Assumptions (color-coded)

Only the following items are **assumptions** (colored blue) — everything else is data.

- Room temperature: $T_{\mathrm{room}} = 25^\circ\mathrm{C}$
- n-BuLi molarity (batch): $c_{\mathrm{nBuLi,\,batch}} = 2.0$ M
- n-BuLi molarity (flow): $c_{\mathrm{nBuLi,\,flow}} = 1.1$ M
- Yield (batch): $Y_{\mathrm{batch}} = 0.70$
- Yield (flow): $Y_{\mathrm{flow}} = 0.85$
- Initial temperature of liquid N_2: $T_{i,\mathrm{LN2}} = -195.8^\circ\mathrm{C}$
- Initial temperature of steam: $T_{i,\mathrm{steam}} = 100^\circ\mathrm{C}$
- Latent heats: $\Delta H_{\mathrm{vap,\,LN2}} = 200$ kJ/kg, $\Delta H_{\mathrm{vap,\,steam}} = 2260$ kJ/kg
- Average heat capacity (mixture): $C_p = 2$ kJ/kg·K
- Exchange rate: 1 \$ = 85
- Labour cleaning: Batch = \$200/cycle, Flow = \$150/cycle
- Estimated CapEx (setup): \$25,000,000

Given Data (symbol list)

- Heat of reaction: $\Delta H_r = 375\ \mathrm{kJ/mol}.$
- Substrate: $m_{\mathrm{sub}} = 100\ \mathrm{kg},\ M_{\mathrm{sub}} = 400\ \mathrm{g/mol},\ \text{price} = \$50/\mathrm{kg}.$
- Product molecular weight: $M_{\mathrm{prod}} = 350\ \mathrm{g/mol}.$
- n-Butyl lithium (given): $V_{\mathrm{nBuLi}} = 250\ \mathrm{L},\ M_{\mathrm{nBuLi}} = 64.06\ \mathrm{g/mol},\ \text{price} = \$10/\mathrm{kg}.$
- Solvents (volumes, densities, prices, recoveries):
  THF: $V_{\mathrm{THF}} = 2000\ \mathrm{L},\ \rho_{\mathrm{THF}} = 0.889\ \mathrm{kg/L},\ \$3/\mathrm{kg}.$
  MeOH: $V_{\mathrm{MeOH}} = 1000\ \mathrm{L},\ \rho_{\mathrm{MeOH}} = 0.792\ \mathrm{kg/L},\ \$0.33/\mathrm{kg},\ \mathrm{rec} = 70\%.$
  DCM: $V_{\mathrm{DCM}} = 2000\ \mathrm{L},\ \rho_{\mathrm{DCM}} = 1.33\ \mathrm{kg/L},\ \$0.4/\mathrm{kg},\ \mathrm{rec} = 70\%.$
  MEK: $V_{\mathrm{MEK}} = 500\ \mathrm{L},\ \rho_{\mathrm{MEK}} = 0.805\ \mathrm{kg/L},\ \$0.9/\mathrm{kg},\ \mathrm{rec} = 70\%.$
  Hexane: $V_{\mathrm{hex}} = 1500\ \mathrm{L},\ \rho_{\mathrm{hex}} = 0.665\ \mathrm{kg/L},\ \$1.2/\mathrm{kg},\ \mathrm{rec} = 70\%.$
- Utilities: Liquid N_2: $12/\mathrm{kg}$. Steam: $5/\mathrm{kg}$.

Costs — Substrate Solvents

Substrate cost:

$$\text{Cost}_{\text{sub}} = m_{\text{sub}} \times \text{Price}_{\text{sub}} \quad \Rightarrow \quad \text{Cost}_{\text{sub}} = 100\ \text{kg} \times \$50/\text{kg} = \boxed{\$5000}$$

Solvent cost line items:

$$\begin{aligned}
\text{THF: } & 2000\ \text{L} \times 0.889\ \text{kg/L} \times \$3/\text{kg} = \boxed{\$5334} \\
\text{MeOH (net after 70\% recovery): } & 1000\ \text{L} \times 0.792\ \text{kg/L} \times \$0.33/\text{kg} \times (1-0.7) = \boxed{\$78.41} \\
\text{DCM (net): } & 2000\ \text{L} \times 1.33\ \text{kg/L} \times \$0.4/\text{kg} \times (1-0.7) = \boxed{\$319.20} \\
\text{MEK (net): } & 500\ \text{L} \times 0.805\ \text{kg/L} \times \$0.9/\text{kg} \times (1-0.7) = \boxed{\$108.67} \\
\text{Hexane (net): } & 1500\ \text{L} \times 0.665\ \text{kg/L} \times \$1.2/\text{kg} \times (1-0.7) = \boxed{\$353.70}
\end{aligned}$$

$$\text{Total solvent cost}: \quad \$5334 + \$78.41 + \$319.20 + \$108.67 + \$353.70 = \boxed{\$6193.98}$$

n-Butyl Lithium — Batch vs Flow

General: $N = c \times V, \; m = N \times \dfrac{M}{1000}, \; \text{Cost} = m \times \$10/\mathrm{kg}.$

