Thermodynamics Based Process Sustainability Evaluation

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Supplementary Material

1. Exergy profit calculation for output stream in case study 1

The calculation for the purge stream:

Assuming a 100 kg/h of purge stream waste is produced from methanol carbonylation and using data from **Table 2**

Exergy of purge stream:
={Mass flowrate of purge stream} × {Total specific exergy content of purge stream}
=100 [kg/h] × (-71.274 [kJ/kg])/3,600
= -1.98 kW
= -0.00198 MW

The specific exergy to be added to the VAM production process is 0.532 MW per 1 t/h of Acetic Acid feed (simulation results). Note that the exergy to separate acetic acid is ignored, as the purpose is to evaluate the potential of waste acetic acid.

If all the content of the purge stream is to be sent to the VAM process, the exergy liability of the purge stream is
= {Exergy of input streams} +{Exergy for the heat and work}
= $\sum_i$ {Mass flowrate of input stream 'i'} × {Total specific exergy of input stream 'i'} + {Mass flowrate of acetic acid feed} × {Specific exergy added to the VAM process}
=100 [kg/h] × (0.0556 × (-152.92[kJ/kg]) + 0.382 × 0.00169 [kJ/kg] + 0.394 × 1.74 [kJ/kg])/3,600,000 + 0.532 [MW/t] × 100 [kg/h]/1,000
= -0.000216 + 0.0532
= 0.0530 MW

Exergy contents/assets of the output products:

= {Exergy of output streams}
= $\sum_j$ ({Mass flowrate of output stream 'j' } × {Total specific exergy of output stream 'j'})
= {Exergy of VAM} + {Exergy of waste water} + {Exergy of waste AA} + {Exergy of purge gas} + {Exergy of waste glycerol}
= 100 [kg/h] × (0.0496 × 7.63 [kJ/kg] + 0.0131 × (-37.572 [kJ/kg]) + 0.0679 × 208.234 [kJ/kg] + 1.64 × (-215.21 [kJ/kg]) + 0.0607 × 155.788 [kJ/kg])/3,600,000
=0.00330 MW

Net Exergy Profit of the purge stream

= 0.0033-0.0530
= -0.0497 MW (original is -0.00198 MW) (increased loss)

2. Exergy profit calculation for input stream in case study 1

Calculation for the acetic acid inlet stream:

Assuming a 100 kg/h of acetic acid inlet stream is input into VAM production process and using data from **Table 1**:

Exergy of the acetic acid stream

= {Mass flowrate of acetic acid stream} × {Total specific exergy content of acetic acid stream}
= 100 [kg/h] × (0.250 [kJ/kg])/3,600
= 0.00694 kW
= 0.000064 MW

The exergy to be added to the methanol carbonylation process is 0.458 MW per 1 t/h of Acetic Acid production [76]

The exergy liability of the acetic acid stream:

= {Exergy of input Methanol} + {Exergy of input CO} + {Exergy losses with: Vent CO +Exergy of propionic acid and the purge stream} + {Exergy for the heat and work}
= 100[kg/h] × (-263.145[kJ/kg] + 60.547[kJ/kg] + 145.745[kJ/kg] + 106.566[kJ/kg]+ 71.247[kJ/kg])/3,600,000 + 0.458[MW/t]*100[kg/h]/1,000
= 0.0034 + 0.0458
=0.0492 MW

Exergy assets of the output products:

= {Exergy of Purge Methanol}
= 100 [kg/h] × (83.209 [kJ/kg])/3,600,000
= 0.0023 MW

Net Exergy Profit of the acetic acid feed stream

= 0.0023 - 0.0492
=-0.0468 MW (a loss)

3. Exergy profit calculation for MSW stream, sending to MBCT system in case study 2

Using data from Table 6, the calculation of exergy of the MSW stream is shown below:
Assuming basis of 1 t/h of MSW, according to Figure 9,
Recyclables = 215 kg/h
Landfill = 157 kg/h
AD inlet = 285 kg/h
Chemical conversion inlet =398 kg/h

Total Exergy to be added to the recycling, landfill, AD and chemical conversion (assuming 8.05 % of plastics in recyclables)

= 215 [kg/h] × (0.0805) × (10.4 [MJ/kg]) + 157 [kg/h] × (0.336 [MJ/kg]) + 285 [kg/h] × (1.09 [MJ/kg]) + 398 [kg/h] × (3.02 [MJ/kg])
= 1744.3 MJ/h
= 0.484 MW

Total Useful Exergy of secondary products from recycling, landfill, AD , and chemical conversion (assuming 8.05 % of plastics in recyclables)

= 215 [kg/h] × (0.0805) × (33.1 [MJ/kg]) + 157 [kg/h] × (0.242 [MJ/kg]) + 285 [kg/h] × (1.41 [MJ/kg]) + 398 [kg/h] × (9.83[MJ/kg])

= 5004 MJ/h

= 1.39 MW

Total Net Exergy Profit

= 1.39-0.484

=0.906 MW

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