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Economic and Environmental Sustainability Assessment

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Green Industrial-Scale Plant Design for Syngas Fermentation to Isopropyl Alcohol and Acetone: Economic and Environmental Sustainability Assessment

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ABSTRACT

Steel mill off gas fermentation presents a promising green alternative to petrochemical isopropyl alcohol (isopropanol, IPA) and acetone production while potentially reducing greenhouse gas emissions. A pilot-scale study stated negative global warming potential (GWP) at 85% gas conversion and 90% product selectivity. However, industrial-scale plant design including detailed techno-economic assessment (TEA) and life cycle assessment (LCA) remain undescribed. Therefore, this study modelled a heat-integrated 47.5 kton/ year gas fermentation process to IPA and acetone, based on pilot-scale data. The downstream processing was designed using vacuum distillation and heat-pump integrated (extractive) distillation to purify the 50 $g_{product}$/ L broth with biomass and acetate as byproducts, to obtain 41.8 kton/ year of 99.6 wt. % IPA and 5.64 kton/ year of 99.0 wt. % acetone. Notably, no steam is consumed and 2.6 MWh of electricity is generated by utilising the energy from the steel mill off gas. The estimated unit production cost (UPC; 0.57 \$/$kg_{product}$) is significantly below market prices (1.65 \$/ kg_{IPA} and 1.45 \$/ $kg_{acetone}$). Moreover, the cradle-to-gate LCA gave GWPs of -1.42 $kg_{CO2\text{-}eq}$/ kg_{IPA} and -1.25 $kg_{CO2\text{-}eq}$/ $kg_{acetone}$, mainly due to avoided steel mill emissions. Other environmental impacts studied were also lower than for petrochemical production. Only the freshwater use is higher (70 L/ kg_{IPA} and 62 L/ $kg_{acetone}$) compared to petrochemical production (16 L/ kg_{IPA} and 28 L/ $kg_{acetone}$). Future research should study the impact of IPA and acetone selectivity and titer on the economic and environmental sustainability of steel mill off gas fermentation to IPA and acetone.

Keywords: Syngas fermentation, Isopropanol, Techno-economic assessment (TEA), Life Cycle Assessment (LCA), Product selectivity, Vacuum distillation, *Clostridium autoethanogenum*

INTRODUCTION

Syngas fermentation of steel mill off gas can provide both (1) a sustainable alternative to petrochemical isopropyl alcohol (isopropanol, IPA) and acetone production and (2) reduce greenhouse gas emissions from the steel industry. Syngas fermentation using *Clostridium autoethanogenum* can convert the energy-rich steel mill off gas (50% CO, 10% H_2, 20% CO_2, 20% N_2) to ethanol on an industrial-scale [1]. Recently, a 120 L pilot producing mainly either isopropyl alcohol (IPA), or acetone or a mixture of both was published [2]. Liew *et al.*, (2022) even claimed negative global warming potential (GWP) for the production of IPA and acetone from steel mill off gas. However, the industrial-scale plant design and its potential techno-economic and environmental performance is yet unknown. Therefore, this study aims to design and model an economically and environmentally sustainable industrial-scale syngas fermentation to produce 47.5 kton/year of >99 wt. % isopropyl alcohol and acetone. Previous work has modelled the syngas fermentation to IPA at a 46 kton/year scale and described the dilution rate, volumetric mass transfer of CO, product selectivity and gas conversion as key sustainability parameters [3]. Besides, an eco-efficient downstream processing has been modelled and described for a gas fermentation broth containing an IPA and acetone mixture [4]. This study fully-integrates the upstream and downstream process design including heat integration and wastewater treatment (anaerobic digestion, CHP and water recycle). Then a techno-economic assessment (TEA) and life cycle assessment (LCA) were performed. Not only considering GWP but also assessing stratospheric ozone depletion, fine particulate matter formation, freshwater eutrophication, marine eutrophication, human carcinogenic toxicity, land use, and freshwater use.

