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DOI
10.1016/B978-0-443-28824-1.50068-5

Publication date
2024

Document Version
Final published version

Published in
Proceedings of the 34th European Symposium on Computer Aided Process Engineering

Citation (APA)
Brouwer, G. J. A., Shijaz, H., & Posada, J. A. (2024). Modelling and Parametric Analysis for Improving Technical Performance of Industrial-Scale Basic Oxygen Furnace Gas Fermentation to Isopropyl Alcohol. In F. Manenti, & G. V. Reklaitis (Eds.), *Proceedings of the 34th European Symposium on Computer Aided Process Engineering: 15th International Symposium on Process Systems Engineering (ESCAPE34/PSE24)* (pp. 403-408). (Computer Aided Chemical Engineering; Vol. 53). Elsevier. https://doi.org/10.1016/B978-0-443-28824-1.50068-5

Flavio Manenti, Gintaras V. Reklaitis (Eds.), Proceedings of the 34th European Symposium on Computer Aided Process Engineering / 15th International Symposium on Process Systems Engineering (ESCAPE34/PSE24), June 2-6, 2024, Florence, Italy
 http://dx.doi.org/10.1016/B978-0-443-28824-1.50068-5

Modelling and Parametric Analysis for Improving Technical Performance of Industrial-Scale Basic Oxygen Furnace Gas Fermentation to Isopropyl Alcohol

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Abstract

The iron and steel industry is responsible for 30% of all industrial CO_2 emissions, largely emitted via hot Basic Oxygen Furnace (BOF) gas (CO, H_2, CO_2). Gas fermentation can convert the BOF gas into valuable chemicals such as the disinfectant and platform chemical isopropyl alcohol (IPA), which is currently only produced with petrochemical cracking. The goal of this research was to model the state-of-the-art industrial-scale BOF gas fermentation to IPA and identify the key process parameters affecting technical performance. The designed and modelled industrial-scale process was based on the published LanzaTech technology with *Clostridium autoethanogenum*. In the process model, the IPA is purified through extractive distillation with pure glycerol as an entrainer. During sensitivity analysis, eleven process parameters were investigated for their effect on the eighteen chosen technical Key Performance Indicators (KPIs). These process parameters are (product selectivity ($Y_{IPA/CO}$), CO volumetric mass transfer rate (VMT_{CO}), CO conversion, reactor dilution rate (D), temperature off-gas condenser, biomass separation liquid loss, extractive distillation glycerol mole fraction, extractive distillation molar reflux ratio, glycerol recycle purge, broth recycle purge and anaerobic digestion waste conversion). The sensitivity analysis identified that the key technical parameters affecting the KPIs are the gas fermentation parameters (CO conversion, VMT_{CO}, $Y_{IPA/CO}$, and D) as well as the biomass filtration liquid loss. Moreover, increasing CO conversion, VMT_{CO}, $Y_{IPA/CO}$ as well as decreasing D and the biomass filtration liquid loss all individually had the greatest positive impact on the KPIs. Thus, this study has successfully synthesised and modelled a state-of-the-art industrial-scale BOF gas fermentation to IPA process and identified the key process parameters to improve its technical process performance. These findings can be used both to optimise the BOF gas fermentation to IPA process, and perform further economic evaluations and environmental impact assessment.

Keywords: BOF gas fermentation, Isopropyl Alcohol (IPA), process modelling, sensitivity analysis, technical performance.

1. Introduction

The iron and steel industry is responsible for 30 % of all industrial CO_2 emissions (IEA, 2020). A large portion of CO_2 is emitted through flaring of the energy-rich off-gas containing CO, H_2 and CO_2 called Basic Oxygen Furnace (BOF) gas. However, BOF gas can be converted, through gas fermentation, into valuable chemicals such as the disinfectant and platform chemical isopropyl alcohol (IPA) (Liew *et al.*, 2022). Currently, there is no green alternative for the polluting petrochemical production of IPA through cracking. BOF gas fermentation to IPA could serve this growing IPA market with a sustainable alternative.

