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Environmental Impact of Simulated Moving Bed (SMB) on the Recovery of 2,3-Butanediol on an Integrated Biorefinery

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ABSTRACT

2,3 butanediol (BDO) has garnered recent interest due to the high titer concentrations that can be obtained through biochemical routes and its potential for efficient conversion into long-chain hydrocarbons. BDO separation, however, is challenging given its low volatility and high affinity towards water. In this study, two BDO separation pathways were compared, single distillation and combined simulated moving bed (SMB) adsorption with distillation. The separations were incorporated into a 2018 biorefinery design developed by the National Renewable Energy Laboratory (NREL) to produce renewable fuels from corn stover, with BDO as an intermediate and adipic acid as the co-product. The comparison was performed on the basis of sustainability, using lifecycle greenhouse gas (GHG) emissions as the metric. It was found that using a single distillation column gives GHG emissions of 48 g_{CO2e}/MJ for the renewable fuel. This is lower than 93 g_{CO2e}/MJ for petroleum fuel but is higher compared to the SMB-based process which achieves 21 g_{CO2e}/MJ. Additionally, the minimum fuel selling price (MFSP) of each pathway was computed. Single distillation gave a minimum MFSP of $2.54/GGE (gallon of gasoline equivalent) of fuel, while SMB reached $2.45/GGE. The SMB's MFSP is lower than the Department of Energy's (DOE) target of $2.50/GGE, demonstrating this pathway is both an economic and sustainable alternative and a sound separation candidate that can enable the viability of the entire biorefinery. The effect of BDO fermentation titer was also considered through a sensitivity analysis.

Keywords: Adsorption, Biofuels, Distillation, Life Cycle Analysis, Technoeconomic Analysis.

INTRODUCTION

2,3 butanediol (BDO) is a molecule of high interest in the chemical and energy industries that is commonly used as an intermediate for added-value products. BDO is commonly produced by the catalytic conversion of C4 components from hydrocarbon mixtures [1]. Although high conversions can be achieved, these pathways have expensive operating costs and still rely on fossil fuels. This has kept BDO from becoming a sustainable and widespread chemical. Recent advances in the biochemical production of BDO from biomass-derived sugars, and high fermentation titers (50-110g/L), have led to an increased attention to this molecule [2].

BDO is seen as a platform to help decarbonize hard-to-abate sectors, such as heavy transportation (trucking and aviation). It has a higher heating value and is less volatile than more commonly produced compounds like ethanol or butanol. Thus, at high purity values it can be used as blendstock or even directly as a drop-in fuel. BDO can also be an intermediate to produce renewable hydrocarbons. Its four carbons and two hydroxyl groups allow the dehydration into high carbon alkenes, which could facilitate subsequent oligomerization and hydrotreating steps. Most notably, in 2018 the National Renewable Energy Laboratory (NREL) [2] developed a process design that details the production of a renewable 50/50 diesel+naphtha fuel product from corn stover. BDO obtained from fermentation is the key intermediate of this process and adipic acid is the main co-product. This design will be referred to as the state-of-technology (SOT). **Figure 1** shows a high-level diagram of the SOT. The insidebattery limit (ISBL) includes alkaline pretreatment, hydrolysis, fermentation, upgrading to fuels and co-product trains. This is an integrated biorefinery, where utilities and other services are provided internally, including combined heat and power (CHP), cooling and wastewater facilities in the outside-battery limit (OSBL).

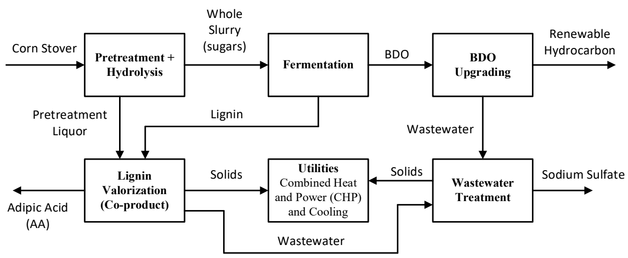

Figure 1. High level diagram of the NREL SOT process. Adapted from Davis et al, 2018 [2]

As seen, the ISBL in the SOT lacks a separation step that recovers BDO post-fermentation. This dilute broth (~100g/L BDO titer) is directly sent to the to the dehydration reaction. In reality, however, is unlikely for the reactor to efficiently upgrade BDO at dilute conditions, making the separation a required step in the plant. **Figure 2** shows a more detailed diagram of the modified upgrading portion of the SOT, with the proposed separation located between fermentation and dehydration to concentrate BDO.

