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Volumetric mass transfer and dilution rate as key parameters for sustainable industrial syngas fermentation to isopropyl alcohol: modeling and parametric assessment

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Abstract: Synthesis gas fermentation is a promising route for the valorization of steel mill off-gas and for replacing conventional fossil-based isopropyl alcohol (IPA) production. A recent 120 L pilot-scale study reported 85% gas conversion at 90% product selectivity and claimed a negative global warming potential (GWP) without detailed process design. The current paper reports a first-of-a-kind industrial-scale syngas fermentation process that was designed using extractive distillation with glycerol to produce 46 kton year^{-1} of 99.1 wt% IPA. The sustainability of an industrial-scale continuous syngas-to-IPA process has not yet been assessed. This study describes the first integrated cradle-to-gate technoeconomic analysis (TEA) and life cycle assessment (LCA), accounting for all emissions scopes, crediting prevented CO_2 emissions from steel mill off gas, and including steel mill heat replacement. Parametric assessment identified higher CO volumetric mass transfer rate (VMT_{CO}) and lower dilution rate (D) as key parameters for enhanced sustainability. For improved process design, economic and environmental tradeoffs were observed for lower glycerol bleed and higher VMT_{CO}. At best, a –44.4% GWP was achieved for a 6.25% increase in VMT_{CO} to 8.5 g L^{-1} h^{-1} (12.2 kgCO_2-eq kg$^{-1}_{IPA}$; Netherlands case) and a –23.2% in IPA production costs for a 30% decrease in glycerol bleed of 7 wt% (USD 3.28 per kg$_{IPA}$, US case) compared with the base-case process. © 2025 The Author(s). *Biofuels, Bioproducts and Biorefining* published by Society of Industrial Chemistry and John Wiley & Sons Ltd.

Supporting information may be found in the online version of this article.

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Key words: basic oxygen furnace (BOF) gas; carbon utilization; isopropanol; extractive distillation; life cycle assessment (LCA); technoeconomic analysis (TEA)

Introduction

To mitigate global warming, 196 countries have committed to reach Net Zero greenhouse gas (GHG) emissions by 2050.[1] The steel industry, responsible for about 7% of global GHG emissions, must reduce its emissions by at least 50% to meet this target.[2] A large portion of these emissions are from flaring energy-rich basic oxygen furnace (BOF) gas. Even in Europe, 25% of the BOF gas is flared without heat or power generation.[3] Basic oxygen furnace gas is a type of synthesis gas (syngas) and the synthetic mixture used by Liew *et al.*[4] consists of 50% CO, 10% H_2, 20% CO_2, and 20% N_2. However, syngas can be converted anaerobically into valuable chemicals by acetogens using the Wood–Ljungdahl pathway through gas fermentation.[5,6] In 2020, steel mill off-gas fermentation to ethanol technology was commercialized using a proprietary,[7] anaerobic acetogen (*Clostridium autoethanogenum*) strain,[6] engineered for prototrophy.[8]

In 2022, a 120 L pilot-scale bioreactor to produce isopropyl alcohol (IPA; also known as isopropanol) from BOF gas was demonstrated with promising results: 85% gas utilization, approximately 3 g L^{-1} h^{-1} productivity, and 90% product selectivity, with a reported cradle-to-gate carbon intensity of −1.17 $kg_{CO2\text{-}eq}$ kg_{IPA}^{-1}.[4] Isopropyl alcohol is used as a solvent, disinfectant and platform chemical and has a USD 3.4 billion market.[4,9] Currently, there is no green alternative for the polluting cracking and reforming of propylene to produce IPA.[10] Therefore, The industrial-scale economic and environmental sustainability of steel mill off-gas fermentation to IPA remain unknown. A fundamental understanding of the consequences of integrating such a carbon capture and utilization (CCU) process with the steel mill, the key gas fermentation parameters, and the associated sustainability tradeoffs is essential to support process optimization.[11]

The integration of economic and environmental sustainability assessments of new bioproduction routes is necessary to identify hotspots and evaluate tradeoffs in alternative process designs. Such tradeoffs are unavoidable and they should be identified at an early stage so that changes have the most impact.[12]

This study contributes to an understanding of the industrial-scale sustainability of steel mill off-gas fermentation to high-purity isopropyl alcohol by proposing a first-of-its-kind integrated process design that combines life cycle assessment (LCA) and technoeconomic analysis (TEA). A sensitivity analysis of 11 varied parameters identifies the key parameters and their associated tradeoffs, supporting the development of more sustainable, integrated gas fermentation process designs.

Materials and methods

Process description and modeling

Liew *et al.*[4] reported a 120 L pilot in which *C. autoethanogenum* fermented 85% of the CO in the synthetic steel mill off-gas mixture (50% CO, 20% CO_2, 20% N_2, and 10% H_2) to isopropyl alcohol with approximately 90% product selectivity ($Y_{IPA/CO}$, $cmol_{IPA}$ mol_{CO}^{-1}). These fermentation parameters were used, including acetate and biomass as byproducts, to model a syngas fermentation plant in Aspen Plus V12.0 with the non-random two-liquid (NRTL) property model to produce 46 kton $year^{-1}$ of 99 wt% IPA.[13] The syngas fermentation was modeled as a stoichiometric reactor with a thermodynamically derived stoichiometry.[14]

Figure 1 provides a schematic overview of the modeled plant, the system boundaries, and the emission scopes of the cradle-to-gate LCA. The systematic approach to account for the LCA and economic consequences of implementing this add-on carbon capture and utilization (CCU) process is shown, including the avoided BOF gas emissions, the process emissions (scope 1), the utility-related emissions (scope 2), and the consequential emissions associated with process implementation (scope 3). For detailed process design and operating conditions, see the Supporting Information (SI) or the original model description.[13] In brief, BOF gas (F1) is fed to the gas fermentation (GF) unit together with pH control reagent (NaOH [2 M]; F2), nitrogen source (NH_4Cl; F3), and water (F4).

The utilities – low pressure steam, high pressure steam, electricity and cooling water (F7) – are used throughout the plant (Fig. 1). Following continuous gas fermentation ($D = 0.1\ h^{-1}$), the broth containing approximately 25 g IPA L^{-1} is separated from the biomass (MF). Most biomass is recycled, whereas the bleed can be treated as waste via anaerobic digestion (AD) or as an animal feed byproduct (P4).

The permeate containing IPA is purified by extractive distillation (C1) with glycerol (F5) a common byproduct of bioprocesses, as proposed by Hartanto *et al.*[15] The IPA

