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Assessment of the Exergy Performance of an Organosolv Process using Aspen Plus®

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Organosolv fractionation is a successful process to separate lignocellulosic biomass in its main component for the preparation of multiple products including biofuels, chemicals, and materials. In this study, the exergetic behaviour of the delignification process of olive tree pruning using ethanol-water as solvent media was evaluated. The experimental equipment consisted of several units, starting with a mixer, a heater, a reactor and, finally, a filtration step for the components separation. Exergetic analysis was used as the decision making tool for the evaluation of the global process efficiency by showing the sources of irreversibilities. The analysis was carried out with Aspen Plus®software. As a result, the total exergy losses found reached around 98 kW, being the heater the main responsible of this quantity, contributing with about 28.75 % of the irreversibility generated in the studied sequence. The obtained information was used as the starting point for the optimization of the process operational conditions for a better energetic behaviour.

1. Introduction

Many studies about exergy analysis to the ethanol production process from lignocellulosic materials has been reported in the literature. Ojeda and Kafarov (2009), carried out an exergetic analysis of the bioethanol production process from sugar cane. Several years later, the same authors carried out an energy and exergy analysis together with process integration methodologies for the evaluation of converting lignocellulosic biomass to bioethanol (Ojeda et al., 2011). Velásquez-Arredondo et al. (2012), analysed the efficiency of biofuels production processes by exergy analysis. In another work, an organosolv biorefinery process has also been evaluated by exergy analysis along with pinch analysis (Garcia et al., 2011).

The goal of this study is to establish a theoretical framework for the exergy analysis of an organo-ethanol process, based on experimental results, to be used as a way for its further optimization. Exergy balances were defined for each component of the process and the exergy destruction rates were calculated, identifying thermodynamic inefficiencies and revealing the potential for further improvement of the process.

2. Organosolv process description

The olive tree pruning was used as feedstock in the studied process, which was treated by ethanol water in the first step of biorefinery process. Figure 1 presents the flowsheet of the organosolv process, where the inputs and outputs are identified. Five main sections can be distinguished: (1) the delignification section, where the lignocellulosic biomass is fractionated with ethanol under well-defined operating conditions, (2) the separation section of the slurry, (3) the cellulosic solid fraction processing (washing), (4) the filtration section and (5) the precipitation of lignin (Gonzalez Alriols et al., 2010). 1 kg/h of dry raw material was mixed with 6 kg/h of ethanol –water (70 % in weight) and fed up to the reactor (200 °C).Then, the slurry from the reactor was sent to a flash unit resulting in a volatile rich vapour stream that would be condensed. Subsequently, the organosolv slurry was filtered to attain the separation of the liquor from the solid fraction. Moreover, the solid

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stream was washed in a two-step unit, using firstly a solution of organic acid and then by water. The black liquor was mixed with water to precipitate the lignin content. Finally, the output stream was filtered in Filter2.

2.1 Simulation of the studied process by Aspen Plus®

The process simulation was performed by Aspen Plus®, on the basis of experimental results obtained by Gonzalez Alriols et al. (2010), to obtain mass and energy balances. The database used for the defining of the biomass components was the one developed by the NREL (Wooley and Putche, 1996).Lignin, cellulose and hemicelluloses were defined by their chemical structure and physical properties, whereas other conventional components were selected from the ASPEN PLUS data bank (Garcia et al., 2012).The selected thermodynamic model for the simulation of the stream properties was NRTL-RK. The present pseudo-components percentages were established as 22.84 wt.% lignin, 13.47 wt.% hemicelluloses and 51.16 wt.% cellulose in the original raw material. The equipment used in the simulation is summarized in Table 1.

