

## Supplementary Information

### **Eco-design approach for an innovative production process of low molar mass dextran**

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## A. Process models for unit operations

Table A.1: Operating parameters and utility requirements for agitation and heating in the batch reactor

| Parameter  | Formulation  |
|--|--|
| <p><i>Electricity consumption for agitation</i><br/>           N=264 rot/min</p>         | $D_R = \sqrt[3]{\frac{4V}{\pi}} \text{ assuming } D_R=H$ <p>H (reactor height in m), V (reactor volume in m<sup>3</sup>)<br/>           D<sub>R</sub> (reactor diameter in m)</p> $P = \rho_{solution} N_p N^3 D_A^5$ <p>P (Agitation - electrical power required in kW)<br/>           ρ<sub>solution</sub> (density of solution in kg.m<sup>-3</sup>),<br/>           N<sub>p</sub> (power number), N (speed of rotation for agitator in rd.min<sup>-1</sup>),<br/>           D<sub>A</sub> (agitator diameter in m) = 1/3 D<sub>R</sub></p> $Re = \frac{\rho_{solution} N D_A^2}{\mu_{solution}}$ <p>Re (Reynolds number)<br/>           μ<sub>solution</sub> (viscosity of solution in cP)</p>   |
| <p>W<sub>R</sub> (Agitation - Electricity required in kWh)</p>                           | $W_R = P \cdot t / 60$ <p>t (time of reaction in min)</p>  |
| <p><i>Heating requirement</i><br/>           Q<sub>R</sub> (Heating required in kWh)</p> | $Q_R = Q_{solution} + Q_{reactor} + Q_{jacket}$ $Q_{solution} = m_s \cdot c_{p,s} \cdot (T_2 - T_e) / 3600$ <p>m<sub>s</sub> (solution mass in kg), c<sub>p,s</sub> (heat capacity of solution in kJ.kg<sup>-1</sup>.K<sup>-1</sup>),<br/>           T<sub>e</sub> (ambient temperature), T<sub>2</sub> (reactor temperature taken at 30°C)</p> $Q_{reactor} = m_r \cdot c_{p,r} \cdot (T_2 - T_e) / 3600$ <p>m<sub>r</sub> (mass of stainless still reactor in kg), c<sub>p,r</sub> (heat capacity of reactor in kJ.kg<sup>-1</sup>.K<sup>-1</sup>)</p> $Q_{jacket} = m_{wj} \cdot c_{p,s} \cdot (T_2 - T_e) / 3600$ <p>m<sub>wj</sub> (mass of water in jacket and hoses in kg), c<sub>p,s</sub> (heat capacity of water in kJ.kg<sup>-1</sup>.K<sup>-1</sup>)</p> |

The agitator used is a pitched blade since the viscosity of the solution at the operating temperature is about 1.4 times the viscosity of water

**Table A.2: Operating parameters and utility requirements for agitation and heating in the batch reactor for enzyme inactivation**

| Parameter                                       | Formulation   |
|---|---|
| <i>Electricity consumption:</i>                 |   |
| $W_I$ (Agitation - Electricity required in kWh) | $W_I = P \cdot t_a / 60$  |
|   | $t_a$ (time of inactivation in min)   |
|   | P (electrical power required in kW – same as for reaction step)   |
| <i>Heating requirement:</i>                     |   |
| $Q_I$ (Heating required in kWh)                 | $Q_I = Q_{solution} + Q_{reactor} + Q_{jacket}$   |
|   | $Q_{solution} = m_s \cdot c_{p,s} \cdot (T_3 - T_2) / 3600$   |
|   | $m_s$ (solution mass in kg), $c_{p,s}$ (heat capacity of solution in $\text{kJ} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$ ),                    |
|   | $T_3$ (inactivation temperature taken at 95°C), $T_2$ (reactor temperature taken at 30°C)   |
|   | $Q_{reactor} = m_r \cdot c_{p,r} \cdot (T_3 - T_2) / 3600$  |
|   | $m_r$ (mass of stainless still reactor in kg), $c_{p,r}$ (heat capacity of reactor in $\text{kJ} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$ )    |
|   | $Q_{jacket} = m_{wj} \cdot c_{p,s} \cdot (T_3 - T_2) / 3600$  |
|   | $m_{wj}$ (mass of water in jacket and hoses in kg), $c_{p,s}$ (heat capacity of water in $\text{kJ} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$ ) |

