



Integrated Design and Control of Reactive and Non-Reactive Distillation Processes

Mansouri, Seyed Soheil; Sales-Cruz, Mauricio; Huusom, Jakob Kjøbsted; Gani, Rafiqul

Publication date:
2015

Document Version
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

Citation (APA):

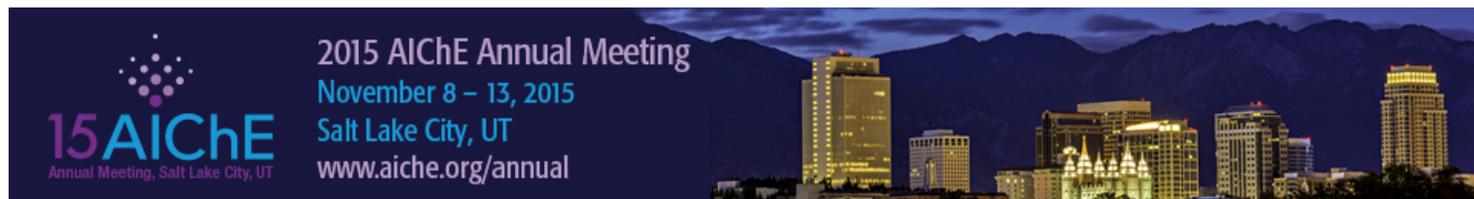
Mansouri, S. S., Sales-Cruz, M., Huusom, J. K., & Gani, R. (2015). *Integrated Design and Control of Reactive and Non-Reactive Distillation Processes*. Abstract from 2015 AIChE Annual Meeting, Salt Lake City, United States. <https://aiche.confex.com/aiche/2015/webprogram/Paper415716.html>

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.



The Global Home of Chemical Engineers

Start

At-A-Glance

Browse by Day

Browse by Topics

Author Index

Keyword Index

Personal Scheduler

415716 Integrated Design and Control of Reactive and Non-Reactive Distillation Processes

Tuesday, November 10, 2015: 9:45 AM

Salon J (Salt Lake Marriott Downtown at City Creek)

Seyed Soheil Mansouri¹, Mauricio Sales-Cruz², Jakob KjØrsted Huusom¹ and Rafiqul Gani¹, (1)Department of Chemical and Biochemical Engineering, Technical University of Denmark, Kgs. Lyngby, Denmark, (2)Departamento de Procesos y Tecnología, Universidad Autónoma Metropolitana-Cuajimalpa, Mexico D.F., Mexico

Process design and process control have been considered as independent problems for many years. In this context, a sequential approach is used where the process is designed first, followed by the control design. However, this sequential approach has its limitations related to dynamic constraint violations, for example, infeasible operating points, process overdesign or under-performance. Therefore, by using this approach, a robust performance is not always guaranteed. Furthermore, process design decisions can influence process control and operation (Huusom, 2015). To overcome these limitations, an alternative approach is to tackle process design and controllability issues simultaneously, in the early stages of process design. This simultaneous synthesis approach provides optimal/near optimal operation and more efficient control of conventional (non-reactive binary distillation columns) (Hamid et al., 2010) as well as complex chemical processes; for example, intensified processes such as reactive distillation (Mansouri et al., 2015). Most importantly, it identifies and eliminates potentially promising design alternatives that may have controllability problems later. To date, a number of methodologies have been proposed and applied on various problems to address the interactions between process design and control, and they range from optimization-based approaches to model-based methods (Sharifzadeh, 2013).

