# ANNOUNCEMENT FOR STUDENT CONTEST PROBLEM COMPETITION 2011

**AWARD 1000 EUR**

**EURECHA - The European Committee for Computers in Chemical Engineering Education**

This contest problem is open to Master/PhD level students.

The participants have approximately three months to prepare and submit solutions to the problem no later than **April the 30th 2011.** Solutions can be prepared by individuals or by team of 2 members.

The written report, not exceeding 15 pages including figures, should follow the formatting rules specified at http://www.escape-21.gr/Content/NEW_ESCAPE-21-template-elsevier.dot
The report, in **pdf** format, and any other file (spreadsheet, simulation input file, etc.), should be packed (**zip** format) and sent to the EURECHA secretariat in electronic form as E-mail attachment to eurecha.secretariat@gmail.com.
The jury will select the best solution, based on technical excellence (i.e. cost effectiveness, energy efficiency, etc.), quality of the report and originality.

The winner will receive:

- A cheque of **1000 EUR** (to cover the travel and accommodation expenses, rest as a gift).
- An invitation to get the award at the ESCAPE 21 symposium
- **Selected solution will be posted on the EURECHA web site.**

# Problem: Design of Bioethanol production from lignocellulosic feedstock

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The problem concerns designing a bioethanol production plant following biochemical route. Hence the process flowsheet must consider the following unit operations as illustrated in Figure 1: pretreatment, enzymatic hydrolysis, fermentation and downstream processes for purification (e.g. flash separation plus distillation). Additional unit operations can also be added such as buffer tanks if necessary. The target design capacity is to process 19600 kg/h of dry biomass, for which corn stover is to be used as the biomass feedstock with the assumption of 30% wt solid concentration. More details about the feedstock characteristics are given in Table 1. The target product purity for ethanol is 99 % wt after the downstream processing.

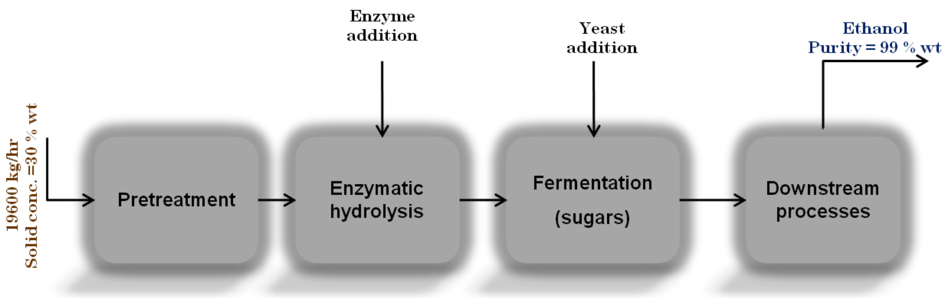


Figure 1. A general process flowsheet of bioethanol production

**Table 1** Feedstock composition on dry basis

| Feature | Value |
|---|---|
| Feedstock | Corn Stover |
| Dry feedstock capacity | 19600 kg/h |
| **% Dry basis composition** | |
| Glucan | 37.4 |
| Xylan | 21.1 |
| Arabinan | 2.9 |
| Lignin | 18 |
| Ash | 5.2 |
| Other compounds | 15.4 |

**Expected outcome from design problem:**
The design report should include: a) process flowsheet, b) detailed mass balance for each unit operation (preferably in excel spreadsheet), c) detailed dimensions of unit operations and equipments (reactor volumes, residence time, temperature, utility (e.g. water consumption), yeast and enzyme addition, etc, (d) approximate cost analysis of the process design. In addition, the following is desired as well: e) sensitivity analysis of design (process configuration) and operational variables and parameters for the best selected process configuration, f) computer-aided platform of the problem solution for verification of results.

The evaluation of the best project will be based on the correctness of the calculations but also on the novelty of the solution such as process configuration, cost and sustainability analysis -not detailed but considerations are welcome. Note that there are several process configurations already in the literature employing different process flowsheets and technologies for lignocellusoic bioethanol production. The participants are welcome to be inspired by them. Also the participants are welcome to use any commercial software in their design and evaluation of the unit operations. However the end simulation results from the software should be transferred to an excel spreadsheet to help with detailed checking of the calculations (see the expected outcome above).