**Table A.3: Operating parameters and utility requirement for enzyme separation by ultrafiltration**

| Parameter                              | Formulation   |
|--|---|
| <i>Washing water and chemicals:</i>    |   |
|  | $V_b = J_{bw} A (t_b F_b t)$  |
|  | $V_s = J_{bw} A t_b$  |
|  | $V_b$ (volume of water used for backwashing in L)   |
|  | $V_s$ (volume of solution used for sanitation in L)   |
|  | $J_{bw} = 2J$ (flux of water used for backwashing in $\text{L} \cdot \text{m}^{-2} \cdot \text{h}^{-1}$ ) |
|  | J (filtrate flux in $\text{L} \cdot \text{m}^{-2} \cdot \text{h}^{-1}$ , J=30)                            |
|  | $F_b$ (backwashing frequency in $\text{h}^{-1}$ , $F_b=4$ )   |
|  | $t_b$ (time of backwashing in h, $t_b = 1/60$ h)  |
|  | t (time of filtration in h)   |
| <i>Electricity consumption:</i>        |   |
| $W_{ES}$ (Electricity required in kWh) | $W_{ES} = W_{filtration} + W_{washing}$   |
|  | $W_{filtration} = \frac{TMP}{\eta} \cdot V \left( \frac{1}{360} \right)$                                  |
|  | $W_{washing} = \frac{2 TMP}{\eta} \cdot (V_b + V_s) \left( \frac{1}{360} \right)$                         |
|  | $W_{filtration}$ (pumping energy for filtration in kWh)   |
|  | $W_{washing}$ (pumping energy for washing in kWh)   |
|  | V (volume of solution to be filtered in L)  |
|  | A (membrane surface in $\text{m}^2$ , A=1 $\text{m}^2$ )  |
|  | TMP (trans-membrane pressure in bar)  |
|  | $\eta$ (pump efficiency within 50-85%)  |

**Table A.4: Operating parameters and utility requirement for dextran separation by ultrafiltration**

| Parameter   | Formulation   |
|---|---|
| Purity of separated dextran:<br>(model from Li et al., 2004)                  | $Purity = \left( 1 + \frac{C_{O,feed0}}{C_{P,feed0}} Y^{((R_P - R_O)/(1 - R_P))} \right)^{-1}$ $R_O = 1 - C_{O,perm}/C_{O,feed}$ $R_P = 1 - C_{P,perm}/C_{P,feed}$ $Y = \left( 1 + \frac{(k - 1) V_{dil}}{k V_{feed0}} \right)^{(R_P - 1)/(k - 1)}$ |
| Where: $R_O$ (rejection coefficient for small molecules, considered constant) |   |
| $R_P$ (rejection coefficient for dextrans, considered constant)               |   |
| $Y$ (recovery rate of dextran, for variable volume diafiltration)             |   |
| $C_O$ (concentration of small molecules in g L <sup>-1</sup> )                |   |
| $C_P$ (concentration of dextrans in g L <sup>-1</sup> )                       |   |
| $V$ (liquid volume in L)  |   |
| $k$ (operation constant, $0 < k < 1$ for variable volume diafiltration)       |   |
| $Q$ (flow in L h <sup>-1</sup> )  |   |
| Subscripts refer to: feed0 – initial conditions in the feed reservoir         |   |
| feed – condition in the feed reservoir  |   |
| dil – dilution liquid used (water)  |   |
| perm – permeate   |   |
| ret - retentate   |   |

Mass balance, energy consumption:

$$Q_{dil} = \frac{V_{dil}}{t}; \quad Q_{feed} = Q_{ret} + Q_{per}$$

$$Q_{dil} = k Q_{per} = k A J_{per}; \quad Q_{ret} = A J_{ret}$$

$$A = \frac{t V_{dil}}{k J_{per}}$$

$$W_{filtration} = t Q_{feed} \frac{TMP}{\eta} \left( \frac{1}{360} \right)$$

$$W_{dilution} = t Q_{dil} \frac{\Delta P}{\eta} \left( \frac{1}{360} \right)$$

$J_{per}$  (permeate flux in L.m<sup>-2</sup>.h<sup>-1</sup>),  $J_{ret}$  (retentate (or recirculation) flux in L.m<sup>-2</sup>.h<sup>-1</sup>), both fixed values  
 $A$  (membrane surface in m<sup>2</sup>),  $t$  (filtration duration in h, fixed value)  
 $W_{filtration}$  (pumping energy for filtration in kWh)  
 $W_{dilution}$  (pumping energy for diluting water in kWh)  
 $\Delta P$  (pressure loss for water pumping in bar)  
 TMP (trans-membrane pressure in bar)  
 $\eta$  (pump efficiency within 50-85%)

Retentate (product) and permeate (effluent) composition :

$$V_{ret} = V_{feed0} + V_{dil} - V_{per}; \quad V_{per} = t Q_{per}$$

$$C_{P,ret} = \frac{C_{P,feed0} V_{feed0}}{V_R + V_P (1 - R_P)}$$

$$C_{O,ret} = C_{P,ret} \left( \frac{1 - Purity}{Purity} \right)$$

$$C_{p,per} = \frac{C_{p,feed0}V_{feed0} - C_{p,ret}V_{ret}}{V_P}$$

$$C_{o,per} = \frac{C_{o,feed0}V_{feed0} - C_{o,ret}V_{ret}}{V_P}$$

Membrane cleaning:

$$V_b = J_{bw} A (t_b F_b t)$$

$$V_s = J_{bw} A t_b$$

$$W_{washing} = \frac{2 TMP}{\eta} \cdot (V_b + V_s) \left( \frac{1}{360} \right)$$

$W_{washing}$  (pumping energy for washing in kWh)

$V_b$  (volume of water used for backwashing in L)

$V_s$  (volume of solution used for sanitation in L)

$J_{bw} = 2J_{per}$  (flux of water used for backwashing in  $L \cdot m^{-2} \cdot h^{-1}$ )

$F_b$  (backwashing frequency in  $h^{-1}$ ,  $F_b=4$ )

$t_b$  (time of backwashing in h,  $t_b = 1/60$  h)

