A Systematic Methodology for Design of Emulsion Based Chemical Products

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1. CHEMICAL PRODUCT DESIGN AND EMULSIONS

- Chemical product design aims to find a product exhibiting a set of desirable or specified behavior
- Chemical industry is shifting from commodities towards higher value added products
- Higher value added products gain their value from a molecular or micro-structure
- Emulsions are largely used as commercial products: food, cosmetic, household and health-care industries
- Surfactant and emulsion properties may require dedicated models

2. A SYSTEMATIC METHODOLOGY

<table>
<thead>
<tr>
<th>Step</th>
<th>Input</th>
<th>Performed Action</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>Step 1</td>
<td>Information about the product</td>
<td>Understanding of needs, translation into target properties in terms of constraints to match</td>
<td>List of main needs, secondary needs and target properties with boundaries</td>
</tr>
<tr>
<td>Step 2</td>
<td>List of main needs</td>
<td>Find chemicals suitable as active ingredient(s), select the most advantageous and search/calculate main properties</td>
<td>Candidate active ingredient with its main properties</td>
</tr>
<tr>
<td>Step 3</td>
<td>Candidate active ingredient with its main properties</td>
<td>Find chemicals suitable as dispersed phase solvents, select the most advantageous and search/calculate main properties</td>
<td>Candidate dispersed phase solvent with its main properties</td>
</tr>
<tr>
<td>Step 4</td>
<td>Candidate active ingredient and dispersed phase solvent with their main properties</td>
<td>Find chemicals suitable as continuous phase solvents, select the most advantageous and search/calculate main properties</td>
<td>Candidate continuous phase solvent with its main properties</td>
</tr>
<tr>
<td>Step 5</td>
<td>Candidate active ingredient dispersed and continuous phase solvents with their main properties</td>
<td>Find chemicals suitable as emulsifiers, select the most advantageous and search/calculate main properties</td>
<td>Candidate emulsifier with its main properties</td>
</tr>
<tr>
<td>Step 6</td>
<td>List of secondary needs, candidate dispersed and continuous phase solvents with their main properties</td>
<td>Find chemicals suitable as additives, select the most advantageous and search/calculate main properties</td>
<td>Candidate additives with its main properties</td>
</tr>
<tr>
<td>Step 7</td>
<td>List of constraints on target properties, all ingredients</td>
<td>Find overall composition of selected ingredients</td>
<td>Product to be experimentally verified (Stage-2)</td>
</tr>
</tbody>
</table>

3. SELECTION CRITERIA

- Constraints
  - Low toxicity → Lethal concentration: LC₅₀ > 3.16
  - Safety → Flash point: FP > 60°C
  - Legislation → Some chemicals are not allowed
  - Critical temperatures → Melting point, boiling point, peculiar critical temperatures of surfactants
  - Stability → Surfactant above critical micelle concentration
- Selection criteria
  - Optimize the effectiveness (it differs ingredient by ingredient and it is estimated mainly with knowledge base)
  - Minimize the cost

4. SURFACTANT PROPERTY MODELING

- Critical micelle concentration (158 data)
  - Non-ionic surfactants, T = 25°C
  - M&G GC⁺ method: \( f(X) = \sum_i N_i C_i + w \sum_j M_j D_j + z \sum_k O_k E_k \)
  - \( R^2 = 0.99 \)

5. A CONCEPTUAL CASE STUDY

- UV sunscreen, emulsified form
- Proposed formulation to be experimentally validated

<table>
<thead>
<tr>
<th>Ingredient</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Avobenzone</td>
<td>0.99%</td>
</tr>
<tr>
<td>Octyl Salicylate</td>
<td>1.22%</td>
</tr>
<tr>
<td>Zinc Oxide</td>
<td>8.56%</td>
</tr>
<tr>
<td>Butyl Acetate</td>
<td>32.4%</td>
</tr>
<tr>
<td>Water</td>
<td>54.9%</td>
</tr>
<tr>
<td>Octyl Esaethylene Oxide</td>
<td>0.09%</td>
</tr>
<tr>
<td>α-Tocopherol</td>
<td>0.34%</td>
</tr>
<tr>
<td>Heptylparaben</td>
<td>0.59%</td>
</tr>
<tr>
<td>laevo-Menthol</td>
<td>0.91%</td>
</tr>
</tbody>
</table>

6. CONCLUSIONS

- A systematic methodology for design of emulsion-based products has been developed
- Its application has been illustrated through the conceptual case study of an emulsified UV sunscreen
- The development of dedicated models for pure compound (surfactant) as well as mixture (emulsion) properties is fundamental
- A second stage, model-experiment based further refinement and/or validation has been considered and needs to be developed
- The work-flow will be implemented into a software to allow virtual product design