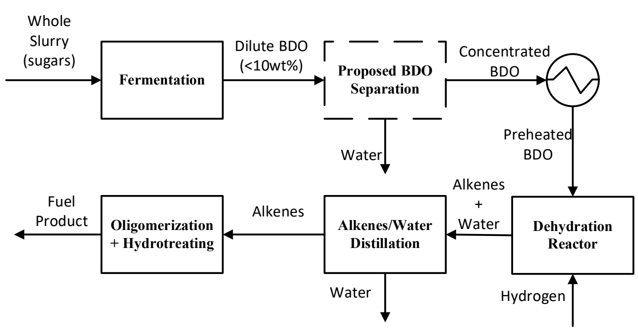

Figure 2. Block diagram based on NREL SOT's [2] main processes downstream of the fermentation

Rejecting water reduces stream size, which directly affects other units. This includes the preheater before dehydration, the dehydration reactor itself and the post-dehydration separation (alkenes/water distillation). The decrease in stream size reduces equipment size, leading to lower capital costs. Most importantly, the BDO preheating energy is also reduced, significantly decreasing operating costs and fuel usage. This leads to much smaller CO2e emissions that can make the fuel product a sustainable substitute of fossil hydrocarbons.

Nevertheless, BDO separation from a dilute aqueous mixture is challenging. BDO's high boiling point (177°C) and affinity towards water make distillation highly energy intensive. Simulated moving bed (SMB) adsorption is proposed as an alternative. Adsorption is a material-based separation, and SMB can enrich BDO to the required purity levels, without incurring in large operating expenses.

The main objective of this study is to compare the lifecycle of two pathways that recover BDO from a fermentation broth: 1) simple distillation and 2) SMB + distillation. Greenhouse gas (GHG) emissions was chosen as the sustainability metric, which is minimized for each pathway through deterministic optimization. To ensure the biorefinery is viable, the resulting design is subject to a minimum economic performance.

PROCESS DESCRIPTION

Single Column Distillation

Figure 3 shows the possible separation alternatives to recover BDO. Single distillation bypasses the SMB and sends the broth directly to the column. This process operates under mild vacuum (0.1-0.5 bar) to prevent high temperatures that could lead to side reactions and sugar degradation. A tray efficiency of 80% was assumed and the number of theoretical stages was fixed at 20. This number was found to offer an optimal balance between capital and operating costs through a sensitivity analysis of the total annualized cost.

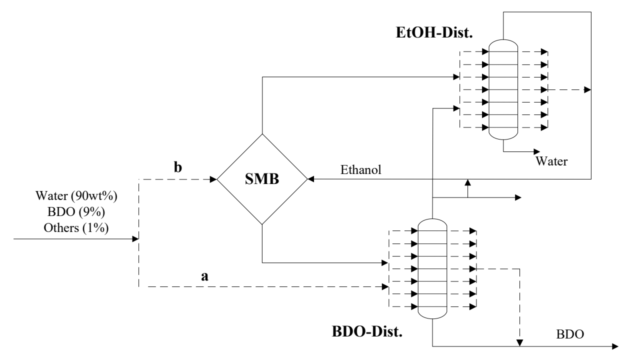

Figure 3. High level process diagram of the proposed BDO separation alternatives: a) single distillation colum and b) SMB + distillation

Water primarily exits the condenser as distillate, while BDO is recovered from the bottoms. The broth impurities leave the column through either the distillate or bottoms, depending on the volatility. Organic acids (malic, lactic and acetic) and inorganic ions (Cl^- and $SO4^{2-}$) are recovered from the distillate. Acetoin, glycerol, xylitol and residual sugars (arabinose, xylose and maltose) are retreived from the bottoms. The concentration of these impurities is very small (<1%) in all streams and their presence is not expected to considerably affect the cost.