$W_{Ds}$  (Total electricity required for dextran separation in kWh)

$Q_{Ds}$  (Heating required in kWh), considering that all liquids are heated from ambient temperature (20°C) to operation temperature (40°C)

$$W_{Ds} = W_{filtration} + W_{dilution} + W_{washing}$$

$$m = V \rho = (V_{feed0} + V_{dil} + V_b + V_s) \rho$$

$$Q_{Ds} = m \cdot c_p \cdot (T_{Ds} - T_a) / (3.6 \cdot 10^6)$$

$m$  (total mass of liquids in kg)

$c_p$  (heat capacity of solution in  $J \cdot kg^{-1} \cdot K^{-1}$ ),

$T_{Ds}$  (operation temperature taken at 40°C),  $T_a$  (ambient temperature taken at 20°C)

**Table A.5: Operating parameters and utility requirement for dextran concentration by ultrafiltration**

| Parameter   | Formulation   |
|---|---|
| <i>Mass balance, energy consumption:</i>  |   |
| A final dextran concentration is targeted,<br>$C_{p,feed}$ = filtration objective (e.g. 130 gL <sup>-1</sup> )<br>in the final volume $V_{feed}$                          | $V_{feed} = \frac{C_{p,feed0} V_{feed0}}{C_{p,feed}}$<br>$V_{per} = V_{feed0} - V_{feed}$   |
|   | $A = \frac{V_{per}}{t J_{per}}$   |
|   | $Q_{per} = A J_{per}; \quad Q_{ret} = A J_{ret}$  |
|   | $Q_{feed} = Q_{ret} + Q_{per}$  |
|   | $W_{filtration} = t Q_{feed} \frac{TMP}{\eta} \left( \frac{1}{360} \right)$   |
|   | V (liquid volume in L)<br>Q (flow in L h <sup>-1</sup> )<br>C <sub>p</sub> (concentration of dextrans in g L <sup>-1</sup> )<br>Subscripts refer to: feed0 – initial conditions in the feed reservoir<br>feed – condition in the feed reservoir<br>perm – permeate<br>ret - retentate<br>t (filtration time in h)     |
| $J_{per}$ (permeate flux in L.m <sup>-2</sup> .h <sup>-1</sup> ), $J_{ret}$ (retentate (or recirculation) flux in L.m <sup>-2</sup> .h <sup>-1</sup> ), both fixed values |   |
| A (membrane surface in m <sup>2</sup> ), t (filtration duration in h, fixed value)  |   |
| $W_{filtration}$ (pumping energy for filtration in kWh)   |   |
| TMP (trans-membrane pressure in bar)  |   |
| $\eta$ (pump efficiency within 50-85%)  |   |
| <i>Membrane cleaning:</i>   |   |
|   | $V_b = J_{bw} A (t_b F_b t)$  |
|   | $V_s = J_{bw} A t_b$  |
|   | $W_{washing} = \frac{2 TMP}{\eta} \cdot (V_b + V_s) \left( \frac{1}{360} \right)$   |
|   | $W_{washing}$ (pumping energy for washing in kWh)<br>$V_b$ (volume of water used for backwashing in L)<br>$V_s$ (volume of solution used for sanitization in L)   |
| $J_{bw} = 2J_{per}$ (flux of water used for backwashing in L.m <sup>-2</sup> .h <sup>-1</sup> )   |   |
|   | $F_b$ (backwashing frequency in h <sup>-1</sup> , $F_b=4$ )<br>$t_b$ (time of backwashing in h, $t_b = 1/60$ h)   |
| $W_{Dc}$ (Total electricity required for dextran concentration in kWh)  | $W_{Dc} = W_{filtration} + W_{washing}$   |
| $Q_{Dc}$ (Heating required in kWh), considering that all liquids are heated from ambient temperature (20°C) to operation temperature (40°C)                               | $m = V \rho = (V_{feed0} + V_b + V_s) \rho$<br>$Q_{Dc} = m \cdot c_p \cdot (T_f - T_i) / (3.6 \cdot 10^6)$<br>m (total mass of liquids in kg)<br>$c_p$ (heat capacity of solution in J.kg <sup>-1</sup> .K <sup>-1</sup> ),<br>$T_f$ (operation temperature taken at 40°C), $T_i$ (ambient temperature taken at 20°C) |

