BAYESIAN BELIEF NETWORK TO PREDICT NANOMATERIAL RELEASE

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FUTURE NANONEEDS (FNN): WP3 EXPOSURE

- Develop a **methodology to forecast environmental releases and emissions** of next-generation nanomaterials (NM) into relevant compartments and in different life cycle stages (LC).

**Tier 1**
- Expected emissions of NM of each life cycle stage using Life Cycle Inventories (LCI) and EUSES
- Identify **focal points** in the life cycle where main release, emission and/or exposure is expected

**Tier 2**
- Directed at a Tier 1 **focal point**: focus on a specific activity or process.
- Identify most significant parameters of release mechanisms, their causal relationships and strengths
- Develop Bayesian network to predict release for future systems
SCOPE WP3

- Nano-enabled products are on the market, the market *share of future applications will increase*. 
- Nanomaterial (NM) flow analysis showed that the end-of-life, especially recycling, of these products is a potential ‘hotspot’ of release/exposure. 
- Shredding is a common process in recycling, however, *data* on the release of nanomaterials during shredding is *very sparse* 
- This poses a forthcoming problem for recycling plants.
FNN VALUE CHAINS

Bayesian Belief Network to predict nanomaterial release

WeEE

Shredded material
→ Assuming most casings, housing, etc are dismantled prior to shredding

Consideration:
Feasibility of combining all these materials in one scenario – considering different shredder designs and size/shape of materials
PEROVSKITES IN PHOTOVOLTAIC PANELS

Tier 1

- Assumption
- OECD, 2004
- CEPE/spERC
- WEEE directive
- spERC
- Other

Spin-coating of perovskite: 59.0% → 1000

1 ton perovskite in solar panels

End of Life

Recycling of perovskite solar panels: 100.0%

Incineration

Landfill

Bayesian Belief Network to predict nanomaterial release
GOAL OF BAYESIAN BELIEF NETWORK

- Predict the **release** of next generation nanomaterials in future and less known applications during end-of-life, specifically shredding, by establishing a Bayesian Belief Network (BBN).

- BBNs have multiple advantages:
  - they provide a coherent framework for making a priori assumptions about **unknowns**
  - present the formal rules to update that knowledge
  - explicitly model the **uncertainty** in the BBN’s release forecasts.

1. Quantify what you already know
2. Construct a relational model for this knowledge
3. Apply Bayes’ rule and predict future situations

**Release** is the liberation of nanomaterial during a natural or technical process at any given LC stage.
PROCESS

1. ‘Hot spots’ or **focal points** analysis for a value chain based on substance flow analysis
2. Expert elicitation to establish relation between nanomaterial release and system parameters:
   a) Activity (shredder) properties
   b) Composite/materials properties
3. Draw relational model of these ‘beliefs’
4. 2\textsuperscript{nd} elicitation round to refine the model
5. Dedicated expert workshop to quantify the relations
6. Followed by telecons to refine model
BELIEFS NETWORK

Bayesian Belief Network to predict nanomaterial release
RESULTS: PRIOR PROBABILITIES

- Experts assessed the likelihood of a nanoparticle being on the surfaces created by shredding.
- They took into account the dispersion state (four classes) and the concentration of nanomaterials in the product’s materials.

For well dispersed NMs and <1% concentration, 90% probability for less than 1% NM on surface.

For layers of NMs and >10% concentration, 61% probability for 10-50% NM on surface.

<table>
<thead>
<tr>
<th>Dispersion_state</th>
<th>Well dispersed</th>
<th>Moderate dispersed</th>
<th>Fully agglomerated</th>
<th>Layered</th>
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</thead>
<tbody>
<tr>
<td>Particles_nano_in_composite</td>
<td>&lt;1 %</td>
<td>1-10 %</td>
<td>&gt;10 %</td>
<td>&lt;1 %</td>
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<tr>
<td>&lt;1%</td>
<td>90.0</td>
<td>16.3</td>
<td>2.3</td>
<td>82.0</td>
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<tr>
<td>1-10%</td>
<td>8.0</td>
<td>73.8</td>
<td>15.3</td>
<td>14.5</td>
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<tr>
<td>10-50%</td>
<td>2.0</td>
<td>9.5</td>
<td>65.0</td>
<td>3.0</td>
</tr>
<tr>
<td>&gt;50%</td>
<td>0.0</td>
<td>0.5</td>
<td>17.5</td>
<td>0.5</td>
</tr>
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</table>
CONCLUSIONS & RECOMMENDATIONS

- BBN acted as a way to understand what drives the release of NM during shredding of WEEE
- The construction of a BBN requires an investment in time
- A BBN expert/facilitator is required to elicit information from experts with different backgrounds
- Multiple expert sessions, and specifically physical meetings, were needed
- The BBN can be adapted for comminution activities like milling or crushing

- The model will be tested using experimental data *(Do you have data available for us?)*

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THANKS TO ALL ‘BELIEVERS’

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<thead>
<tr>
<th>Name</th>
<th>From</th>
<th>Contribution as</th>
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<tbody>
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THANK YOU FOR YOUR ATTENTION

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It is proposed to consider the fraction of NM that is captured or forms residue in the process and ventilation systems (which may enter the WIP, recycling, etc.), which determines the effectiveness of Risk Management Measures (RMM) and resulting emissions.
BAYESIAN BELIEF NETWORK

- Probabilistic graphical model
  - Directed Acyclic Graph & causal network
  - Nodes represent random variables
  - Edges represent conditional dependency (strength of relations)

- Represent knowledge about an uncertain domain
  - Considered to reflect our degree of belief whether an event will occur
  - Uses knowledge of the past / expert opinions (priors)
  - Recognizes the need to update knowledge in light of observations

Bayesian Belief Network to predict nanomaterial release
- Quantify what you know before getting data:
  \[ P(X) \quad \text{("prior")} \]
- Build a model for your data
  \[ P(Y \mid X) \quad \text{("model")} \]
- Apply Bayes’ rule
  \[ P(X \mid Y) = \frac{P(Y \mid X)P(X)}{P(Y)} \quad \text{("posterior")} \]