Furfural production through two bioconversion routes: experimental optimization and process simulation

S.G.C. Almeida[1], G.F. Mello[1], T.K. Kovacs[1], D.D.V. Silva[2], M.A.M. Costa[1], K.J. Dussán[1,3]

[1]Department of Engineering, Physics and Mathematics, Institute of Chemistry, São Paulo State University-UNESP, Araraquara, São Paulo, 14.800-900, Brazil.
[2]Department of Biochemistry and Organic Chemistry, Institute of Chemistry, São Paulo State University-UNESP, Araraquara, São Paulo, 14.800-900, Brazil.
[3]São Paulo State University (Unesp), Bioenergy Research Institute (IPBEN), Araraquara, Sao Paulo, 14800-060, Brazil

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Presenting author email: kelly.medina@unesp.br

Furfural is a furanic aldehyde obtained from the acid treatment of pentoses found in lignocellulosic material. It has excellent physical and chemical properties that allow its application in the generation of fertilizers, antacids, plastics, paints, fungicides, besides having importance as precursor of derivatives for the chemical industry, such as furfuryl alcohol and tetrahydrofuran. The objective of this study was to optimize operational conditions (temperature, solid/liquid ratio, time, and acid catalyst concentration) of the production of furfural from sugarcane biomass (50% bagasse and 50% straw) and simulate the optimal condition in Aspen Plus® under two conditions: in the first, pre-treatment and reaction occur separately (case 1); in the second, both occur in the same equipment (case 2). For the case 1: the pre-treatment of sugarcane biomass was performed in 2L reactor at 120ºC, solid/liquid ratio of 1:5, 2% (v/v) H_2SO_4 for 70 min. In this stage was obtained a hemicellulosic hydrolysate with 42 g/L total sugars. The optimization of furfural production in both cases were reached using a central composite rotational design. For the case 1: the optimal conditions of acid concentration, temperature and time were: 1.24% (v/v), 194°C and 46 min, obtaining 7.0 g/L furfural. For the case 2: the optimal conditions of acid concentration, temperature, solid/liquid ratio, and time were: 1% (w/v) sulfuric acid, 200°C, 3 S/L ratio and 70 min and it was obtained 14 g/L furfural. Both cases were simulated using an initial flow of 166.67 ton/h of biomass, leading to the yield of 15.43 ton/h of furfural in case 1, with an energy requirement of around 65 MJ per kg of pure product obtained, and 22.25 ton/h of furfural in case 2, with a requirement of around 400 MJ per kg of product. Thus, the energy integration of the process streams was made using the Aspen Energy Analyzer tool, obtaining a thermal exchange network for each case, with energy savings of approximately 85% in case 1 and 67% in case 2. In addition, the economic assessment of both cases was performed using the Aspen Economic Analyzer. All values used were indexed for the period from July to December 2018. For this period, an average exchange rate of R$ 3.884 was considered. An operating period of 200 days/year was considered. It was also considered autonomous distilleries in which the demands of heat, electricity and mechanical energy are assembled by the cogeneration plant that consumes 1/3 of the residual biomass generated in the sugar and ethanol production process. By proposing a scenario for furfural production from sugarcane biomass, revenues of US$ 164.65 million and US$ 180.55 million are generated for a co-product (sugarcane biomass) that currently only one third is being used for power generation. For case 1 the use of the solid fraction (95 t/h), obtained after hemicellulose extraction, for bioelectricity generation will increase the revenues of the current mills that will have in its portfolio besides sugar, alcohol, furfural, and bioelectricity. Furthermore, the integration of furfural production to the second-generation ethanol production chain could give sustainability to the process, favoring the full use of biomass, with the generation of higher value-added bioproduct.

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