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Publication date:
2012

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

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Wednesday, October 31, 2012: 8:30 AM

Oakmont (Omni)

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Process Intensification by Membrane-Assisted Reactive Separation Processes: A Design Tool based on Process Analysis and Optimization

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Due to decreasing fossil fuel reserves, sustainability is an important factor in the chemical industry that has to be considered when new processes are developed. One opportunity to reach higher efficiencies in the production of bulk chemicals is the use of intensified processes. Two promising examples from the field of process intensification are (1) reactive distillation (RD) combining reaction and distillation within one apparatus and (2) hybrid separation processes, for instance the external integration of distillation with membrane separation. In both cases, synergetic effects lead to an increased sustainability in means of economics and ecologics. The use of a multifunctional reactor such as reactive distillation within a hybrid separation process promises even higher benefits. Despite all advantages, the potential of those and other intensified processes is hardly exploited in industry. The main reasons are a lack of process know-how and missing process synthesis tools.

Here, a combined methodology for process intensification is proposed consisting of four integrated blocks which are starting with the general design problem as input followed by “system identification & analysis”, a “synthesis/design” and finally a “model-based validation/verification” to identify a near optimal intensified process[1)]. Whenever and wherever necessary, knowledge from experiments are generated and transferred by the block “experimental validation/verification”.

In the “system identification & analysis”, the process under investigation is analysed to identify limitations and/or identify critical phenomena which need to be intensified for the targeted performance improvement. Based on these results, criteria are used to identify which workflow(s) is/are followed for “synthesis/design” of the intensified process. The synthesis/design workflows are a knowledge based approach (KBS), a unit-operation based workflow (UBS) and/or phenomena based approach (PBS). While the complexity and the time spent to obtain a solution arises from KBS to PBS, also the novelty and potentially the achieved process improvement increases. The results of the “synthesis/design” which are a small number of potentially promising (intensified) process options are verified in the “model-based validation/verification” to identify the best process option.

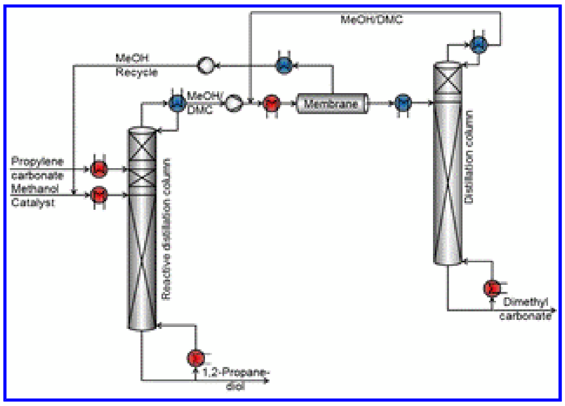

Figure 1: Simplified flowsheet of the developed membrane-assisted reactive separation process

In this contribution, the whole combined methodology will be presented and highlighted through the application to a case study which is the chemical equilibrium-limited transesterification of propylene carbonate with two molecules of methanol to produce the target product dimethyl carbonate and the byproduct 1,2-propanediol. The objective is to minimize the production costs per ton of dimethyl carbonate. Two synthesis/design workflows will be highlighted which are KBS and UBS. It will be shown that the use of the UBS workflow lead to the development of a membrane-assisted reactive separation processes that consists of an RD column, a vapor permeation membrane and a conventional distillation column (see Figure 1). Finally, in the “model-based validation/verification” an evolutionary algorithm based on the “modified differential evolution” approach is used to solve the reduced optimization problem of the remaining process options from the UBS and KBS workflow by determining apparatus dimensions and operating conditions for the minimal objective function. The results for the membrane-assisted reactive separation process compared to the base-case process obtained from KBS for the production of dimethyl carbonate comprises high savings in capital and energy use leading to lower production costs.

References:

[1)]: Lutze, P. et al.: Phenomena-based Process Synthesis and Design to achieve Process Intensification; Proc. 21st European Symposium on Computer Aided Process Engineering – ESCAPE 21, 2011, Greece

Acknowledgements:

The financial support of the German Federal Ministry of Education and Research for the project “Energy Efficiency Management and Benchmarking in the Process Industry” is gratefully acknowledged.

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