

Production of Furfuryl Alcohol

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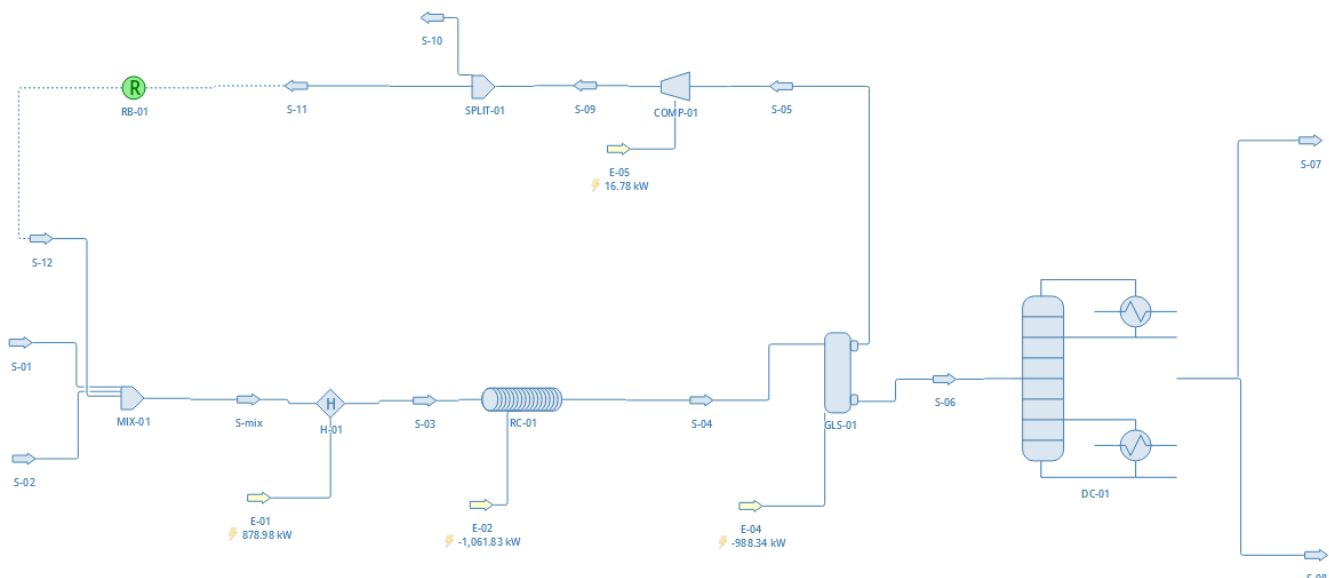
Background & Description:

The Furfuryl Alcohol (FAL) is an industrial chemical used in binders for foundry sands in the manufacture of cores and molds in metallurgy. It can be produced by gas-phase hydrogenation of Furfural with a copper chromite catalyst. Furfural is hydrogenated to Furfuryl Alcohol in a packed bed react.

Streams S-01 (51.3 kmol/h) and S-02 (51.3 kmol/h) are fed to the mixer and preheated to a temperature of 135 C prior to entering the reactor, to promote the formation of FAL. In the Flow Reactor (PFR), 2 reactions (Hydrogenation of Furfural and Production of 2- Methylfuran) of heterogeneous catalysis occur, where a conversion of FAL (C_FAL) of 99.33% is reached with a residence time of 11.31 s. Subsequently, the reaction products enter a liquid-gas separator that operates at a temperature of 40 C and 1.04 bar. The gas phase from the separator is recirculated and compressed and a part of the stream enters the mixer, where it mixes with streams S-01 and S-02. The liquid phase enters a distillation column (12 stages) that operates at a pressure of 0.27 in the lower stage (T = 133.15 C) and 0.2 in the upper stage (T = 77.3 C). The final concentration of FOL (X_FOL) at the bottom of the distillation column is 0.990, while the distillate has a concentration of H₂O (X_H₂O) of 0.516.

Thermodynamic package: Material Streams (Raoult's Law), Distillation Column (Gamma-Phi/Hayden O'Connell/NRTL/T correlation/Ideal)

Flowsheet:



Results:

The results of the simulation obtained are shown in Table 1-2, they are in agreement with those obtained by Tseng et al., (2015), who used Aspen Plus for the design and simulation of the process.

Table 1: Simulation results

Production of Furfuryl Alcohol									
Object	S-01	S-02	S-03	S-04	S-05	S-06	S-07	S-08	
Temperature	323.15	408.15	408.15	408.15	313.15	313.15	350.487	406.306	K
Pressure	130000	130000	110000	109416	104000	104000	20000	27000	Pa
Mass Flow	1.34695	0.0285583	1.50909	1.50909	0.133151	1.37594	0.147102	1.22884	kg/s
Molar Flow	14.25	14.1667	57.3056	43.4338	27.9354	15.4984	2.94659	12.5518	mol/s
Molar Fraction (Mixture) / Furfural	0.98	0	0.243694	0.0021457	5.06971E-05	0.0059219	0.000169627	0.00727227	
Molar Fraction (Mixture) / Furfuryl Alcohol	0	0	0.000510257	0.290877	0.00103564	0.813308	0.0590148	0.990383	
Molar Fraction (Mixture) / Hydrogen	0	1	0.73225	0.617562	0.960174	1.29274E-05	6.7995E-05	5.64562E-19	
Molar Fraction (Mixture) / Water	0.02	0	0.00843132	0.0402988	0.00711916	0.100104	0.516797	0.00228367	
Molar Fraction (Mixture) / 2-Methylfuran	0	0	0.0151146	0.0491166	0.0316208	0.0806524	0.423951	6.12016E-05	

Table 2: Reactor Results

Reactor (RC)		
Property	Value	Unit
Residence time	11.3135	s
FAL conversion	99.3326	%
H ₂ conversion	36.0778	%
Thermal load	-1061.83	kw

After obtaining the results through the simulation in DWSIM, it is necessary to validate the results obtained with the scientific reference, by comparing the results to calculate the percentage error. The article used for the validation of the results was carried out by Tseng et al., (2015). In the validation of the results, the most relevant results were considered. Table 2 shows the validation results.

Table 2: Simulation validation (% Error)

Variable	Description	Units	DWSIM	Tseng et al. (2015)	Error (%)
X_FOL	FOL - Molar fraction at the bottom of the column.		0.990	0.992	0.163
C_FAL	FAL - % conversion in the reaction.	%	99	99.33	0.332
F_S-03	Molar flow at the inlet of the reactor.	mol/s	57.306	60.092	4.636
F_S-04	Molar flow at the reactor outlet.	mol/s	43.434	46.264	6.117
F_S-05	Molar flow out of the separator (Reflow).	mol/s	27.935	31.995	12.688
F_S-06	Molar flow at the column inlet.	mol/s	15.498	14.269	8.614
F_S-08	Molar flow at the bottom of the column.	mol/s	12.552	13.889	9.627

References:

TSENG, Y.T., WANG, W.J., WARD, J.D. y LEE, H.Y., 2015. Design and control of a process to produce furfuryl alcohol. Journal of the Taiwan Institute of Chemical Engineers, vol. 51, pp. 44-52. ISSN 18761070. DOI 10.1016/j.jtice.2015.01.001. Disponible en: <http://dx.doi.org/10.1016/j.jtice.2015.01.001>.