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Assessing Distillation Processes through Sustainability Indicators Aligned with the Sustainable Development Goals

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ABSTRACT

A generally applicable framework for the evaluation of the sustainability of distillation processes is proposed by aligning indicators directly to selected sustainable development goals (SDGs) created by the United Nations. The indicators are related to the goals good health and well-being (SDG 3), clear water and sanitation (SDG 6), affordable and clean energy (SDG 7), decent work and economic growth (SDG 8), industry, innovation and infrastructure (SDG 9), responsible consumption and production (SDG 12), climate action (SDG 13) and life below water (SDG 14). A total of 12 sustainability indicators, including human toxicity potential, wastewater generation, water consumption, renewable energy share, energy demand, material footprint, profit, waste generation, recycling ratio of waste, greenhouse gas emission, eutrophication potential and acidification potential are assigned to selected SDGs. The application of the indicators is illustrated by two case studies: a batch (BD) and a continuous (pressure-swing) distillation process. Case BD6, where the CO_2 emission was minimized, proves to be the most sustainable BD process. It has the lowest greenhouse gas emission, acidification potential and waste generation. Although it has the lowest profit, the variations across the BD cases are minimal. By the pressure-swing distillation, L4 (feeding into low-pressure column, heat integration with optimization) is the best case, with the highest profit and the lowest energy demand, material footprint and greenhouse gas emission values.

Keywords: Distillation, Continuous Distillation, Batch Distillation, Environment, Energy, Sustainability

INTRODUCTION

There has been a growing interest in sustainability in chemical engineering as industries aim to reduce their environmental footprint without compromising economic performance. This research proposes a set of sustainability indicators aligned with the United Nations' Sustainable Development Goals (SDGs) [1] for the evaluation of the sustainability of distillation processes, offering a structured way to assess and improve these systems. The use of these indicators is illustrated in two case studies: (1) a continuous pressure-swing distillation (PSD) of a maximum-azeotropic mixture without and with heat integration and (2) the recovery of acetone from a waste solvent mixture by batch distillation (BD). These processes were selected due to their widespread industrial use, their potential to benefit from improvements in their sustainability, and to show the general applicability of the indicators proposed.

Distillation is one of the most commonly used methods for the separation of liquid mixtures. It is performed in a continuous way when large processing capacities are needed (e.g. refining). Batch distillation is also used frequently (e.g. in the pharmaceutical industry) because of its flexibility in separating mixtures with varying quantity and composition, including waste solvent mixtures. However, distillation is very energy-intensive, leading to high operational costs and greenhouse gas emissions. In fact, distillation stands out as the most energy-consuming process in the chemical industry, using more than 40% of the total energy demand of an industry itself responsible for 30% of industrial energy usage in the US.

This study aims to address these issues by propos-

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ing sustainability indicators that account for environmental, economic and social aspects. By aligning these indicators with the SDGs, as globally recognized sustainability standards, the research also aims to encourage industries towards more sustainable practices. To our knowledge, this work is the first to propose sustainability indicators aligned with SDGs in the field of distillation.

The case studies illustrate how to apply the proposed indicators to evaluate the sustainability aspects of distillation processes. In the PSD example [3], the process was optimized without and with heat integration, which led to a significant decrease in both the total annual cost (TAC) and environmental impact (CO_2 emission). In the acetone recovery by BD case [4], either the profit or the CO_2 emissions were optimized. In this work, we determined how the proposed sustainability indicators improved due to the optimization and heat integration performed in these previous works.

This study focuses on addressing a key gap by aligning the evaluation of distillation processes directly with the SDGs. This ensures that the results contribute not only to advancing methodological approaches but also directly support global sustainability goals. Therefore, in this study, we propose a set of sustainability indicators aligned with SDGs.

Another key novelty of this study is that, while traditional techno-economic analysis (TEA) focuses on economic feasibility and life cycle assessment (LCA) on environmental impact, our approach simultaneously incorporates both dimensions.