In 2020, LanzaTech commercialised industrial-scale BOF gas fermentation to ethanol using a genetically engineered and patented (Simpson *et al.*, 2012), prototrophic (Annan *et al.*, 2019), anaerobic acetogen (*Clostridium autoethanogenum*, *C. autoethanogenum*) (Köpke and Simpson, 2020). Usually, the gas-liquid mass transfer is limiting the reaction rate and volumetric productivity (q_i) of gas fermentations. However, alcohols like ethanol have gas-liquid mass transfer enhancing properties (Puiman *et al.*, 2022a), giving a CO volumetric mass transfer rate (VMT_{CO}) up to 8.5 g_{CO}/L/h for the industrial-scale external-loop gas-lift reactor used by LanzaTech (Puiman *et al.*, 2022b). The effect of IPA on the mass transfer was not investigated, but according to Keitel and Onken (1982, p. 94) the mass transfer-enhancing properties of ethanol and isopropanol (i.e., IPA) are similar. More recently, LanzaTech published promising results of a pilot-scale process to produce IPA from BOF gas (Liew *et al.*, 2022). Nonetheless, the industrial-scale IPA process and the key parameters affecting its performance are not yet known. Therefore, the goal of this research was to model the state-of-the-art industrial-scale BOF gas fermentation to IPA and identify the key process parameters affecting technical performance. First, the 46,000 $kton_{IPA}$/year (Liew *et al.*, 2022) industrial-scale production process was modelled (see section 2) and its technical performance assessed (see section 3). Then, a sensitivity analysis was performed to identify the key process parameters to improve technical process performance (see section 4). Lastly, conclusions and recommendations are given (see section 5).

2. Modelling of Industrial-Scale Basic Oxygen Furnace Gas Fermentation to Isopropyl Alcohol

This section describes the modelling of the industrial-scale state-of-the-art BOF gas fermentation to IPA, including heat integration and recycles, in Aspen Plus V12.0. The most relevant process units and conditions are schematically given (see Figure 1). The property method used is Non-Random Two-Liquid (NRTL), with Mix Non-Conventional (MIXNC) for the gas fermentation and biomass filtration. The model was based on the published LanzaTech technology (Liew *et al.*, 2022; Köpke and Simpson, 2020; Handler *et al.*, 2016) with the genetically engineered, prototrophic *C. autoethanogenum* (Simpson *et al.*, 2012; Annan *et al.*, 2019). The gas fermentation stoichiometry was approached as a black box and obtained through thermodynamics (Heijnen and Van Dijken, 1992), assuming only acetic acid and biomass as by-products. This resulted in an overall black box stoichiometry (see Equation 1) as input for the stoichiometric reactor (RStoich) in the model. Acetone and ethanol were not included as by-products due to their minor fraction produced (Liew *et. al.*, 2022), but were accounted for with the other by-products. Besides, reaction kinetics were not included, since the gas fermentation was assumed limited by the volumetric mass transfer of CO (VMT_{CO}; Liew *et al.*, 2022).

$$-8.24\,CO - 1.58\,H_2 - 2.63\,H_2O - 0.0462\,NH_3 - 0.111\,NaOH \rightarrow 0.185\,CH_{1.75}O_{0.5}N_{0.25} + 1.00\,IPA + 4.83\,CO_2 + 0.111\,Acetic\ Acid + 0.111\,Na^+ \qquad (1)$$

The applied industrial-scale reactor conditions and mass transfer rate were described by Puiman *et al.* (2022b). The product recovery mentioned by Liew *et al.* (2022) was split into biomass cross-flow filtration and extractive distillation (Simpson *et al.*, 2012), with pure glycerol as an entrainer (see Figure 1). The purges, to prevent accumulation of impurities, were anaerobically digested (Figure 1; Liew *et al.*, 2022). The biogas resulting from the anaerobic digestion and the fermenter off-gas is combusted with an excess of O_2, to generate heat as a utility for internal use (see Figure 1).