**Design basis**

- Identify for each unit operations what the design variables are, which one should be calculated and how (see below point).
- For dimensioning reactors state clearly the assumptions for the design (e.g. residence time is t hr under T temperature, p pressure, C catalyst for the pretreatment unit). State also clearly the source of the assumptions; it could be a research study from literature or a report form internet (search literature and internet).
- You may use steady-state models to calculate yields and conversion efficiency in each unit operations (pretreatment, hydrolysis, fermentation). Alternatively you may also use dynamic models (see the appendix or other published in literature). We understand implementation of dynamic models is too complex so this is not obliged but given as an option.
- State clearly the safety factors used for each unit operations.
- State clearly how the unit operation is designed and to be operated, e.g. as batch, fed-batch or continuous processing. In case fed-batch and continuous units are involved in a process flowsheet, define clearly how the continuous operation will handle this (add necessary timers or buffer tanks or alike if necessary).
- Make necessary assumptions for the cost calculations. In addition, make any other assumptions deemed necessary for technical dimensioning (again provide the reasoning).

## Appendix

Please use Table 2 as starting point and not necessary as the final dimensioning of your unit operations. The assumptions for each of the unit operations are stated in Morales-Rodriguez et al 2010. The participants are motivated to come up with their own design.

Table 2. Process characteristic and suggested conditions for the different unit operations from Morales-Rodriguez et al 2010.

| **Feature** | **Value** | **Pretreatment** | |
|---|---|---|---|
| Feedstock* | Corn Stover | Reactive* | Diluted sulfuric acid |
| Dry feedstock capacity* | 19600 kg/h | Concentration % (wt/v)* | 1.1 |
| | | Residence time* | 2 minutes |
| **% Dry basis composition** | | Temperature | 443 K |
| Glucan* | 37.4 | Solid in the reactor % (wt/v)* | 30 |
| Xylan* | 21.1 | | |
| Arabinan* | 2.9 | | |
| Lignin* | 18 | | |
| Ash* | 5.2 | | |
| Other compounds | 15.4 | | |
| **Enzymatic hydrolysis** | | **Co-Fermentation** | |
| Temperature* | 338 K | Temperature | 303 K |
| Initial solid concentration % (wt/v) | 20 | Inoculum level** | 10% |
| Size of the vessels* | 3596 $m^3$ | Size of the vessels* | 3596 $m^3$ |
| Enzyme | Cellulases (EG, CBH and BDG) | Organism | *Saccharomyces cerevisiae* strain1400 (pLNH33) |
| **SSCF** | | | |
| Temperature | 308 K | | |
| Inoculum level** | 10% | | |
| Size of the vessels* | 3596 $m^3$ | | |
| Enzymes | Cellulases (EG, CBH and BDG) | | |
| Organism | *Saccharomyces cerevisiae* strain1400 (pLNH33) | | |

*NREL Report (Aden et al., 2002)

Table 1. Pretreatment mathematical model (Lavarack et al. 2002).

| Compound | Equation | No. Eq. |
|---|---|---|
| Glucan (cellulose) $g/kg\cdot h$ | $r_{Gn,PT}=-k_{1,G}^{PT}C_{Gn}$ | Eq. (1) |
| Glucose $g/kg\cdot h$ | $r_{G,PT}=k_{1,G}^{PT}C_{Gn}-\phi k_{2,G}^{PT}C_{G}$ | Eq. (2) |
| Xylan $g/kg\cdot h$ | $r_{Xn,PT}=-k_{1,Xy}^{PT}C_{Xn}$ | Eq. (3) |
| Xylose $g/kg\cdot h$ | $r_{Xy,PT}=k_{1,Xy}^{PT}C_{Xn}-\phi k_{2,Xy}^{PT}C_{Xy}$ | Eq. (4) |
| Arabinan $g/kg\cdot h$ | $r_{An,PT}=-k_{1,A}^{PT}C_{An}$ | Eq. (5) |
| Arabinose $g/kg\cdot h$ | $r_{A,PT}=k_{1,A}^{PT}C_{An}-\phi k_{2,A}^{PT}C_{A}$ | Eq. (6) |
| Lignin $g/kg\cdot h$ | $r_{Ln,PT}=-k_{1,ASL}^{PT}C_{Ln}$ | Eq. (7) |
| Acid-Soluble lignin $g/kg\cdot h$ | $r_{ASL,PT}=k_{1,ASL}^{PT}C_{Ln}-\phi k_{2,ASL}^{PT}C_{ASL}$ | Eq. (8) |
| Other comps. | $r_{OC,PT}=\phi\ \ k_{2,G}^{PT}C_{G}+k_{2,Xy}^{PT}C_{Xy}+k_{2,A}^{PT}C_{A}+k_{2,ASL}^{PT}C_{ASL}-k_{3,ASL}^{PT}C_{OC}$ | Eq. (9) |