METHODS

Process modelling

The process was modelled in Aspen Plus V12.0 for a total production of IPA and acetone of 47.5 kton/y (see Figure 1). Whereas, the gas fermentation was modelled as previously described [3] using the 120 L pilot data [2], with adaptation of the (optimistic) CO volumetric mass transfer rate to 14.9 g/L/h. A CO volumetric mass transfer up to 8.5 g/L/h was deemed feasible for ethanol [5] at a lower overhead pressure (1.1 bar vs 1.4 bar). Additionally, IPA decreases the bubble size already at lower concentrations [6]. This resulted in a product titer of about 50 g/L, which can give a ~33% lower biomass growth rate [7]. The downstream processing was modelled based on [4]. Vacuum distillation was employed to capture volatile products while recycling the broth back to the fermenter. The product stream was further purified using heat pump-assisted distillation, incorporating heat integration from the hot steel mill off-gas. Additionally, Combined Heat and Power (CHP) generation and wastewater treatment with recycling were implemented [8]. All decisions during process design were made to minimise energy requirements.

Techno-economic assessment (TEA)

The techno-economic assessment was performed according to the National Renewable Energy Laboratory (NREL) methodology to determine the capital expenses (CAPEX) and operating expenses (OPEX) [9]. The CAPEX includes the equipment and installation costs as well as indirect costs for home office and construction, field expenses, proratable expenses, project contingency, working capital, site development, additional piping, warehouse and initial water and solvent costs. The installed costs for the equipment, except the bioreactor was determined according to [10], [11] and using the Marshall & Swift cost index value of 1773.4 (end of 2021). Whereas the bioreactor (external-loop gas lift reactor) installed costs were determined based on a direct quotation, a scaling factor of 0.60, an installation factor of 2.00 [9], and a Chemical Engineering Plant Cost Index (CEPCI) of 800.3 (2024). In principle, the assessment was done for a plant located in the US. The assumed plant lifetime was 10 years.

For the OPEX, the costs for the steel mill off gas were assumed 14.64 $/ton based on low-pressure steam costs (7.78 $/GJ) for replacing the otherwise captured heat from flaring (38% efficiency) and the CHP costs were assumed 2.1 $/MWh (2024) [12]. The costs of wastewater treatment for recycle was done using data from [8]. The unit production costs (UPC) were calculated in US$ per kg of product (isopropyl alcohol or acetone) and the profit margin was calculated based on the market prices (1.65 $/ kg_{IPA} and 1.45 $/ $kg_{acetone}$).

Life cycle assessment (LCA)

The Life Cycle Assessment was performed cradle-to-gate (see Figure 1) using the ReCiPe 2016 Midpoint Hierarchical method (V1.04) and the US life cycle impacts from the Ecoinvent database V3.11. Including scope 1, 2, and 3 emissions. The assessed midpoint indicator categories are: (I) Global warming potential (GWP in $kg_{CO2\text{-}eq}$/ $kg_{product}$), (II) Stratospheric ozone depletion (SOD in $kg_{CFC11\text{-}eq}$/ $kg_{product}$, (III) Fine particulate matter formation (FPMF in $kg_{PM2,5\text{-}eq}$/ $kg_{product}$), (IV) Freshwater eutrophication (FWE in $kg_{P\text{-}eq}$/ $kg_{product}$), (V) Marine eutrophication (ME in $kg_{N\text{-}eq}$/ $kg_{product}$), (VI) Human Carcinogenic Toxicity (HCT in $kg_{1,4\text{-}DCB\text{-}eq}$/ $kg_{product}$), (VII) Land use ($m^2_{crop\text{-}eq}$/ $kg_{product}$), and (VIII) Freshwater use (m^3/ $kg_{product}$).

The environmental impacts are economically allocated to IPA and acetone based on their market price. Besides, production of other byproducts (i.e., biomass as a feed and electricity generation) is accounted for using substitution.