**Table A.6: Operating parameters and utility requirements for the chromatography unit**

| Parameter  | Formulation   |
|--|---|
| <i>Operating parameters:</i>   |   |
|  | $V_c = H_c \cdot S_c$   |
|  | $V_0 = \varepsilon \cdot V_c$   |
|  | $u = Q_w / (3600 \cdot S_c)$  |
|  | assuming $H_c = 10 \cdot D_c$   |
| $H_c$ (column height in m), $D_c$ (column diameter in m), $S_c = \pi \left(\frac{D_c^2}{4}\right)$ (column section in m <sup>2</sup> ) |   |
|  | $V_c$ (ion-exchange column volume in m <sup>3</sup> )   |
|  | $\varepsilon$ (column external porosity)  |
|  | $V_0$ (Void volume in m <sup>3</sup> )  |
| $Q_w$ (Water flow rate in m <sup>3</sup> .h <sup>-1</sup> ) in experimental range 0.08-0.2 m <sup>3</sup> .h <sup>-1</sup>             |   |
|  | $u$ (Percolation velocity in m.s <sup>-1</sup> )  |
|  | $\Delta t_{tot} = \Delta t_O + \Delta t_P$  |
|  | $V_w = \Delta t_{tot} \cdot Q_w$  |
|  | $\Delta t_{tot}$ (Total elution time in h)  |
|  | $\Delta t_P = n_i \left(2 \frac{V_0}{Q_w}\right)$ (Elution time of fraction 1= polymers, in h)  |
|  | $\Delta t_O = n_i \left(4 \frac{V_0}{Q_w}\right)$ (Elution time of fraction 2 = oligomers, in h)  |
| $n_i = V / V_i$ (injection number), $V$ (solution volume in m <sup>3</sup> ), $V_i = 5\% V_c$ (injection volume in m <sup>3</sup> )    |   |
|  | $V_w$ (Water volume required in m <sup>3</sup> )  |
| <i>Electricity consumption:</i>  |   |
|  | Ergun formula for pressure loss in packed bed   |
|  | $\frac{\Delta P}{H_c} = \frac{150 \cdot \mu_{sol} \cdot u \cdot (1 - \varepsilon)^2}{(\varphi_s \times d_p)^2 \cdot \varepsilon^3} + (1.75) \frac{\rho_{sol} \cdot u^2 \cdot (1 - \varepsilon)}{\varphi_s \cdot d_p \cdot \varepsilon^3}$ |
|  | $\Delta P$ (Pressure loss caused by the packed bed in Pa)   |
| $\mu_{sol}$ (viscosity of solution in Pa.s), $d_p$ (diameter of resin particles in m)  |   |
|  | $\varphi_s = 1$ (shape coefficient, particles considered spherical)   |
|  | $\rho_{sol}$ (solution density in kg.m <sup>-3</sup> )  |
|  | $\Delta P_d = \frac{Q_w \cdot \mu_{sol} \cdot L_d}{(3600) \cdot K \cdot S_c}$   |
|  | $K = \frac{\varepsilon_d \cdot d_{p,d}^2}{32}$  |
| $\Delta P_d$ (Pressure loss caused by the porous disc supporting the packed bed, in Pa)  |   |
| $L_d$ (Disc length in m), $K$ (proportionality constant in m <sup>2</sup> )  |   |
| $\varepsilon_d$ (disc porosity), $d_{p,d}$ (pore diameter of the disc in m)  |   |
| $W_C$ (Electricity required for chromatographic separation in kWh)   | $W_C = (\Delta P + \Delta P_d) \cdot Q_w \cdot \Delta t_{tot} / (3.6 \cdot 10^6)$   |
| <i>Heating requirement:</i>  |   |
| $Q_C$ (Heating required in kWh)  | $Q_C = m_s \cdot c_{p,s} \cdot (T_C - T_a) / (3.6 \cdot 10^6)$  |
|  | $m_s$ (solution mass in kg), $c_{p,s}$ (heat capacity of solution in J.kg <sup>-1</sup> .K <sup>-1</sup> ),   |
|  | $T_C$ (Chromatography temperature taken at 50°C), $T_a$ (ambient temperature, 20°C)   |

**Table A.7: Energy requirements and calculations for the lyophilization (\*)**

| Parameter  | Formulation  |
|--|--|
| $Q_{L,cool}$ (Energy for freezing step in kWh)   | $Q_{cool} = Q_{c1} + Q_f + Q_{c2} + Q_s$ <p style="text-align: right;">Where, <math>Q_{c1} = m_t \cdot c_{p,l} \cdot (T_f - T_e)/3600</math><br/> <math>Q_f = m_t \cdot L_f/3600</math><br/> <math>Q_{c2} = m_t \cdot c_{p,i} \cdot (T_{sf} - T_f)/3600</math><br/> <math>Q_s = m_s \cdot c_{p,s} \cdot (T_{sf} - T_e)/3600</math></p> <p style="text-align: center;"><math>m_t</math> (total mass of dextran solution leaving the chromatography in kg)<br/> <math>m_s = 10 \times m_t</math> (mass of stainless steel in kg, factor 10 being the scaling factor)<br/> <math>c_{p,l}</math> (heat capacity of liquid water in <math>J \cdot kg^{-1} \cdot K^{-1}</math>), <math>c_{p,i}</math> (heat capacity of ice in <math>J \cdot kg^{-1} \cdot K^{-1}</math>)<br/> <math>L_f</math> (latent heat of freezing in <math>J \cdot kg^{-1}</math>), <math>c_{p,s}</math> (heat capacity of stainless steel in <math>J \cdot kg^{-1} \cdot K^{-1}</math>)<br/> <math>T_f</math> (freezing temperature of water), <math>T_{sf}</math> (sub-freezing temperature = <math>-40^\circ C</math>)</p> |
| $N_{vacuum}$ (Vacuum power <sup>(*)</sup> in kW) | $N_{vacuum} = S_{th}(P_v - P_a + C')(3 \times 10^{-5})$ <p style="text-align: center;"><math>S_{th}</math> (theoretical pumping speed in <math>m^3 \cdot h^{-1}</math>), <math>C'</math> (mechanical loss constant in mbar)<br/> <math>P_v</math> (forevacuum pressure in mbar), <math>P_a</math> (Intake pressure in mbar)<br/> (*) Rotary oil pump</p>   |
| $Q_{L,heat}$ (Energy for drying step in kWh)     | $Q_{heat} = Q_{sub} + Q_h + Q_s$ <p style="text-align: right;">With, <math>Q_{sub} = m_t \cdot L_s/3600</math><br/> <math>Q_h = m_t \cdot c_{p,v} \cdot (T_{od} - T_{sf})/3600</math><br/> <math>Q_s = m_s \cdot c_{p,s} \cdot (T_{od} - T_{sf})</math></p> <p style="text-align: center;"><math>m_p</math> (total mass of dextrans in kg)<br/> <math>c_{p,v}</math> (heat capacity of vapor water in <math>J \cdot kg^{-1} \cdot K^{-1}</math>), <math>T_{od}</math> (over drying temperature = <math>40^\circ C</math>)</p>  |
| $t_d$ (Drying time in h)                         | $t_d = Q_{heat}/(c_d \cdot \eta)$ <p style="text-align: right;"><math>c_d</math> (drying capacity in kW), <math>\eta</math> (drying efficiency)</p>  |
| $S_d$ (Drying surface requirements in $m^2$ )    | $S_d = m_t/(c_s \cdot DT)$ <p style="text-align: right;"><math>c_s</math> (sublimation capacity = <math>1kg \cdot water \cdot m^{-2} \cdot h^{-1}</math>)</p>  |