This framework could also be applied to any process with well-defined inputs and outputs where emissions and products are generated.

METHODOLOGY

The following potentially distillation-related SDGs are selected: good health and well-being (3), clean water and sanitation (6), affordable and clean energy (7), decent work and economic growth (8), industry, innovation and infrastructure (9), responsible consumption and production (12), climate action (13), life below water (14). For each SDG, the UN has selected different targets, each of which has one or more numerical indicators assigned. However, these SDG indicators can only be interpreted at regional or higher levels, making them unsuitable for assessment of technological processes. Within the selected SDGs, the following relevant targets are identified: reduction of deaths and illnesses from hazardous chemicals and environmental pollution (3.9), improving water quality by reducing pollution and increasing water-use efficiency across all sectors (6.3 and 6.4), increasing the share of renewable energy in the global energy mix and improvement of energy efficiency by 2030 (7.2 and 7.3), improving global resource efficiency in consumption and production (8.4 and 12.2), added manufacturing value (9.2), reduction of CO_2 emission and greenhouse gases (9.4, 13.2), proportion of hazardous waste treated (12.4), recycling rate (12.5), marine pollution by eutrophication (14.1) and acidification (14.3) [1].

After selecting the relevant targets and the more specific SDG indicators proposed by the UN that could be linked to distillation studies, sustainability indicators were aligned to the SDG indicators and defined. The selected SDG indicators and their aligned sustainability indicators can be found in Table 1.

The indicators could be expressed either as absolute or relative (specific) values. In the latter case, which is selected here, they are expressed relative to the total mass or mass flow rate of the product(s) (m_p). It must be noted that many of the quantities used for the calculation of the indicators have different units depending on whether the process is batch or continuous. In the former case, masses are used, in the latter, mass flow rates. Nevertheless, the indicators always have the same units.

Human toxicity potential (HTP) [5] weighs thethe masses of potentially toxic components (for components i=1…n, where n is the number of components) in the waste streams with their characterization factor (CF). Wastewater generation (WwG) and water consumption (WC) contain the total wastewater mass flow rate (m_{ww}) and the total mass flow rate of water used in the process, respectively. Renewable energy share (RES) is the ratio of total energy from renewable energy sources (E_r) to total energy demand (E); the latter value is used in the energy demand (ED).

The material footprint (MF) takes into account the mass of equipment (m_{eq}) and additional materials consumed during the operation, such as entrainer or reagents. Since the installation of the equipment only happens once, the mass of additional materials and m_p should be calculated for the lifetime of the plant to ensure a fair comparison. Profit (P) is calculated by net income (I) after the costs (C). I typically includes the value of the products. Waste generation (WG) contains the total mass of liquid waste (m_{lw}). Recycling ratio of waste (RRW) is the ratio of the mass of the recycled waste (m_r) to m_{lw}. The greenhouse gas emission (GHG) [6] expresses the total mass emissions of the process in CO_2 equivalents. This value could be calculated with different time horizons of GWP (e.g., 20 y). CO_2 emissions as an indicator could be aligned with 9.4.1, but it would be redundant as it is already included in GHG. By the eutrophication potential (EP) [7] the emissions of components in waste streams are weighted by their potency factor (PF). The acidification potential (AP) [6] refers to only the aquatic acidification potential, calculated from the total mass of released H^+ ions (m_{H^+}), as we assume, as a worst-case scenario from the point of view of aquatic life, that gaseous emissions would be completely absorbed in surface waters.

Table 1: Selected UN SDG indicators and their aligned indicators with the equations.