RESULTS AND DISCUSSION

Process

IPA and acetone are produced from the hot steel mill off gas (syngas) through gas fermentation (see Figure 1) at a capacity of 5,278 kg_{IPA}/h of 99.57 wt. % IPA and 706 kg_{Ac}/h of 99 wt. % acetone. After the gas fermentation followed the broth and the volatile products are separated and purified through vacuum distillation (C1), acetone distillation (C2), pre-concentration (C3), and extractive distillation with ethylene glycol (C4 and C5). The heat pump integration of the distillation columns and the utilisation of the heat from the syngas feed showed that the process at a CO conversion of 85%, product selectivity of 90% and a product titer (IPA + acetone) of about 50 g/L is utilising no steam and producing net 2.6 MWh of electricity. Whereas, Liew *et al.* [2] reported ~5 $MJ_{electricity}$/$kg_{product}$ for both products and for IPA the need for 6.28 MJ_{steam}/kg_{IPA}. Thus, the modelled process is more energy efficient than the model used for the 120 L pilot [2], possibly due to the optimistic CO volumetric mass transfer rate of 14.9 g/L/h resulting in a 50 g/L product titer in

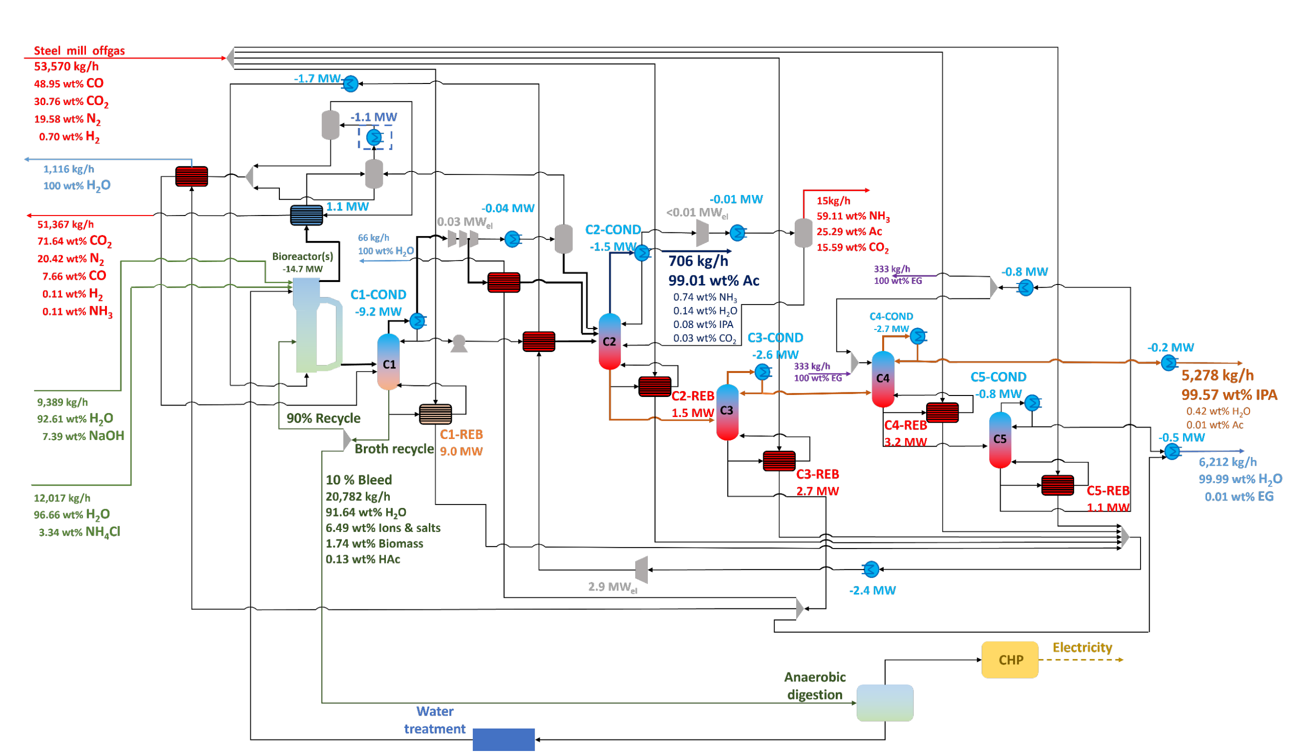

Figure 1: Overview of the 47.5 kton/year syngas fermentation (41.8 $kton_{IPA}$/y, 5.64 $kton_{acetone}$/y). The green inflows to the bioreactor are the pH control and nitrogen source, whereas the red in- and outflows are the gas streams. The inflowing syngas (at 1373 K/ 1100 °C) is used for heat exchange before it is compressed (3.84 bar) and fed to the bioreactor. Multi-stage heatpump integrated distillation is used to obtain 99.01 wt. % Ac (C2, dark blue) and 99.57 wt. % IPA (C4, orange). First the broth is separated from the volatile products (C1) by vacuum distillation. Followed by acetone distillation (C2), pre-concentration of IPA (C3), extractive distillation of IPA with ethylene glycol (EG) (C4), and EG recovery (C5). The anaerobic digestion, combined heat and power generation (CHP), and water treatment to demiwater are included within the system boundaries for the economic and environmental assessment.