(\*) Lyophilization or Freeze-drying includes: (1) Freezing: The product has to be frozen at a temperature below the melting temperature of the water; (2) Vacuum: The purpose is to lower the pressure by means of vacuum pumps. The type of vacuum pump in freeze drying is the rotary oil pump. Rotary oil pump are able to achieve vacuum as low as about micro-m Hg; (3) Primary desiccation or sublimation: During the sublimation phase, water passes directly from the solid to the gaseous state, mass transfer and heat transfer occur simultaneously; (4) Secondary desorption or desiccation: Desorption is the phase that immediately follows to the sublimation. After the last crystal has disappeared by sublimation, the remaining water is in absorbed form in the product and in the vapor state (saturating vapor of the water). This absorbed water, on the finely porous product, must be eliminated because it would be detrimental to the good preservation of the lyophilized product. This lyophilization step corresponds to an isothermal desorption during which the water is removed from the product in molecular form at constant pressure and temperature; (5) Return to atmospheric pressure: When returning to atmospheric pressure or breaking the vacuum, a neutral gas (nitrogen or carbon dioxide) is most often used in order to prevent the lyophilized product from reabsorbing water because the lyophilized product has to be removed and packaged in an environment with low relative humidity.



## B. LCA results

Table B.1: Results of ReCiPe Endpoint impact method with details on impact categories (Results are expressed for 1 kg of dextran produced – functional unit)

| Impact / points              | Benchmark 1     | Benchmark 2     | Benchmark 3     |
|------------------------------|-----------------|-----------------|-----------------|
| <b>ecosystem quality</b>     |                 |                 |                 |
| climate change, ecosystems   | 5.93E+00        | 9.44E-01        | 3.56E-01        |
| terrestrial acidification    | 2.33E-02        | 4.20E-03        | 1.90E-03        |
| freshwater eutrophication    | 1.56E-02        | 3.03E-03        | 9.70E-04        |
| terrestrial ecotoxicity      | 1.69E-02        | 3.95E-03        | 2.13E-03        |
| freshwater ecotoxicity       | 1.76E-03        | 2.80E-04        | 9.50E-05        |
| marine ecotoxicity           | 5.91E-06        | 8.51E-07        | 2.31E-07        |
| agricultural land occupation | 9.35E-01        | 8.00E-01        | 7.84E-01        |
| urban land occupation        | 9.00E-02        | 1.64E-02        | 6.29E-03        |
| natural land transformation  | 1.45E-01        | 2.21E-02        | 8.62E-03        |
| <b>total</b>                 | <b>7.16E+00</b> | <b>1.79E+00</b> | <b>1.16E+00</b> |
| <b>human health</b>          |                 |                 |                 |
| climate change, human health | 9.07E+00        | 1.44E+00        | 5.45E-01        |
| ozone depletion              | 9.10E-04        | 1.73E-04        | 7.16E-05        |
| human toxicity               | 2.76E+00        | 3.72E-01        | 9.81E-02        |
| photochem. oxidant form.     | 8.09E-04        | 1.29E-04        | 4.84E-05        |
| particulate matter formation | 3.41E+00        | 5.40E-01        | 2.04E-01        |
| ionising radiation           | 1.26E+00        | 1.45E-01        | 3.75E-02        |
| <b>total</b>                 | <b>1.65E+01</b> | <b>2.50E+00</b> | <b>8.85E-01</b> |
| <b>resources</b>             |                 |                 |                 |
| metal depletion              | 1.01E-02        | 2.00E-03        | 5.58E-04        |
| fossil depletion             | 1.07E+01        | 1.67E+00        | 5.87E-01        |
| <b>total</b>                 | <b>1.07E+01</b> | <b>1.67E+00</b> | <b>5.88E-01</b> |
| <b>total</b>                 | <b>3.44E+01</b> | <b>5.96E+00</b> | <b>2.63E+00</b> |

## C. Life Cycle Inventory for dextran production and purification

The LCI for the three benchmarks studied is based on an initial sucrose concentration of 200 g L<sup>-1</sup>. The selected LCI datasets are from ecoinvent 2.2, as shown in Table C.1 and Table C.2. Table C1 contains also the amount of materials used in the sensitivity analysis.