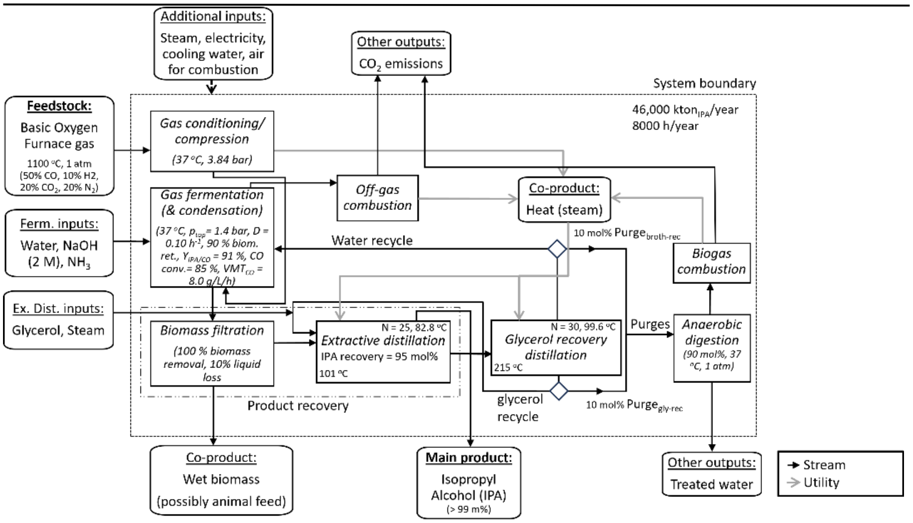

Figure 1: The schematic overview of the Basic Oxygen Furnace gas fermentation to isopropyl alcohol (IPA) adapted and extended from Liew *et al.* (2022). D: dilution rate, biom. ret.: biomass retention, $Y_{IPA/CO}$: product selectivity, CO conv.: CO conversion, VMT_{CO}: volumetric mass transfer rate of CO in the reactor, N: number of distillation stages.

3. Technical Performance Assessment of the Industrial-Scale Basic Oxygen Furnace Gas Fermentation to Isopropyl Alcohol

The key performance indicators (KPIs) were selected based on their indication of gas fermentation performance, overall substrate-to-product performance, or technical performance. Besides productivity and carbon efficiency, this leads to KPIs such as the consumption of chemicals/ substrates, the consumption of utilities, as well as the generation of wastes and process-related CO_2 emissions. Moreover, KPIs that influence economics are the required reactor volume ($V_{Reactor}$) and the IPA titer. Together, these eighteen KPIs indicate the overall technical process performance (see Table 1).

Table 1: Key Performance Indicator (KPI) results of the base case scenario of the BOF gas fermentation to IPA process model. Furthermore, the VMT_{CO}: CO volumetric mass transfer rate, R_{IPA}: IPA production rate, $V_{Reactor}$: required reactor volume, q_{IPA}: volumetric productivity, and $glycerol_{MF\text{-}ED}$: mole fraction of glycerol at the extractive distillation.

Parameters	Base Case	Units	KPI Results	Base Case	Units	KPI Results	Base Case	Units
Set parameters:			***Process KPIs:***			***Emission & waste:***		
VMT_{CO}	8.000	g_{CO}/L/h	R_{IPA}	5755	kg_{IPA}/h	CO_2 Off-gas	$4.387e^{+4}$	kg/h
CO conversion	0.850	Mole frac.	Carbon Efficiency	$3.022e^{-1}$	Mole frac.	CO_2 Biogas	9778	kg/h
CO Feed (BOF gas)	$2.662e^{+4}$	kg/h	$V_{Reactor}$	2829	m^3	Process CO_2 emission	$5.364e^{+4}$	kg/h
$Glycerol_{MF\text{-}ED}$	$5.131e^{-2}$	Mole frac.	q_{IPA}	2.083	g_{IPA}/L/h	Waste in Wastewater	1459	kg/h
Dilution rate	0.100	h^{-1}	IPA titer	22.30	g/L	Biomass Out	457.9	kg/h
Product selectivity	$9.101e^{-1}$	Cmole frac.						
Purities:			***Feeds:***			***Utility consumption:***		
IPA purity	$9.913e^{-1}$	mass%	Feed Glycerol	7440	kg/h	Electricity	8835	kW
Glycerol rec. purity	$9.590e^{-1}$	mass%	Feed Water	28.35	m^3/h	Cooling water	1050	-GJ/h
			Feed NaOH	435.8	kg/h	LP-Steam	118.1	GJ/h
			Feed NH_3	102.2	kg/h	HP-Steam	424.3	GJ/h

