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Ecotoxicity of Selected Solvents: A Comparative Study between Conventional and Non-Conventional Candidates

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Abstract
Solvent extraction is a common chemical process in which a compound is exploited to extract the undesired substances from a feed stream. One of the main drawbacks of industrial solvents is that they pose short and long term environmental impacts due to their high toxicity and persistent in the ecosystem once released. In this study, aquatic toxicity data for two common industrial solvents as well as two ionic liquids, as non-conventional solvents, were collected and compared. The results undermine the importance of the selection of solvents not only based on their toxicity data but also based on their physical properties.

Keywords: Solvent, Toxicity, Aquatic organisms, ionic liquids

1. Introduction
Solvent extraction is one of the widely-used chemical processes in which compounds will be withdrawn from a feed stream by means of a chemical solvent whose solubility is high towards the component of interest, but not towards other compounds in the solution. As an example, in oil refineries, heavy aromatic compounds must be extracted from the oil to improve the quality of final products. Daily, a large amount of solvent from all different categories are being used in industrial plants worldwide, pointing towards the need for paying attention to the adverse environmental impacts these compounds can carry with themselves.

One of the issues with industrial solvents comes from their incomplete recycling and regenerating after each cycle of use, increasing the chance of their release into the aquatic environment such as freshwater bodies. Furfural and Sulfolane are two widely used organic solvents, being well-known for their high selectivity towards aromatic compounds. These solvents are mostly used in aromatic-aliphatic separation processes since their solubility towards aliphatic hydrocarbons is not as high, so they almost selectively dissolve only aromatic compounds.

Relatively higher boiling points of these solvents, compared to that of more volatile solvents such as acetone, makes their regeneration process through distillation quite
challenging. Both compounds are -to some extent- soluble in water making their existence in water bodies more likely.

On the other side, two ionic liquids with high solubility towards aromatic compounds, due to the high polarity of these compounds, were selected. Ionic liquids are complex organic salts, usually in liquid state, which can be customized to have good solvent properties. Ionic liquids with low melting point and acceptable viscosity can be good candidates for liquid-liquid extraction processes.21-23

2. Methods
To study the environmental impacts arising from the use of industrial solvents, two common solvents, namely Sulfolane and Furfural, and two non-conventional compounds, n-butylpyridinium chloride, [BPy] Cl, and 1-butyl-3-methylimidazolium tetrafluoroborate, [Bmim] BF₄ ionic liquids were studied for their impacts on aquatic organisms. Aquatic toxicity data as well as bioaccumulation factor, BCF, were used as indices to compare the greenness of these compounds. BCF factor shows the extent to which a chemical gets into the body of living organisms in water, biota, especially on fish.

3. Results and discussions
The important physical properties of solvents affecting their long-term environmental impacts are listed in Table 1.

<table>
<thead>
<tr>
<th>Solvents</th>
<th>Boiling Point (°C)</th>
<th>Vapor Pressure @ 25°C [kPa]</th>
<th>Water solubility @ 25°C [g/l]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Furfural</td>
<td>162</td>
<td>0.3</td>
<td>83</td>
</tr>
<tr>
<td>Sulfolane</td>
<td>285</td>
<td>Negligible</td>
<td>Miscible</td>
</tr>
<tr>
<td>[BPy] Cl</td>
<td>&gt;400</td>
<td>Negligible</td>
<td>43.2</td>
</tr>
<tr>
<td>[Bmim] BF₄</td>
<td>&gt;400</td>
<td>Negligible</td>
<td>Miscible</td>
</tr>
</tbody>
</table>

As it can be observed from Table 1, all the solvents selected, have high boiling points and negligible vapor pressures, lowering the risk of air pollution, significantly.

To study the impacts of solvents in this study, their toxicity data towards aquatic organisms, namely fish, Daphnia Magna and a green algae (PKS) were collected from the literature as listed in Table 2.21, 24-27
It can be seen from Table 2 that ionic liquids can be more toxic than their organic counterparts, as [BPy] Cl in this study is considerably more toxic towards Daphnia Magna compared to sulfolane. However, much lower values for the bioaccumulation factor, BCF, of ionic liquids point towards this fact that their exposure to biota can be significantly lower than organic solvents making them better candidates for this purposes. Studies show that the solvent power of ionic liquids which good solvent properties, are very much comparable to that of conventional solvents meaning that, approximately, same amount of solvent would be needed to accomplish an extraction task.

4. Conclusions:

- Ionic liquids are not always greener than their organic solvents counterparts when they are compared to one another based on same application.
- Large size of cations and anions in ionic liquids is probably the reason of them not diffusing into the bodies of freshwater organisms, making their bioaccumulation factors meaningfully small.
- Ionic liquids are less likely to pose a risk to fish population since although their high toxicity values, their exposure can be negligible.

References:


