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Supplementary Information

Techno-economic assessment for the large-scale production of colloidal lignin particles

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Process equipment sizing

The area of the heat exchangers is determined based on the heat duty (Q), overall heat transfer coefficient (U) and the logarithmic mean temperature (ΔT_{LM}) using equation 1.

$$A = \frac{Q}{U * \Delta T_{LM}} \tag{1}$$

The overall heat transfer coefficient values are calculated based on the individual heat transfer coefficients for the shell (h_1) and tube side (h_2) using Equation 2.

$$\frac{1}{U} = \frac{1}{h_1} + \frac{1}{h_2} \tag{2}$$

The pumps are designed as centrifugal pumps and the work done by the pump in J/kg is calculated using Equation 3.

$$W = \frac{P_{out} - P_{in}}{\rho_{out}} + \frac{Pressure\ drop}{\rho_{out}} \tag{3}$$

where P_{out}, P_{in} are the pressure values in Pa at the outlet and inlet respectively and ρ_{out} is the density of the outlet process stream. The power required in $Watt$ is calculated by multiplying work with mass flowrate in kg/s and dividing with the pump efficiency (0.8).

The distillation column design is based on tray by tray modelling (rigorous modelling) approach using Aspen plus. The column diameter is calculated by utilizing the tray sizing option in aspen plus. The height of the distillation column is determined using Equation 4. The diameter of the top section is considered as 2 times the column diameter and the diameter of the bottom section is taken to be same as the column diameter

$$H = d_c + 2d_c + d_c \tag{4}$$

where d_c is the diameter of the column in m

The spray drier is designed based on the volume (V_d), diameter (d_s) and height (h_d) of the drier. The volume is calculated using Equations 5 and the residence time is taken as 5 seconds.

$$V_d = Air\ flow\ rate\ (cfs) * residence\ time \tag{5}$$

Once the volume is determined, the diameter is calculated using Equation 6. The height is assumed to be four times the diameter and the angle of the cone is considered as 60°.

$$V_d = 4 * d_s * \left(\frac{\pi * d_s^2}{4}\right) + \frac{0.866\pi d_s^3}{12} \tag{6}$$

Ultrafiltration unit is designed based on the membrane area and the flux speed. The design data was provided by the company Valmet. With a membrane area of 756 m^2 and a flux speed of 100 $L/m^2/h$, the unit can filter 75600 L/h of feed.

A small-scale tubular reactor was designed and developed by us at Aalto University. It consists of tubes with mixing elements that aid in the formation of a stable and uniform dispersion. The tubular reactor will be discussed in detail in a future publication.

The mixers are designed as cylindrical vessels by calculating the volume, diameter and height. The volume of the mixer is determined by multiplying the volumetric flow rate with the residence time. The residence time is taken as 15 min in the calculations. The diameter of the mixer (d_m) can be calculated from volume (V) using Equation 7. The height (h_m) is taken as two times the diameter.

$$d_m = \left(\frac{2*V}{\pi}\right)^{1/3} \tag{7}$$

The flash drum is designed as a vertical vapor liquid separator without demister pad as described by Sinnot.[1] A liquid hold up time of five minutes is assumed and the equipment is sized as shown in Equation 8 -12

$$u_t = 0.07 * \left[\frac{(\rho_{liquid} - \rho_{vapor}}{\rho_{vapor}}\right]^{0.5} \tag{8}$$

$$D_v = \left(\frac{4*\dot{v}_{vapor}}{\pi*u_t}\right)^{0.5} \tag{9}$$

$$H_{liquid} = \dot{v}_{vapor} * 60 * 5 \tag{10}$$

$$h_{liquid} = \frac{H_{liquid}}{\pi*\left(\frac{D^2}{4}\right)} \tag{11}$$

$$Height = h_{liquid} + \frac{D_v}{2} + D_v \tag{12}$$

where ρ_{liquid} and ρ_{vapor} are liquid and vapor density in kg/m^3, u_t is the settling velocity in m/s, $\dot{v}_{vapor}$ is the vapor phase volumetric flow rate in m^3/s, D_v is the minimum allowable diameter in m, H_{liquid} is the liquid hold-up volume in m^3 and h_{liquid} is the liquid hold-up in m

Equipment cost estimation

The purchase price of process equipment is determined based on the equations given by Brown et al.[2] The prices are for year 2005 and in US dollars. These are converted to year 2017 prices in Euros by considering the chemical engineering plant cost indexes (CEPCI) and currency conversion as shown in Equation 13.

$$Price_{2017} = Price_{2005}(\$) * \frac{CEPCI_{2017}}{CEPCI_{2005}} * 0.84\ \frac{€}{\$} \tag{13}$$

The purchase cost of tanks is calculated by using Equation 14.

$$Price_{2005}\ (\$) = 800 * \left(\frac{gallons}{1000}\right)^{0.8} * mf \tag{14}$$

where mf is the material factor and is taken as 2.4 for stainless steel.