4. Sensitivity Analysis of the Industrial-Scale Basic Oxygen Furnace Gas Fermentation to Isopropyl Alcohol

4.1. Parameters Investigated During the Sensitivity Analysis

The goal of the sensitivity analysis was to highlight the key parameters of the industrial-scale BOF gas to IPA process (model) (Figure 1) to improve technical performance (see Table 1). The sensitivity analysis was performed on eleven process parameters which were expected most influential on the technical performance or process design choices (see Table 2). During the sensitivity analysis, the process parameter investigated was typically varied ±30 % unless there were theoretical restrictions. At the same time, the other parameters studied and conditions of the process were kept constant (see Table 2).

4.2. Sensitivity Analysis Results

The overview of the sensitivity analysis results (Table 2) shows which KPIs are sensitive. A KPI was considered sensitive for a parameter, when a parameter change (±Δ%) resulted in at least ±0.90 Δ% for that KPI. For example, q_{IPA} is sensitive to VMT_{CO}, since +30 % VMT_{co} resulted in +30 % q_{IPA}. The sensitivity analysis helped identify five process parameters that show the biggest overall effect on the KPIs across all KPI groups (see Table 2). These key process parameters are the fermentation parameters of CO conversion and product selectivity ($Y_{IPA/CO}$), the CO volumetric mass transfer rate (VMT_{CO}), and the dilution rate (D), as well as the biomass filtration liq-to-liq phase fraction (= 1 - liquid loss). These key process parameters have the biggest effect on technical performance of the industrial-scale BOF gas-to-IPA fermentation process and are a good focus point to improve technical performance. Based on the sensitivity analyses, the following trends were found:

Higher CO conversion and $Y_{IPA/CO}$ improve technical performance (see Table 2). Both CO conversion and $Y_{IPA/CO}$ influence most KPIs (Table 2) of which the most important economic indicators are R_{IPA}, carbon efficiency and $V_{Reactor}$. However, $V_{Reactor}$ increases along with R_{IPA} and results in more utility consumption. Therefore, at higher CO conversion the indicated q_{IPA} does not increase, only relatively more BOF gas is used. Besides, technical performance improves at a higher $Y_{IPA/CO}$ and less by-product is formed, consequently reducing the utility consumption, waste and process-related CO_2 emissions (Table 2). Lower dilution rate seems to improve technical performance (see Table 2). Overall, utility consumption, waste and process-related CO_2 emissions increase with increasing D, while the R_{IPA} decreases and vice versa (Table 2). However, the increase in HP-steam, water, and glycerol consumption at a lower D might provide a trade-off against the R_{IPA} and carbon efficiency. Also, at lower D an IPA titer above 25 gIPA/L (Köpke *et al.*, 2016) can, in reality, limit process performance due to product inhibition. Additionally, Wang *et al.* (2023) has shown that an alcohol titer has an optimum mass transfer enhancing effect, where a higher titer reduces the mass transfer. Thus, for this process, the IPA titer likely has an optimum around 25 g_{IPA}/L. Higher CO volumetric mass transfer rate improved technical performance (see Table 2). Overall, at a higher VMT_{CO} the KPIs indicate increased technical performance, generating less waste and relatively more product (q_{IPA}) in a more concentrated process (lower $V_{Reactor}$) (Table 2). Lower biomass filtration liquid loss seems to improve technical performance (see Table 2). A lower biomass filtration liquid loss (liq-to-liq frac., Table 2) resulted in the KPIs indicating improved technical performance. Because of the reduction of broth loss, consequently less product loss. As a result, the R_{IPA} increased and the consumption of fresh feeds reduced. However, utility consumption increased, possibly giving a trade-off if the utility consumption increases more than the R_{IPA}. Extractive distillation affects technical performance, with a lower molar reflux ratio ($RR_{mol,ED}$) indicating improved technical performance (see Table 2). The investigated parameters of the extractive distillation ($Gly_{MF\text{-}ED}$ and $RR_{mol,ED}$) showed that the $C_{IPA,Reactor}$, glycerol feed, and CO_2 biogas are sensitive to the $Gly_{MF\text{-}ED}$ (Table 2). Whereas, only the LP-steam consumption is sensitive to the $RR_{mol,ED}$. A 30 % lower $RR_{mol,ED}$ decreases the LP-steam 1.38 times as much, while R_{IPA} and carbon efficiency only change -1.13 % (Table 2). Combining these insights, the extractive distillation itself is considered important for process performance.

