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SUSSOL - Sustainable Solvents Selection and Substitution Software

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PURPOSE OF THE ABSTRACT

Solvents are used in many industrial applications, e.g. paints and coatings, cleaning agents and chemical reactions. Traditional solvents are often toxic, volatile, highly flammable, non-biodegradable and non-renewable. Substitution of a traditional non-aqueous solvent with a ?green' solvent is a time-consuming process. Moreover, it requires knowledge about the chemical and physical properties of the said solvents. Existing selection/substitution tools and models focus mainly on the SHE (Safety, Health & Environment) aspects of solvents, without taking into account the physicochemical properties. However, these physicochemical properties determine whether a given solvent is appropriate for a particular application [1].
In addition, the selection of solvents in the past was based all too often on ?trial and error', in which the choice for a particular solvent was primarily determined by the experience of the person making the selection. Chemists often do not look beyond the solvents that they already have used, or solvents which are readily available (the solvents present in the lab storage) [1].

Solvent substitution/selection software has been developed to facilitate the process of solvent selection. Using machine learning algorithms [2], the software accommodates the search for the best performing and most sustainable solvent for a specific industrial application. Three industrial case studies were used to validate the software. The cases concerned the selection of solvents for a coating formulation, industrial cleaning agents and a contact adhesive respectively. Employing an extensive dataset of physicochemical data, cluster analyses were performed to select a series of promising solvents for each application. Based on the CHEM21 approach [3], a simplified greenness evaluation was executed, resulting in a shortlist of sustainable solvents for each application. Screening experiments were performed to assess the best performing solvent. A successful validation was obtained for the described application, since for all three case studies a sustainable alternative was found.

FIGURES

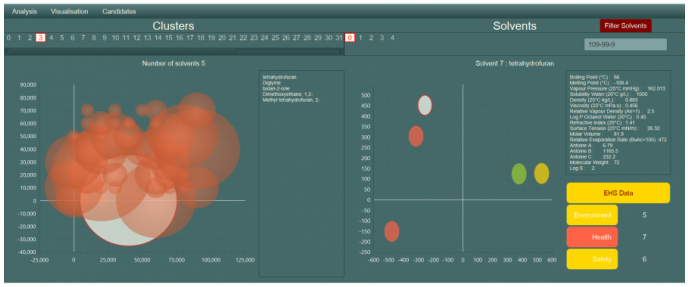

FIGURE 1
SUSSOL application
Clustering screen

FIGURE 2

KEYWORDS
solvent selection | machine learning | neural network | sustainable solvents

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