combination with the energy-efficient DSP design.

Techno-economic assessment (TEA)

Capital Expenses (CAPEX): Bioreactor as main cost component and minimal expenses for the distillation columns

The NREL method [9] gave a factor of 1.84 for the modelled syngas fermentation process to get to the CAPEX of 103.7 M$, from the total installed equipment costs (56.3 M$, see Figure 2A). At a plant lifetime of 10 years, the **CAPEX** is about **0.22 $/$kg_{product}$**. The total installed equipment costs are dominated by the bioreactor costs (57.9%, see Figure 2A) which were estimated to have a working volume of 565 m^3 [5]. Besides the bioreactor, the compressors (17.8%) and the combined heat and power generation (CHP, 13.4%) contribute most to the total installed equipment costs. 38% of the compressor CAPEX are to compress the gas feed to 3.84 bar before fermentation. Whereas, all distillation columns only make up 5.5% of the CAPEX, because of separating the volatile products directly from the broth through vacuum distillation [4]. This reduces the mass flow to the distillation columns by 88.4%.

Operating Expenses (OPEX): Minimised through heat integration of the hot steel mill off gas

The **OPEX** (see Figure 2B) are only 16.82 M$/y, which is **0.35 $/$kg_{product}$**. Traditional fermentation processes have OPEX dominated by feedstock expenses. However, the use of the steel-mill “waste” off-gas only contributes 0.04% to the OPEX. The steel mill off gas costs were assumed based on the otherwise obtained heat from flaring. In addition, no consumption of heat utilities and the net generation of 2.6 MWh electricity greatly reduce the OPEX. Moreover, the efficient recycle of the broth and components due to vacuum distillation allows for 90 % broth recycle as well as efficient downstream processing of the products. Therefore, typically minor expenses like labour and pH control together contribute to 67% of the OPEX.