In this work, integrated design and control of non-reactive distillation, ternary compound reactive distillation and multi-component reactive distillation processes is considered systematically through a computer-aided framework. To assure that design decisions give the optimum operational and economic performance, operability and controllability issues are considered simultaneously with the process design issues. Operability issues are addressed to ensure a stable and reliable process design at pre-defined operational conditions whereas controllability is considered to maintain desired operating points of the process at any kind of imposed disturbance under normal operating conditions. First, to design non-reactive binary distillation columns, a set of conventional and simple design methods such as McCabe-Thiele and driving force approach (Bek-Pedersen and Gani, 2004) are selected. Next, these design methods are extended using element concept to also include ternary as well as multicomponent reactive distillation processes. The element concept (Pérez Cisneros et al., 1997) is used to translate a ternary system of compounds ($A + B \leftrightarrow C$) to a binary system of element (W_A and W_B). In the case of multicomponent reactive distillation processes the equivalent element concept is used to translate a multicomponent (multi-element) system (Jantharasuk et al., 2011) of compounds ($A + B \leftrightarrow C + D(\text{inert})$) to a binary system of key elements (elements W_{HK} and W_{LK}). For an energy-efficient design, non-reactive driving force (for binary non-reactive distillation), reactive driving force (for ternary compound reactive distillation) and binary-equivalent driving force (for multicomponent reactive distillation) were employed. For both the McCabe-Thiele and driving force method, vapor-liquid equilibrium data are based on elements (except for binary non-reactive distillation column). ICAS-PDS is used to compute the reactive vapor-liquid equilibrium data set by consecutive calculation of reactive bubble points. It has been shown previously that designing a reactive distillation column at the maximum driving force will result in the minimum energy consumption (Bek-Pedersen and Gani, 2004). Note that the same principles that apply to

energy consumption (Bek-Pedersen and Gani, 2004). Note, that the same principles that apply to a binary non-reactive compound system are valid also for a binary-element or a binary-key-element system. Therefore, it is advantageous to employ the element based method for multicomponent reaction-separation systems.

The operation of the non-reactive distillation column, ternary reactive distillation column (binary-element) and multicomponent reactive distillation column (binary-key-element) is investigated at the highest driving force and other candidate points. It is shown analytically and through rigorous dynamic process simulation (using ICAS process simulation software and Aspen Plus) for all three cases that the sensitivity of the system to the disturbances in the feed at the highest driving force is less than any other candidate point. By application of this approach, it is shown that designing the non-reactive and reactive distillation processes at the maximum driving force results in an optimal design in terms of controllability and operability as well as an optimal/near optimal design from an energy point of view. It is verified that the reactive distillation design option is less sensitive to the disturbances in the feed at the highest driving force and has the inherent ability to reject disturbances.

References:

Bek-Pedersen, E., Gani, R., 2004. Design and synthesis of distillation systems using a driving-force-based approach. *Chem. Eng. Process. Process Intensif.* 43, 251–262. doi:10.1016/S0255-2701(03)00120-X

Hamid, M.K.A., Sin, G., Gani, R., 2010. Integration of process design and controller design for chemical processes using model-based methodology. *Comput. Chem. Eng.* 34, 683–699. doi:10.1016/j.compchemeng.2010.01.016

Huusom, J.K., 2015. Challenges and opportunities in integration of design and control. *Comput. Chem. Eng.* doi:10.1016/j.compchemeng.2015.03.019

Jantharasuk, A., Gani, R., Górak, A., Assabumrungrat, S., 2011. Methodology for design and analysis of reactive distillation involving multielement systems. *Chem. Eng. Res. Des.* 89, 1295–1307. doi:10.1016/j.cherd.2011.04.016

Mansouri, S.S., Sales-Cruz, M., Huusom, J.K., Woodley, J.M., Gani, R., 2015. Integrated Process Design and Control of Reactive Distillation Processes, in: 9th International Symposium on Advanced Control of Chemical Processes.

Pérez Cisneros, E.S., Gani, R., Michelsen, M.L., 1997. Reactive separation systems—I. Computation of physical and chemical equilibrium. *Chem. Eng. Sci.* 52, 527–543. doi:10.1016/S0009-2509(96)00424-1

Sharifzadeh, M., 2013. Integration of process design and control: A review. *Chem. Eng. Res. Des.* doi:10.1016/j.cherd.2013.05.007

Extended Abstract: File Not Uploaded

See more of this Session: [Process Intensification By Process Integration](#)

See more of this Group/Topical: [Process Development Division](#)

Follow Us

[LinkedIn](#)

[Twitter](#)

[Facebook](#)

[YouTube](#)

[Flickr](#)

[Slide Share](#)

[About](#) | [Join AIChE](#) | [Global](#) | [Contact](#) | [Advertise](#) | [Tools](#) | [Press](#) | [Privacy & Security](#) | [Code of Ethics](#) | [Sitemap](#) |

Copyright © American Institute of Chemical Engineers. All rights reserved.