SDG Indicators	Indicator Name	Indicators	Formula	
3.9.1	Air pollution mortality rate	Human toxicity potential (HTP)	$HTP = \frac{\sum_{i=1}^{n}(m_i \cdot CF_i)}{m_p}$	(1)
3.9.3	Unintentional poisoning mortality			
3.9.2	Water and sanitation mortality rate	Wastewater generation (WwG)	$WwG = \frac{m_{ww}}{m_p}$	(2)
6.3.1	Wastewater treated safely			
6.3.2	Good ambient water quality			
6.4.1	Water-use efficiency change	Water consumption (WC)	$WC = \frac{m_w}{m_p}$	(3)
6.4.2	Water stress level			
7.2.1	Renewable energy share	Renewable energy share (RES)	$RES = \frac{E_r}{E}$	(4)
7.3.1	Energy intensity	Energy demand (ED)	$ED = \frac{E}{m_p}$	(5)
8.4.1	Material footprint	Material footprint (MF)	$MF = \frac{m_{eq} + m_a}{m_p}$	(6)
9.2.1	Manufacturing value added	Profit (P)	$\mathrm{P} = \frac{I - C}{m_p}$	(7)
12.2.1	Material footprint			
12.4.2	Hazardous waste generation	Waste generation (WG)	$\mathrm{WG} = \frac{m_{lw}}{m_p}$	(8)
12.5.1	Recycling rate	Recycling ratio of waste (RRW)	$RRW = \frac{m_r}{m_{lw}}$	(9)
9.4.1	CO_2 emission	Greenhouse gas emission (GHG)	$GHG = \frac{\sum_{i}^{n}(m_{GHG,i} \cdot GWP_i)}{m_p}$	(10)
13.2.2	Total GHG emission			
14.1.1	Coastal eutrophication	Eutrophication potential (EP)	$EP = \frac{\sum_{i}^{n}(m_i \cdot PF_i)}{m_p}$	(11)
14.3.1	Marine acidity	Acidification potential (AP)	$AP = \frac{m_{H^+}}{m_p}$	(12)

RES and WC are not calculated, as renewable energy sources and freshwater were not used in the case studies. However, they were added as indicators to propose a framework that could be applied to all distillation processes.

CASE STUDIES

Pressure-swing distillation

A maximum-boiling azeotropic water(A)–ethylenediamine(B) mixture is separated by PSD [3]. The flow rate of the fresh feed is 100 kmol/h with a composition of 35 mol% A. As calculated by the UNIQUAC model, the azeotrope contains 44.1% A at 0.10 bar and 25.6 % A at 2.02 bar, which are the two column pressures. Since the feed composition is between the azeotropic ones, it can enter either the high- (HPC) or the low-pressure column (LPC), resulting in two possible sequences: HP-LP (Figure 1) and LP-HP. The distillate of HPC is A with a purity of 99.5 %. The bottom product of HPC is fed into LPC, where B is produced as distillate in a purity of 99.5 %, and the bottom product, whose composition is near the azeotropic one at the pressure of LPC, is recycled to HPC.

By the PSD cases (Table 2), H and L identify the column sequences HP-LP and LP-HP. H1 and L1 refer to cases without heat integration (NHI) and optimization, and H2 and L2 mean optimized NHI cases. H3 and L3 denote the application of heat integration to the optimal NHI without further optimization, while H4 and L4 refer to optimized heat-integrated cases. TAC was the objective function. Heat integration is achieved by heating the reboiler of the LPC by condensing the top vapor of HPC. The integration is partial in all cases except H4, meaning that an auxiliary condenser is needed to fully condense the vapor. By H4, full heat integration is optimal, where the heat duties of the condenser of HPC and reboiler of

LPC are equal.

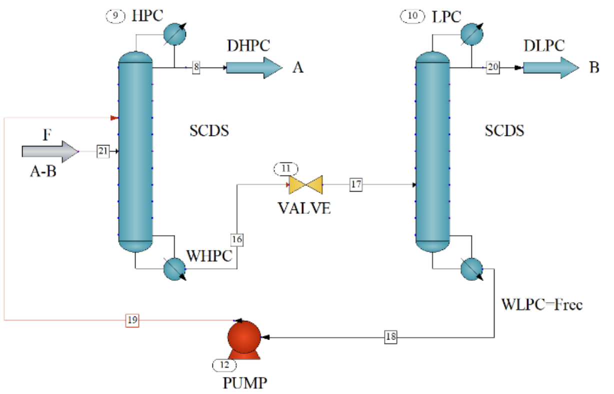

Figure 1. ChemCAD flowsheet for the separation of the A-B mixture with feeding into HPC.