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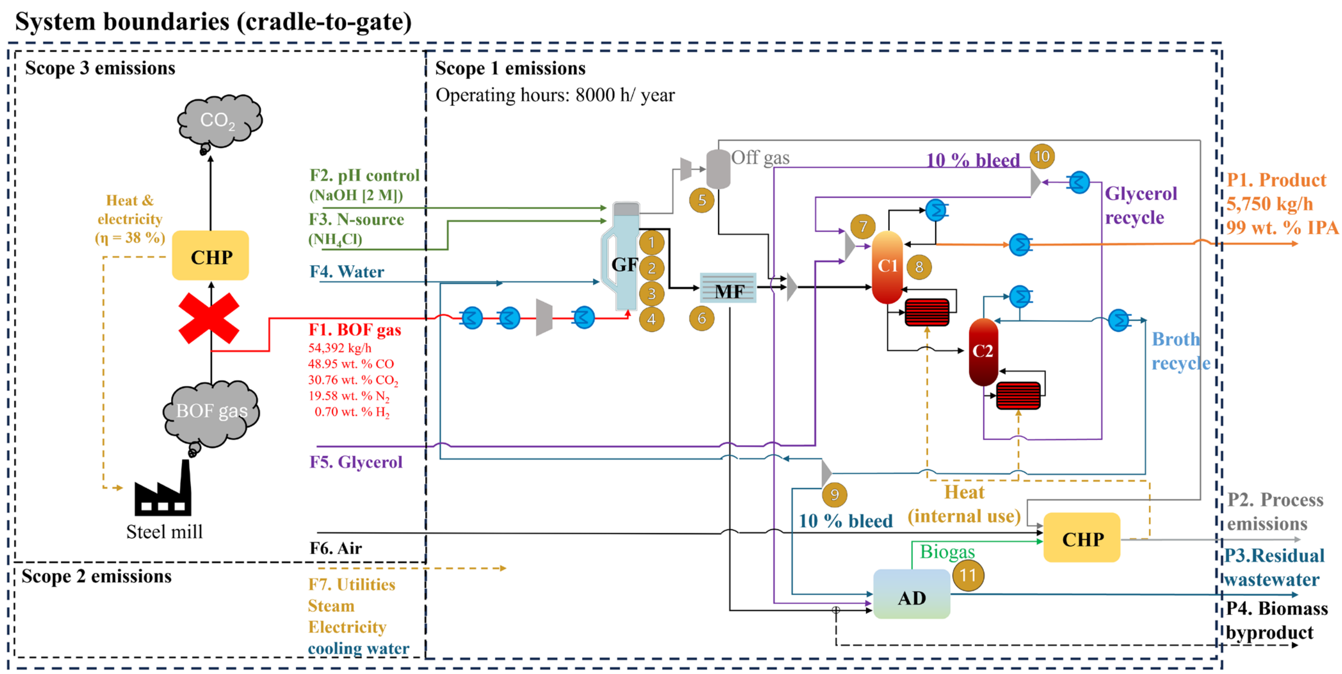

Figure 1. Schematic overview of the modeled BOF gas fermentation to isopropyl alcohol (IPA; isopropanol), including the system boundaries and emission scopes considered in the cradle-to-gate life cycle assessment (LCA). 1. Carbon monoxide volumetric mass transfer rate (8 g L^{-1} h^{-1}). 2. Carbon monoxide conversion (85%). 3. Product selectivity IPA/CO (YIPA/CO; 0.91 mol IPA mol CO^{-1}). 4. Dilution rate (0.1 h^{-1}). 5. Temperature off-gas condenser (278.15 K). 6. Biomass filtration liquid fraction in permeate (0.99). 7. Glycerol mole fraction during extractive distillation (5.13×10^{-2}). 8. Extractive distillation reflux ratio (40). 9. Water bleed (10%). 10. Glycerol bleed (10%). 11. Anaerobic digestion conversion (0.90).

product (>99 wt%) is collected from the top of the extractive distillation. The bottom stream with glycerol is rectified for recycle (C2) and produces a medium flow of water with trace elements for broth recycle to the gas fermentation (GF). Anaerobic digestion (AD) treats the organics in wastewater from the recycle bleeds (Figs 1, 9 and 10) and generates biogas, which is combusted to generate process heat.

Heat integration utilizes the hot BOF gas (F1; 1100 °C / 1373 K / 2012 °F) and the biogas and fermenter off-gas streams. Air (F6) is supplied for combustion in the combined heat and power (CHP) system, producing process CO_2 emissions. The numbered circles in Fig. 1 indicate the eleven process parameters analyzed in this study (see the section on improved process designs below).

Modeling assumptions

For this study, the process was modeled as a continuous steady-state system, with a CO volumetric mass transfer rate of up to 8.5 g L^{-1} h^{-1} as the rate-limiting parameter,[16] and no steel mill off-gas clean-up required prior to fermentation.[6] The metabolic stability of the *C. autoethanogenum* strain is assumed upon recycle, and the scalability of the parameters obtained from the 120 L pilot is assumed.[4] Biomass and acetate are considered the only significant fermentation byproducts, with isopropyl alcohol assumed inhibitory only above 50 g L^{-1}.[17]

Life cycle assessment

The process life cycle was assessed as a cradle-to-gate system, including process emissions (scope 1), utility-related emissions (scope 2), and scope 3 emissions associated with the use of BOF gas (Fig. 1). As the BOF gas is diverted to gas fermentation, the energy normally recovered through flaring is replaced by the costs and environmental impacts of low-pressure steam generated from natural gas combustion.

This approach assigns a monetary value to BOF gas (Supporting Information, Section S5.4) and attributes scope 3 emissions to the BOF gas fermentation process. Although this approach may affect the economic and environmental performance of the gas fermentation plant, it provides a consistent basis for assessing changes in a traditional steel mill, enabling a comparable sustainability assessment of this novel integrated bioprocess.

The LCA was conducted using the ReCiPe 2016 Midpoint (H) V.1.03/World (2010) H with the Ecoinvent 3.10 life cycle impact database, for both the Netherlands and the USA. Two potential applications for the biomass byproduct were assessed: anaerobic digestion followed by heat integration from biogas combustion and use as a soybean meal replacement for fish feed.

Previously, only the global warming potential (GWP) of BOF gas fermentation to IPA was reported.[4] This study extends the LCA to seven midpoint indicator categories considered most relevant for bioprocesses:

- global warming potential (GWP) ($kg_{CO2\text{-}eq}\ kg^{-1}{}_{p}$);
- fine particulate matter formation (FPMF) ($kg_{PM2,5\text{-}eq}\ kg^{-1}{}_{p}$);
- freshwater eutrophication (FWE) ($kg_{P\text{-}eq}\ kg^{-1}{}_{p}$);
- marine eutrophication (ME) ($kg_{N\text{-}eq}\ kg^{-1}{}_{p}$);
- human carcinogenic toxicity (HCT in $kg_{1,4\text{-}DCB\text{-}eq}\ kg^{-1}{}_{p}$);
- arable land use ($m^2{}_{crop\text{-}eq}\ kg^{-1}{}_{p}$);
- freshwater use ($m^3\ kg^{-1}{}_{p}$).

Parametric sensitivity analysis

The technical, economic, and environmental performance of the BOF gas-fermentation-to-IPA plant depends on the conditions in each processing unit. In a previous study we performed a sensitivity analysis to elucidate both: (i) the influence of key process parameters on technoeconomic and environmental plant performance, and (ii) the technical, economic, and environmental hotspots, as described by Brouwer *et al.*[13] In the study we considered:

- VMT_{CO}: CO volumetric mass transfer rate;
- CO conv: CO conversion (fraction);
- $Y_{IPA/CO}$: product selectivity of the CO converted to IPA (fraction);
- D: dilution rate of the fermentation;
- T off-gas cond.: temperature of the off-gas condenser;
- Biom. Filt. L-L: Fraction of the feed liquid in the biomass filtration step ending in the permeate;
- MF_{Gly}: the mole fraction of glycerol during the extractive distillation;
- RR_{ED}: the extractive distillation reflux ratio;
- Water bleed: water sent to the wastewater treatment (fraction);
- glycerol bleed: glycerol sent to the wastewater treatment (fraction);
- AD efficiency: the fractional conversion of organics during anaerobic digestion.

Parameters were typically varied by ±30%, unless constrained by theoretical or physical limits, to explore industrially relevant conditions (see Supporting Information, Table S4.1). The sensitivity analysis assessed two economic indicators – unit production cost (UPC) and total investment cost (TIC) – and seven environmental impact categories (see the previous section).

Plant location

Both the economic and environmental impacts depend on the location of the process. The study includes the USA, as previous work has reported LCA results for this region,[4] and compares the results with the Netherlands to identify location-dependent opportunities and barriers.