**Table C.1: Ecoinvent modules used for the Life Cycle Inventory of the production and purification of dextrans (Quantities are expressed for 1kg dextran produced)**

| Material/energy  | Benchmark 1          | Benchmark 2         | Benchmark 3          |
|--|----------------------|---------------------|----------------------|
| Sugar, from sugar beet, at sugar refinery, [CH], kg                      | 2.38                 | 2.38                | 2.38                 |
| Water, completely softened, at plant [RER], kg                           | 517.7                | 809.1               | 15.13                |
| Water, deionized, at plant [CH], kg                                      | 0.12                 | 2.78                | 0.272                |
| Water, ultrapure [GLO], kg   | 10.5                 | 10.5                | 10.5                 |
| Electricity mix [FR], kWh  | 418.8                | 47.75               | 12.21                |
| Hydrogen peroxide, 50% in water, at plant [RER], kg                      | 0.013                | 0.308               | 0.030                |
| Treatment, sewage, to wastewater treatment, class 4 [CH], m <sup>3</sup> | 0.518                | 0.812               | 0.026                |
| Enzyme, kg   | 0.000167             | 0.000167            | 0.000167             |
| <b>Material included in sensitivity analysis</b>                         |                      |                     |                      |
| Chemical plant, organics [RER]*, units                                   | 4 10 <sup>-10</sup>  | 4 10 <sup>-10</sup> | 4 10 <sup>-10</sup>  |
| Molasses, from sugar beet, at sugar refinery [CH], kg                    | 7.14                 | 7.14                | 7.14                 |
| Polysulfone [CH]**, kg   | 1.3 10 <sup>-5</sup> | 4 10 <sup>-4</sup>  | 2.2 10 <sup>-5</sup> |

RER (Rest of Europe Region excluding Switzerland data); GLO (global data); CH (Switzerland data); FR (French data)

\*generic dataset for a chemical plant for organic substances production. One plant = 1 unit, corresponding to an average production during the plant lifetime (30 years).

\*\* polysulfone is the generic polymer used for UF membrane fabrication. Data adapted from ecoinvent 3.5

The data in ecoinvent are representative of production of several enzymes (Alpha-amylase; Glucoamylase; Cellulase). In the ecoinvent module for enzyme production, it is assumed that the enzymes are produced from potato starch and a bacterial strain. The production of bacterial strain is not taken into account (not significant for the overall utility consumption). The heat and power consumption for production are based on the work of Dunn et al. (2012). Impacts related to the use of enzyme for dextran production are presented in SI, Table D.1. The ReCiPe Endpoint represents less than 0.03% from the total Endpoint, and less than 0.03% of the total climate change impact, regardless of the benchmark.

**Table C.2: Ecoinvent data for the production of 1 kg enzyme (corresponding to 6000 kg dextran produced)**

| Consumable   | for 1kg enzyme      |
|--|---------------------|
| Potato starch, at plant [DE]                             | 4.17 kg / kg enzyme |
| Heat, unspecified, in chemical plant [RER]               | 8.3 MJ / kg enzyme  |
| Electricity, medium voltage, production FR, at grid [FR] | 6.3 kWh / kg enzyme |

## D. Sensitivity analysis

### D.1 Raw material: use of molasses instead of sugar

Table D.1: Impact calculation results for 2 raw materials: sugar (A), molasses (B) (Results are expressed for 1 kg of dextran produced)

| A                    |              |              |              |
|----------------------|--------------|--------------|--------------|
| ReCiPe Endpoint      | Benchmark 1  | Benchmark2   | Benchmark 3  |
| sugar                | 1.97E-01     | 1.97E-01     | 2.02E-01     |
| electricity          | 3.87E+00     | 4.41E-01     | 1.15E-01     |
| process water        | 1.84E-03     | 2.70E-03     | 7.70E-04     |
| enzyme production    | 1.07E-04     | 1.07E-04     | 1.10E-04     |
| wastewater treatment | 2.11E-02     | 3.31E-02     | 1.08E-03     |
| chemicals            | 1.62E-03     | 3.66E-02     | 3.64E-03     |
| <b>total</b>         | <b>4.092</b> | <b>0.710</b> | <b>0.322</b> |

| B                    |              |              |              |
|----------------------|--------------|--------------|--------------|
| ReCiPe Endpoint      | Benchmark 1  | Benchmark2   | Benchmark 3  |
| molasses             | 1.26E-01     | 1.26E-01     | 1.29E-01     |
| electricity          | 3.87E+00     | 4.41E-01     | 1.15E-01     |
| process water        | 1.84E-03     | 2.70E-03     | 7.70E-04     |
| enzyme production    | 1.07E-04     | 1.07E-04     | 1.10E-04     |
| wastewater treatment | 2.11E-02     | 3.31E-02     | 1.08E-03     |
| chemicals            | 1.62E-03     | 3.66E-02     | 3.64E-03     |
| <b>total</b>         | <b>4.021</b> | <b>0.640</b> | <b>0.250</b> |
| <b>(A-B)/A %</b>     | <b>1.7</b>   | <b>9.9</b>   | <b>35.9</b>  |