Table 2. Kinetic expressions of the enzymatic hydrolysis model (Kadam et al., 2004).

| Compound | Equation | No. Eq. |
|---|---|---|
| Cellulose to cellobiose, $g/kg \cdot h$ | $r_{1,EH} = \frac{k_{G2}^{EH} C_{E_{1B}} R_{Gn} C_{Gn}}{1 + \frac{C_{G_2}}{K_{1IG2}^{EH}} + \frac{C_G}{K_{1IG}^{EH}} + \frac{C_{Xy}}{K_{1IXy}^{EH}}}$ | Eq. (10) |
| Cellulose to glucose , $g/kg \cdot h$ | $r_{2,EH} = \frac{k_{1,G}^{EH} \; C_{E_{1B}} + C_{E_{2B}} \; R_{Gn} C_{Gn}}{1 + \frac{C_{G_2}}{K_{2IG2}^{EH}} + \frac{C_G}{K_{2IG}^{EH}} + \frac{C_{Xy}}{K_{2IXy}^{EH}}}$ | Eq. (11) |
| Cellobiose to glucose, $g/kg \cdot h$ | $r_{3,EH} = \frac{k_{2,G}^{EH} C_{E_{2F}} C_{G_2}}{K_M \left(1 + \frac{C_G}{K_{3IG}^{EH}} + \frac{C_{Xy}}{K_{3IXy}^{EH}}\right) + C_{G_2}}$ | Eq. (12) |
| Enzyme Adsorption, $g/kg \cdot h$ | $C_{E_{iB}} = \frac{E_{i\max} K_{\mathrm{iad}} C_{E_{iF}} C_{Gn}}{1 + K_{\mathrm{iad}} C_{E_{iF}}}$ | Eq. (13) |
| Enzyme, $g/kg$ | $C_{E_{Ti}} = C_{E_{Fi}} + C_{E_{Bi}}$ | Eq. (14) |
| Substrate reactivity | $R_{Gn} = \alpha \, C_{Gn} / C_{Gn}^0$ | Eq. (15) |
| Temp. dependence | $k_{ir(T2)} = k_{ir(T1)} e^{-E_{ai}/R \; 1/T1 - 1/T2}$ , $30°C \leq T \leq 55°C$ | Eq. (16) |
| Cellulose kinetic, $g/kg \cdot h$ | $r_{Gn,EH} = -r_{1,EH} - r_{2,EH}$ | Eq. (17) |
| Cellobiose kinetic, $g/kg \cdot h$ | $r_{G_2,EH} = 1.056 r_{1,EH} - r_{3,EH}$ | Eq. (18) |
| Glucose kinetic, $g/kg \cdot h$ | $r_{G,EH} = 1.111 r_{2,EH} + 1.053 r_{3,EH}$ | Eq. (19) |
| Water kinetic, $g/kg \cdot h$ | $r_{W,EH} = -0.055 r_{1,EH} - 0.111 r_{2,EH} - 1.05263 r_{3,EH}$ | Eq. (20) |

Table 3. Kinetic expressions of the co-fermentation model (Krishnan et al., 1999).