Simulated Moving Bed + Distillation

The core of the proposed novel separation is the simulated moving bed (SMB) adsorption unit. SMB adsorption is a technology that mimics movement of solid throughout the bed by fixing the adsorbent and rotating instead the inlet and outlet ports. A 4-4-4-4 SMB is considered, where each column is packed with pure silica MFI-type zeolite, a highly hydrophobic material that is very selective towards BDO. Ethanol was chosen as the SMB desorbent. It has enough affinity with the adsorbent to efficiently displace the adsorbed BDO, and is highly volatile, facilitating its recovery via distillation. Following the SMB are two distillation columns, one to recover BDO from the extract and the other to recover ethanol from the raffinate.

A case study for PAREX [3], a well-known industry-scale SMB process, was used to guide column size (length and diameter), maximum column velocity, Peclet number and other high level operating decisions. Both distillation columns were modelled with the same approach as the single column. A tray efficiency of 50% was assumed for ethanol/water. Through a total annualized cost sensitivity analysis , 30 theoretical stages were found to offer the optimal trade-off between capital and operating costs for both columns.

METHODOLOGY

Physical Parameters

Figure 4 shows the stepwise approach that was followed to perform the comparative study. For either case, the first step was obtaining the key physical parameters needed to model either separation unit. For distillation, UNIQUAC was used to compute activity coefficients. The ASPEN Plus V.12. database [4] was used to retrieve the interaction parameters of the binary pairs. These coefficients are based on experimental vapor liquid equilibrium (VLE) data. This database was also used to retrieve the coefficients needed to calculate vapor pressure, heat capacity and reference enthalpy of each component.

For adsorption, a linear driving force (LDF) assumption was used to model the mass transfer from the bulk liquid into the solid adsorbent. The equilibrium in the adsorbent was represented with a Mixed Linear + Langmuir (MLL) isotherm. The relevant parameters are then the apparent mass transfer coefficient, $k_{app,i}$, Henry's linear constant, H_i, saturation capacity, $q_{m,i}$, and Langmuir's affinity, K_i, where i represents each component. These parameters were obtained by fitting experimental data of a lab-scale SMB pilot plant.

Mathematical Models

Next, the obtained parameters were used to solve the mathematical equations that represent each system. Distillation was rigorously modeled, meaning mass and energy balances were performed in each stage, while enforcing phase equilibrium for each component. For adsorption, the mass balance, the convection-diffusion equation was used with axial dispersion values estimates from the Peclet number. It was assumed that the SMB stayed constant at 50°C, as this was the temperature of the pilot-plant experiments. The boundary conditions, flow balances at each node and enforcement of cyclic steady state (CSS) conditions constitute the remainder of the SMB equations.

This led to a system of partial differential algebraic equations (PDAEs) that were modelled as a non-linear programming (NLP) problem. Pyomo.DAE 6.5. [5] was used to discretize the PDAEs and the system was solved using Ipopt 3.12.13 [6].

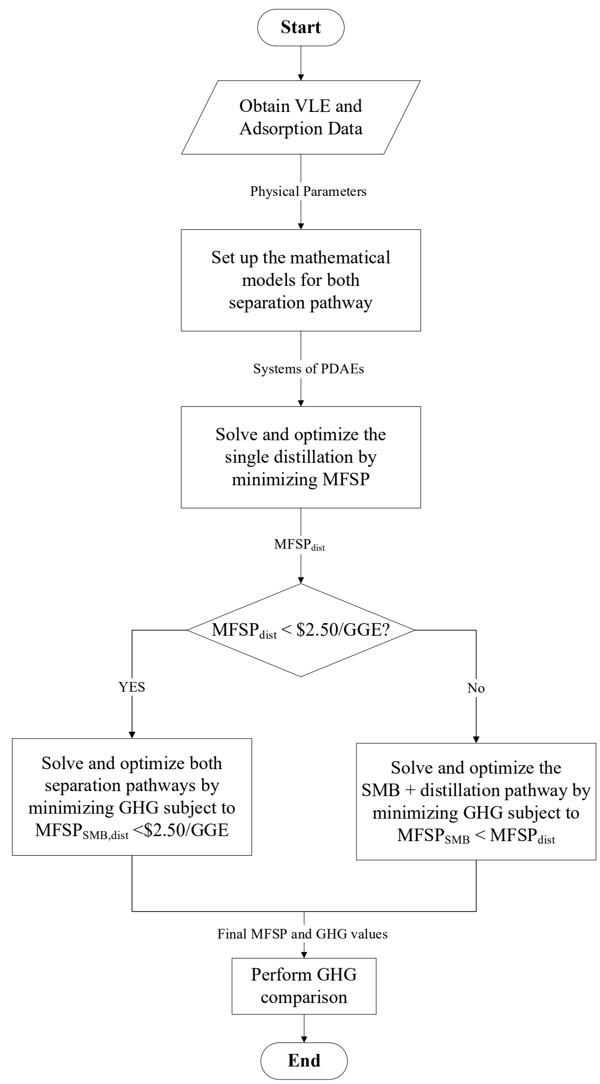

Figure 4. Proposed stepwise approach to develop the comparative study between separation pathways

