Use of LCA tools in the early stages of a research project - A case study about an innovative process for cellulose nanocrystals extraction

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Birth of a new unit at Materia Nova

Justification of environmental added value asked to obtain grants for a new project

Many projects meant to have environmental dimension (biobased plastics, biotechnologies, solar cells...)

High interest in making a priori and a posteriori environmental impact studies for our projects

Creation of a new environmental impact unit
Cellulose nanocrystals extraction

Cellulose Fiber → Cellulose Nanocrystals

- **H$_2$SO$_4$**
- **Heating**
- **Centrifugation**
- **Dialysis**

**Steps:**
1. **H$_2$SO$_4$** treatment
2. Heating
3. Centrifugation
4. Dialysis

**Materials:**
- Cellulose
- Cellulose Nanocrystals

**Techniques:**
- Microfibril
- Fiber
Cellulose nanocrystals extraction

**Cellulose nanocrystals:**

- High Young’s Modulus (=steel)
- Interesting shape/aspect ratio (needle like)
- Extracted from biomass (potentially from local biomass)

**Green nanoparticles**

High consumption of acid and water

**Process not so green**
Cellulose nanocrystals extraction

Ionic Liquids are presented as green solvents of cellulose:

- Recyclability
- Low VOC emissions
- Good solvation of lignocellulose

- Reuse of reagent
- Low amount of sulfuric acid
- Decrease of water consumption during purification
Background of the study

- Environmental cost of IL production?
  
  Currently not industrial scale product

- How much recycling to improve our process?
  
  How many cycles needed for environmental benefit?

  How many possible to keep a good extraction?

  The success of nanocrystals extraction at bench will not directly provide information about the greenness of the process

  First bench results coupled with Simple LCA can help to pinpoint critical points
Background of the study

Evaluation of the “greenness” potential of the study

Simultaneous kick-off as first lab experiments

→ Identification of hotspots
Comparison needs data for **same scale of production**

**Virtual upscaling** of the new process (industrial scale)

Need to **recover** values of s-o-a process

No data on detailed or described industrial process

Comparison of **lab scale** processes s-o-a and experimental data

**NEW STRATEGY**
Highly simplified hypotheses

Identical yields and raw materials → fibers out of system boundaries

Same nanocrystal quality → FU = treatment for 1 kg of CNC

Same energetic input → not taken into account

No intrinsic impact of BMIM Recycling → modeled by input division

No effluent treatment → treated as emission to water
# Data collection / choice of the method

<table>
<thead>
<tr>
<th>Description</th>
<th>Details</th>
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</thead>
<tbody>
<tr>
<td>LCA literature negligible about IL or CNC, non existent for the combination</td>
<td></td>
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<tr>
<td>No IL in the DB, neither as process nor as substance</td>
<td></td>
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<tr>
<td>1 publication about LCA of [BMIM]Cl production</td>
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<tr>
<td>DB : no waste water treatment for a comparable process</td>
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<tr>
<td>Emissions : Choice of a proxy based on toxicology literature (phenol)</td>
<td></td>
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<tr>
<td>Material inputs: firsts lab tests estimation</td>
<td></td>
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<tr>
<td>Calculation method:</td>
<td>- including phenol and $\text{H}_2\text{SO}_4$ emissions</td>
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<tr>
<td></td>
<td>- including a “water depletion” category</td>
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<td></td>
<td>→ restricted choice: ILCD 2011 Midpoint</td>
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</tbody>
</table>
BMIM-CI modelisation

From literature, Righi 2011

Single score, Eco-indicator
Impacts of the different processes

ILCD calculation
Major impact contributors for « BMIM » process
Optimisation way of BMIM process

IL recycling optimization

ILCD calculation
Optimisation way of BMIM process

BMIM-Cl synthesis optimization (yield)

48% → 90%

ILCD calculation
Conclusions

First results
- environmental benefit is not automatic

Numerous ways of improvement:
- IL recycling (> 20 cycles in some publications)
- “greener” production of [BMIM]Cl (or other ILs) ?
  (not matured production, scale effect, biosourcing…)
- Yield and quality of CNC ? → FU modification ?
  (theoretical better thermal resistance)

Necessity to refine the model:
- treatment/ recycling of the acid
- intrinsic impact of recycling of ionic liquid (if cycles nb increased)

Scientific contribution of the project is not in balance with LCA
Thanks for your attention

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