chemengineering

Supplementary Materials

Circumventing Unintended Impacts of Waste N95 Facemask Generated during the COVID-19 Pandemic: A Conceptual Design Approach

Economic assumptions, CAPEX and OPEX estimation approaches

Table S1. Economic assumptions employed in the study.

Parameters	Value	Remark
Economic indicator	Net present value	
Annual operating hours	7200 h	300 days per year
Project life	30 y	
Discount rate	10% for real term DCF analysis	
Equity	100%	
Income tax rate	30%	Income tax rate for the USA as of 2019
Depreciation	Straight line	
Salvage value	0	
Working capital	5% of fixed capital investment,	
Cost year	2020	
Selling price ethanol	US$0.735 per kg	[1] (average selling prices before COVID-19 pandemic)
Selling price of HTL oil product	US$0.92 per kg	[1] (average selling prices before COVID-19 pandemic, pure gasoline is US$0.967)
Selling price of low pressure steam	US$ 5.83 per ton	[2]
Chemical Engineering Plant Cost Index (CEPCI), year 2020	607.5	

Table S2. Capital cost components employed in TCI (CAPEX) determination [3,4].

Cost component	Estimation approach
Warehouse (W)	4% of SIC
Site Development (SD)	9% of SIC
Additional Piping (AP)	4.5% of SIC
Total direct cost (TDC)	AP+SD+W+TEIC
Prorateable Expenses (PE)	10% of TDC
Field Expenses (FE)	10% of TDC
Home Office & Construction (HC)	20% of TDC
Project Contingency (PC)	10% of TDC
Other Costs (O)	10% of TDC
Total Indirect Cost (TIC)	
Fixed Capital Investment (FCI)	TDC+TIC
Location Factor (plant assumed to be sited in USA)	1
Working Capital (WC)	5% of sum of FCI
Total Capital Investment (TCI)	Sum of FCI+WC

9 **Table S3.** Operating cost components employed in TOC (OPEX) determination (all costs used are
10 available in the associated reference sources).

Cost component	Estimation approach	Some notes	Remarks	Reference
Salaries for labour and supervision (LS)	N_w ×average individual salary	$N_W = \left(6.29 + 31.7p^2 + 0.23n\right)^{0.5}$ N_w denotes the number of workers, p is the number of processing steps involving solids and n is the number of other processing steps.	Workers paid USD12.29 per h	[5]
Labour burden (LB)	90% of total salaries	Additional labour costs in addition to the salary.	It may include costs such as retirement benefits, health benefits etc.	[6]
Maintenance (M)	3% of purchased equipment cost	Cost necessary to maintain the plant for sustained productivity		[7]
Property insurance (PI)	0.7% of Sum of FCI	Cost incurred to insure the plant		[3,4]
Fixed operating cost (FOC)	PI+M+LB+LS			
Raw materials	Based on unit market prices and mass consumed	Cost of feedstock, chemical, organic and inorganic inputs		[8]
Utilities	Based on unit market prices and energy and mass consumed	Cost of high pressure steam and electricity	Electricity cost: USD0.11 per kwh, High pressure steam: USD6.71 per ton	[1,2,9]
Waste disposal	Based on unit market prices and energy and mass consumed	Additional cost incurred in facilitating the disposal of any wastewater stream	USD1.31 per ton	[9]
Variable operating cost (VOC)				
Total operating Cost (TOC)	FOC + VOC			

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Table S4. Data employed in developing the cash flow table.

Waste N95 facemask conversion case	**Fixed capital investment (US$)**	**Working capital (US$)**	**Annual sales (US$)**	**Operating cost (US$)**
Waste N95 facemask conversion to the heat energy and electrical power	7239530.2	361976.5	8330841.3	1741429
Waste N95 facemask conversion to an energy dense (gasoline-like) oil product	4079630.6	203981.5	11382012.1	2749306.9
Waste N95 facemask conversion to ethanol via syngas fermentation	8355826.1	417791.3	7615485.8	13396192.7

14 **Table S5.** Thermodynamic model inputs and major reaction equations.

Major equipment	Model Specifications
Gasification process	ASPEN reactor models (RYIELD reactor for de-volatilisation: splitting the feed into elements as determined by ultimate analysis results in Table 1 and RGIBBS reactor for approximating gasification reaction steps; i.e. $C + O_2 \rightarrow CO_2$, $C + 0.5O_2 \rightarrow CO$, $C + CO_2 \rightarrow 2CO$, $C + H_2O \rightarrow CO_2 + H_2$, $C + H_2O \rightarrow CO + H_2$ Pressure: 1.013 bar Hydrate check: rigorous Temperature: 1000 °C Phase equilibrium and chemical equilibrium assumed Products: CO_2, CO and H_2
<u>Cogeneration system</u>	
Heat generation	Fuel (syngas)combustion: RSTOIC reactor model with reaction equations imposed as follows; $2CO + O_2 \rightarrow 2CO_2$; fractional conversion of CO: 1 $2H_2 + O_2 \rightarrow 2H_2O$; fractional conversion of H_2: 1 Valid phases: Vapor-Liquid Temperature: 1000 °C Pressure: 1.013 bar
High pressure pump for water supply	Pressure: 100 bar Flash option: liquid only Pump efficiency: 0.9
Heater for boiler	Operating at a pressure: 100 bar. Heat supplied from the combustion reactor
Turbines	Method used : Isentropic using ASME method Discharge pressure: 25 bar (turbine 1), 1.013 bar (turbine 2). Isentropic efficiency: 1 Valid phases: Vapor-Liquid
Fermentation reactor	Temperature: 37 °C Pressure: 1.013 bar Reactor model: RSTOIC Reactions [10] $4CO + 2H_2O \rightarrow CH_3COOH + 2CO_2$, fractional conversion of CO: 0.9 $2CO_2 + 4H_2 \rightarrow CH_3COOH + 2H_2O$, fractional conversion of H_2: 0.7 $6CO + 3H_2O \rightarrow C_2H_5OH + 4CO_2$, fractional conversion of CO: 0.9 $2CO_2 + 6H_2 \rightarrow C_2H_5OH + 3H_2O$, fractional conversion of H_2: 0.7
First distillation column (concentration of ethanol in the distillate 83.5 wt.%)	Number of stages: 10 Condenser type: Total Calculation type: Equilibrium type Pressure in the column: 1.013 bar Valid phases: Vapor-liquid Reflux ratio: 1 (mole basis) Boilup ratio: 1 (mole basis)
Second distillation column (concentration of ethanol in the distillate 89.4 wt.%)	Number of stages: 10 Condenser type: Total Calculation type: Equilibrium type Pressure in the column: 1.013 bar

	Valid phases: Vapor-liquid Distillate rate: 1246.7 kg/h (mass basis) Boilup ratio: 1 (mole basis)
Hydrothermal liquefaction reactor	Temperature: 425 ^{o}C Pressure: 230 bar Reactor model: RGIBBS Valid phases: Vapor-liquid ASPEN models (RYIELD reactor for de-volatilisation: splitting the feed into elements as determined by ultimate analysis results in Table 1 and RGIBBS reactor for approximating complex polymerisation reactions i.e.

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