Techno-economic analysis

Capital expenses

Total capital expenses (CAPEX) include direct costs for equipment purchase and installation as well as other capital costs. Equipment costs were obtained from literature or known cost correlations,[18,19] and the bioreactor cost (USD 3.45 million for 250 m^3 working volume) was based on a direct 2024 quotation. All equipment costs were adjusted to 2023 prices using the Chemical Engineering Plant Cost Index (CEPCI). Installed equipment costs were calculated following the US National Renewable Energy Laboratory (NREL) methodology.[20]

The total investment cost (TIC) of the plant was estimated by adding costs for home office and construction, field expenses, prorateable expenses, project contingency, site development, warehouse, and other costs to the total installed equipment cost (TIEC), resulting in a TIC equal to 1.97 × TIEC (see Supporting Information, Table S5.2).[20] Total capital expenses were annualized using straight-line depreciation, assuming a 20-year project lifetime and a 10% interest rate. Further details are provided in Supporting Information, Section S5.

Operating expenses

Total operating expenses (OPEX) include the labor, utilities, feedstocks, chemicals, and maintenance costs. Feedstock and chemical prices were obtained from UN Comtrade and IPA prices of USD 1.31 per kg_{IPA} for the USA and USD 1.63 per kg_{IPA} for the Netherlands were used (see Supporting Information, Table S5.6).[21,22] However, the cost of BOF gas (USD 14.64 per ton BOF gas) was calculated based on the value of the process heat it could provide to the steel mill when flared. The 2023 utilities prices for the USA and Netherlands were estimated according to Ulrich and Vasudevan,[23] and corrected for water losses, assuming 30% loss for steam and 7% loss for cooling water (see Supporting Information, Table S1).[24,25] Labor costs and annual maintenance costs (10% of the TIC) were estimated using US wages of USD 40 per h and Netherlands wages of USD 32 per h.[25–27] For more details see the Supporting Information, Section S5.

Unit production costs

The total annualized costs divided by the production capacity of 46 $kton_{IPA}$ $year^{-1}$ gave the UPC (USD $kg^{-1}{}_{IPA}$), which was used as the main indicator of economic sustainability. The effect of selling spent biomass as a soybean meal replacement was determined using a soybean meal price of USD 0.807 per kg.[28]

Results and discussion

The industrial-scale BOF gas fermentation to IPA process was evaluated for its technoeconomic and environmental sustainability potential and parametric tradeoffs.
Then, improved process designs were proposed and assessed on the basis of the parametric analysis.

Base case process producing 46 kt of isopropyl alcohol per year

The base case process was modeled with 85% gas conversion,[4] 91% $Y_{IPA/CO}$,[4] an 8 g L^{-1} h^{-1} volumetric mass transfer rate (VMT_{CO}),[16] a dilution rate (D) of 0.1 h^{-1},[4] and 90% biomass recycling ($\mu = 0.01$ h^{-1}). The model yielded a product titer (C_{IPA}) of 22.3 g L^{-1}, which is below the reported growth inhibiting concentration of 50 g L^{-1}. The modeled production rate (q_{IPA}) was 2.08 g L^{-1} h^{-1} with a downstream processing yield (Y_{DSP}) of 97.7%, whereas, for the pilot, the reported q_{IPA} was 3 g L^{-1} h^{-1},[4] producing 46 $kton_{IPA}$ $year^{-1}$ at 99.13 wt% IPA (8000 h at 5755 kg_{IPA} h^{-1}). Other relevant base-case parameters are described in the parametric sensitivity analysis of this paper and in Brouwer *et al.*[13]

The long-term metabolic stability of the microbial cells was assumed – as was reported for ethanol production.[6] However, metabolic stability for the production of isopropyl alcohol might be lower – as indicated by the lower theoretical biomass yield in comparison with acetate production (Supporting Information, Table S2.3) – but this is beyond the scope for this study.

Base case technoeconomics

As expected for the gas-fermentation plant, the fermenters are the largest contributor to the total installed equipment cost (TIEC) (USD 111.9 million), accounting for about 46%. The total capital investment is USD 259.7 million for the USA (annualized: USD 30.5 million $year^{-1}$) and USD 309.1 million for the Netherlands (annualized: USD 36.3 million $year^{-1}$). For CAPEX details and country-specific breakdowns, see Supporting Information, Section S6. The OPEX dominates the annual costs, at USD 170.6 million for the USA and USD 355.5 million for the Netherlands (Fig. 2). For the same process, steam and glycerol represent 51% and 6.6% of the OPEX in the Netherlands, whereas they contribute 15.3% and 24.3% in the USA. These differences show that location substantially influences the major cost drivers and priorities for process optimization.

The base case UPC (Fig. 3) for the USA (USD 4.27 per kg_{IPA}) is approximately half that for the Netherlands (USD 8.38 per kg). The higher Dutch UPC reflects the higher utility costs in the Netherlands (Fig. 2). Even so, the US base case yields a UPC of more than three times the market price (USD 1.31 per kg_{IPA}).[22] Using expected 2030 green energy prices for both locations lowers the UPC for the Netherlands case to USD 5.42 per kg_{IPA} (−35%) and increases the US price to USD 5.71 per kg_{IPA} (+33%) (Fig. 3). This comparison does not consider the expected CAPEX increase associated with an electric or hybrid system.[29] If biomass is treated as waste rather than being sold as a fish feed byproduct, the UPC increases by USD 0.06 per kg_{IPA}. This assumes that regulations would permit *C. autoethanogenum* biomass to be used as fish feed. The UPC is highly sensitive to utility prices: in the Netherlands, steam and cooling water contribute 0.7 Δ%UPC/Δ%price, and (cooling) water, 0.4 Δ%UPC/Δ%price) for the Netherlands and the glycerol for the USA (0.2 Δ%UPC/Δ%price) (Supporting Information, Section S7). These values indicate the relative contributions to OPEX.

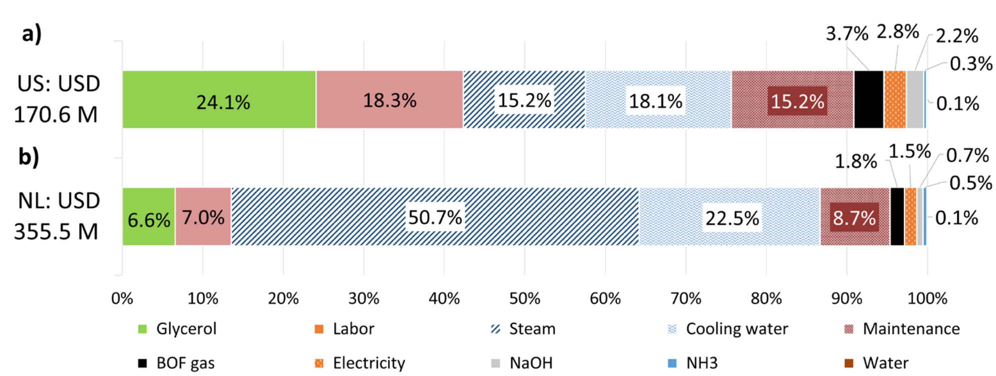

Figure 2. Operational expense (OPEX) distributions for USA and Netherlands conditions and prices.