| Climate change       |               |              |              |
|----------------------|---------------|--------------|--------------|
| ReCiPe Endpoint      | Benchmark 1   | Benchmark 2  | Benchmark 3  |
| sugar                | 1.21E+00      | 1.21E+00     | 1.24E+00     |
| electricity          | 3.75E+01      | 4.27E+00     | 1.11E+00     |
| process water        | 1.99E-02      | 2.91E-02     | 7.93E-03     |
| enzyme production    | 7.34E-04      | 7.34E-04     | 7.54E-04     |
| wastewater treatment | 2.19E-01      | 3.44E-01     | 1.12E-02     |
| chemicals            | 1.53E-02      | 3.47E-01     | 3.45E-02     |
| <b>total</b>         | <b>38.944</b> | <b>6.200</b> | <b>2.404</b> |

| Climate change       |               |              |              |
|----------------------|---------------|--------------|--------------|
| ReCiPe Endpoint      | Benchmark 1   | Benchmark 2  | Benchmark 3  |
| molasses             | 7.74E-01      | 7.74E-01     | 7.95E-01     |
| electricity          | 3.75E+01      | 4.27E+00     | 1.11E+00     |
| process water        | 1.99E-02      | 2.91E-02     | 7.93E-03     |
| enzyme production    | 7.34E-04      | 7.34E-04     | 7.54E-04     |
| wastewater treatment | 2.19E-01      | 3.44E-01     | 1.12E-02     |
| chemicals            | 1.53E-02      | 3.47E-01     | 3.45E-02     |
| <b>total</b>         | <b>38.510</b> | <b>5.767</b> | <b>1.959</b> |
| <b>(A-B)/A %</b>     | <b>1.1</b>    | <b>7.0</b>   | <b>18.5</b>  |

In the simulations, 3 kg of molasses (from sugar beet) replace 1 kg of sugar, based on the saccharide content of molasses (33%). The use of molasses as raw material has less impact than sugar. The relative differences between the impacts obtained with molasses (B) and sugar (A) are negligible in the case of benchmark 1, 7 to 10 % for benchmark 2 and much larger (18 to 36%) for benchmark 3. This result is explained by the low contribution of raw materials to overall impacts especially for benchmark 1 where energy consumption is the major contributor.

### D.2 Sensitivity of environmental performances to the initial sucrose concentration

1) Results are expressed for 1kg of dextran produced in Benchmark 2.

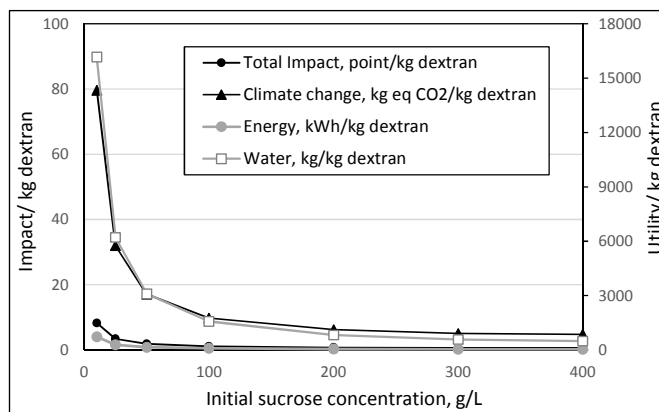


Figure D.1. Impact calculation results and utilities for Benchmark 2 for different sucrose concentration

2) Influence of the initial sucrose concentration on utility consumption and impact results (Results are expressed for 1 batch, i.e. 100L of initial sucrose solution).