Overall economics

The estimated **unit production costs (UPC)** are only

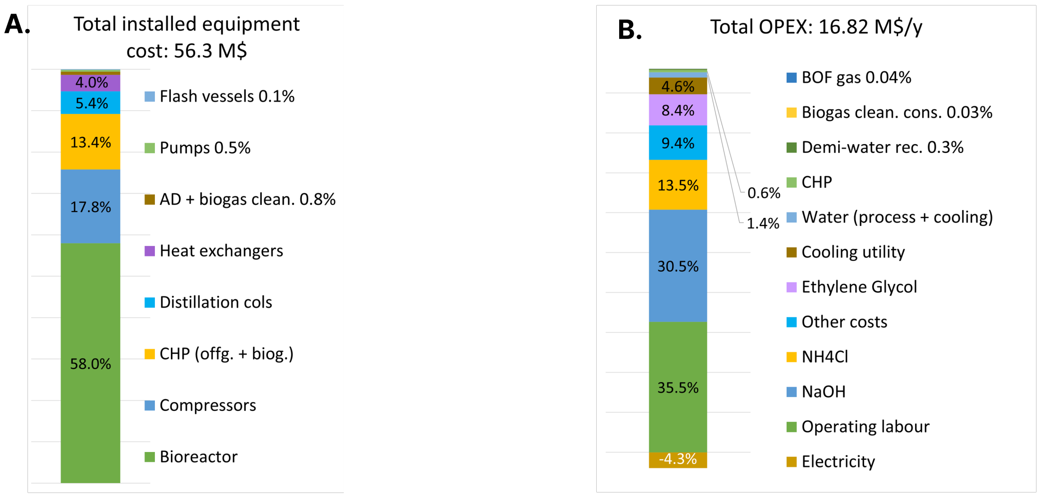

Figure 2: Economic assessment of the modelled syngas fermentation to 47.5 kton/y of isopropyl alcohol and acetone process. The calculated CAPEX is 103.7 M$ assuming a plant lifetime of 10 years of which 54.3% is the total installed equipment costs (A), the operating expenses are 16.82 M$/year (B). The excess energy produced from the CHP is assumed to be sold as electricity to the grid. AD is anaerobic digestion, CHP is combined heat and power generation, and BOF gas is the steel mill offgas (basic oxygen furnace gas) from the steel mill.

0.57 $/kg$_{\text{product}}$ (isopropyl alcohol or acetone). whereas the market price for these products is 1.65 $/kg$_{IPA}$ and 1.45 $/kg$_{Ac}$ [13]. This leaves a margin between the production costs and the 2024 market price of 1.08 $/kg$_{IPA}$ (65.6%) and 0.88 $/kg$_{Ac}$ (60.8%), respectively. Thus, having an estimated **margin** of **over 60%** using the modelled, heat-integrated, gas fermentation process. Moreover, when the biomass byproduct is not anaerobically digested but sold as an animal feed, the overall UPC decreases with an additional 8.8% (0.05 $/kg$_{\text{product}}$).

Cradle-to-gate life cycle assessment (LCA)

The global warming potential can be net zero when considering the converted steel mill off gas as prevented emissions

The cradle-to-gate LCA gave net zero GWP for IPA and acetone production, when considering it as preventing the steel mill off gas related emissions (see Figure 3 & Table 1). The environmental impacts are economically allocated to the products and gave GWPs similar to the pilot-scale study [2] (see Figure 3). However, the results for acetone of Liew *et al.* [2] are on the high acetone selectivity (~85%), whereas this study uses high IPA selectivity with only 12 wt. % acetone produced. Besides, comparison of the GWPs from this study to the petrochemical IPA and acetone production indicates a potential GWP reduction of 160% for IPA and 147% for acetone. Still, the GWP is dependent on the mitigated CO_2 emissions by converting steel mill off gas into IPA and acetone. Additionally, utilising both the latent energy of the steel mill off gas before gas fermentation and combusting the residual off gas enables lower GWPs because of zero steam consumption and net electricity production (see Table 1). Additionally, the gas fermentation process prevents the direct use of fossil fuels for IPA and acetone production.

Table 1: Global Warming Potential (GWP) contributions for the modelled syngas fermentation to 47.5 kton$_{prod}$/year of >99 wt. % isopropyl alcohol (IPA) and acetone (Ac).

	Isopropy alcohol (kg$_{CO2\text{-}eq}$/kg$_{IPA}$)	**Acetone** (kg$_{CO2\text{-}eq}$/kg$_{Ac}$)
Process emissions	7.64	6.70
Heat replacement	0.636	0.558
NaOH	0.147	0.129
Ethylene Glycol	0.120	0.105
NH4Cl	0.090	0.079
Water	0.069	0.061
NaCl	8.87×10^{-4}	7.79×10^{-4}
Steam	0.000	0.000
Electricity (produced)	-0.255	-0.224
CO2 prevented from flaring	-9.86	-8.66
Total	**-1.42**	**-1.25**

Other environmental impacts most relevant to fermentation processes

Comparison of the modelled syngas fermentation process with conventional petrochemical production (see Table 2) also gave lower impacts for the stratospheric ozone depletion, marine eutrophication human carcinogenic toxicity. In addition, the calculated fine particulate