Economic Analysis

Separation Scheme

After solving the PDAEs, the resulting mass and energy balances were used to size the equipment and estimate operating expenses. The distillation columns were sized as tray towers under vacuum conditions. The columns had constant diameter, which was estimated using a correlation based on internal vapor flow. A stage spacing of 1.5 ft was assumed. For SMB, each adsorption column had the same fixed diameter of 4m. This value is in accordance with other large-scale SMB designs found in literature [7,8]. The length of the columns was set as a free variable to be determined from the optimization. After sizing, the columns of distillation and SMB were both costed as empty vertical vessels [9].

The condensers and reboilers were sized as shell-and-tube heat exchangers. The area was estimated assuming counter-current operation and a constant overall heat transfer coefficient. A single stage liquid-ring pump was used to generate vacuum in the distillation columns and centrifugal pumps were used for pressure rise. All aforementioned correlations for purchased and installed costs were obtained from Seider et al. [9], except for the rotary valve, which was obtained from a case study of a large-scale petrochemical plant [10].

Besides utilities, which are mostly satisfied internally, the main operating expenses are related to the purchase of make-up ethanol and adsorbent. The unit cost of adsorbent was based on the cost of its synthesis raw materials. This cost was scaled to the biorefinery level using the six-tenths factor rule. The obtained price was $20/kg and a replacement time of 5 years was assumed. Given the discrepancy in size between the lab bench and the biorefinery, there is an inherent degree of uncertainty in these values that could be addressed through sensitivity analysis. However, this was considered outside of the scope of this work.

Next, the "Discounted Cash Flow Analysis" model from NREL [11] was implemented in the NLP problem. This model is based on U.S. Department of Energy (DOE) recommendations for renewable energy systems. It includes values for interest rate, equity, depreciation, plant lifetime and taxes. The most important metric from the model is the minimum fuel selling price (MFSP) of the fuel. This is a key metric used to assess the viability of biofuels. DOE has set a MFSP target of $2.50/GGE (gallon of gasoline equivalent) or less to be reached by 2030. With the current assumptions, the SOT reaches a MFSP value of $2.47/GGE.

Utilities of the Biorefinery

As mentioned, the main effect of BDO separation is reducing operating expenses of the biorefinery. Most notably, the broth is raised to 250°C and 60 atm prior to the dehydration reactor, and by removing water and reducing the BDO stream size, the energy load also significantly decreases. This saves around 90% of the high-pressure steam (HPS) internally produced, which can instead be used to generate additional power in the turbine and reduce imported electricity. Altogether, this leads to a power output of 32.9 MW and a ~50% import reduction from the grid compared to the SOT. This value was corroborated by Liu et al. [12] in a previous study.

Next, heat duties associated with the separation scheme were considered. The distillation reboilers are the main consumers of energy in either pathway. These columns use low-pressure steam (LPS), which requires withdrawal from the turbine system. Without changes to the existing design, this withdrawal would reduce the turbine's power output. Thus, as a simplification, natural gas is imported in order to generate additional steam needed to meet these duties and still maintain the turbine output of 32.9 MW.

Greenhouse Gas Emissions System Boundary

The fuel's lifecycle analysis was then considered, with GHG emissions (in g_{CO2e}/MJ_{fuel}) as the key metric. A technical report in 2020 was developed by the Argonne National Lab (ANL) [13], where the SOT's well-to-wheel emissions were calculated. The system boundary in this report encompasses all processes between the corn stover collection in the field and the production of fuel and co-product from the biorefinery. The functional unit of the system is a GGE of fuel.

For this study GHGs were estimated using the displacement method. Through this method lifecycle emissions are attributed entirely to the fuel and none to the co-product. The fuel, however, receives credit for the emissions associated with the co-product's conventional fossil pathway. This remains consistent with the economic model of the SOT, where adipic acid production revenue is credited to the fuel's MFSP. The ANL 2020 report was used as a guideline and the GREET tool [14] was used to develop expressions for GHG emissions. The reader is encouraged to read this report for more details regarding the lifecycle assumptions.