Table 1: Description of the equipment used in the simulation

Equipment	Description	Aspen module	Specifications
Mixer	Mixer	Mixer	1 bar
Heater	Heater	Heater	200 °C, 0 vapour fraction
Reactor	Reactor	RSTOIC	200 °C, 0 vapour fraction
Flash	Flash	Flash2	1 bar, adiabatic
Condenser	Cooler	Heater	1 bar, 0 vapour fraction
Cooler	Cooler	Heater	25 °C, 1 bar
Filter	Filter	SSplit	Solid stream at 90 % wt. of consistency
Wash	Washer	Swash	Liquid to solid mass ratio:1 Mixing efficiency :1
Wash2	Washer	Swash	Liquid to solid mass ratio:1 Mixing efficiency:1
Tank	Tank	Mixer	1 bar
Precip	Precipitation	RSTOIC	25 °C, adiabatic
Filter	Filter	SSplit	25 °C, solid stream dry

The delignification reactor was simulated by RSTOIC model, in which the reactions occurred during this step are summarized in Table 2.

Table 2: Reactions used to represent the lignocellulosic fractionation.

Reactions	Yield (%)
Cellulose (solid) cellulose (mixed)	0.34
Lignin(solid) 0.681lgnsol(mixed)+0.319lignin2(solid)	1
Xylan (solid) xylan (mixed)	0.08
Cellulose (mixed) +H2OGlucose (mixed)	0.95
Ash (solid) Ash (mixed)	0.638
Xylan (mixed) +H2Oxylose (mixed)	0.248
Extrac (solid) Extrac (mixed)	0.648

Part of the solid cellulose, cellulose (solid), was firstly converted into dissolved cellulose, cellulose (mixed). Then cellulose (mixed) was hydrated to form dissolved glucose (mixed). Similarly, the hemicelluloses that were defined as xylan were partly transformed into xylose (mixed). The lignin (solid) presented in the lignocellulosic feedstock was converted partly into dissolved ligsol (mixed) and part remained in the pulp as lignin2(solid), whereas, extractives were assumed to be exclusively formed by β-sitosterol.

2.2 Theoretical background –Formulations

The energy balance for a general steady-flow process neglecting the contribution of kinetic and potential energy, assuming steady state, can be defined by Eqs(1) and (2):

$$Energy\ input - Energy\ output = Energy\ accumulation \qquad (1)$$

$$0 = Q + W + \sum_i F_i H_i - \sum_e F_e H_e \tag{2}$$

Q and W are the heat and work added to the process, respectively, and H and F are the specific enthalpy of the material stream and the molar flow rate, respectively. Subscripts i and e refer to the inlet and outlet streams, respectively (Kaushika et al, 2011). Energy cannot be created or destroyed; it can be converted from one form to another. Exergy Flow Analysis provides a way for process assessment that can be used as a tool for identifying material wastes and energy loss, detecting areas needing technological improvements. Exergy is also a useful indicator for measuring material potential reactivity and quality, comparing different production processes of product substitutes that are especially useful when comparing renewable sources of energy (Demir et al, 2011). The exergy balance for a flow process in a system during a finite interval may be defined by Eq(3):

$$\mathit{Exergy\ input} - \mathit{Exergy\ output} - \mathit{Exergy\ consumption} = \mathit{Exergy\ accumulation} \tag{3}$$

The ‘exergy consumption’ terms in Eq(3) results from the generation of entropy within the system hence the degradation of some part of the ‘quality energy’ of the resources within the system. This destruction of exergy can also be named ‘irreversibility’ or exergy loss and it can be defined by Eq(4): (Ofori-Boateng and Lee, 2014):

$$\sum (1 - \frac{T_0}{T}) Q - W + (\sum_i m_i Ex_i)_{in} - (\sum_i m_i Ex_i)_{out} = Ex_{destruction} = T_0 S_{generation} = I \tag{4}$$