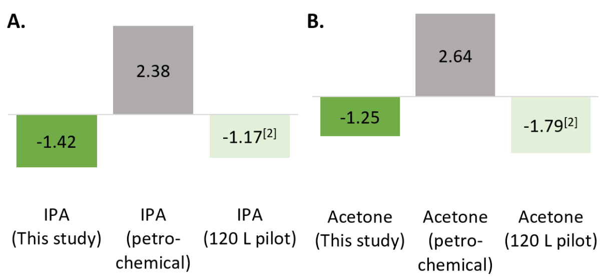

Figure 3: The cradle-to-gate global warming potential of the modelled syngas fermentation to 47.5 kton/year of >99 w% isopropyl alcohol and acetone (left, dark green) compared to the GWP of petrochemical-derived IPA (middle, grey) from ECOINVENT V3.11, and the reported 120 L pilot-scale based LCA [2]. Both this study and [2] assumed the steel mill offgas to be prevented carbon emissions.

matter formation and land use are about one order of magnitude smaller for the syngas fermentation process. On top of that, the freshwater eutrophication could be net zero due to the prevented steel mill emissions and net electricity generation. A common concern for fermentation processes is the high fresh water use. However, for the modelled gas fermentation process the freshwater use is only about threefold that of the petrochemical processes, ranging from 62-70 L/$kg_{product}$ (see Table 2). The designed process already has about maximum fresh water recycle and reuse. Therefore, efficient water management is important for developing more sustainable chemical production through (syngas) fermentation.

CONCLUSIONS

- Converting steel mill off gas through (syn)gas fermentation at a product titer of 50 g/L and 85% gas conversion can produce high purity (>99 wt. %) isopropyl alcohol (isopropanol, IPA) and acetone. This process is both economically sustainable (unit production costs ≈ 1/3 market price) and environmentally sustainable, potentially achieving net zero GWP.
- Effective downstream processing of the volatile products, isopropyl alcohol (isopropanol, IPA) and acetone, can be obtained through vacuum distillation with broth recycling, followed by acetone distillation, pre-concentration, and extractive distillation of IPA with ethylene glycol.
- Effective heat integration, utilising both the latent and chemical energy of the steel mill off gas, results in net zero steam consumption and net electricity generation (2 MWh) in the modelled syngas fermentation process, producing 47.5 $kton_{product}$/ year.
- The method of accounting for the environmental impacts and substitution, when utilising a waste stream or generating a byproduct, respectively, is crucial to the LCA outcome. When the steel mill off gas is considered as prevented emissions, the modelled syngas fermentation process can have a net zero GWP.

Table 2: Environmental impacts, besides the global warming potential for the cradle-to-gate LCA of the modelled syngas fermentation of steel mill off gas to 47.5 kton/year of >99 wt. % isopropyl alcohol (IPA) and acetone (Ac).

Product:	**Isopropyl alcohol** (This study)	**Petrochemical IPA** (ECOINVENT V3.11)	**Acetone** (This study)	**Petrochemical Acetone** (ECOINVENT V3.11)
Stratospheric ozone depletion ($kg_{CFC11-eq}$ / $kg_{product}$)	4.17E-07	4.60E-07	3.66E-07	3.24E-07
Fine particulate matter formation ($kg_{PM2.5-eq}$ / $kg_{product}$)	3.23E-04	2.77E-03	2.84E-04	3.31E-03
Freshwater eutrophication (kg_{P-eq} / $kg_{product}$)	-2.89E-05	4.15E-04	-2.54E-05	4.28E-04
Marine eutrophication (kg_{N-eq} / $kg_{product}$)	9.12E-05	2.59E-05	8.01E-05	2.33E-05
Human carcinogenic toxicity ($kg_{1,4-DCB-eq}$ / $kg_{product}$)	0.021	0.057	0.018	0.061
Land use ($m^2_{crop-eq}$ / $kg_{product}$)	4.94E-03	1.81E-02	4.34E-03	1.61E-02
Water consumption (m^3 / $kg_{product}$)	0.070	0.016	0.062	0.028

RECOMMENDATIONS

- To evaluate the effect of titer and product selectivity on the downstream process design, techno-economic performance and environmental sustainability of syngas fermentation, future work should look into both lower isopropyl alcohol and acetone product titer and higher acetone selectivity.
- To study the influence of different (volatile) by-products on the process performance.
- To perform experimental studies on the effect of isopropyl alcohol concentration on the volumetric mass transfer.

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