Supplementary materials for:

A Technoeconomic Platform for Early-Stage Process Design and Cost Estimation of Joint Fermentative–Catalytic Bioprocessing

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Table S1. Catalysis modeling in ESTEA2 — User inputs and heuristics used by the tool

Process inputs (User)		
Selectivity (%)		
Conversion (%)		
Mean Residence Time (min)		
Solubility (mg/L)		
Process assumptions		
Quantity	**Value**	**Reference**
Tube Height, H_{Tube}	4.88 m	[20] (Figure 14–18) (Year — 2002)
Tube Diameter, D_{Tube}	0.019 m	
Tube Volume, V_{Tube}	0.00138 m^3	
Base Size, $BS_{Catalysis}$	100 m^2	
Base Cost, $BC_{Catalysis}$	$12,000	
Scaling Exponent, $SE_{Catalysis}$	0.44	

Table S2. Catalysis modeling in ESTEA2 – stepwise calculations as performed by the tool

A. Catalyst Void Fraction, Φ $1 - \left(\frac{\text{Bulk density}}{\text{Particle density}}\right) \times 100$
B. Working volume, V_w (m^3) Volumetric flow−IN (m^3/h) × Mean residence time (min) × 0.0167 (h/min)
C. Total volume, V_{Total} (m^3) $\left(\frac{V_w}{\Phi}\right)$
D. Catalyst required, C_{req} (kg) V_{Total} (m^3) × ϱ_{Bulk} (kg/m^3)
E. Number of tubes, N_{Tubes} $\left(\frac{V_{Total}}{V_{Tube}}\right)$
F. Number of reactors, $N_{Reactors}$ $\left(\frac{N_{Tubes}}{\text{Tubes per reactor}}\right)$

Table S3. Dryer modeling in ESTEA2 — User inputs and heuristics used by the tool

Process inputs (User)		
Final product moisture content (%)		
Residence time (min)		
Product Yield (%)		
Process assumptions		
Parameter	**Value**	**Reference**
Air in T	110°C	[27] (Example: 9.10)
Air in H	0.008 lb/lb	
Air in Enthalpy	162.35 kJ.kg	
Air in V	1.09 m^3/kg	
Air out T	37.78 °C	
Air out H	0.0375 lb/lb	
V out	0.93 m^3/kg	
Exit enthalpy	355 kJ/kg	
Enthalpy loss	9.77 kJ/kg	
Base Size	60 m^3	[20] (Figure 15–34) (Year — 2002)
Base Cost	$400,000	
Cost Exponent	0.5	

Table S4. Dryer modeling in ESTEA2 – stepwise calculations as performed by the tool

A. Air rate into the dryer, AR_{Dryer}(kg/h) $\frac{\text{Mass flow IN (kg/h) - Mass flow OUT (kg/h)} \times \text{Average}[V_{Air\ IN}(m^3/kg) - V_{Air\ IN}(m^3/kg)]}{(H_{Air\ OUT} - H_{Air\ IN})}$
B. Dryer volume, V_{Dryer} (m^3) AR_{Dryer} (kg/h) × Residence time (min) × 0.0167 h/min
C. Heat requirement, (MMBtu) AR_{Dryer} (kg/h) × [$T_{Air\ IN}$ - $T_{Air\ OUT}$]°C × $Air_{Specific\ Heat}$ (KJ/kg°C) × POH (h) x 9.47 × 10^{-10} MMBtu/J

Table S5. Batch reactor modeling in ESTEA2 — User inputs and heuristics used by the tool

Process inputs (User)		
Acid/Base mass ratio		
Product purity (%)		
Product yield (%)		
Residence time (h)		
ΔT (°C)		
Process assumptions		
Parameter	**Value**	**Reference**
Base size (smaller capacity)	4 m^3	[20] (Figure 13–15) (Year — 2002)
Base cost	$30,000	
Cost exponent	0.56	
Base size (large capacity)	10 m^3	
Base cost	$50,000	
Cost exponent	0.56	
Process downtime	1 h	

Table S6. Batch reactor modeling in ESTEA2 – stepwise calculations as performed by the tool

A. Acid/Base volume, $V_{A/B}$ (m³) $\frac{\text{Acid/Base mass ratio} \times \text{Product mass flow-In (kg/h)} \times \text{POH (h)}}{\text{Acid/Base density (kg/m}^3\text{)}}$
B. Working volume, V_w (m³/batch) (Volumetric flow (m³/h) × Residence time (min) × 0.0167 (min/h)) + $V_{A/B}$ (m³)
C. Number of Units $\frac{\text{Working volume (m}^3\text{)}}{\text{Base size (m}^3\text{)}}$

Table S7. Electricity, water, energy and labor cost comparison between ESTEA2 and literature for the ethanol process model

Factor	Source	Value	ESTEA2: Source
Electricity	ESTEA2	$0.0012/kg	-
	Claypool and Raman	$0.0013/kg	(−) 8%
	Duffield	$0.0014/kg	(−) 15%
	Hofstrand	$0.0013/kg	(−) 8%
	Shapouri and Gallagher	$0.0013/kg	(−) 8%
Water	ESTEA2	$0.0034/kg	-
	SuperPro	$0.0038/kg	(−) 10%
	Kwiatkowski	$0.0041/kg	(−) 17%
	Hofstrand	$0.0041/kg	(−) 18%
Energy	ESTEA2	$0.035/kg	-
	SuperPro	$0.039/kg	(−) 10%
	Kwiatkowski	$0.069/kg	(−) 49%
	Shapouri and Gallagher	$0.067/kg	(−) 47%
Labor	ESTEA2	$0.024/kg	-
	Claypool and Raman	$0.020/kg	(+) 20%
	Kwiatkowski	$0.019/kg	(−) 26%