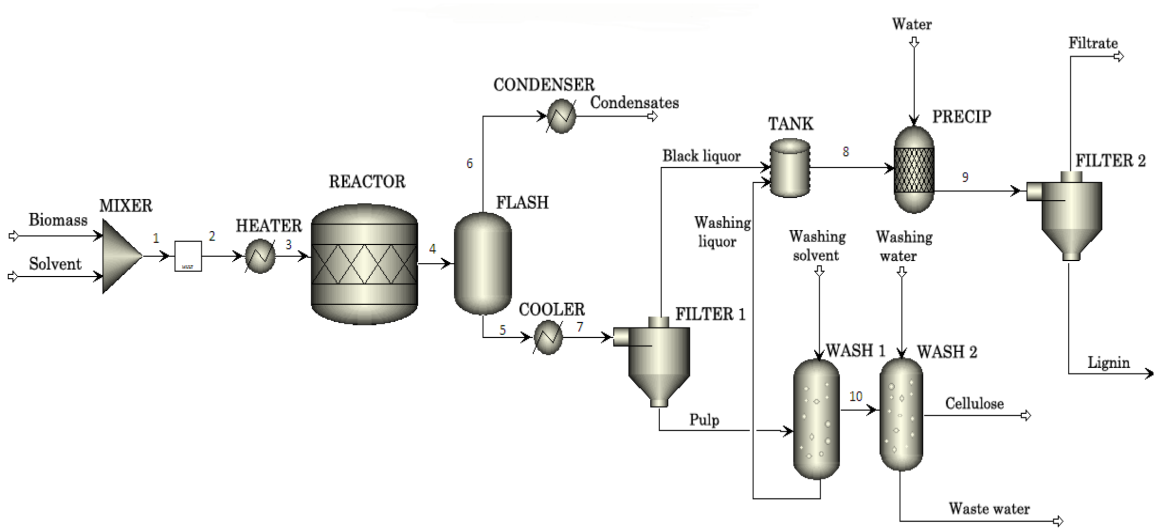

Figure1: Flowsheet of the organosolv process

3. Results

3.1 Energy analysis

The results of the main input and output streams obtained from the simulation of the studied process are presented in Table 3. The calculation basis was 100 kg/h of biomass. Mass flow (F, kmol/s), temperature (T, °C), pressure (P, bar) and energy flow (EF, kW) are shown for each stream.

The lignocellusic biomass, solvent, washing solvent and the washing water were defined as input. Otherwise, condensates, cellulose; waste water, filtrate and lignin were considered as output streams. Thus, the simulated organosolv process yield, regarding the amount of dissolved lignocellulosic feedstock, was around 53 %.

Table 3: Inlet and outlet parameters of energy flow rates of the process

Stream	F (kg/h)	T (°C)	P (bar)	EF (kW)
Solvent	600.0	25	1	1,494
Biomass	106.5	25	1	143.5
Condensates	380.8	78.8	1	841.2
Washing Water	388.7	25	1	1,710
Washing solvent	118.9	25	1	296.1
Wastewater	388.7	25.4	1	1,699
Cellulose	60.37	25.4	1	21.64
Water	758.4	25	1	3,337
Filtrate	1125	26.5	1	4,319
Lignin	12.97	26.5	1	47.37

3.2 Exergy Analysis

Materials, energy and exergy balances were calculated for each stream.
Figure 2 presents the exergy losses distribution in the process equipment.

