

Education in the Principles of Green Engineering. “How to Choose a Safer Solvent”

Lourdes Calvo^{1*}, Albertina Cabañas²

*lcalvo@ucm.es

¹ Universidad Complutense de Madrid, Departamento de Ingeniería Química y de Materiales

² Universidad Complutense de Madrid, Departamento de Química Física
Facultad de Ciencias Químicas, Avda. Complutense s/n, Madrid, 28040 España

Keywords: Education; Green engineering; Metrics; Solvent selection; Life Cycle Analysis

Abstract

In the subject of Separation Operations, a compulsory subject in the 3rd year of the Chemical Engineering degree, within the chapter of Extraction, we have introduced a seminar on safer solvents. It is devoted to the selection of solvents using the criteria: higher extraction yield/selectivity and lower environmental impact. This latter aspect is based on the criteria adopted by the best guides published mainly in the pharmaceutical sector, such as GSK or ACS. We also use the concept of **Life Cycle Assessment (LCA)**. In the context of solvents, the cradle-to-grave LCA must include raw material and energy requirements for manufacturing, generated emissions and waste, transport, and final disposal (as represented in Figure 1). Besides, we present the concept of **bio-solvents** as opposed to petrochemical derivatives; and of **neoteric solvents** (ionic liquids, deep eutectic solvents and supercritical fluids) as alternatives to common organic diluents.

For the selection of a solvent, we use the concept of “**Like dissolves like**”, with several examples. This implies that the solvent must reduce the activity coefficients of the solute. One way to evaluate this is based on group interaction criteria. Alternatively, Hansen Solubility Parameters, HSP, are a practical way to understand issues of solubility. A good solvent for a specific compound can be well characterised by three parameters: δ_D for Dispersion (van der Waals), δ_P for Polarity (related to dipole moment) and δ_H for hydrogen bonding.

On a concrete example of traditional extraction, we propose several solvents. Students must choose the two or three best ones according to the partition constants and selectivity, to maximize yield, minimize solvent consumption and reduce the downstream processing of the extract. They must then apply health, safety (consulting the safety data sheet, SDS) and environmental impact criteria (with the help of the above-mentioned guides) to choose the best one. A very relevant aspect is its recovery, as it is normally done by distillation. This operation is expensive and energy-consuming, so the students must consult the boiling point of the solvents in relation to the boiling point of the extract. Lastly, they must consult the market price and availability for the final discussion.

In this way, students become aware of the complexity of choosing a good solvent, as green as possible to make a chemical process economically viable. It is difficult but it is its obligation as future chemical engineers.

This seminar is part of a workplan of our group (<https://www.ucm.es/leffs/>) to promote **Sustainable Chemistry and Chemical Engineering** in formation. We aim at introducing **green concepts** in several subjects and in training workshops for Undergraduate, Master and PhD students.

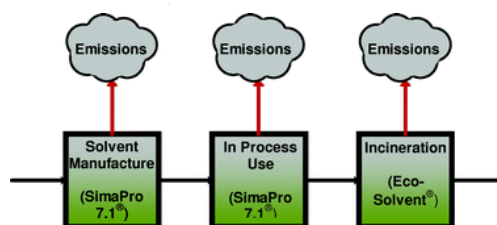


Figure 1. Outline of the Life Cycle Analysis of a solvent (Green Chemistry, RCS publishing)

Acknowledgements. UCM Innovation Project, n° 172, Training in Sustainable Chemistry and its relationship with the Sustainable Development Goals.