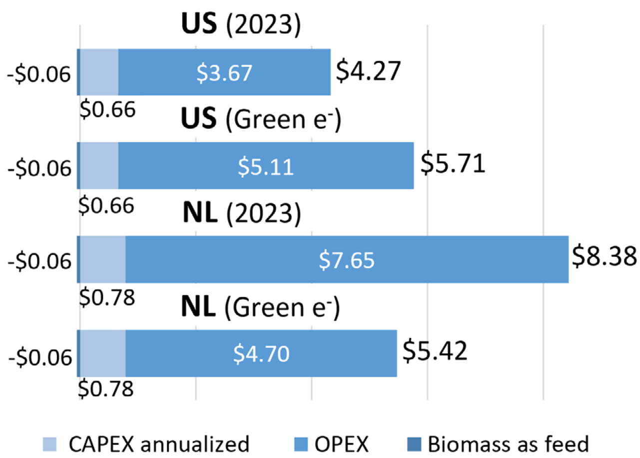

Figure 3. The Netherlands and USA unit production costs for 1 kg of isopropyl alcohol (IPA) produced from basic oxygen furnace (BOF) gas.

Base case environmental impacts

Comparing the USA and Netherlands, the US base-case process exhibits higher environmental impacts: the GWP is 13% higher (24.73 kgCO_2-eq), the FPMF 35% higher, and the freshwater eutrophication (FWE) 7% higher (Fig. 4). These increases are attributable to the higher environmental impacts of US steam and electricity (Fig. 4).

The US process exhibits lower impacts in ME, HCT, arable land use, and freshwater use compared with the Netherlands. Specifically, ME is 24% lower, HCT 9% lower, land use 13% lower, and water use 36% lower, primarily due to the lower environmental impacts of US-based glycerol. Most environmental impacts of the BOF gas fermentation to IPA process arise from steam and glycerol consumption (Fig. 4). Process CO_2 emissions are not captured. These

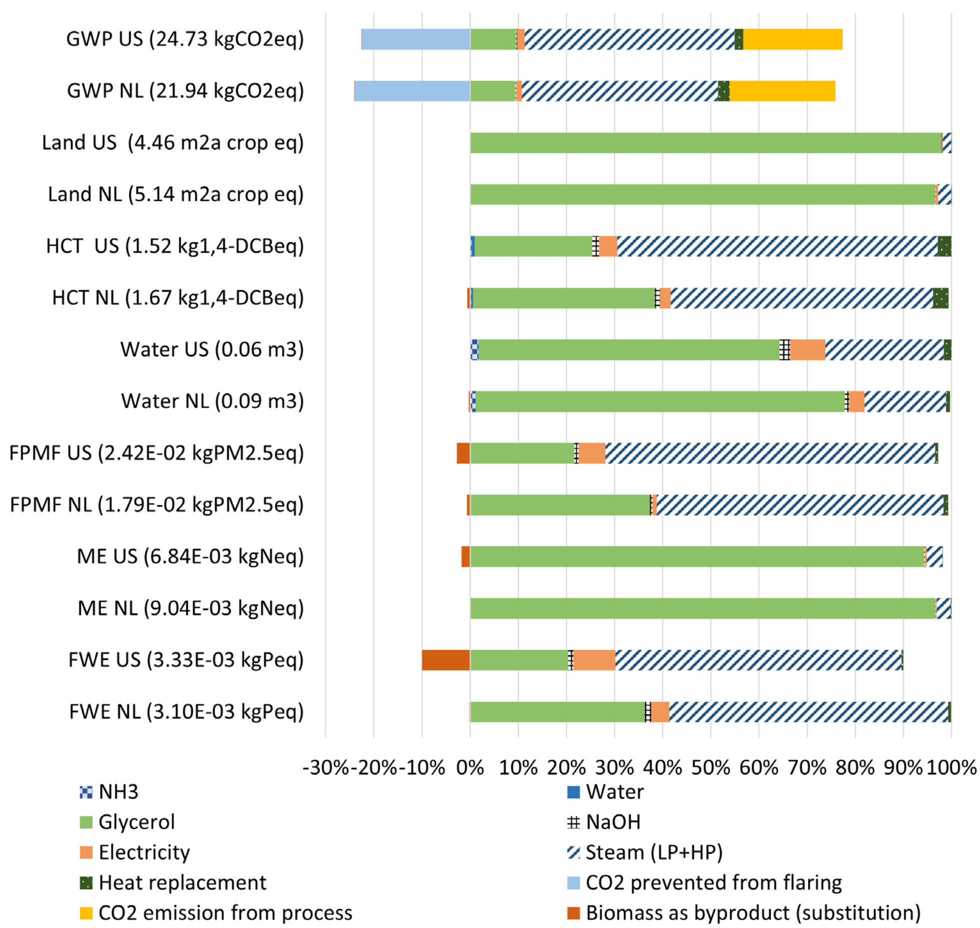

Figure 4. Environmental impacts and contributions for the basic oxygen furnace (BOF) gas fermentation to isopropyl alcohol (IPA) process per kg of IPA produced for the USA and Netherlands cases. FPMF, fine particulate matter formation; FWE, freshwater eutrophication; GWP, global warming potential; HCT, human carcinogenic toxicity; ME, marine eutrophication.

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emissions could, however, be stored or utilized if the off-gas is upgraded to syngas using green electricity.

To examine mitigation options, scenarios with lower steam consumption, lower glycerol consumption, and CO_2 off-gas capture were studied (Fig. 5 and Supporting Information, Section S9). Eliminating steam or glycerol consumption individually results in GWP reductions of 78.5% and 17.8%, respectively. When these options are combined, the Netherlands process – having the lowest GWP – can approach cradle-to-gate Net Zero carbon emissions, accounting for all three scopes, if glycerol and steam consumption are reduced by more than 50% and CO_2 off-gas is captured (Figs. 1 and 5).

We conclude that steam, cooling water, and glycerol consumption govern both the economic and environmental performance of the modeled base-case process.

Parametric sensitivity analysis

Economic key process parameters

Considering the relative economic sensitivity (Δ%UPC per Δ%), based on the different process parameters (see Fig. 6 and Supporting Information, Table S4.1) we identified the three parameters with the highest impact on the UPC of IPA: the CO volumetric mass transfer rate (VMT_{CO}), the bioreactor dilution rate (D), and the biomass filtration liquid permeate fraction (Biom. filt. L-L; i.e., the liquid loss). Each of these parameters has a relative impact greater than 0.51 Δ%UPC/Δ% parameter, and therefore strongly influences the economic sustainability of the process (Fig. 6 and Supporting Information, Section S7).

In contrast, CO conversion (CO conv.), glycerol bleed (Gly bleed), and the extractive distillation glycerol molefraction

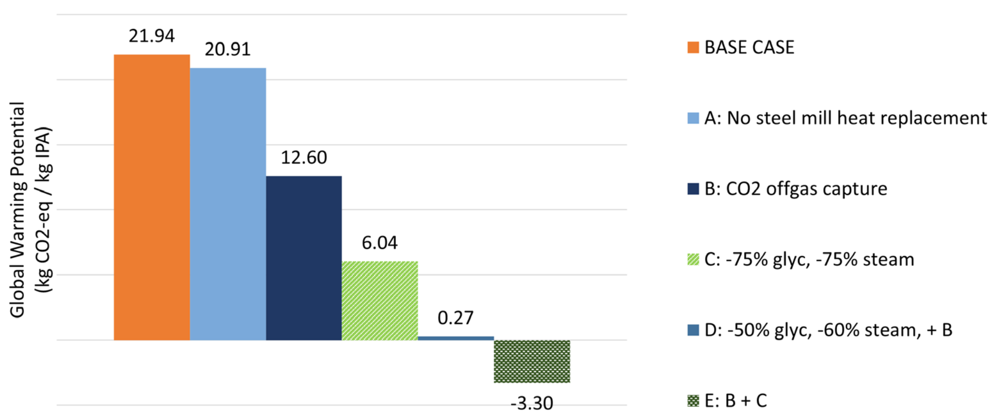

Figure 5. The change in the global warming potential (GWP) ($kg_{CO2\text{-}eq}$ $kg^{-1}{}_{IPA}$) for the Netherlands when the glycerol and/or steam consumption per kg_{IPA} produced is decreased. Effects of capturing process emissions. The GWP is calculated based on the 2024 Dutch electricity mix and includes heat replacement for the steel mill.