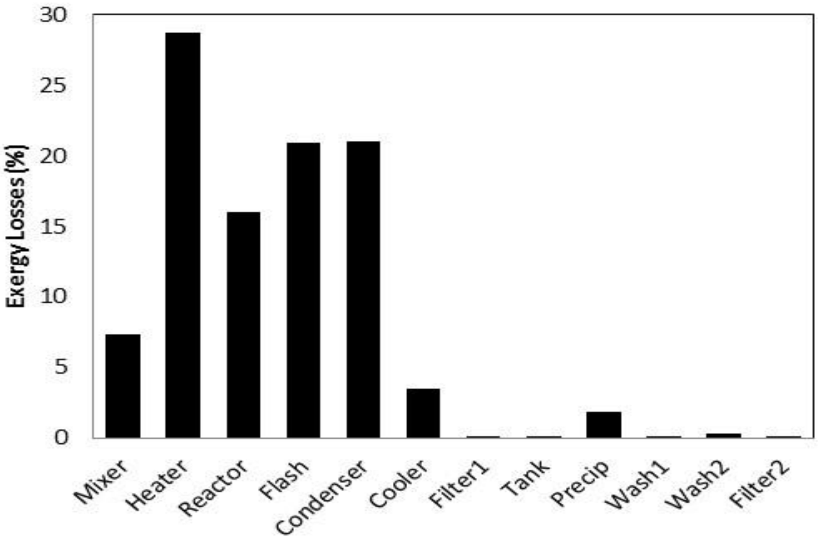

Figure 2: Exergy losses distribution

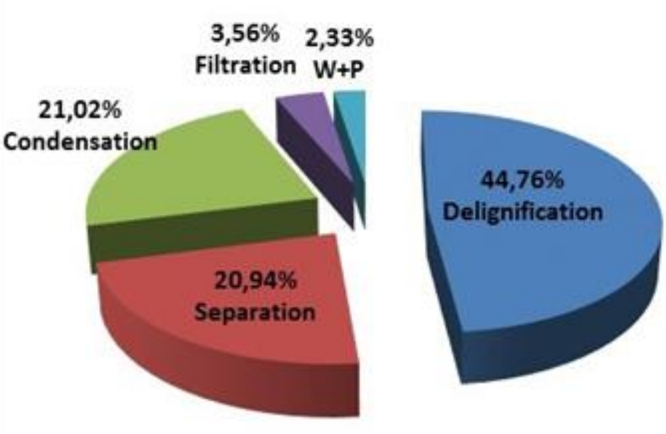

Figure3: Exergy losses contribution per sections

In fact, the exergy analysis showed that the total exergy losses of the organo-ethanol process were about 98 swathe delignification section is responsible for 44 % of the total irreversibility generated, in which the heater contributed with a 28 % and the reactor with a 16 %.The separation and condensation section contributed, respectively, with a 20.9 % and 21 % of the total losses, whereas, the exergy losses in the other sections were found negligible. Thus, the heater was found to be the main responsible of the total losses in this unit. These losses are inevitable due to the higher heat transfer between the input and output stream. Furthermore, the irreversibility generated in the reactor was considered significant as well, despite the reactions' kinetics were not considered in the study.

Table 4 presents the exergy rates.

The contribution of exergy losses in the five sections presented is summarized in Figure 3.

Table 4: Inlet and outlet parameters of exergy flow rates of the process

Stream	F (kmol/s)	T (°C)	P (bar)	Ex (kW)
Solvent	19108	25	1	3.84
Biomass	0.004	25	1	0.24
1	0.195	25	1	11.35
2	19.48	25	1	1,135
3	19.48	200	30.2	1,107
4	19.66	200	29.5	1,122
5	8.604	81.7	1	545
6	11.05	81.7	1	598
Condensates	11.05	78.8	1	619
7	8.604	25	1	548
Black Liquor	8.388	25	1	535
Pulp	0. 214	25	1	13.6
Washing Water	20.92	25	1	1,383
Washing Liquor	3. 816	24.97	1	222.7
Washing solvent	19108	25	1	220.1
10	$5.26 \times 10^{-0.5}$	24.97	1	11.07
Wastewater	5.77×10^{-03}	25.38	1	1,372
Cellulose	20.77	25.38	1	21.64
8	0.328	24.97	1	757.6
Water	12.20	25	1	2,783
9	42.10	26.48	1	3,539
Filtrate	54.20	26.48	1	3,539
Lignin	54.20	26.48	1	0.16

4. Conclusions

In this study, the exergy analysis of an organo-ethanol process, based on experimental data was performed. The results have shown that the delignification step was responsible of a 44 % of the total losses in the process, in which the heater contributed with 28 % and the reactor with a 16 %.Thus, the combination of an exergy analysis and the optimization of the process operational conditions showed to be a powerful tool to assess process feasibility and to improve its energetic performance.

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