Chemical Engineering and Processing 105 (2016) 10–20

Contents lists available at ScienceDirect

Chemical Engineering and Processing: Process Intensification

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

Design and control of a continuous multi-product process with product distribution switching: Sustainable manufacture of furfuryl alcohol and 2-methylfuran

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ARTICLE INFO

Article history:
Received 14 December 2015
Received in revised form 15 March 2016
Accepted 11 April 2016
Available online 12 April 2016

Keywords:
Furfuryl alcohol
2-Methylfuran
Process design
Process control
Product distributions transition

ABSTRACT

A process for the sustainable simultaneous manufacture of furfuryl alcohol (FOL) and 2-methylfuran (2-MF) is designed using commercial process simulation software. The process is designed to produce 50 kmol/hr of product, and the nominal (base case) design produces 40 kmol/h of furfuryl alcohol and 10 kmol/h of 2-methylfuran. The process is designed to permit the adjustment of the product distribution from 35/15 to 45/5 furfuryl alcohol/2-methylfuran. Energy consumption is reduced by employing a feed-effluent heat exchanger and employing a 3-phase distillate receiver at the top of the distillation column and refluxing only the organic phase. Control studies suggest that a simple decentralized control structure without controller parameter scheduling can accommodate changes in the production rate and feed composition and can also transition smoothly between product distributions.

1. Introduction

As the most widely produced chemical from lignocellulosic biomass, furfural (FAL) has received considerable attention as a platform for the sustainable production of chemicals and fuels from renewable feedstocks including agricultural waste [1–4]. About 60–70% of furfural produced worldwide is converted to furfuryl alcohol, which is the major ingredient in furan foundry binders [4]. Other chemicals produced from furfural include furan, tetrahydrofurfuryl alcohol, furfurylamine, tetrahydrofurfuryl-amine, 2-methylfuran, methyltetrahydrofuran and furoic acid [4]. Tseng et al. [5] previously studied the design of a process to produce furfuryl alcohol from furfural.

2-Methylfuran is used as a solvent and as a precursor in the manufacture of various specialty chemicals. Because the demand for 2-methylfuran is considerably less than the demand for furfuryl alcohol, and because 2-methylfuran is produced as a byproduct (coproduct) in the production of furfuryl alcohol, it is not economical to produce 2-methylfuran with a dedicated process. Instead, furfuryl alcohol and 2-methylfuran are produced in the same process by the hydrogenation of furfural.

When two or more products are produced in the same process, it is desirable to control the product distribution as well as the overall production rate so that the distribution can be adjusted depending on market conditions. Planning and scheduling of multi-product batch processes has received considerable attention in the literature [6]; however, the design and control of multi-product continuous processes has received much less attention. Kapilakarn and Luyben [7,8] studied the plantwide design and control of continuous multi-product processes; however, their examples used fictitious species. Other authors have studied steady-state optimization [9] and scheduling [10,11] of multi-product continuous processes, but not dynamics and control. Therefore it is of interest to study the design and control of a realistic process with multiple products including product distribution switching.

In this work, the design and control of a process for the simultaneous production of furfuryl alcohol and 2-methlfuran including product distribution switching is considered. Steady-state process design is simulated using Aspen Plus 7.3, and process dynamics and control are modeled using Aspen Plus Dynamics 7.3.

The remainder of this work is organized as follows: in Section 2, the kinetic and thermodynamic models used in this work are presented and discussed. In Section 3, the steady state design of the process is presented, and improvements to the base-case design are presented and discussed. In Section 4, control structures are developed for the base-case and improved process and the

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http://dx.doi.org/10.1016/j.cep.2016.04.003
0255-2701/

dynamic responses including the responses to product distribution changes are reported. Finally in Section 5 conclusions are presented.

2. Kinetic and thermodynamic models

Furfuryl alcohol and 2-methylfuran can be produced by the hydrogenation of furfural in the gas phase. The reactions are:

$$\text{Furfural(FAL)} + H_2 \rightarrow \text{Furfuryl Alchohol(FOL)}$$

$$\text{Furfuryl alcohol(FOL)} + H_2 \rightarrow 2-\text{methylfuran}(2-\text{MF}) + H_2O$$