| Compound | Equation | No. Eq. |
|---|---|---|
| Biomass Glucose, $g/L\cdot h$ | $r_{1,CF}=\frac{dC_{X_G}}{dt}=\frac{\mu_{\max,G}C_G}{K_{1G}^{CF}+C_G+\frac{C_G^{\ 2}}{K_{1X_G IG}^{CF}}}\left(1-\left(\frac{C_{Et_G}}{Et_{\max,G}}\right)^{\beta_G}\right)$ | Eq. (21) |
| Biomass Xylose, $g/L\cdot h$ | $r_{2,CF}=\frac{dC_{X_{Xy}}}{dt}=\frac{\mu_{\max,Xy}C_{Xy}}{K_{2Xy}^{CF}+C_{Xy}+\frac{C_{Xy}^{\ 2}}{K_{2IXy}^{CF}}}\left(1-\left(\frac{C_{Et_{Xy}}}{Et_{\max,Xy}}\right)^{\beta_{Xy}}\right)$ | Eq. (22) |
| Biomass kinetic, $g/L\cdot h$ | $r_{X,TOT}=x_G r_{1,CF}+x_{Xy}r_{2,CF}$ | Eq. (23) |
| Glucose, $g/L\cdot h$ | $-r_{3,CF}=\frac{1}{Y_{Et_G/G}}\frac{dC_{Et_G}}{dt}=\frac{1}{Y_{X_G/G}}\frac{dC_{X_G}}{dt}+m_G C_{X_G}$ | Eq. (24) |
| Xylose, $g/L\cdot h$ | $-r_{4,CF}=\frac{1}{Y_{Et_{Xy}/Xy}}\frac{dC_{Et_{Xy}}}{dt}=\frac{1}{Y_{X_{Xy}/Xy}}\frac{dC_{X_{Xy}}}{dt}+m_{Xy}C_{X_{Xy}}$ | Eq.(25) |
| Ethanol Glucose, $g/L\cdot h$ | $r_{5,CF}=\frac{1}{C_{X_G}}\frac{dC_{Et_G}}{dt}=\frac{\nu_{\max,G}C_G}{K'^{CF}_{5G}+C_G+\frac{C_G^{\ 2}}{K'^{CF}_{5IG}}}\left(1-\left(\frac{C_{Et_G}}{Et'_{\max,G}}\right)^{\gamma_G}\right)$ | Eq.(26) |
| Ethanol Xylose, $g/L\cdot h$ | $r_{6,CF}=\frac{1}{C_{X_{Xy}}}\frac{dC_{Et_{Xy}}}{dt}=\frac{\nu_{\max,Xy}C_{Xy}}{K'^{CF}_{6Xy}+C_{Xy}+\frac{C_{Xy}^{\ 2}}{K'^{CF}_{6IXy}}}\left(1-\left(\frac{C_{Et_{Xy}}}{Et'_{\max,Xy}}\right)^{\gamma_{Xy}}\right)$ | Eq.(27) |
| Ethanol kinetic, $g/L\cdot h$ | $r_{Et,TOT}=r_{5,CF}+r_{6,CF}$ | Eq.(28) |