By L2, surrogate model-based optimization was used with models fitted to the simulation results by using ALAMO. By H2, H4 and L4, TAC was minimized by an elitist, real-coded genetic algorithm.

HTP is not calculated since CF of B is not available. The only waste stream is the distillate of HPC, and it is considered as wastewater. Thus, WG equals WwG. The total energy demand is the sum of the two reboiler duties. MF takes the shell weight of the columns (calculated by CHEMCAD) into account during their lifetime (assumed to be 10 y), while GHG consists of the CO_2 emissions related to the production of heating steam. RRW is zero since there is no waste recycling. AP is also zero because the waste stream is basic. P was calculated as the yearly income minus TAC, the former of which is the mass of the B product and the price of B (1682 US$/t [8]). For the calculation of EP, the mass of B in the waste is multiplied by its COD value and PF of 0.022, as well as its nitrogen content with a PF of 0.42 [9].

Recovery of acetone by batch distillation

From an aqueous waste solvent mixture containing dichloromethane (A) and methyl tert-butyl ether (B) as pollutants, acetone (C) is recovered by BD [4]. The composition of the feed is 1 mass% A, 1% B, 49% C and 49% water (D). The purity requirements for the acetone product are: ≤0.1 mass% A, ≤0.1% B and ≤ 0.25% D.

The components form three minimum-boiling (A-D, B-C, B-D) and one maximum-boiling (A-B) binary azeotropes, as well as a ternary saddle azeotrope (A-B-C). The VLLE calculations were performed by UNIQUAC.

The recovery of C is performed in a BD column with 25 theoretical trays (not including the reboiler and the condenser) at atmospheric pressure. The volume of the charge is 20 m^3 (17,785.9 kg). The reboiler duty is 1800 MJ/h. The steps of the process are as follows:

1. A and the majority of B are removed in Fore-cut1, although with a considerable loss of C due to the B-C azeotrope. This fore-cut is incinerated. The reflux ratio of the step (R_1) and its stopping criteria (Cr_1) are optimized.
2. Fore-cut2 is taken to remove the remaining amount of B. It is recycled to recover its C content. R_2 and Cr_2 are parameters optimized.
3. The main cut is high purity C. A relatively high R_3 (optimized) is needed due to the C-D tangent azeotrope.
4. The C content of the still residue (wastewater) is decreased to the necessary extent (0.2 %) for biological purification by taking an after-cut. R_4 is optimized.

The cases of BD (Table 3) are as follows: by BD1 Fore-cuts 1 and 2 are taken as a single fore-cut. By BD2 the fore-cut is divided into two parts with no other modification. BD3 and BD4, respectively, denote the cases with the highest profit and lowest specific CO_2 emission obtained by modifying a single input variable by sensitivity studies. BD5 and BD6 refer to cases with maximum P and minimum CO_2, optimized by the complex method.

In HTP, the HCl emission (CF=24) from the incineration of the A content of the fore-cut and the C emission (CF=0.079) in the still residue are taken into account [9]. WwG includes the wastewater from the still residue. MF was calculated by the shell weight of the column (1727 kg) divided by the total mass of the product for the lifetime of the plant (10 y). In WG, the total mass of liquid waste includes the fore-cut(s), the after-cut and the still residue. To calculate RRW, the recycling of the after-cut and second fore-cut was considered. GHG considers the CO_2 emissions resulting from the incineration of the fore-cut and that from the generation of heating steam. EP is calculated from the emission of C in the still residue multiplied by its COD value and PF=0.022. For AP, the mass of H^+ ions was calculated from the HCl emission.

