Membrane separation and membrane reactors: Methodological approach in process design

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Highlights

- A criterion describing Reactor-Separator-Recycle systems and membrane reactors is established.
- A global efficiency is determined as a function of equipment efficiencies.
- Most efficient recycling structures can be determined.

1. Introduction

Choosing unit operations is one of the most critical and early steps in process design. It will define the technologies, utilities, control strategy, by-products, etc. By this way, choosing the process steps set substantially the OPEX and CAPEX in overall project.

Integrated processes, coupled units and intensified pieces of equipment have been largely described in the last decades. Despite they are often used as tools for cost minimization and plant optimization, they are not included in conventional process design approach[1].

The main objective of this project is to identify quantitative criteria and/or rules of thumb in order to choose the most interesting operation arrangement even in the very early phases of the process synthesis approach. To do so, two specific cases are studied: membrane separator in a reactor-separator-recycle loop and its integrated equivalent: a membrane reactor.

A second stage in this work is to analyze numerical and qualitative criteria in order to decide the nature of the reactor, to determine the recycles in the sub-flowsheet and to suggest the recycling ratio optimizing the performance of the system. At the end, an algorithm defining the best superstructure and some optimal operative conditions will be designed.

2. Methods

The problem is treated in two steps, the first one is the study of conventional unit operation based system presented on the right in Figure 1. It enables to establish the nature of the decision criteria (numerical, qualitative, economical, technical, etc.) and the basic information needed to choose between an intensified and a common reactor[2]. As a secondary result in this stage, it is possible to determine the recycle ratios that maximize the global efficiency in the reactor-separator-recycle system.

The second step is the study of the integrated membrane reactor (on the left in Figure 1): it includes the mathematical modeling and characterization of transport and reaction phenomena[3]. In addition the parameters identified before as output variables or decision criteria are evaluated in order to guarantee a relevant comparison. Actually the same information is kept as input and the same variables are used as output in the coupled reactor model.

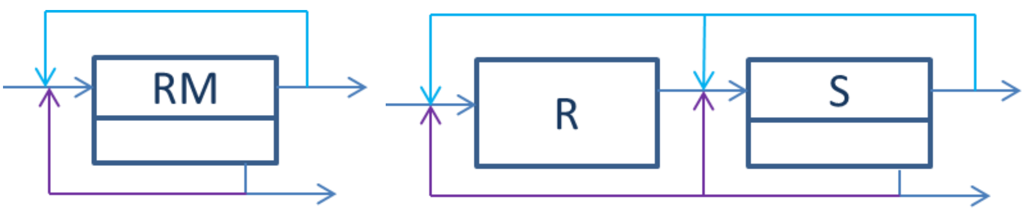

Figure 1. Superstructures studied in this work.

Finally, phenomena modeling, coupling and approach validation are performed by using numerical and simulation tools, such as Matlab, ProII, and Aspen HYSYS.

3. Results and discussion

In the first instance, the uncoupled case is studied and a technical criterion is chosen: the global efficiency. In this way, an equation to obtain the global efficiency from the local ones is deduced. This equation enables to describe the global performance of all possible structures in the reactor-separator-recycle system.

In parallel, the case study of membrane reactor has been established and equations describing a preliminary performance index have been written for the simplest cases. In both cases, it is possible to determine the global efficiency from some basic information on the reaction-separation problem: reaction kinetics, membrane selectivity and permeability and feed composition.

Also, the two expressions allow identifying the optimal arrangement of recycling streams. It is possible to determine the optimal recycling ratio for permeate and retentate in both structures. By this way, a classification of the different structures is made: it is possible to associate one of the structures depending on the reaction and separation performances. Indeed a specific unit and recycles arrangement can be chosen as a function of the basic information of the problem.

4. Conclusions

In the first part of this work, general equations describing the global efficiency of a membrane reactor and a reactor-separator-recycle were determined. For both cases, the input information was established too. By using these general expressions, it is possible to determine the feasibility of a coupled reactor, the maximum attainable efficiency and the best structure (including or not recycles of permeate and retentate) to solve a generic reaction separation problem.

Even if the global efficiency described in this work could be an important parameter in the decision-making procedure for process design, further works should focus on including economic aspects as a driving criterion to make a final choice between a coupled or an independent reactor.

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Keywords
Reactor-Separator-Recycle System; Membrane reactor; Process synthesis.