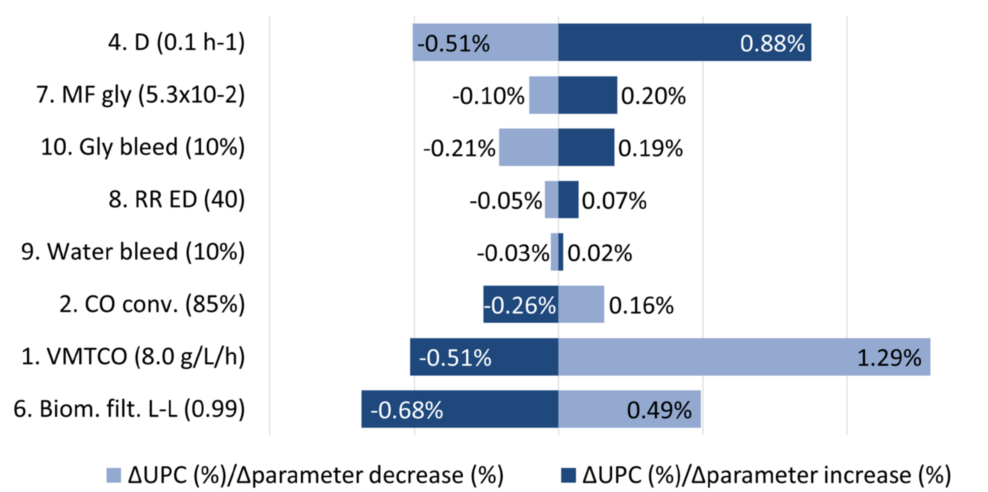

Figure 6. Parametric sensitivity analysis showing the change in UPC (%) for each parameter when increased. Parameters were varied by ±30%, except for CO conversion (CO conv., ±5%) and biomass filtration liquid permeate fraction (biomass filt. L-L, ±1%). See Fig. 1 for parameter definitions and the process overview.

(MF_{gly}) have a smaller relative influence on the UPC of 0.10–0.21 Δ%UPC/Δ% parameter (Fig. 6 and Supporting Information, Section S7). This impact is at most half that of biom. filt. L-L, D and VMT_{CO} across the ranges that were studied.

Environmental key process parameters

The parametric sensitivity analysis (Fig. 7 and Supporting Information, Fig. S10.1) indicates that similar patterns occur across environmental midpoint impact categories when process parameters are varied. The parameters with the largest impacts are: VMT_{CO}, $Y_{IPA/CO}$, D, RR_{ED}, and glycerol bleed, with consistent effects across categories. A more sustainable process is achieved with higher VMT_{CO} and $Y_{IPA/CO}$ whereas lower D, RR_{ED}, and MF_{Gly} also enhance sustainability.

Process parameter tradeoffs for improving economic and environmental sustainability

When analyzing the influence of process parameters on economic and environmental sustainability, a higher VMT_{CO} and lower D emerge as key factors (see Table 1). A higher VMT_{CO} and a lower D create a more concentrated process because fermenter volumetric productivity is assumed to be limited by the VMT_{CO} rather than biological conversion. At constant VMT_{CO}, a lower D reduces broth outflow while maintaining higher steady-state biomass concentrations and similar product yields. Previous studies also identified the dilution rate[30] and gas mass transfer[16,31] as important process parameters. However, a lower D may reduce cell viability.

The VMT_{CO} was based on ethanol at lower overhead pressure,[31] whereas propanol reduces bubble size more than ethanol, and increased pressure also enhances mass transfer.[32] This suggests that higher VMT_{CO} values could be achievable. Alternatively, VMT_{CO} could be increased through bioreactor or sparging design to extend gas residence time, and/or enlarge the gas–liquid interface with smaller bubbles.

Improved process designs

When evaluating parameter changes to improve process performance, all key parameters except D and VMT_{CO} are near their theoretical limit (Table 1). The feasible parameter

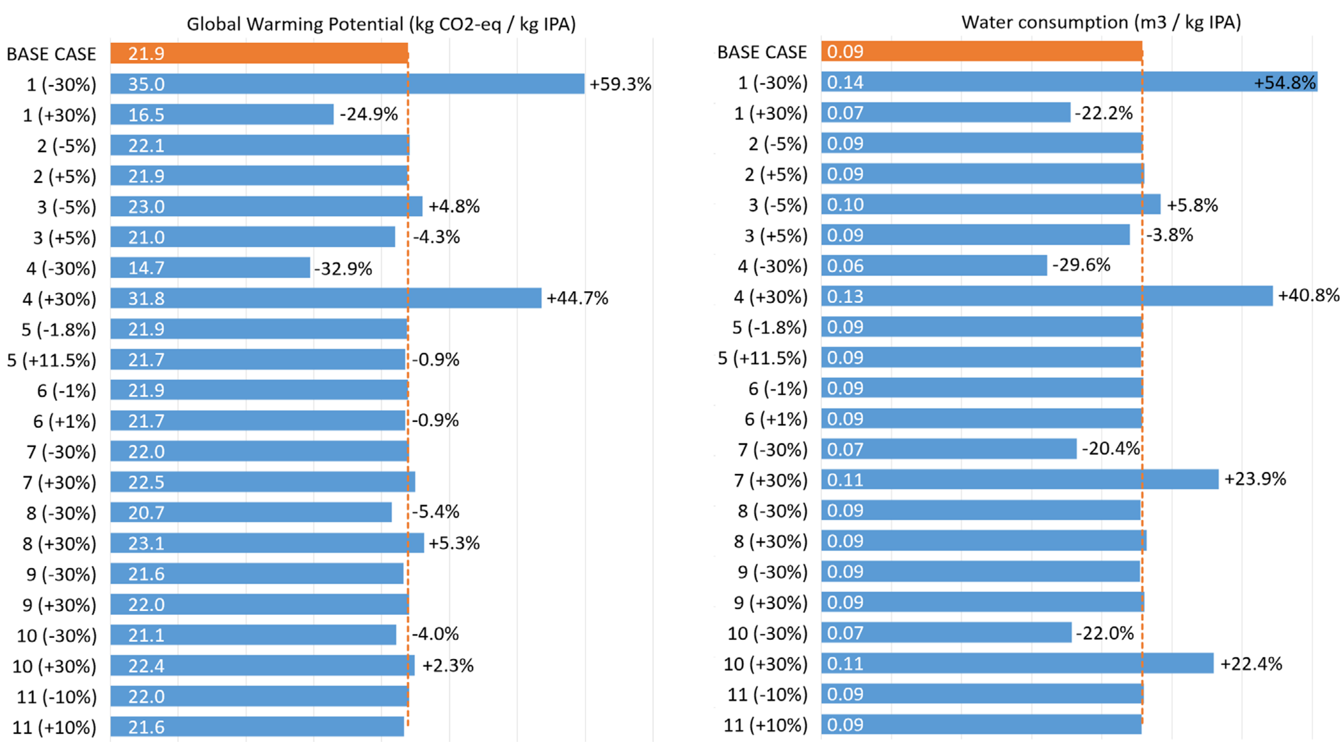

Figure 7. Sensitivity of the global warming potential ($kg_{CO2\text{-}eq}\ kg^{-1}_{IPA}$) and freshwater consumption ($m^3\ kg^{-1}$ IPA) to process parameters. All parameter changes are evaluated relative to the base case Netherlands scenario with biomass as a byproduct (vertical dashed line). The varied process parameters and their base values are: CO volumetric mass transfer rate (8 g $L^{-1}\ h^{-1}$); CO conversion (85%); product selectivity IPA/CO ($Y_{IPA/CO}$; 0.91 mol mol^{-1}); dilution rate (0.1 h^{-1}); off-gas condenser temperature (278.15 K); biomass filtration liquid permeate fraction (0.99); glycerol mole fraction during extractive distillation (5.13×10^{-2}); extractive distillation reflux ratio (40); water bleed (10%), glycerol bleed (10%); and anaerobic digestion conversion (0.90).