The purchase price of mixers and flash drum is determined by considering them as pressure vessels and using Equation 15.

$$Price_{2005}\ (\$) = 5180 * \left(\frac{gallons}{1000}\right)^{0.67} * mf * (0.0023 * p + 0.66) \tag{15}$$

Where p is the pressure in psi and mf is the material factor with a value of 2.6 for stainless steel

The purchase price of heat exchangers is calculated using Equation 16. Shell and tube heat exchangers are used in the process.

$$Price_{2005}\ (\$) = 462 * (Area,\ ft^2)^{0.5} * 2 \tag{16}$$

where mf is the material factor with a value of 2 for stainless steel

For estimating the price of a distillation column, first the price of the column is determined based on the Equation 17 given for pressure vessels and then this is price is multiplied with a distillation column factor (F) which is calculated using equation A5.

$$F = L/D * (Diameter,\ ft^2)^{-0.47},\ \text{L/D} < 5 \tag{17}$$

where L/D is the ratio of column height to column diameter

Bubble cap trays are used in the distillation column and its price is calculated using Equation 18.

$$Price_{2005}\ (\$) = 73.1 * (diameter, ft)^{1.8} * 2 * mf * qf \tag{18}$$

where mf is material factor with a value of 1.9 for stainless steel and qf is the quantity factor with a value of 1.4 for a distillation column with 12 stages.

The purchase price of pump is calculated based on the mass flowrate ($\dot{m}$) in gpm and the pump head developed (h_p) in feet using Equation 19. The pump type is centrifugal and stainless steel is chosen as the material of construction.

$$Price_{2005}\ (\$) = 2070 * \left(\frac{\dot{m} * h_p}{1000}\right)^{0.27} * mf * pf \quad (19)$$

where mf is the material factor with a value of 1.9 for stainless steel and pf is the pressure factor with a value of 1 since the pump is operating below 150 psig.

The purchase price of the ultrafiltration unit was provided by the vendor. Since the tubular reactor consists of tubes with static mixing elements placed inside them, its purchase cost is calculated as the sum of the piping cost and the cost of the mixing elements. The piping cost is calculated using Equation 20 and the mixing element cost is obtained from the vendor.

$$Piping\ cost = 1000 * (0.1 * F + 0.924) * D^{0.83} * mf \quad (20)$$

Where F represents the number of fittings/1000 ft of pipe, D is the nominal pipe diameter in $inches$ and mf is the material factor with a value of 1.4 for stainless steel.

The purchase price of the hopper conveyor system and product packaging unit was determined based on vendor quotes.

Profitability assessment

The profitability of the process is evaluated based on the payback period, return on investment(ROI) and internal rate of return (IRR). The equations used in the calculation of NPV, ROI and payback period are listed below:

$$Earnings\ before\ interest\ and\ tax\ (EBIT) = Revenue - Annual\ operating\ cost \quad (21)$$

$$Depriciation = 0.1 * Fixed\ capital\ investment \quad (22)$$

$$Profit\ before\ tax\ (PBT) = EBIT - Depriciation \quad (23)$$

$$Interest = 0.02 * Total\ investment \quad (24)$$

$$Taxes = 0.20 * PBT \quad (25)$$

$$Profit\ after\ tax\ (PAT) = PBT - Taxes - Interest \quad (26)$$

$$Net\ present\ value\ at\ year\ 0 = -Total\ investment \quad (27)$$

$$NPV_i = NPV_{i-1} + (PAT + Depriciation)/(1 + 0.1)^i \quad (28)$$

$$Return\ on\ investment\ (\%) = \left(\frac{PAT}{Total\ investment}\right) * 100 \quad (29)$$

$$Payback\ period = \frac{Total\ investment}{PAT} \tag{30}$$

References

1 J. M. Coulson, R. K. Sinnott and J. Richardson, *Coulson & Richardson's Chemical Engineering Volume 6: Chemical Engineering Design*, 2005, vol. 2.

2 T. Brown, *Engineering Economics and Economic Design for Process Engineers*, 2006.