Optimization

Below are the expressions of the NLP problem. Pyomo and Ipopt were also used for the optimization.

$$
\begin{gathered}
\min_{\boldsymbol{x}} \boldsymbol{y} \\
s.t. \boldsymbol{f}(\boldsymbol{u}, \boldsymbol{x}\,;) = \boldsymbol{0} \\
\boldsymbol{g}(\boldsymbol{u}, \boldsymbol{x}\,;) \geq \boldsymbol{0} \\
\boldsymbol{y} = \boldsymbol{h}(\boldsymbol{u}, \boldsymbol{x}\,;\, \theta) \\
\boldsymbol{x}_{\boldsymbol{min}} \leq \boldsymbol{x} \leq \boldsymbol{x}_{\boldsymbol{max}}
\end{gathered}
$$

The objective function $\boldsymbol{y}$ can be either MFSP or GHG minimization. The equality constraints, $\boldsymbol{f}$, are represented by the system of PDAEs and the discounted cash flow model. The only inequality constraints, $\boldsymbol{g}$, in this problem are the maximum allowable MFSP and minimum BDO purity post-distillation. The main decision variables, $\boldsymbol{x}$, of the SMB are the length of each adsorption column, the velocity in each zone and step time. For distillation variables are pressure, reflux ratio and reboiler duty. With appropriate initialization, the stage location of each feed stream can also be determined without resorting to MINLP. The state variables are represented by u and the physical parameters by θ.

RESULTS

Baseline GHG Emissions

Using GREET and the displacement method, it was found that the lifecycle GHG of the SOT's fuel product is 23.0 g_{CO2e}/MJ. From this value 121.4 g_{CO2e}/MJ is attributed to the fuel and 98.4 g_{CO2e}/MJ is credit from producing adipic acid. This represents a significant decrease from 93.0 g_{CO2e}/MJ for petroleum-derived diesel [14]. It should be noted that we assumed a carbon footprint of adipic acid (AA) of 4.3 kg_{CO2e}/kg_{AA}. This does not consider GHG-100 emissions from nitrous oxide (N_2O) and is a more conservative estimate than the ANL 2020 report, which assumed 11.6 kg_{CO2e}/kg_{AA} and led to net emissions of -148 g_{CO2e}/MJ for the SOT.

Next, an expression was developed to relate GHG with the relevant mass and energy flows (natural gas import and make-up ethanol). First, GHG emissions were re-calculated based on the updated grid electricity import. As mentioned, turbine output increases from 11.8 MW to 32.9 MW, reducing import from 41.5 MW to 20.4 MW. This resulted in 103.3 g_{CO2e}/MJ attributed to fuel and after considering adipic acid credit, a net value of 4.9 g_{CO2e}/MJ was obtained. Then, natural gas (NG) and make-up ethanol (EtOH) import were varied in GREET to estimate how GHG changes, resulting in the following linear expression:

$$GHG = 4.9 \times \frac{1}{R} + 0.1362 \times NG + 0.0023 \times EtOH \qquad (1)$$

R represents BDO recovery. This ranges from 0 to 1 and serves as a scaling factor to make-up for BDO lost during separation. GHG is expressed in g_{CO2e}/MJ, NG in MMBTU/hr and EtOH in kg/hr. This was the expression used in the objective function for minimizing GHG. It should be clarified that NG and EtOH are the added imports that result from incorporating the separation to the biorefinery. Natural gas (58 MMBTU/hr) and ethanol (37 kg/hr) are both imported in the SOT, but those are already accounted in the 4.9 g_{CO2e}/MJ calculation.

Approach Implementation

The proposed approach was implemented and for both pathways, the binary feed is 10wt% BDO (~100g/L titer), while the minimum purity requirement of the exit stream is 85 wt% BDO. **Figure 5a** shows the mass balances of the optimal configuration of the single distillation pathway. This configuration achieved a $MFSP_{dist}$ of $2.54/GGE. **Figure 5b** shows the obtained optimal configuration for the SMB pathway. This configuration was obtained with a $MFSP_{SMB}$<=$2.54/GGE constraint.