Table 1. Parameter influence and importance for economic and environmental sustainability of the basic oxygen furnace (BOF) gas fermentation to isopropyl alcohol (IPA).

Parameter	Lower IPA production costs (USD $kg^{-1}{}_{IPA}$)	Lower overall environmental impacts	Relative theoretical/technical limit
1. VMT_{CO}	⇧⇧⇧	⇧⇧⇧	+6.25%
2. CO conv.	⇧⇧	⇧	+17.6%
3. $Y_{IPA/CO}$	⇧	⇧⇧	+9.9%
4. D	⇩⇩⇩	⇩⇩⇩	About −30%
5. $T_{off\text{-}gas\ cond\cdot}$	⇧	⇧	Technical tradeoff
6. Biom. Filt. L-L	⇧⇧	⇧	1%
7. MF_{Gly}	⇩⇩	⇩	Technical tradeoff
8. RR_{ED}	⇩	⇩	Technical tradeoff
9. Water bleed	⇩	⇩	Technical tradeoff
10. Glycerol bleed	⇩⇩	⇩⇩	Technical tradeoff
11. AD efficiency	⇧	⇧	+11.11%

The direction and number of arrows give the direction of improved sustainability and the relative influence of the parameter. The technical/theoretical limitations of the parameter are taken into account for these influences.

Table 2. Parameter changes introduced for the three improved process designs (IMP), compared with the base case basic oxygen furnace (BOF) gas fermentation to isopropyl alcohol (IPA) process.

	IMP1	IMP2	IMP3
1. VMT_{CO} (+6.25%; 8.5 g/L/h)	✗	✓	✓
4. D (−30%; 0.07 h^{-1})	✓	✓	✓
5. $T_{off\text{-}gas\ cond\cdot}$ (+11.50%; 310.15 K)	✓	✓	✓
8. RR (−30%; 28)	✓	✓	✓
10. Glycerol bleed (−30%; 0.07)	✓	✓	✗

Table 3. Base case consumption, emissions and waste production per kg isopropyl alcohol (IPA) and the change compared to the improved process designs. The two biggest differences between improved 1 (IMP1) and improved 3 (IMP3) are given in bold.

	Base case ($kg_i\ kg^{-1}{}_{IPA}$)	IMP1	IMP3
NH_3	1.78×10^{-2}	−15.4%	−14.9%
Water	5.86	−42.8%	−46.1%
Glycerol	1.29	**−52.1%**	−35.5%
NaOH	7.57×10^{-2}	−0.08%	0.56%
Electricity (kWh)	1.22	−18.9%	−16.1%
Steam	54.8	−36.8%	**−45.2%**
CO_2-eq prevented	10.18	−0.7%	−0.05%
Process CO_2 emissions	9.32	−9.2%	−5.45%
Waste in wastewater	2.54×10^{-1}	−35.8%	−27.8%
Biomass	7.96×10^{-2}	−15.4%	−14.9%

IMP1: D −30%, $T_{off\text{-}gas\text{-}cond}$ +11.50%, RR_{ED} −30% and glycerol bleed −30%; IMP3: combination of VMT_{CO} +6.25%, D −30%, $T_{off\text{-}gas\text{-}cond}$ +11.50%, RR_{ED} −30%.

changes were combined and evaluated in three improved process designs (IMP1–3), incorporating tradeoffs between glycerol bleed (IMP1 and 2) and VMT_{CO} (IMP2 and 3) (Table 2).

These modifications resulted in changes in key consumptions and emissions, as summarized in Table 3. IMP1 and IMP3 achieved substantial reductions in water, glycerol, and steam use. IMP2 is not shown, as it did not reach the required IPA purity of 99 wt%. A tradeoff between the glycerol bleed and VMT_{CO} is clear: glycerol consumption is reduced by 52.1% in IMP1, while steam consumption decreases by 45.2% in IMP3 relative to the base case (Table 3)The IPA titers remain below the reported growth-inhibiting concentration of 50 g L^{-1}, with 33.3 g L^{-1} for IMP1 and 35.5 g L^{-1} for IMP3.[17]

Improved process economics

This tradeoff between IMP1, with lower glycerol consumption, and IMP3, with lower steam consumption, is reflected in the UPC per case (Fig. 8). IMP1 provides the most favorable economic outcome for the USA, with a UPC of USD 3.28 per kg_{IPA} (−23.2%), whereas IMP3 yields the lowest UPC for the Netherlands, at USD 5.62 per kg_{IPA} (−32.9%). These differences correspond to the relative economic contributions of steam and glycerol (Fig. 2) and

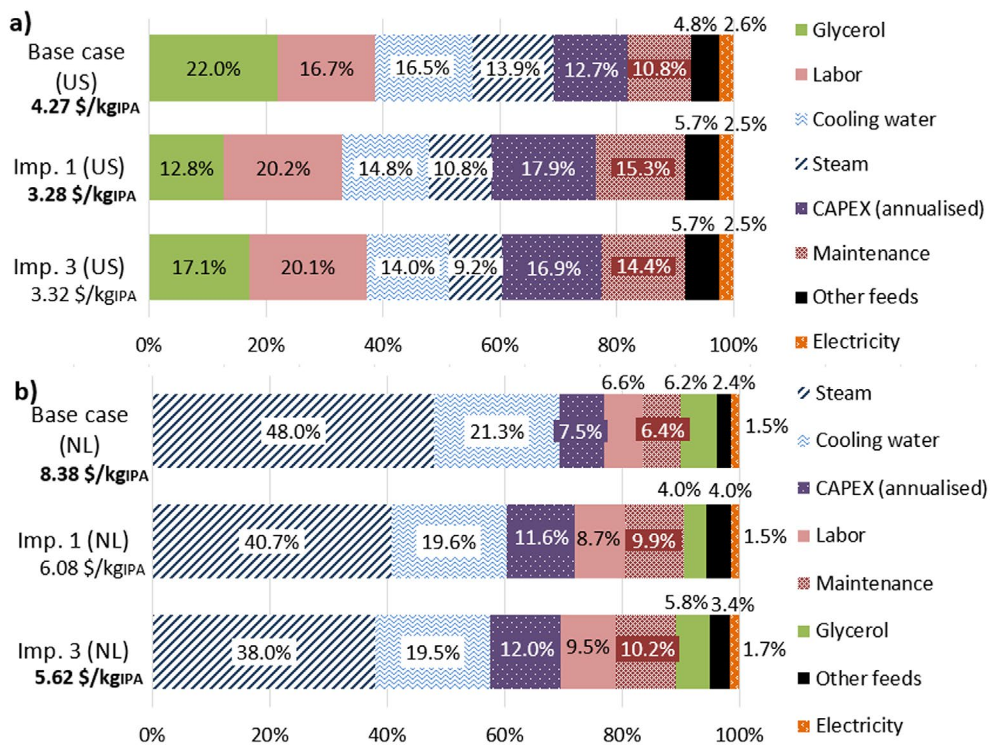

Figure 8. The unit production costs of 1 kg isopropyl alcohol (IPA) from basic oxygen furnace (BOF) gas fermentation for improved process designs when based in (a) the USA or (b) the Netherlands.

whether a +6.25% change in VMT_{CO} has greater impact than a −30% glycerol bleed. Overall, the lowest UPC of USD 3.28 per kg_{IPA} is achieved in the US IMP1 case, which remains more than twice the US market price of USD 1.31 kg $_{IPA}$.[22]

Environmental assessment combined parameters

In terms of GWP (Fig. 9(a)), IMP3 achieves up to a 44.4% reduction relative to the base case. For IMP1, reductions across impact categories range from 40.2% for HCT to 51.5% for ME, with GWP reduced by 42.4% (Fig. 9(a,c,f)). In IMP3, all impact categories decrease between 35.4% (water use) and 44.4% (GWP) (Fig. 9(a–g), SI, Table S11.1). The sustainability of each improved process design is location-dependent due to higher emissions per unit of utilities in the Netherlands (steam from natural gas) and lower impacts for US glycerol (biobased). IMP3 is considered the most sustainable design for both locations, yielding 12.20 and 13.71 kg CO_2-eq kg^{-1} IPA for the Netherlands and USA, respectively.

