Chemical Engineering & Processing: Process Intensification 128 (2018) 188–198

Contents lists available at ScienceDirect

Chemical Engineering & Processing: Process Intensification

journal homepage: www.elsevier.com/locate/cep

Effects of intensification on process features and control properties of lignocellulosic bioethanol separation and dehydration systems

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ARTICLE INFO

Keywords:
Lignocellulosic bioethanol
Separation
Dehydration
Intensification
Control properties

ABSTRACT

Separation and dehydration process is a key step to reduce the total production cost of lignocellulosic bioethanol. In the earlier work (Torres-Ortega and Rong, 2016), we have obtained new intensified systems for lignocellulosic bioethanol separation and dehydration through dividing wall columns, which have considerable reduction to both capital and energy costs. This work presents the analysis of process features and control properties of the intensified systems with similar capital reduction and energy savings. The control properties were based on singular value decomposition (SVD) and dynamic performances under mild disturbances and changes of set point in Aspen Dynamics V8.8. The control properties and dynamic responses of the intensified separation systems were examined against the reference system for their structural changes during intensification by thermal couplings and column section recombination. The simultaneous analysis of process feature changes by intensification and their control properties achieved the intensified systems with both cost savings and competitive control properties.

1. Introduction

Separation and dehydration of lignocellulosic bioethanol typically starts from a fermentation broth with 5 wt. % of bioethanol, and a mixture of water, soluble organic matter, gases and insoluble solids. Once bioethanol is concentrated, it needs to be dehydrated to a purity of 99.5 wt %. However, a bioethanol-water azeotrope (95.63 wt. % bioethanol) hinders the use of conventional distillation.

Regarding separation and dehydration of lignocellulosic bioethanol, distillation and extractive distillation have attracted attention for their capability to work with large flow rates [2]; however, they are high-energy consumption technologies. In this regard, process intensification can play a significant role. We understand intensification as any process modification achieving higher efficiency, lower expenses, more environmentally friendly operation, size reduction, or any combination of the above. Examples of process intensification in distillation are membrane distillation [3], HiGee distillation [4], cyclic distillation [5], dividing wall column (DWC) [6–9], and dividing wall extractive distillation [1,10–12], among others. In spite of the potential savings, intensified separation systems still represent a minor proportion on distillation sequences due to a more challenging control know-how [13].

Control property analysis by using condition number and minimum singular values, and dynamic responses studies have shown that intensified separation systems, including DWC and Petlyuk systems, can outperform conventional column systems [14–17].

In a previous work, through systematic process synthesis and intensification using thermal couplings and column section recombination, we generated different intensified separation systems for the lignocellulosic bioethanol separation problem [1]. A column section stands for a set of trays or packing where no external mass or heat transfer takes place [18]. The selected intensified systems presented comparable total annual cost (TAC) savings with respect to a reference

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Abbreviations: σ^*, Maximum singular values; σ_*, Minimum singular value; AC, Absorption Column; CF, Centrifuge Filter; CSD, Control Structure Design; DAP, Diammonium Phosphate; DC, Distillation Column; DWC, Divided Wall Column; F, Flash; HMF, Hydroxymethylfurfural; IAE, Integral of the Absolute Error; *L*, Reflux Flowrate; NREL, National Renewable Energy Laboratory; NRTL, Non-Random Two-Liquid Model; PI, Proportional-Integral; SC, Stripping Column; SVD, Singular Value Decomposition; TAC, Total Annual Cost [USD year^{-1}]; TUC, Total Utility Coss [USD year^{-1}]; U, Direction of the process outputs; V, Direction of the process inputs; V, vapor boilup rate; wt.%, Mass Percentage; σ, Singular Values; Σ, Diagonal Matrix; γ, Condition number

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https://doi.org/10.1016/j.cep.2018.04.031
Received 28 January 2018; Received in revised form 23 April 2018; Accepted 26 April 2018

system (using conventional distillation columns). However, they had different separation train and diameters sizes, number and mass flowrate of recycles and total utilities costs (TUC) savings. Understanding how this intensification procedure (thermal couplings and column section recombination) modified these process features and their effect on control properties and dynamic responses can give further insights about which process features have more effect on control properties, and therefore suggest where the intensification should focus on. Moreover, it may also contribute to accelerate the selection from among intensified separation systems by using control shortcuts and analyzing process features in a relatively straightforward way.

Contrary to the conventional distillation process, control properties of intensified distillation columns have been little explored in the published literature, although some authors have attacked this problem. Jimenez et al. [19] have demonstrated the application of the singular value decomposition (SVD) technique to compare the controllability properties of intensified distillation structures. It is important to highlight that the dynamic model used in each equilibrium stage, for application of SVD, includes transient total mass balance, transient component mass balances, equilibrium relationship, summation constraints and transient energy balance. Similar control studies [20–22] have performed control analysis in studies of complex distillation systems. As far as we know, no study has been reported on the control properties in highly intensified distillation systems in the production of biofuels.

