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# Sustainable Isopropanol, Acetone or Mixed Production from Steel Mill Offgas: Modelling and Assessment of Syngas Fermentation at Different Titer and Yields

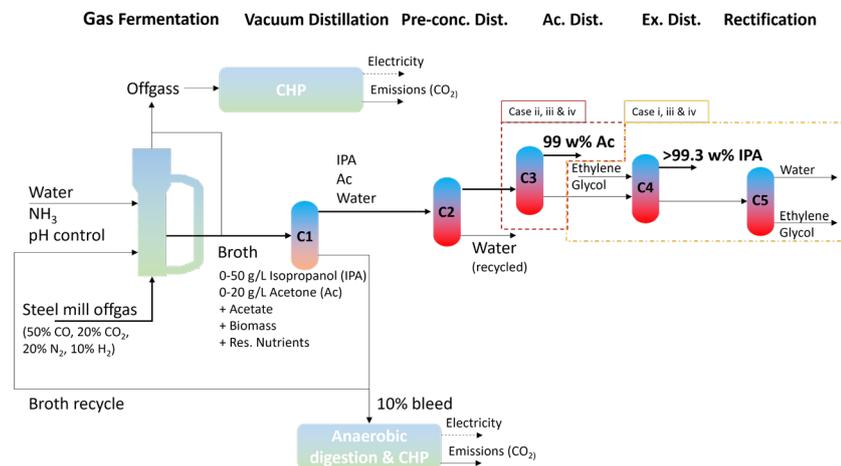
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Syngas fermentation of steel mill offgas presents a sustainable alternative to petrochemical-based isopropanol and acetone production, while utilising greenhouse gas emissions. *Clostridium autoethanogenum* (*C. autoethanogenum*) can convert energy-rich steel mill offgas into isopropanol (also: isopropyl alcohol, IPA) and/ or acetone with up to 90% product yields<sup>1</sup>. Bioprocess optimization typically prioritizes Titer, Rate, and Yield (TRY), whereas the potential for multi-product fermentation is often overlooked. Therefore, this study evaluates the impact of syngas fermentation product yields and titers on downstream processing (DSP) and the economic and environmental sustainability of an, 47.5 metric tonne per year, industrial-scale process. Four cases were modelled in Aspen Plus V12.0 based on pilot-scale data<sup>1</sup> and integrating detailed syngas fermentation modelling<sup>2</sup> and DSP design using vacuum distillation and further heat-pump assisted (extractive) distillation depending on the

Gas Fermentation  
 Vacuum Distillation  
 Pre-conc. Dist.  
 Ac. Dist.  
 Ex. Dist.  
 Rectification



**Figure 1.** Simplified scheme of the modelled 47.5 kton/ year syngas fermentation plant design with the different configurations based on the case studied (i-iv). C3 is only required for acetone (case ii-iv) and C4 & C5 are only required for isopropanol (case i, iii, iv). Where the product titer depends on the case: (i-iii) ~20 gP/L, (iv) 37 gP/L.

products<sup>3</sup>. The cases studied are: (i) 90% isopropanol yield, (ii) 90% acetone yield, and (iii) an isopropanol-acetone mixture at 80%:10% product yield, respectively (see Figure 1). Additionally, case (iv) is case (iii) at a high CO volumetric mass transfer rate (VMTCO) of 14.9 g<sub>CO</sub>/L/h (i-iii is 10 g<sub>CO</sub>/L/h).

For the syngas fermentation processes designed (see Figure 1), all cases are thermally self-sufficient utilising heat from the hot steel mill offgas and heat-pump integration. Additionally, (iv) even generates 2.6 MWh electricity through the offgas combustion and anaerobic digestion coupled to power generation (CHP, see Figure 1). **Techno-economic assessment** (TEA) showed that the Unit Production Costs (UPC) decrease by 19-23% from 0.70 \$/kg<sub>p</sub> (iii) and 0.74 \$/kg<sub>p</sub> (i-ii) to 0.57 \$/kg<sub>p</sub> (iv) at a higher VMTCO and titer. Still, the syngas fermentation to IPA and/ or acetone is economically viable for each case studied giving a 49.1-65.3% margin compared to the current fossil-derived market prices (1.45 \$/kg<sub>Ac</sub>, 1.65 \$/kg<sub>IPA</sub>). Additionally, selling biomass as a byproduct would decrease the UPC with ~0.05 \$/kg<sub>p</sub>. Environmental sustainability was assessed through a cradle-to-gate **life cycle assessment** (LCA) based on ReCiPe 2016 (H). Giving a Global Warming Potential (GWP) of -1.05 kg<sub>CO<sub>2</sub>-eq</sub>/kg<sub>IPA</sub> (i) to -1.42 kg<sub>CO<sub>2</sub>-eq</sub>/kg<sub>IPA</sub> (iv), when accounting for the steel mill offgas emissions reduced and not taking into account the end-of-life of IPA and Acetone. Which is in correspondence with the reported -1.17 kg<sub>CO<sub>2</sub>-eq</sub>/kg<sub>IPA</sub><sup>1</sup> and a 144-164% GWP reduction compared to fossil IPA (2.38 kg<sub>CO<sub>2</sub>-eq</sub>/kg<sub>IPA</sub>; ECOINVENT V3.11). For acetone the GWP is from -1.01 to -1.29 kg<sub>CO<sub>2</sub>-eq</sub>/kg<sub>Ac</sub> which is a GWP reduction of 144-150% compared to fossil acetone production (2.64 kg<sub>CO<sub>2</sub>-eq</sub>/kg<sub>Ac</sub>; ECOINVENT V3.11). Thus, this study shows that the sustainable isopropanol and acetone production is obtained already at ~20 g<sub>p</sub>/L but is most sustainable when produced as a mixture and at a higher titer.

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2. Brouwer, G. J. A., Shijaz, H. & Posada, J. A. Modelling and Parametric Analysis for Improving Technical Performance of Industrial-Scale Basic Oxygen Furnace Gas Fermentation to Isopropyl Alcohol. in *Computer Aided Chemical Engineering* (eds. Manenti, F. & Reklaitis, G. V) vol. 53 403–408 (Elsevier, 2024).
3. Janković, T., Straathof, A. J. J. & Kiss, A. A. Advanced purification of isopropanol and acetone from syngas fermentation. *Journal of Chemical Technology and Biotechnology* **99**, 714–726 (2024).