Higher temperature of the off-gas condenser and a lower purified glycerol purge fraction improved technical performance (see Table 2). The off-gas condenser showed less utility consumption and little reduction in performance at increased temperature, thus higher $T_{off\text{-}gas\ cond.}$ could improve technical performance (see Table 2). Whereas, technical performance improved for a lower glycerol purge fraction, giving less glycerol consumption, waste production, and process-related CO_2 emissions (see Table 2). Usually, there is a trade-off in KPIs for each parameter. These KPIs have opposite trends and both affect the technical process performance. This makes the overall effect of a parameter change hard to predict.

Table 2: Sensitivity analysis results. The lower boundary, base case, and upper boundary results were linearly fitted. If the adjusted $R_2 \geq 0.95$, then the linear fit slope is given. Otherwise, the resulting Δ%. VMT_{CO}: CO volumetric mass transfer rate, the liq-to-liq frac.: 1 - liquid loss during biomass filtration, $Gly_{MF\text{-}ED}$: extractive distillation glycerol molefraction, $RR_{mol,ED}$: molar reflux ratio during extractive distillation. R_{IPA}: IPA production rate, q_{IPA} volumetric productivity, LP-steam: low-pressure steam, and HP-steam: high-pressure steam. A sensitivity > ±0.90 Δ% of the parameter is bold.