Comparing plant locations, the Netherlands generally shows the lowest GWP, FPMF, and FWE, whereas the USA, specifically IMP1, achieves the lowest ME, land use, and water use. Overall, lower water use and HCT are typically observed for the USA.

We conclude that the most sustainable process design and location depend on the priority assigned to specific impact categories. If GWP is prioritized, IMP3 is the most sustainable (Fig. 9(a)), whereas IMP1 is preferred for all other impact categories (Fig. 9(b–g)). This reflects a tradeoff between CO volumetric mass transfer rate (VMT_{CO}, +6.25%, 8.5 g L^{-1} h^{-1}) and glycerol bleed (−30%, 0.07). Further reductions in environmental impact could be achieved with a higher VMT_{CO} and by redesigning the downstream processing (DSP) to improve energy and glycerol efficiency or by using an alternative to glycerol.

Comparison of improved processes with pilot data and petrochemical IPA production

The improved process UPC (Fig. 10) shows that, for the Netherlands case, with the current energy grid, IMP3 has the lowest UPC of 5.62, whereas with a future green electricity grid this could drop to USD 3.96 USD per kg_{IPA}. The market price is USD 1.31 per kg_{IPA} and USD 1.63 per kg_{IPA} for the USA and Netherlands, respectively.[22] Low-carbon utilities are beneficial for the GWP of this process (see Fig. 10). We believe that, with alternative DSP designs and further optimization, the current state-of-the-art BOF gas fermentation to IPA could achieve both more competitive

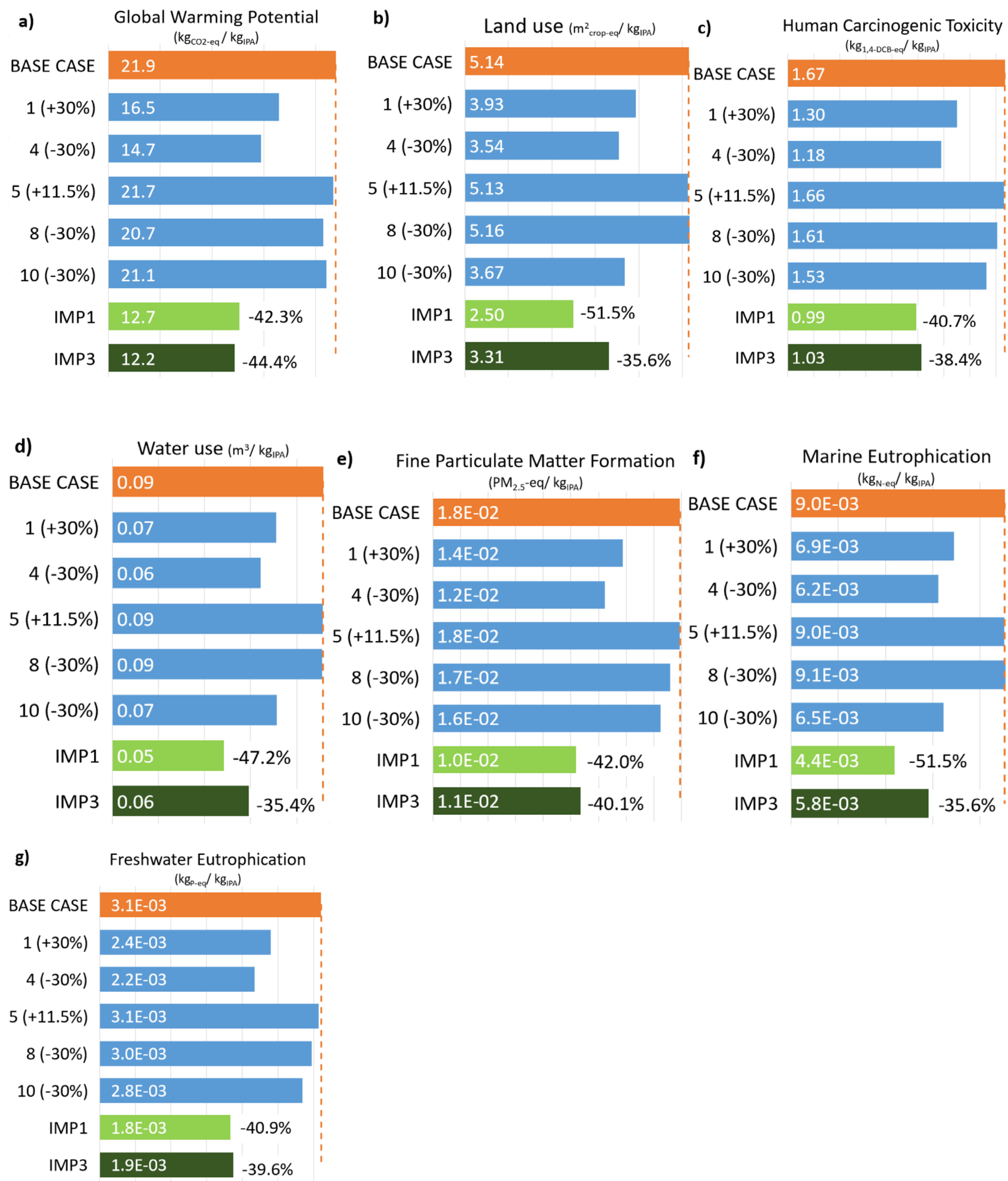

Figure 9. The environmental impacts in the Netherlands for (a) global warming potential (GWP), (b) land use, (c) human carcinogenic toxicity (HCT), (d) water use, (e) fine particulate matter formation (FPMF), (f) marine eutrophication (ME), (g) freshwater eutrophication (FWE) change compared to the base case (orange bar and dashed line) when the different process parameters are varied. The parameter changes, compared with the base case, are: CO volumetric mass transfer rate increased by 30% (1), dilution rate decreased by 30% (4), off-gas condenser temperature increased by 11.50% (5), extractive distillation reflux ratio decreased by 30% (8), and glycerol bleed decreased by 30% (10). IMP1 combines a 30% decrease in dilution rate, an 11.50% increase in off-gas condenser temperature, a 30% decrease in reflux ratio, and a 30% decrease in glycerol bleed. IMP3 combines a 6.25% increase in CO volumetric mass transfer rate, a 30% decrease in dilution rate, an 11.50% increase in off-gas condenser temperature, and a 30% decrease in reflux ratio.