Batch:

$$N_{\mathrm{nBuLi,batch}} = 2.0\ \mathrm{M} \times 250\ \mathrm{L} = \boxed{500\ \mathrm{mol}}$$

$$m_{\mathrm{nBuLi,batch}} = 500\ \mathrm{mol} \times 0.064\ \mathrm{kg/mol} = \boxed{32\ \mathrm{kg}}$$

$$\text{Cost}_{\mathrm{nBuLi,batch}} = 32\ \mathrm{kg} \times \$10/\mathrm{kg} = \boxed{\$320}$$

Flow:

$$N_{\mathrm{nBuLi,flow}} = 1.1\ \mathrm{M} \times 250\ \mathrm{L} = \boxed{275\ \mathrm{mol}}$$

$$m_{\mathrm{nBuLi,flow}} = 275\ \mathrm{mol} \times 0.064\ \mathrm{kg/mol} = \boxed{17.61\ \mathrm{kg}}$$

$$\text{Cost}_{\mathrm{nBuLi,flow}} = 17.61\ \mathrm{kg} \times \$10/\mathrm{kg} = \boxed{\$176.10}$$

Product Mass

Assume 1:1 stoichiometry substrate $\rightarrow$ product.
Moles of substrate:

$$N_{\mathrm{sub}} = \frac{m_{\mathrm{sub}} \times 1000}{M_{\mathrm{sub}}} \quad \Rightarrow \quad N_{\mathrm{sub}} = \frac{100\ \mathrm{kg} \times 1000}{400\ \mathrm{g/mol}} = \boxed{250\ \mathrm{mol}}$$

Theoretical product mass:

$$m_{\mathrm{prod,th}} = N_{\mathrm{sub}} \times \frac{M_{\mathrm{prod}}}{1000} \quad \Rightarrow \quad m_{\mathrm{prod,th}} = 250\ \mathrm{mol} \times \frac{350\ \mathrm{g/mol}}{1000} = \boxed{87.50\ \mathrm{kg}}$$

Yields:

$$m_{\mathrm{prod,batch}} = m_{\mathrm{prod,th}} \times 0.70 = \boxed{61.25\ \mathrm{kg}} \qquad m_{\mathrm{prod,flow}} = m_{\mathrm{prod,th}} \times 0.85 = \boxed{74.37\ \mathrm{kg}}$$

Cryogenics (Liquid N_2) and Steam Costs

Liquid N_2 — calculations:

Cooling mass required:

$$\frac{(m_{\text{sub}} + m_{\text{THF}})\, C_p\, \Delta T}{\Delta H_{\text{vap,LN2}}} \Rightarrow \frac{(100 + (2000 \times 0.889)) \times 2 \times 100}{200} = \boxed{1878 \text{ kg}}$$

Maintenance:

$$\frac{\Delta H \times N_{\text{sub}}}{\Delta H_{\text{vap,LN2}}} \Rightarrow \frac{375 \times 250}{200} = \boxed{465 \text{ kg}}$$

Total LN_2 mass:

$$m_{\text{LN2,total}} = 1878 + 465 = \boxed{2343 \text{ kg}}$$

Cost (conversion):

$$\text{Cost}_{\text{LN2}} = 2343 \text{ kg} \times 12/\text{kg} = \boxed{28{,}116 = \frac{28{,}116}{85} = \$330.77}$$

Steam — calculations:

Mass of steam:

$$m_{\text{steam}} = \frac{1894 \times 2 \times 25}{2260} + \frac{2686 \times 2 \times 75}{2260} + \frac{500 \times 2 \times 20}{2260} = \boxed{230.96 \text{ kg}}$$

Cost:

$$\text{Cost}_{\text{steam}} = 230.96 \text{ kg} \times 5/\text{kg} = \boxed{1{,}154.80 = \$13.58}$$