In the present work, we evaluated the control properties using SVD and dynamic responses (mild disturbances and set point changes) of different separation systems, as well as the effect of using thermal couplings and column section recombination as intensification tools with respect to the process features: diameter sizes, TUC savings and number and mass flowrate of recycles. This control test do not consider this process stage, indeed, analysis of operating procedures such as startup and shutdown strategies, which are transient and discontinuous by nature, so it can be considered as a separate study [23].

We expect to obtain good control properties and dynamic responses for the intensified separation systems, identify promising separation systems, and relate key process features with control properties and dynamic responses for the lignocellulosic bioethanol separation problem.

First, we explained how we selected the intensified separations systems; then, we described the evaluation methodologies followed by the most relevant results, and finally, we concluded with our observations regarding the relation between process features, and control properties and dynamic responses for the present case study.

2. Synthesis of new intensified separation systems for lignocellulosic bioethanol separation and dehydration

2.1. Separation problem and reference separation system

The separation stream of this work consisted in a mixture of gas (4.78 wt%), water and bioethanol (79.17 wt%) and soluble organic compounds (16.15 wt%). This mixture is the solids-free fermentation broth presented in previous works [1,2]. The composition and flow rate of the separation stream is described in Table 1. The reference separation system [1], is depicted in Fig. 1.

Shortly in Fig. 1, the solids-free lignocellulosic bioethanol stream was fed to the distillation column (DC-1) where most of the water and organic matter, in the way of stillage, were separated as bottom product, and the top stream sent to a set of two flashes (F-2 and F-3). F-2 and F-3 operated at different conditions and separated the gases producing a hydrous bioethanol stream sent to an extractive distillation column EDC-5. An absorption column (AC-4) recovered bioethanol dragged with the gases and sent it back to DC-1. Bioethanol purity specification was achieved when glycerol and the hydrous bioethanol were fed in EDC-5. Finally, the recovery of glycerol was done by a combination of a flash (F-6) and a stripping column (SC-7). Finally, the recovered solvent can be recycled back to EDC-5.

Table 1
Mass composition (wt%) of the lignocellulosic bioethanol separation problem.

Lignocellulosic bioethanol (solids-free)		Grouped-components	
NH_3	0.01%	**Main gas components**	4.68%
O_2	0.01%		
CO_2	4.67%		
Bioethanol H_2O	4.89% 74.28%	**Bioethanol + water**	79.17%
Glucose	0.67%	**Soluble organic components**	16.15%
Xylose	0.61%		
Extractive	1.68%		
Soluble Lignin	0.33%		
HMF	0.24%		
Furfural	0.02%		
Lactic Acid	0.15%		
Xylitol	0.05%		
Glycerol	0.01%		
Succinic Acid	0.02%		
$(NH_4)_2SO_4$	11.76%		
NH_4 acetate	0.55%		
DAP	0.07%		
Total mass flow rate:		421,064 kg/h	

2.2. Design and simulation of the separation systems

We used the process simulator Aspen Plus V8.8, thermodynamic package NRTL, Henry gaseous components, NREL physical property data (components not included in Aspen properties database) [24] and RadFrac modules to simulate the separation systems. Design parameters and operating conditions were taken from Torres-Ortega and Rong [1].

We evaluated total annual cost (TAC) according to the modular methodology of Guthrie [25,26] using the simplified expression depicted in Eq. (1), considering five years of return of investment. We defined the total utilities cost (TUC) as the summation of each equipment utilities cost, Eq. (2).

$$TAC = \sum\left[\left(\frac{Capital\ Cost_i}{Time\ of\ investment}\right) + Utility\ cos\ ts\right] \tag{1}$$

$$TUC = \Sigma[Cos\ t\ Re\ b.\ duty_i + Cos\ t\ Cond.\ duty_i + Cos\ t\ Pump\ \&\ Comp\ power_i + Cos\ t\ Solvent_i] \tag{2}$$

We approximated DWC and other intensified systems modeling by using column sections system model, Fig. 2. This model reflects better the actual situation and allows for maximum flexibility regarding specifications, and vapor and liquid splits for control studies [6]. Equivalent approximated models have been experimental validated in several studies [27–30].

2.3. Intensification procedure for separation systems

We used thermal couplings and column section recombination as major intensification tools due to the possibility to have a sequential (synthesis and design) procedure that simplifies the whole task. That is, we start with a "conventional" separation system using conventional columns and designs, and then we can synthesize further intensified separation systems based on the previous conventional system. The details of the general procedure are thoroughly discussed somewhere else [1,31–36], to name a few.

The summary of the reference and intensified separation systems results of the work presented by Torres-Ortega and Rong [1] are depicted in Fig. 3. Briefly, process intensification was applied in the separation section (to obtain hydrous bioethanol) –in blue-, dehydration section (to obtain final product) –in green-and both separation and