RESULTS

Pressure-swing distillation

Table 2 shows the results of PSD cases. WwG=WG and EP were constant (0.163 kg/kg and 3.10 mg/kg) in all cases as the waste stream and m_p were the same. Therefore, these values are not given in Table 2.

H1 had the highest ED, making it the most energy-intensive case. H1 also had the lowest P and highest GHG. While MF remained high due to larger diameters and shell weight of the columns. These factors indicate that H1 is the least favorable case in terms of overall sustainability. This is due to the fact that it did not benefit either from the heat integration or from the optimization.

L1 performed slightly better than H1 with a reduced ED (by 15%) because of lower heat duties while maintaining a comparable P. It also showed a lower GHG(by 15%) due to its reduced ED, reducing its overall environmental footprint.

By H2, the optimization reduced both the capital cost and the heat duties of the columns. H2 had a much

Table 2: Calculated sustainability indicators for PSD cases.

Indicators	**PSD cases**							
	H1	**L1**	**H2**	**L2**	**H3**	**L3**	**H4**	**L4**
ED, MJ/kg	8.71	7.38	7.26	6.97	4.60	4.20	4.44	4.18
MF, mg/kg	285	294	293	240	293	240	269	178
P, $/kg	1.59	1.60	1.60	1.61	1.63	1.63	1.63	1.63
GHG, kg/kg	0.13	0.11	0.11	0.11	0.07	0.06	0.07	0.06

lower ED (by 17%) than H1 and a slightly higher P. It also had a much lower GHG (by 15%), while its MF increased slightly (by 3%).

L2 had a lower ED (by 5%) and a reduced MF(by 18%) compared to L1. Its P was slightly (by 1%) higher than that of L1, with a similar GHG value. L2 is more favorable than H2 in all respects.

H3 had a much lower ED (by 47% and 17%) compared to H1 and H2 due to the usage of the top vapor of HPC to heat the reboiler of LPC. Thus, compared to H2, it also had a higher P (by 3%) while. its GHG () was significantly (by 36%) reduced, making it one of the better cases. However, MF remained high.

L3 showed further improvement, having a lower ED (by 40%) compared to L2 due to the heat integration. It maintained a high P and a similar MF, as well. With the second lowest GHG, L3 emerges as one of the most environmentally sustainable cases, balancing profitability and reduced emissions.

H4 had an even lower ED (by 3%) than H3, although it was still higher than that of L3. It maintained a high P and its MF was also lower than that of H1 (by 6%) or H2 (by 9%) but still higher than L2. Its GHG was comparable to H3, showing a good sustainability performance.

L4 was the most sustainable case, with the lowest ED (7.86 MJ/kg), MF (178 mg/kg), and GHG (0.06 kg/kg) values, while its P (1.63 $/kg) was the highest. These factors indicated that L4, benefiting from both heat integration and optimization, is the most sustainable option.

Batch distillation

Table 3 shows the results of BD cases. As it had the highest amount of incinerated fore-cut, BD1 had the highest HTP among all cases. For the same reason, it also had the highest GHG, making it the least sustainable in terms of environmental impact. WwG was 1.12 kg/kg. It had the second lowest P and RRW. It had a high MF and a relatively moderate EP and the highest AP. Additionally, BD1 generated the second most waste and had a high ED, contributing to its lower sustainability profile. These results could be explained by the fact that BD1 had a single fore-cut that was incinerated, thus causing more environmental impact and incineration cost.

BD2 showed a significantly lower HTP (by 14%) since the amount of incinerated material decreased. It had the highest P due to the high m_p and lower incineration cost. The values of WwG, ED, WG, MF, EP, and AP did not change compared to BD1. RRW was the highest among all cases. Its GHG was reduced considerably (by 26%) compared to BD1 because less fore-cut was incinerated. BD3, where R_2 was considerably decreased, benefited from the sensitivity study and had slightly lower HTP and WwG values than BD1 and BD2. It had the lowest ED, one of the lowest MF and WG, and performed slightly better in terms of GHG (by 5%) than BD2. P was between BD1 and BD2. It also had a reduced AP (by 6%) and EP (by 3%) compared to BD2, indicating a more sustainable process than BD1 and BD2. These changes can be explained by a higher m_p and lower operation time.