**Nomenclature**

| | |
|---|---|
| $C_A$ | Arabinose concentration, $g/kg$ |
| $C_{An}$ | Arabinan concentration, $g/kg$ . |
| $C_{ASL}$ | Acid-soluble lignin concentration, $g/kg$ |
| $C_{Ln}$ | Lignin concentration, $g/kg$ . |
| $C_{E_{iT}}$ | Total enzyme concentration, $g/kg$ |
| $C_{E_{1B}}$ | Bound concentration of CHB and EG, $g/kg$ |
| $C_{E_{2B}}$ | Bound concentration of $\beta$-glucosidase, $g/kg$ |
| $C_{E_{1F}}$ | Free enzyme concentration of CHB and EG in solution, $g/kg$ |
| $C_{E_{2F}}$ | Free enzyme concentration of $\beta$-glucosidase in solution, $g/kg$ |
| $C_{Et_G}$ | Ethanol concentration from glucose fermentation, $g/kg$ |
| $C_{Et_{Xy}}$ | Ethanol concentration from xylose fermentation, $g/kg$ |
| $C_{Et_{Xy}}$ | Ethanol concentration, $g/kg$ |
| $C_G$ | Glucose concentration, $g/kg$ |
| $C_{G_2}$ | Cellobiose concentration, $g/kg$ |
| $C_{Xy}$ | Xylose concentration, $g/kg$ |
| $C_{Xn}$ | Xylan concentration, $g/kg$ |
| $C_{Gn}$ | Glucan (cellulose) concentration, $g/kg$ |
| $C_{OC}$ | Other compounds concentration, $g/kg$ |
| $C_{X_G}$ | Cell dry weight in glucose fermentation, $g/L$ |
| $C_{X_{Xy}}$ | Cell dry weight in xylose fermentation, $g/L$ |
| $E_a$ | Activation energy = -5540 $cal/mol$ |
| $E_{1\max}$ | Maximum mass of enzyme 1 that can be adsorbed onto a unit mass of substrate, 0.06 $g\ protein/g\ substrate$. |
| $E_{2\max}$ | Maximum mass of enzyme 2 that can be adsorbed onto a unit mass of substrate, 0.01 $g\ protein/g\ substrate$. |
| $Et_{\max,G}$ | Ethanol concentration above which cells do not grow in glucose fermentation, $95.40\ for\ \mathrm{Et} \le 95.4\ g/L$, $129.90\ for\ 95.4 < Et \le 129.9\ g/L$ |
| $Et_{\max,Xy}$ | Ethanol concentration above which cells do not grow in xylose fermentation = 59.040 $g/L$. |
| $Et'_{\max,G}$ | Ethanol concentration above which cells do not produce ethanol in glucose fermentation, $103\ for\ \mathrm{Et} \le 103\ g/L$, $136.40\ for\ 103 < Et \le 136.4\ g/L$ |
| $Et'_{\max,Xy}$ | Ethanol concentration above which cells do not produce ethanol in xylose fermentation = 60.20 $g/L$ |
| $K_{1ad}$ | Dissociation constant for enzyme 1 = 0.4 $g\ protein/g\ substrate$ |
| $K_{2ad}$ | Dissociation constant for enzyme 2 = 0.1 $g\ protein/g\ substrate$ |
| $k_{1,G}^{EH}$ | Reaction rate constant for glucose 1 in the enzymatic hydrolysis = 7.18 $g/mg \cdot h$ |
| $k_{2,G}^{EH}$ | Reaction rate constant for glucose 1 in the enzymatic hydrolysis = 285.5 $h^{-1}$ |
| $k_{G2}^{EH}$ | Reaction rate constant for cellobiose in the enzymatic hydrolysis = 22.3 $g/mg \cdot h$ |

| | |
|---|---|
| $K_{1IEt}^{EH}$ | Inhibition constant for ethanol 1 in the SSCF unit = 0.15 $g/kg$ |
| $K_{1IG}^{EH}$ | Inhibition constant for glucose 1 = 0.1 $g/kg$ |
| $K_{2IG}^{EH}$ | Inhibition constant for glucose 2 = 0.04 $g/kg$ |
| $K_{3IG}^{EH}$ | Inhibition constant for glucose 3 = 3.9 $g/kg$ |
| $K_{1IG2}^{EH}$ | Inhibition constant for cellobiose 1 = 0.015 $g/kg$ |
| $K_{2IG2}^{EH}$ | Inhibition constant for cellobiose 2 = 132.0 $g/kg$ |
| $K_{1IXy}^{EH}$ | Inhibition constant for xylose 1 = 0.1 $g/kg$ |
| $K_{2IXy}^{EH}$ | Inhibition constant for xylose 2 = 0.2 $g/kg$ |
| $K_{3IXy}^{EH}$ | Inhibition constant for xylose 3 = 201.0 $g/kg$ |
| $K_M$ | Substrate (cellobiose) saturation constant = 24.3 $g/kg$ |
| $K_{1G}^{CF}$ | Monod constant, for growth on glucose = 0.565 $g/L$ |
| $K_{2Xy}^{CF}$ | Monod constant, for growth on xylose =3.4 $g/L$ |
| $K'^{CF}_{5IG}$ | Inhibition constant, for product formation from glucose = 4890.0 $g/L$ |
| $K'^{CF}_{6IXy}$ | Inhibition constant, for product formation from xylose = 81.30 $g/L$ |
| $K'^{CF}_{5G}$ | Monod constant, for product formation from glucose = 1.342 $g/L$ |
| $K'^{CF}_{6Xy}$ | Monod constant, for product formation from xylose = 3.4 $g/L$ |
| $K_{1X_GIG}^{CF}$ | Inhibition constant, for growth on glucose = 283.7 $g/L$ |
| $K_{2IXy}^{CF}$ | Inhibition constant, for growth on xylose = 18.1 $g/L$ |
| $k_{1,A}^{PT}$ | Reaction rate constant for arabinose formation in the pretreatment = $0.0021\,h^{-1}$ |
| $k_{2,A}^{PT}$ | Reaction rate constant for arabinose degradation in the pretreatment = $0.0064\,h^{-1}$ |
| $k_{2,ASL}^{PT}$ | Reaction rate constant for acid-soluble lignin degradation in the pretreatment = $0.0021\,h^{-1}$ |
| $k_{3,ASL}^{PT}$ | Reaction rate constant for other compounds degradation in acid-soluble lignin reaction for the pretreatment = $3.6767\times10^{-4}\ h^{-1}$ |
| $k_{1,G}^{PT}$ | Reaction rate constant for glucose formation in the pretreatment = $9.6291\times10^{-4}\ h^{-1}$ |
| $k_{2,G}^{PT}$ | Reaction rate constant for glucose degradation in the pretreatment = $8.6451\times10^{-4}\ h^{-1}$ |
| $k_{1,Xy}^{PT}$ | Reaction rate constant for xylose formation in the pretreatment = $0.0056\,h^{-1}$ |
| $k_{2,Xy}^{PT}$ | Reaction rate constant for xylose degradation in the pretreatment = $0.0192\,h^{-1}$ |
| $k_{1,ASL}^{PT}$ | Reaction rate constant for acid-soluble lignin formation in the pretreatment = $6.1345\times10^{-5}\ h^{-1}$ |
| $m_G$ | Maintenance coefficient in glucose fermentation = 0.097 $h^{-1}$ |
| $m_{Xy}$ | Maintenance coefficient in xylose fermentation =0.067 $h^{-1}$ |
| $r_{i,j}$ | Reaction rate of compound $i$ for the different unit operations, $g/kg\cdot h$ = $g/L\cdot h$, $\rho_{mixture}=1\ kg/L$ |