Total Manufacturing Costs

Batch Reactor — total cost:

$$\begin{aligned}\mathsf{Total}_{\mathrm{batch}} &= \mathsf{Cost}_{\mathrm{sub}} + \mathsf{Cost}_{\mathrm{solvents}} + \mathsf{Cost}_{\mathrm{nBuLi,batch}} \\ &\quad + \mathsf{Cost}_{\mathrm{LN2}} + \mathsf{Cost}_{\mathrm{steam}} + \mathsf{Labour\&Cleaning}_{\mathrm{batch}} \\ &= \$5000 + \$6193.98 + \$320 + \$330.77 + \$13.58 + \$200 \\ &= \boxed{\$12{,}058.33}\end{aligned}$$

Cost per kg of product (batch):

$$c_{\mathrm{batch}} = \frac{\mathsf{Total}_{\mathrm{batch}}}{m_{\mathrm{prod,batch}}} = \frac{\$12{,}058.33}{61.25\ \mathrm{kg}} = \boxed{\$196.87/\mathrm{kg}}$$

Scale to 100 metric tonnes:

$$\mathsf{Cost}_{100\ \mathrm{MT,\ batch}} = 100{,}000 \times \$196.87 = \boxed{\$19{,}687{,}000}$$

Flow Reactor — totals savings

Flow Reactor — total cost:

$$\begin{aligned}\text{Total}_{\text{flow}} &= \$5000 + \$6193.98 + \$176.10 + \$330.77 + \$13.58 + \$150 \\ &= \boxed{\$11{,}864.43}\end{aligned}$$

Cost per kg of product (flow):

$$c_{\text{flow}} = \frac{\text{Total}_{\text{flow}}}{m_{\text{prod,flow}}} = \frac{\$11{,}864.43}{74.37\ \text{kg}} = \boxed{\$159.53/\text{kg}}$$

Scale to 100 metric tonnes:

$$\text{Cost}_{100\ \text{MT, flow}} = 100{,}000 \times \$159.53 = \boxed{\$15{,}953{,}000}$$

Annual saving (batch $\to$ flow):

$$\boxed{\text{Annual Saving} = \$19{,}687{,}000 - \$15{,}953{,}000 = \$3{,}734{,}000}$$

ROI (per-kg and Annual with CapEx)

Per-kg ROI formula:

$$\mathrm{ROI}_{\mathrm{per\ kg}} = \frac{\text{Selling price} - \text{Manufacturing cost}}{\text{Manufacturing cost}} \times 100\%$$

Using Selling price = \$200/kg:

$$\mathrm{ROI}_{\mathrm{batch}} = \frac{200 - 196.87}{196.87} \times 100\% = \boxed{1.58\%}$$

$$\mathrm{ROI}_{\mathrm{flow}} = \frac{200 - 159.53}{159.53} \times 100\% = \boxed{25.36\%}$$

CapEx = \$25,000,000 amortized over 10 years ⇒ Annual amortization = \$2,500,000.
Net Profit:

$$\text{Net Profit} = \text{Annual Revenue} - (\text{Production Cost}_{\mathrm{flow}} + \text{Annual Amortization})$$

Substitute:

$$\text{Net Profit} = \$20{,}000{,}000 - (\$15{,}953{,}000 + \$2{,}500{,}000) = \boxed{\$1{,}547{,}000}$$

Annual ROI:

$$\mathrm{ROI}_{\mathrm{annual}} = \frac{\$1{,}547{,}000}{\$25{,}000{,}000} \times 100\% = \boxed{6.18\%}$$

Summary — Part A (cost items)

Item	Final value
Substrate cost	$\boxed{\$5000}$
Total solvent cost	$\boxed{\$6193.98}$
n-BuLi cost (batch)	$\boxed{\$320}$
n-BuLi cost (flow)	$\boxed{\$176.10}$
Liquid N_2 cost	$\boxed{\text{INR } 28{,}116 = \$330.77}$
Steam cost	$\boxed{\text{INR } 1{,}154.80 = \$13.58}$
Total cost (batch)	$\boxed{\$12{,}058.33}$

Summary — Part B (yields, unit economics, ROI)

Item	**Final value**
Product mass (batch)	$\boxed{61.25\ \mathrm{kg}}$
Cost/kg (batch)	$\boxed{\$196.87/\mathrm{kg}}$
Total cost (flow)	$\boxed{\$11{,}864.43}$
Product mass (flow)	$\boxed{74.37\ \mathrm{kg}}$
Cost/kg (flow)	$\boxed{\$159.53/\mathrm{kg}}$
100 MT cost (batch)	$\boxed{\$19{,}687{,}000}$
100 MT cost (flow)	$\boxed{\$15{,}953{,}000}$
Annual saving (batch→flow)	$\boxed{\$3{,}734{,}000}$
Per-kg ROI (batch / flow)	$\boxed{1.58\%\ ;\ 25.36\%}$
Annual ROI (flow, w/CapEx)	$\boxed{6.18\%}$