Table 3: Calculated sustainability indicators for BD cases.

Inds.	**BD cases**					
	BD1	**BD2**	**BD3**	**BD4**	**BD5**	**BD6**
HTP, kg/kg	0.56	0.48	0.46	0.47	0.46	0.46
WwG, kg/kg	1.12	1.12	1.09	1.10	1.08	1.08
ED, MJ/kg	5.84	5.84	5.29	5.87	5.37	5.90
MF, mg/kg	95.3	95.3	92.5	93.7	92.1	92.4
P, $/kg	1.18	1.21	1.19	1.20	1.19	1.17
WG, kg/kg	1.33	1.33	1.26	1.29	1.23	1.23
RRW, kg/kg	0.03	0.07	0.05	0.07	0.03	0.05
GHG, kg/kg	0.44	0.32	0.31	0.30	0.29	0.26
EP, mg/kg	0.35	0.35	0.34	0.33	0.41	0.25
AP, mg/kg	83.0	71.0	66.9	68.6	66.3	66.7

By BD4, R1 was increased compared to its value by BD2. This decreased the mass of both fore-cuts and increased m_p. BD4 had a similar HTP to BD3. It also had the second-highest ED value due to a slight increase in the operation time. MF and WwG were both slightly (by 2%) lower than by BD2. It had a lower GHG (by 6%), as well as slightly reduced WG (3%) and AP (by 3%) compared to

BD2. It had the second-highest P and the second-lowest EP.

By BD5, the profit (in $) was maximized. It had the lowest HTP and WG, and the second lowest ED. WwG was relatively low. P was very similar to BD3. Its GHG value was relatively low. While it showed the lowest AP, its EP was the highest. Overall, BD5 is favorable in terms of sustainability.

BD6, where the CO_2 emission was minimized, emerged as the most sustainable case. It had the lowest GHG and EP, second-lowest HTP and AP WG values. However, it had the highest ED and lowest P value mostly because of the increased operation time. However, the difference in P among the BD cases was very small.

CONCLUSIONS

To assess the sustainability of distillation processes, a set of sustainability indicators, directly linked to sustainable development indicators of the United Nations, were proposed. Sustainable development goals (SDGs), targets and, finally, the sustainable development indicators were selected by considering their fit to distillation studies.

8 out of 17 SDGs were selected, and they include good health and well-being, clear water and sanitation, affordable and clean energy, decent work and economic growth, industry, innovation and infrastructure, responsible consumption and production, climate action and life below water.

A set of (12) sustainability indicators aligned with those of UN's included human toxicity potential (HTP), wastewater generation (WwG), water consumption (WC), renewable energy share (RES), energy demand (ED), material footprint (MF), profit (P), waste generation (WG), recycling ratio of waste (RRW), greenhouse gas emissions (GHG), eutrophication potential (EP) and acidification potential (AP).

This framework was applied to a batch (BD) and a continuous (pressure-swing, PSD) distillation case study to evaluate their performance in terms of sustainability. Six cases were studied for BD evaluating the effects of the division of the fore-cut, sensitivity studies and optimization of the profit or the CO_2 emissions. PSD cases include scenarios such as no heat integration and no optimization, optimized without heat integration, heat integration without optimization, and optimal heat integration. These scenarios were studied for two column sequences differing in whether the feed was introduced into high- or the low-pressure column.

In the case of PSD, the most sustainable operation was L4 (heat-integrated and optimized by GA, feeding into the low-pressure column). It had the lowest ED, MF and GHG, while the highest P value. Among the BD cases, BD6 (minimized CO_2 emission) had the best overall sustainability: lowest GHG, WwG and EP and second lowest HTP, MF, WG and AP values.

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