| | |
|---|---|
| $r_{X,TOT}$ | Total reaction rate for the biomass, $g/L\cdot h$ |
| $r_{Et,TOT}$ | Total reaction rate for ethanol, $g/L\cdot h$ |
| $R$ | Universal gas constant, 1.9872 $cal/mol\cdot K$ |
| $R_{Gn}$ | Substrate reactivity |
| $T$ | Temperature, $K$ |
| $V$ | Reaction volume, $kg-slurry$ |
| $x_i$ | Mass fraction of glucose or xylose in the glucose and xylose mixture = $C_G/C_G+C_{Xy}$ and $C_{Xy}/C_G+C_{Xy}$ , respectively. |
| $Y_{Et_G/G}$ | Product yield constant (g-ethanol/g-glucose) = 0.470 $g/g$ |
| $Y_{Et_{Xy}/Xy}$ | Product yield constant (g-ethanol/g-xylose) = 0.400 $g/g$ |
| $Y_{X_G/G}$ | Cell yield constant from glucose (g-cells/g-substrate) =0.115 $g/g$ |
| $Y_{X_{Xy}/Xy}$ | Cell yield constant from xylose (g-cells/g-substrate) =0.162 $g/g$ |

Greek letters

| | |
|---|---|
| $\alpha$ | Constant relating substrate reactivity with degree of hydrolysis, 1. |
| $\beta_G$ | constants in product inhibition model in glucose fermentation $1.29\ for\ \mathrm{Et}\le 95.4\,g/L,\ 0.25\ for\ 95.4<Et\le 129.9\,g/L$ |
| $\beta_{Xy}$ | Constant in the product inhibition model in xylose fermentation = 1.036 $g/L$ |
| $\gamma^G$ | Maximum specific rate of glucose formation $1.42\ for\ \mathrm{Et}\le 95.4\ g/L,$ |
| $\gamma^{Xy}$ | Maximum specific rate of xylose formation = 0.608 $g/L$ |
| $\phi$ | Fraction ratio of solid material to liquid in the pretreatment. |
| $\mu_{\max,G}$ | Maximum specific growth rate in glucose fermentation = 0.662 $h^{-1}$ |
| $\mu_{\max,Xy}$ | Maximum specific growth rate in xylose fermentation = 0.190 $h^{-1}$ |
| $v_{\max,G}$ | Maximum specific rate of glucose formation = 2.005 $h^{-1}$ |
| $v_{\max,Xy}$ | Maximum specific rate of xylose formation = 0.250 $h^{-1}$ |

## References


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