A number of researchers have studied the hydrogenation of furfural over various catalysts; unfortunately, few of them also considered the reaction that produces 2-methylfuran. The most widely-used catalyst for the production of furfuryl alcohol is copper chromite. Brown and Hixon [12] present data for the yield of furfuryl alcohol and 2-methlfuran in a reactor packed with copper chromite catalyst at temperatures between 100 and 164 °C. Based on their data, the following kinetic model was identified:

$$r_{FOL} = 9.98 \times 10^7 \exp\left(-\frac{4166}{T}\right) C_{FAL} C_{H_2}^2 \quad (1)$$

$$r_{2-MF} = 4.09 \times 10^{15} \exp\left(-\frac{14838}{T}\right) C_{FOL} C_{H_2} \quad (2)$$

where concentrations are in mol/L (kmol/m^3) and the reaction rates are kmol/s-m^3. Values of pre-exponential factors and activation energies were determined from data presented by Brown and Hixon given in Table 1. Using these data, Arrhenius plots were constructed for both reactions and the activation energies and pre-exponential factors of both reactions were determined as shown in Fig. 1. The form of Eq. (1) was suggested by Borts et al. [13] while the form of Eq. (2) assumes a first order dependence on the concentration of both reactants.

Vapor-liquid and vapor-liquid-liquid equilibria were modeled with the NRTL equation in Aspen Plus. Values of the NRTL parameters used in this work are given in Table 2. Sources of the binary parameters are given in Table 3. Interaction parameters between furfural and furfuryl alcohol and between water and furfural and water and furfuryl alcohol were available in the Aspen databank. Other sets of binary interaction parameters were regressed based on data taken from the literature as indicated in the footnotes to in Table 3. The stationary points including azeotropes predicted by Aspen Plus using the thermodynamic model are shown in Table 4. In addition to the pure components, there are binary azeotropes between furfural and water and 2-methylfuran and water. T-xy diagrams for all pairs of condensable species predicted by the model are shown in Fig. 2. Furfural and water and 2-methylfuran and water have large 2-liquid regions.

Table 1
Reaction rates at different temperatures.

Reaction 1	
T (K)	k_1 (sec^{-1} mol^{-2} L^2)
373.0	1500
381.5	1735
389.0	2110
394.3	2427
401.0	3365
Reaction 2	
T (K)	k_2 (sec^{-1} mol^{-1} L)
408.2	0.59
414.9	1.36
422.7	2.61
434.0	3.88
434.2	5.41

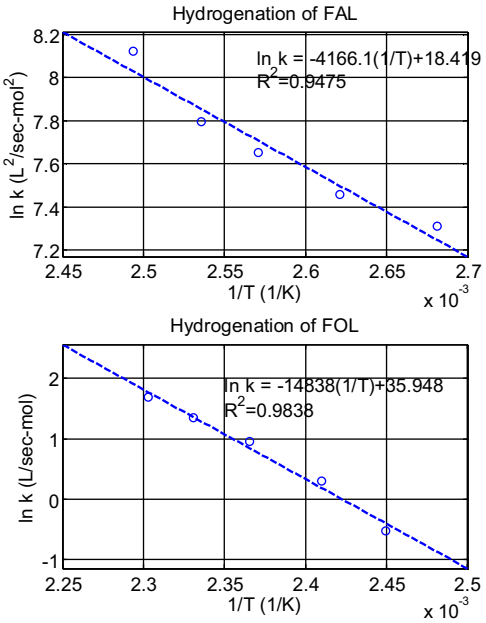

Fig. 1. Arrhenius plot of two reactions.

Table 2
NRTL binary parameters.

Component i Component j	FAL FOL	FAL H_2O	FOL H_2O	MF FOL	MF FAL	MF H_2O
a_{ij}	0	−4.7563	0	1.6859	0.007942	−14.53
a_{ji}	0	4.2362	0	0.1097	−0.001577	−1.17
b_{ij} (K)	69.0160	1911.4222	60.3941	−154.3	1319.0490	5516.6
B_{ji} (K)	24.0213	−262.2408	845.5429	−126.8	−279.9706	1432.99
α_{ij}	0.3	0.3	0.3	0.3	0.3	0.2

Table 3
Sources of binary interaction parameters.

	Furfural	Furfuryl alcohol	2-methylfuran
Furfuryl alcohol	Aspen Databank		
2-methylfuran	Regressed[a]	Regressed[b]	
Water	Aspen Databank	Aspen Databank	Regressed[c]

[a] Regressed from data reported by Holdren and Hixon [14].
[b] Regressed from data reported by Tai [15].
[c] Regressed from data reported by Tetrisyanda [16].

Table 4
Thermodynamic stationary points at 0.1 bar in the process.

Temp (°C)	Classification	FAL	FOL	MF	H2O
107.72	Stable node	0	1	0	0
92.48	Saddle	1	0	0	0
45.80	Saddle	0	0	0	1
43.40	Saddle	0.1347	0	0	0.8653
7.09	Saddle	0	0	1	0
−2.52	Unstable node	0	0	0.7743	0.2257