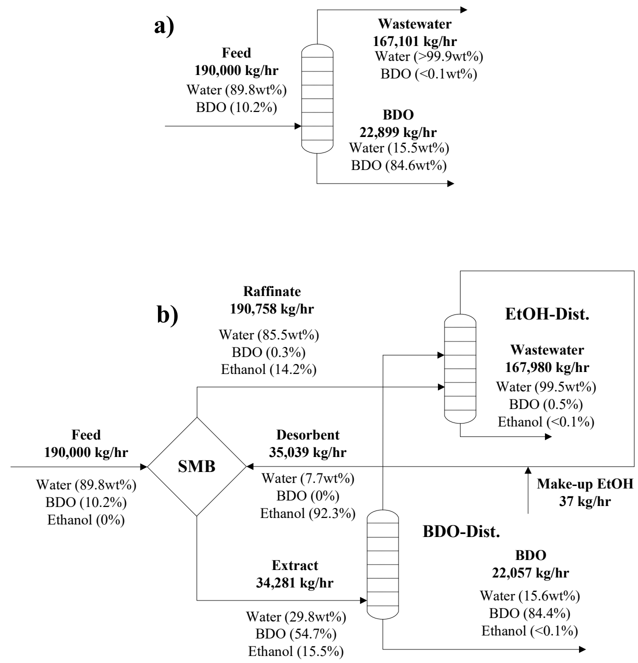

Figure 5. Resulting optimal process designs of: a) the single distillation column and b) SMB + distillation

The optimization problems were solved using the true moving bed (TMB) approximation model for the SMB and an IPOPT convergence tolerance of $1x10^{-3}$. It should also be noted that the distillate of the EtOH-dist column is ~92 wt% ethanol. Thus, the ethanol/water azeotrope at this vacuum pressure (~96 wt%) is not expected to be encountered.

Comparison of the Proposed Pathways

Table 1 shows the comparison between the distillation columns for both pathways. As seen the most significant difference is the duty of the reboiler and condenser units for each pathway. Most notably, it is shown that the combined reboiler duty from the two columns in the SMB pathway is much lower than single distillation. This further establishes adsorption as a far more effective separation alternative in this context.

In all cases a lower boundary of 0.10 bar was imposed to the column pressure. For single distillation, the optimal pressure was slightly higher at 0.22 bar, since this raises the temperature of the wastewater from the tops, which was used for heat integration with the feed.

Table 1. Results operating conditions of the single distillation, and BDO and EtOH recovery columns

Distillation Column	Single Dist.	BDO Dist.	EtOH Dist.
Number of Stages	20	30	30
Feed Stage(s)	19	29	10/18
Pressure (bar)	0.22	0.10	0.30
Reflux Ratio (mole)	0.06	0.02	1.77
Reboiler Duty (MW)	118.2	6.5	24.3
Condenser Duty (MW)	116.2	6.2	26.5

Table 2 shows the comparison between the alternatives evaluated in this study. The ideal separation represents the SOT with BDO recovery, but without incurring in capital or operating costs yet (i.e., the maximum potential of BDO separation [12]).

Table 2. Results operating conditions of the single distillation, and BDO and EtOH recovery columns

Process	SOT	Ideal Sep.	Single Dist.	SMB+ Dist.
Natural Gas Import (MMBTU/hr)	58	58	379	174
Grid Import (MW)	41.5	20.4	20.4	20.4
MFSP ($/GGE)	2.47	2.11	2.54	2.54
GHG (g_{CO2e}/MJ)	23.0	4.9	48.7	20.5

Single distillation, as expected, had poor economic and sustainability performance. Its large MFSP and GHG values render the entire process unfeasible, and thus, simple distillation cannot be considered a viable alternative to recover BDO in this biorefinery. In comparison, SMB+distillation gave lower GHG, demonstrating the effectiveness of the proposed hybrid separation and its potential to be incorporated in the biorefinery.

Sensitivity Analyses

In the proposed approach, either MFSP or GHG is minimized, but not both simultaneously. This does not provide a complete outlook and Pareto fronts were build to allow a more thorough comparison. **Figure 6** shows the Pareto optimal curves for the single distillation and SMB processes. In the case of single distillation, the leftmost point represents the result from minimizing MFSP without GHG restriction, while the rightmost point is the minimization of GHG without MFSP restrictions.