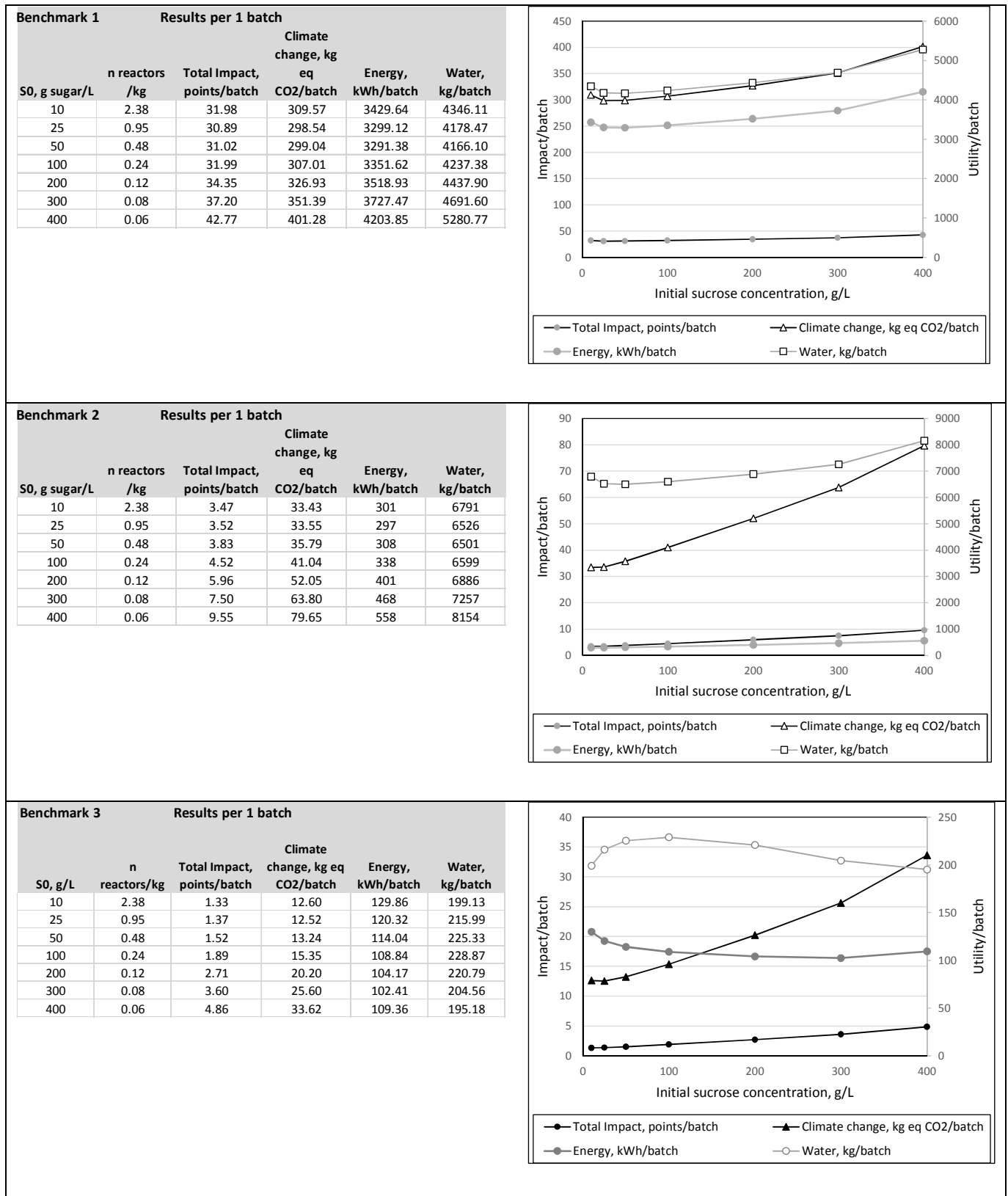


Figure D.2. Impact results and utilities for the 3 benchmarks, for different sucrose concentrations. Results expressed for 100L of initial solution.

### D.3 Infrastructure contribution to total impact ReCiPe and to climate change impact

The infrastructure contribution is higher for Benchmark 3 due to the lower total impact compared to Benchmark 1.

**Table D.2: Contribution of infrastructure to impact results for Benchmark 1 and 3 (Results are expressed for 1 kg of dextran produced)**

| Benchmark 1                      |                                    | Benchmark 3                      |                                    |
|----------------------------------|------------------------------------|----------------------------------|------------------------------------|
| % infrastructure in Total impact | % infrastructure in Climate change | % infrastructure in Total impact | % infrastructure in Climate change |
| 0.11                             | 0.08                               | 2.54                             | 1.95                               |
| 0.12                             | 0.09                               | 2.57                             | 2.04                               |
| 0.14                             | 0.10                               | 2.78                             | 2.31                               |
| 0.18                             | 0.14                               | 2.97                             | 2.64                               |
| 0.17                             | 0.13                               | 2.10                             | 2.02                               |
| 0.23                             | 0.18                               | 2.36                             | 2.38                               |
| 0.27                             | 0.21                               | 2.33                             | 2.42                               |

### D.4 Membrane replacement and contribution of chromatography resin to total ReCiPe impact and climate change impact

Replacement was envisaged every 1 year, with a productivity of 1680 kg of dextran per year (corresponding to a production line with a nominal 100L reactor).

**Table D.3: Contribution of membrane and resin replacements to impact results for the three benchmarks (Results are expressed for 1 kg of dextran produced)**

| Impact                                 | Benchmark 1          | Benchmark 2 | Benchmark 3 |
|--|----------------------|-------------|-------------|
|  | Membrane replacement |             |             |
| total Endpoint impact                  | 8.2E-05              | 2.4E-03     | 1.4E-04     |
| % from benchmark impact                | 2.0E-03              | 3.4E-01     | 4.3E-02     |
|  | Resin replacement    |             |             |
| total Endpoint impact                  | 8.3E-03              | 8.3E-03     | 0.0E+00     |
| % from benchmark impact                | 2.0E-01              | 1.2E+00     | 0.0E+00     |
|  | Membrane replacement |             |             |
| climate change, kg CO <sub>2</sub> -eq | 6.2E-04              | 1.9E-02     | 1.1E-03     |
| % from benchmark impact                | 1.6E-03              | 3.0E-01     | 4.4E-02     |
|  | Resin replacement    |             |             |
| climate change, kg CO <sub>2</sub> -eq | 6.6E-02              | 6.6E-02     | 0.0E+00     |
| % from benchmark impact                | 1.7E-01              | 1.1E+00     | 0.0E+00     |