation systems. The optimisation technique proposed by the authors in Ochoa-Estopier et al. (2013) is applied to increase net profit considering: 1) operational optimisation of the heat-integrated system; and 2) operational optimisation for the distillation column while proposing retrofit modifications for the associated heat exchanger network. The selection of the degrees of freedom of the distillation model was made based on knowledge that product yields dominate process economics and pump-around specifications have a major impact on heat recovery. Samples generated from rigorous models simulations are used to regress and validate the reduced model structured as an ANN. Results are illustrated in Table 1.

Table 1: Optimisation results for the crude oil distillation system

Item	Units	Base case	Case one: operational optimisation	Case two: operational optimisation and HEN retrofit
Retrofit modifications		-	-	Additional area and one new heat exchange unit
Operating cost	(M$/y)	2,876.0	2,875.6	2,875.4
Additional area	(m^2)	-	-	193.8
Annual capital cost	(M$/y)	-	-	0.05
Product income	(M$/y)	2,879.2	2,894.2	2,897.6
Net profit	(M$/y)	3.2	18.6	22.2

M$ denotes millions of US dollars. Results for case study two are taken from Ochoa-Estopier et al., (2013)

In both cases, yields of the most valuable distillation products are increased and energy requirements decreased to achieve considerable economic improvements. As indicated in Table 1, greater economic benefits are obtained when including retrofit modifications for the HEN, compared to only performing operational optimisation. HEN retrofit provides more degrees of freedom and hence more flexibility to perform optimisation.

Conclusions

To obtain the best results from the optimisation of heat integrated processes, the process model and heat exchanger network model need to be optimized simultaneously. For the process models, there are three general classes of model that can be used; rigorous, simplified and statistical. Rigorous process models for many cases cannot be used effectively. The process model needs to be simple and robust enough to be included in an optimisation with a model of heat recovery network that includes all of the network details. One of the big challenges to progress the application of this approach is the effective generation of reduced process models for use in such applications. This paper has reviewed the different approaches and highlighted the areas of application of the different approaches to producing reduced models.

Acknowledgements

The authors would like to thank the Mexican National Council of Science and Technology (CONACYT, no. 204362/308621) and the Roberto Rocca Education Program (RREP) for financial support granted for the development of this work.

References

Chen, L., 2008, Heat-Integrated Crude Oil Distillation Design. PhD Thesis, University of Manchester, Manchester, UK.

Hartmann, J.C.M., 2001, Determine the Optimum Crude Intake Level - a Case History, Hydrocarbon Processing, 80(6), 77-84.

Liau, L.C.-K., Yang, T.C.-K., Tsai, M.-T., 2004, Expert System of a Crude Oil Distillation Unit for Process Optimization using Neural Networks, Expert Systems with Applications, 26(2), 247–255.

López, D.C., Mahecha, C., 2009, Optimization Model of a System of Crude Oil Distillation Units with Heat Integration and Metamodeling, Ciencia, Tecnología y Futuro, 3, 159–174.

Motlaghi, S., Jalali, F., Ahmadabadi, M., 2008, An Expert System Design for a Crude Oil Distillation Column with the Neural Networks Model and the Process Optimization using Genetic Algorithm Framework, Expert Systems with Applications, 35(4), 1540–1545.

Ochoa-Estopier, L.M., Jobson, M., Smith, R., 2013, Retrofit of Heat Exchanger Networks for Optimising Crude Oil Distillation Operation. Chemical Engineering Transactions, 34.

Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., Saisana, M., Tarantola, S., 2008, Global Sensitivity Analysis: the Primer, John Wiley & Sons, Ltd, California, USA.

Suphanit, B., 1999, Design of Complex Distillation Systems. PhD Thesis, University of Manchester Institute of Science and Technology, Manchester, UK.

Zhang, N., Smith, R., Bulatov, I., Klemeš, J. J., 2013, Sustaining High Energy Efficiency in Existing Processes with Advanced Process Integration Technology, Applied Energy, 101, 26–32.