Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supplementary Document

The specific total cost (STC) are the sum of specific investment costs (SIC) and the specific operation costs (SOC). The specific investment costs include terms related with decomposition, membrane separation, PSA process, and compressors, as shown in Equation* MERGEFORMAT (2). The specific operation costs include terms related with ammonia feed, decomposition catalyst, membrane, adsorbent and electricity, as shown in Equation* MERGEFORMAT (3).

$$STC = \sum_i SIC_i + \sum_j SOC_j$$ * MERGEFORMAT (1)

$$\sum_i SIC_i = SIC_{decomp} + SIC_{mem} + SIC_{PSA} + SIC_{comp}$$ * MERGEFORMAT (2)

$$\sum_j SOC_j = SOC_{feed} + SOC_{decomp} + SOC_{PSA} + SOC_{mem} + SOC_{elec}$$ * MERGEFORMAT (3)

The specific investment costs are calculated with the annual hydrogen productivity and the equivalent annual investment costs which is calculated according to the even yearly cash flow during the plant lifetime[34]., as shown in Equation* MERGEFORMAT (4).

$$SIC_i = \frac{IC_i}{m_{\mathrm{H2},year}} \frac{r}{1-\frac{1}{(1+r)^{t_{Plant}}}}$$ * MERGEFORMAT (4)

The specific operation costs are calculated with the annual hydrogen productivity and the yearly operation costs, as shown in Equation* MERGEFORMAT (5).

$$SOC_i = \frac{OC_i}{m_{\mathrm{H2},year}}$$ * MERGEFORMAT (5)

It is assumed that, the investment costs for compressors and membrane units scale linearly with the compressor work and the membrane area, respectively. The investment costs of PSA unit includes the costs for pressure vessels and the costs for adsorbents, as shown in Equation* MERGEFORMAT (6).

$$IC_{comp} = P_{comp} \cdot p_{comp}$$ * MERGEFORMAT (6)

$$IC_{mem} = A_{mem} \cdot p_{mem}$$ * MERGEFORMAT (7)

$$IC_{PSA} = IC_{PSA-vessel} + IC_{PSA-ads}$$ * MERGEFORMAT (8)

The Guthrie-Ulrich base cost method[35] was chosen for the pressure vessels, as shown in Equation* MERGEFORMAT (9), in which f_{update}, f_{pressure}, f_{module}, f_{valve} are factor of update, factor of material pressure correction, factor of module and factor of valves, respectively. The base cost of vessel is calculated by Equation* MERGEFORMAT (10). The investment costs of adsorbent scale linearly with the mass of adsorbent, as shown in Equation* MERGEFORMAT (11). The investment costs of ammonia decomposition reactor are calculated in a similar way as the adsorption bed.

$$IC_{PSA-vessel} = f_{update} IC_{vessel,base} \left(f_{pressure} + f_{module} - 1\right) f_{valve}$$ * MERGEFOR

$$IC_{vessel,base} = IC_{vessel,0} \cdot \left(\frac{L}{L_0}\right)^w \cdot \left(\frac{D}{D_0}\right)^e$$ * MERGEFORMAT

$$IC_{ads} = p_{ads} \cdot m_{ads}$$ * MERGEFORMAT (11)

The costs of feed gas is based on the price of anhydrous NH_3. The operation costs for compression work is based on electricity price. The costs for membrane replacement are calculated by dividing the membrane investment costs by its lifetime, and so are the costs for adsorbent service. The operation cost of NH3 decomposition is related with catalyst, which is calculated in a similar way as the adsorbent. The costs of NH3 removal is neglecting in this study.

$$OC_{feed} = m_{NH3} p_{NH3}$$ * MERGEFORMAT (12)

$$OC_{elec} = P_{comp} p_{elec}$$ * MERGEFORMAT (13)

$$OC_{mem} = IC_{mem} / t_{mem}$$ * MERGEFORMAT (14)

$$OC_{PSA} = IC_{ads} / t_{ads}$$ * MERGEFORMAT (15)