		Gas Fermentation				Off-gas treatment	Microfiltration
KPI Group	**KPI**	**CO conv. (±5 %)**	**VMT_{CO} (±30 %)**	**Product selectivity (±5 %)**	**Dilution rate (±30 %)**	**$T_{off\text{-}gas\ cond.}$ (K, -1.80 %, +11.50 %)**	**liq-to-liq frac. (±1 %)**
Process KPIs	R_{IPA}	**0.99 (R^2= 1.000)**	LB -10.16 %; UB -0.25 %	**1.02 (R^2= 0.990)**	LB +0.47 %; UB -9.94 %	LB -0.02 %; UB +0.07 %	**1.04 (R^2= 1.000)**
	Carbon efficiency	**0.99 (R^2= 1.000)**	LB -10.16 %; UB -0.25 %	**1.02 (R^2= 0.990)**	LB +0.47 %; UB -9.94 %	LB -0.02 %; UB +0.07 %	**1.04 (R^2= 1.000)**
	q_{IPA}	No effect	**1.00 (R^2= 1.000)**	**1.00 (R^2= 1.000)**	-0.02 (R^2= 0.965)	No effect	No effect
	IPA titer	0.06 (R^2= 1.000)	LB +23.73 %; UB **+33.80** %	LB +1.04 %; UB **+8.29** %	LB **+47.34** %; UB **+32.39** %	-0.13 (R^2= 0.978)	0.74 (R^2= 0.997)
	$V_{Reactor}$	**1.00 (R^2= 1.000)**	LB **+42.86** %; UB -23.07 %	No effect	No effect	No effect	No effect
Feeds	Water feed	**0.98 (R^2= 1.000)**	**-1.14 (R^2= 0.953)**	**3.70 (R^2= 1.000)**	**1.04 (R^2= 0.999)**	LB -0.08 %; UB 1.78 %	**-8.56 (R^2= 1.000)**
	Glycerol feed	**0.99 (R^2= 1.000)**	**-1.10 (R^2= 0.950)**	0.13 (R^2= 0.992)	**1.00 (R^2= 0.999)**	LB 0.00 %; UB -0.10 %	0.86 (R^2= 1.000)
	NaOH feed	**1.00 (R^2= 1.000)**	No effect	**-16.97 (R^2= 1.000)**	LB +0.61 %; UB +0.03 %	No effect	No effect
	NH_3 feed	**1.00 (R^2= 1.000)**	No effect	-0.70 (R^2= 1.000)	LB -14.85 %; UB +0.03 %	No effect	No effect
Utility consumption	Electricity	-0.18 (R^2= 0.999)	-0.12 (R^2= 0.961)	-0.10 (R^2= 0.995)	0.11 (R^2= 0.997)	-0.77 (R^2= 0.983)	0.13 (R^2= 1.000)
	Cooling water	**0.98 (R^2= 1.000)**	-0.65 (R^2= 0.958)	0.30 (R^2= 0.992)	0.59 (R^2= 0.997)	LB 0.00 %; UB -0.07 %	0.70 (R^2= 1.000)
	LP-steam	**1.28 (R^2= 1.000)**	LB -14.39 %; UB +4.24 %	LB **-5.23** %; UB **+12.68** %	-0.33 (R^2= 0.952)	LB +0.05 %; UB -0.32 %	**1.64 (R^2= 1.000)**
	HP-steam	**1.85 (R^2= 1.000)**	**-1.33 (R^2= 0.968)**	LB **-4.83** %; UB +1.32 %	**1.21 (R^2= 0.991)**	LB 0.00 %; UB -0.14 %	0.77 (R^2= 1.000)
Emission & waste	CO_2 off-gas	-0.34 (R^2= 1.000)	No effect	0.09 (R^2= 0.999)	**0.99 (R^2= 1.000)**	LB 0.00 %; UB +0.11 %	No effect
	CO_2 biogas	**1.00 (R^2= 1.000)**	LB **+49.17** %; UB -21.36 %	**-1.26 (R^2= 0.990)**	**1.07 (R^2= 0.988)**	LB 0.04 %; UB -0.56 %	**1.61 (R^2= 0.999)**
	Process CO_2 emission	-0.09 (R^2= 1.000)	LB +8.96 %; UB -3.89 %	-0.16 (R^2= 0.976)	0.19 (R^2= 0.987)	LB 0.00 %; UB -0.01 %	0.29 (R^2= 0.999)
	Waste in wastewater	**0.99 (R^2= 1.000)**	LB **+36.37** %; UB -18.69 %	**-3.48 (R^2= 1.000)**	0.83 (R^2= 0.999)	LB 0.02 %; UB -0.30 %	**1.24 (R^2= 1.000)**
	Biomass Out	**1.00 (R^2= 1.000)**	No effect	-0.70 (R^2= 0.999)	0.43 (R^2= 0.984)	No effect	No effect

