



Comparison of intensified reactive distillation configurations for the synthesis of diphenyl carbonate



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ABSTRACT

Reactive Distillation is one of the most representative examples of Process Intensification due this technology allows to simplify and to unify the reaction and separation processes in only one equipment, reducing in this way the total cost of the process. However, the RD technology can be improved through energy integration in order to reduce the energy consumption, increasing energy efficiency and economic benefits compared with conventional reactive distillation. In this paper, four intensified reactive distillation configurations for the Synthesis of Diphenyl Carbonate are compared. A conventional reactive distillation (CRD), a thermally coupled reactive distillation (TCRD) and two novel configurations with energy integration, which consist in a reactive distillation with vapor recompression (VRRD) and the second one in a hybrid process that involve thermally coupling in a reactive distillation with vapor recompression (VTCR). Economic and controllability aspects were evaluated for all of the configurations. The results show that the processes with energy integration provide significant energy savings compare with the CRD process. The result of the condition number shows that the control properties are better in the intensified process compare with the conventional process. In addition, the TCRD is the process that provides the best control properties and economic benefits.

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1. Introduction

Polycarbonate is an important engineering plastic, and it is widely utilized because of its excellent properties in the manufacturing of a wide range of products such as those found in the automotive, consumer electronics, and packaging industries. In recent decades, significant research has been devoted to the search for environmentally friendly processes and new routes to produce polycarbonate; these processes are free from highly toxic compounds, e.g. phosgene and chlorine, found in the phosgene process for polycarbonate manufacturing. One of the most relevant green routes involves the reaction between dimethyl carbonate (DMC) and phenol to carry out the transformation of DMC into diphenyl carbonate (DPC), which reacts with bisphenol-A to produce

polycarbonate. However, this route is limited because of low selectivity to DPC, side reactions, and azeotrope formation [1]. Some authors [2,3] have proposed an improved route to produce DPC and methyl acetate (MA) through the reaction between DMC and phenyl acetate (PA) to overcome the limitations mentioned above because the later route avoids azeotrope formation, and it provides a high equilibrium constant value in the reaction between DMC and PA.

In recent years, Process Intensification (PI) has become an attractive research area in academia and industry providing alternatives to develop and implement more efficient, sustainable and safe processes [4,5]. Reactive distillation (RD) is one of the best examples of PI, in RD it is possible to perform the reaction and separation operations simultaneously in a single device, this can offer significant advantages with respect to the traditional process of reaction and separation [6]. One of the most relevant advantages at the operational level of RD is the ability to increase the overall conversion and the selectivity by the continuous removal of

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reaction products from the reaction zone unit; this is particularly useful for reactions where the thermodynamic reaction equilibrium prevents high conversions. Literature offers relevant works that show the advantages that reactive distillation can provide including the potential to reduce capital investment and consumption of utilities [7–9]. In the context of PI, there is room for further development of RD by introducing more complexity in its operation. For example, by implementing heat-integrated reactive separation configurations, improvements in energy efficiency and further advantages in economic terms than conventional reactive distillation can be attained. It has been widely documented [10–13] that in separation configurations without reaction (e.g. heat-integrated configurations, thermally coupled distillation configurations) have proven to provide significant energy savings and higher energy efficiency than conventional separation configurations. However, the full implementation of these schemes has not been entirely achieved because of the operational and controllability issues and the complex control structures of these configurations, even conventional reactive distillation may pose a significant challenge when approaching a suitable control strategy.

Considering all the above, new proposals for improving RD by implementing heat integration should take into account not only economic aspects of the process but also a preliminary evaluation of controllability issues. To study the economic performance and to evaluate the controllability of intensified reactive distillation configurations through the introduction of heat integration in reactive distillation, this work compares four intensified reactive distillation configurations. The alternatives comprise two new reactive distillation configurations involving vapor recompression and thermally coupled vapor recompression, a thermally coupled reactive configuration, and a conventional reactive configuration without heat integration. To the best of our knowledge, there is no a study that involves vapor recompression and reactive distillation to synthesize DPC. The total annual cost and the calculation of a controllability index, namely the condition number for a preliminary evaluation of controllability of these designs were performed.