For the SMB process, the leftmost point is also MFSP minimization without GHG constraint. However, the rightmost end is not bounded, given that the SMB can be as large as needed. This indefinitely increases the quantity of adsorbent, decreasing desorbent use and energy load. Thus, GHG also decrease indefinitely but at the expense of a prohibitive adsorbent purchasing cost.

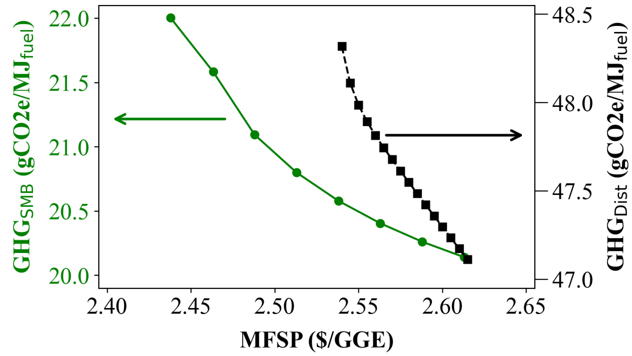

Figure 6. Pareto Fronts of the Separation Alternatives

It should be noted, that for either front, GHG is not very sensitive to the MFSP. The most important observation, however, is that the SMB-process can improve the SOT's economic and sustainability performance. As shown, for any MFSP under $2.47/GGE, GHG remains below 23 g_{CO2e}/MJ, proving again the viability of this separation alternative.

Finally, a sensitivity analysis was developed by varying BDO titer. The fermentation in the SOT is an ongoing research topic and is not clear that a titer of 100g/L is optimal for the overall flowsheet. **Figure 7** shows the effect of BDO titer on GHG and MFSP by applying the proposed approach. As seen, GHG emissions of single distillation considerably increase with decrease in titer. This is an expected result, given that a large and dilute stream leads to a higher energy demand that increases both GHG and MFSP.

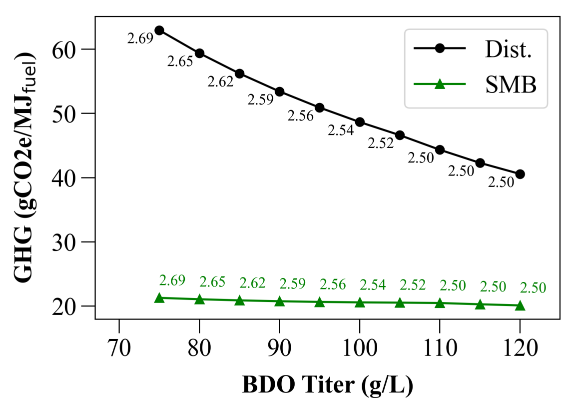

Figure 7. Effect of BDO titer concentration on the GHG emissions for both separation pathways (the annotated values represent the MFSP at each point in $/GGE)

Remarkably, however, the change of GHG emissions in SMB is almost negligible. To understand this better we can further explore the 75 g/L titer point. After optimizing the NLP problem with GHG as the objective function, the obtained MFSP is $2.69/GGE, and the quantity of adsorbent is 1392 tonnes. However, the at this titer level MFSP minimization gives $2.46/GGE, and a much lower adsorbent quantity of 342 tonnes. Implementing a very large quantity of adsorbent is clearly a suboptimal economic decision, but it greatly reduces desorbent use and energy duties, all of which help improve GHG. Thus, SMB size is allowed to increase almost indefinitely in order to accommodate varying titers, and only marginal changes in GHG are observed.

CONCLUSIONS

A comparative study was performed between two separation technologies to recover BDO from a fermentation broth. Single distillation was compared to a novel SMB+distillation separation scheme on the basis of GHG emissions. Both separations were incorporated in a biorefinery design developed by NREL that produces renewable fuels with corn stover as feedstock and dilute (10wt%) BDO as an intermediate.

The comparison was done by following a stepwise optimization approach where GHG is minimized. The resulting design achieved GHG emissions of 20 g_{CO2e}/MJ for SMB+distillation, lower than 48 g_{CO2e}/MJ for single distillation and 93 g_{CO2e}/MJ for petroleum fuel.

The effect of BDO fermentation titer was also considered. As expected, for single distillation, decreasing titer significantly increased energy consumption and, thus, worsened MFSP and GHG emissions. However, for SMB, the GHG emissions were not sensitive to titer.

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