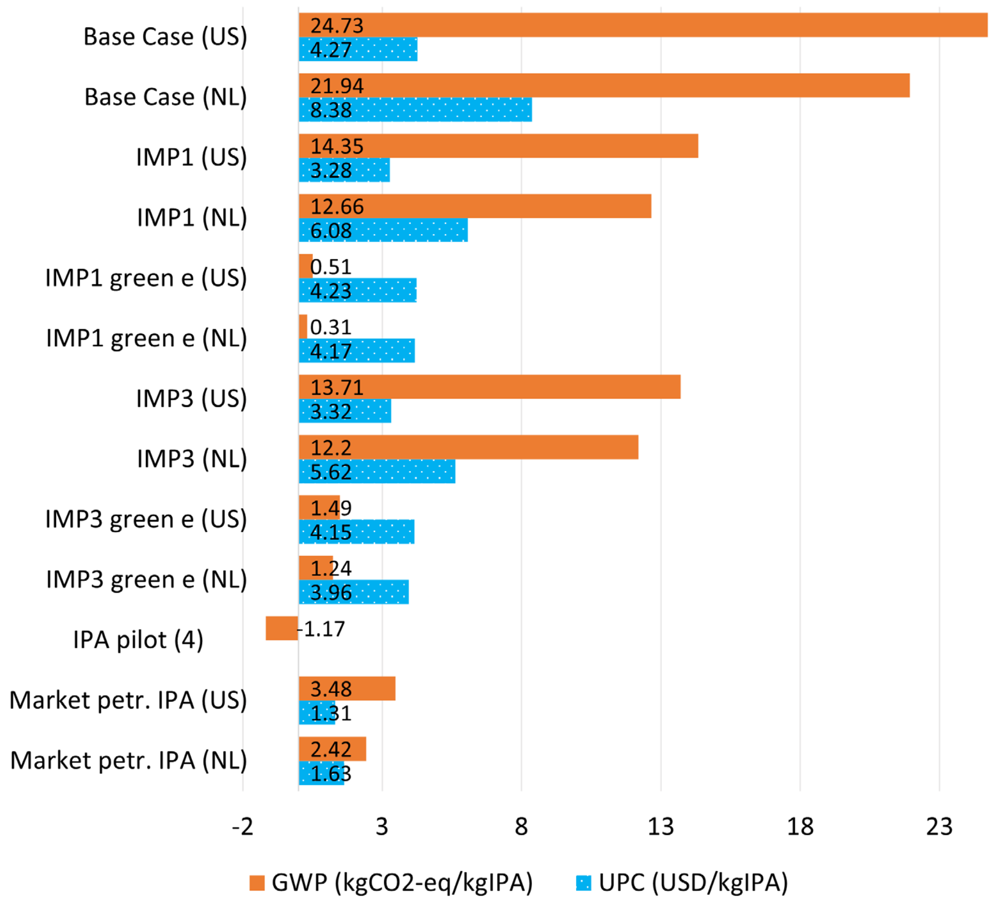

Figure 10. Comparison of the unit production costs (UPCs) and global warming potentials (GWPs) of the base case, improved process 1 (IMP1), improved process 3 (IMP3), and current petrochemical isopropyl alcohol (IPA) market price and emissions. All process designs include selling the microbial biomass as a soybean meal feed replacement (USD –0.06 per kg_{IPA}).

economics and improved environmental performance compared with fossil IPA.

Considering the cradle-to-gate LCA, the base case shows a substantially higher GWP than the emissions reported for the pilot-scale study by Liew *et al.*[4] (24.73 $kg_{CO2\text{-}eq}\ kg^{-1}{}_{IPA}$ compared with −1.17 $kg_{CO2\text{-}eq}\ kg^{-1}{}_{IPA}$) (Fig. 10). This difference is mainly driven by the steam and glycerol consumption associated with downstream processing (see Fig. 4).

For a gate-to-gate assessment of the gas fermentation stage, the modeled process yields GHG emissions of −0.86 $kg_{CO2}\ kg^{-1}{}_{IPA}$, because it avoids CO_2 emissions from flaring the BOF gas. Liew *et al.*[4] reported a GWP of −1.17 $kg_{CO2}\ kg^{-1}{}_{IPA}$.

Conclusions

A novel, integrated gas fermentation process was designed, modeled, and improved to produce 46 kton $year^{-1}$ of IPA (>99 wt%) from BOF gas. This study combined economic and environmental assessments across seven midpoint impact categories to evaluate sustainability trade-offs and to account for the implications of integrating this CCU-type process at the steel mill.

Parametric sensitivity analysis shows that a higher CO volumetric mass transfer rate (0.52 $\Delta\%UPC/\Delta\%VMT_{co}$) and lower dilution rate (0.51 $\Delta\%UPC/\Delta\%D$) are the key parameters for improving sustainability. Combining individually beneficial parameter changes introduced tradeoffs and, in some cases, reduced technical performance.

The economic and environmental sustainability tradeoffs are related to plant location, glycerol and steam price, and their respective life cycle environmental impacts. As a consequence, the best economics are obtained for IMP1 in the USA (UPC: USD 3.28 per kg_{IPA}; −23% from base case), still exceeding the market price of USD 1.31 per kg; whereas the lowest GWP is obtained for IMP3 in the Netherlands (12.2 $kg_{CO2\text{-}eq}\ kg^{-1}{}_{IPA}$; −44.4% from the base case). The current process design requires more energy- and glycerol-efficient downstream processing to be economically competitive and achieve Net Zero GWP.

Future recommendations

To further identify options for improving sustainable processing, we suggest the following lines of investigation:

- Reducing utility use, particularly steam, and lowering glycerol consumption during IPA production from BOF gas fermentation. Future work could also assess a redesigned DSP scheme using vacuum distillation[33] and evaluate its economic and environmental implications.
- Assessing the influence of product selectivity and acetone byproduct formation (the precursor of IPA) on industrial-scale process performance.
- Examining the mass-transfer-enhancing effect of IPA through experimental studies and *in silico* evaluation, and determining its impact on overall technoeconomic and environmental performance at industrial scale.

Abbreviations

AD efficiency	The fractional conversion of organics during anaerobic digestion.
Biom. Filt. L-L	Fraction of the feed liquid in the biomass filtration step ending in the permeate.
BOF gas	Basic oxygen furnace gas, a form of syngas from a steel mill.
CAPEX	Capital expenses.
COconv	Carbon monoxide conversion (fraction).
D	Dilution rate of the fermentation.
Glycerol bleed	Glycerol sent to the wastewater treatment (fraction).
IPA	Isopropyl alcohol/isopropanol.
LCA	Life cycle assessment.
MF_{Gly}	The relative mole fraction of glycerol compared to the liquid feed during the extractive distillation.
μ	Biomass growth rate (h^{-1}).
OPEX	Operating expenses.
RR_{ED}	The extractive distillation reflux ratio.
Syngas	Synthesis gas, a gas mixture of CO, CO_2, H_2 and N_2.
T off-gas cond.	Temperature of the off-gas condenser.
TEA	Techno-economic analysis.
TIC	Total investment cost.
TIEC	Total installed equipment cost.
VMT_{CO}	Carbon monoxide volumetric mass transfer rate of the vapor-to-liquid phase.
Water bleed	Water sent to the wastewater treatment (fraction).
Y_{DSP}	Downstream processing yield.
$Y_{IPA/CO}$	Product selectivity ($cmol_{IPA}\ mol_{CO}^{-1}$) of the carbon from CO ending in the IPA product.

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Conflict of interest statement

The authors declare no conflict of interest.

Data availability statement

The authors confirm that the data supporting the findings of this study are available within the article and its supplementary materials. Additional data are available from the corresponding author upon reasonable request.

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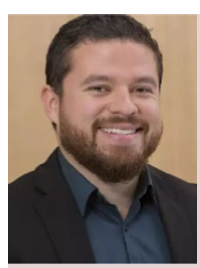

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