		Extractive distillation		Purges before recycle		Anaerobic digestion
KPI Group	**KPI**	**$Gly_{MF\text{-}ED}$ (±30 %)**	**$RR_{mol,ED}$ (±30 %)**	**Glycerol Purge (±30 %)**	**Broth Purge (±30 %)**	**Waste conv. frac. (±10 %)**
Process KPIs	R_{IPA}	LB -4.51 %; UB +0.24 %	LB -1.13 %; UB +0.08 %	LB -0.06 %; UB +0.03 %	No effect	No effect
	Carbon efficiency	LB -4.51 %; UB +0.24 %	LB -1.13 %; UB +0.08 %	LB -0.06 %; UB +0.03 %	No effect	No effect
	q_{IPA}	No effect	No effect	No effect	No effect	No effect
	IPA titer	LB **+34.80** %; UB -1.81 %	LB +8.69 %; UB -0.63 %	-0.01 (R^2= 0.950)	-0.09 (R^2= 0.956)	No effect
	$V_{Reactor}$	No effect	No effect	No effect	No effect	No effect
Feeds	Water feed	LB -1.23 %; UB +0.24 %	LB -0.36 %; UB +0.03 %	LB -0.08 %; UB 0.27 %	**0.95 (R^2= 1.000)**	No effect
	Glycerol feed	**1.07 (R^2= 1.000)**	LB -0.27 %; UB +0.02 %	**1.00 (R^2= 1.000)**	LB -0.63 %; UB +0.35 %	No effect
	NaOH feed	No effect	No effect	No effect	No effect	No effect
	NH_3 feed	No effect	No effect	No effect	No effect	No effect
Utility consumption	Electricity	0.12 (R^2= 0.999)	LB -0.06 %; UB 0.00 %	0.11 (R^2= 1.000)	LB 0.00 %; UB -0.13 %	0.12 (R^2= 1.000)
	Cooling water	LB -1.70 %; UB +0.69 %	0.16 (R^2= 1.000)	0.02 (R^2= 1.000)	LB -0.33 %; UB 0.16 %	0.02 (R^2= 1.000)
	LP-steam	-0.14 (R^2= 0.998)	**1.38 (R^2= 1.000)**	LB +1.09 %; UB +2.25 %	LB +0.96 %; UB -0.23 %	-0.06 (R^2= 1.000)
	HP-steam	LB +2.21 %; UB -7.10 %	LB -0.69 %; UB 0.03 %	-0.27 (R^2= 0.997)	0.05 (R^2= 0.979)	-0.28 (R^2= 1.000)
Emission & waste	CO_2 off-gas	No effect	No effect	No effect	No effect	No effect
	CO_2 biogas	**0.96 (R^2= 0.994)**	LB 0.97 %; UB -0.07 %	**0.97 (R^2= 1.000)**	-0.04 (R^2= 0.985)	**1.10 (R^2= 1.000)**
	Process CO_2 emission	0.18 (R^2= 0.994)	LB 0.18 %; UB -0.01 %	0.18 (R^2= 1.000)	-0.01 (R^2= 0.985)	0.20 (R^2= 1.000)
	Waste in wastewater	0.54 (R^2= 0.998)	LB 0.15 %; UB -0.01 %	0.53 (R^2= 1.000)	0.27 (R^2= 1.000)	**-5.14 (R^2= 1.000)**
	Biomass Out	No effect	No effect	No effect	No effect	No effect

5. Conclusions

A state-of-the-art industrial-scale BOF gas fermentation to IPA was modelled based on the LanzaTech pilot reported in the literature. IPA purification using extractive distillation is an energy- and glycerol-intensive process with room for improvement. Besides, the process KPIs (R_{IPA}, carbon efficiency, $V_{Reactor}$, q_{IPA}, IPA titer), feeds, utility consumption, process-related CO_2 emission, and waste generated could be used to identify the key parameters of the BOF gas fermentation to IPA. The key parameters identified are the gas fermentation parameters (CO conversion, VMT_{CO}, $Y_{IPA/CO}$, and D) and the liquid loss during biomass filtration. The technical process performance could be improved by increasing either the CO conversion, VMT_{CO}, or $Y_{IPA/CO}$, and decreasing D or the biomass filtration liquid loss. These key parameters can be used to optimise the technical process performance. However, this is just an indication based on the process KPIs, feeds, utility consumption, process-related CO_2 emissions and waste generated. To further assess the process performance, a Techno-Economic Evaluation and Life-Cycle Assessment should be done. These insights can be combined to assess the overall (i.e., technical, economic and environmental) performance of the BOF gas fermentation to IPA process.

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