This paper is organized in the following sections. Section 2 provides the modeling fundamentals, including the chemical kinetics and thermodynamics of the reactive system, the details of the total annual cost calculation (TAC), and the description of the simulation of the intensified reactive distillation configurations. Section 3 contains the methodology utilized for the minimization of the TAC and condition number calculation; Section 4 offers the results of this study, and the conclusions of this work are stated in Section 5.

2. Modeling fundamentals

A comprehensive revision of the fundamentals, constraints, and specifications of the process was necessary. Thus, a proper thermodynamic model that adequately describes phase equilibria of the reactive systems was selected. Also, a suitable kinetic model for the chemical reactions in the process was selected. The simulation of each different reactive configuration was carried out using steady-state equilibrium-stage simulations using Aspen Plus V8.4[®] software. The raw materials and product specifications used during the simulations were the same for all the intensified reactive configurations under comparison.

2.1. Chemical kinetics

The synthesis of DPC from DMC and PA involves a homogenous catalyst tetra-*n*-butyl orthotitanate, the reaction has a two-step reaction that takes place through formation of the intermediate,

MPC. The first step is the transesterification of DMC and PA to the intermediate Methyl Phenyl Carbonate (MPC) and the by-product MA as in Equation (1). Two possible routes exist for the second step: The transesterification of MPC and PA to DPC and MA (See Equation (2)) or the disproportionation of MPC yielding DPC and DMC as in Equation (3):



The overall reaction is defined:



The rate expressions for the reversible reactions of Equations (1)–(3) are respectively as follows:

$$r_1 = k_1 C_{\text{PA}} C_{\text{DMC}} - k_{-1} C_{\text{MPC}} C_{\text{MA}} \quad (5)$$

$$r_2 = k_2 C_{\text{PA}} C_{\text{MPC}} - k_{-2} C_{\text{DPC}} C_{\text{MA}} \quad (6)$$

$$r_3 = k_3 C_{\text{MPC}}^2 - k_{-3} C_{\text{DPC}} C_{\text{DMC}} \quad (7)$$

The kinetic constants of the three reversible reactions are related in Equation (8).

$$\frac{k_2}{k_{-2}} = \frac{k_1}{k_{-1}} \cdot \frac{k_3}{k_{-3}} \quad (8)$$

Table 1 shows the kinetic parameters that fit with the Arrhenius Equation, this data consist in the pre exponential factor k_0 and activation energy E_a , and are necessary to the calculation of kinetic constants k_i in function of the temperature. This data were taken from previous work of Cheng et al. [2].

2.2. Thermodynamics

The reactive system consists of five components, DPC, MPC, PA, DMC, and MA; Yao [14] showed experimentally that the equilibrium liquid-vapor can be fit with the ideal model, due the boiling point temperature difference of any combination of two components in the system is large enough. Therefore the mixture exhibits ideal behavior, which can be represented by an ideal thermodynamic, so an ideal model can be suitable for the estimation of the vapor-liquid equilibrium in this system.

2.3. Total annual cost calculation

In order to objectively compare the different reactive configurations, two relevant aspects were defined in this paper. The first is the process economics, this involves the Total Annual Cost (TAC) calculation; the second aspect is the evaluation of the

Table 1
Kinetic parameters for reaction rate coefficients.

	$k_0(\text{m}^3/\text{kmol s})$	$E_a(\text{kJ}/\text{kmol})$
k_1	135	5.42×10^4
k_{-1}	52	5.49×10^4
k_2	1210	6.15×10^4
k_{-2}	611	5.62×10^4
k_3	8.20×10^4	7.68×10^4
k_{-3}	1.09×10^5	7.08×10^4

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