

SUSSOL – Using AI for the selection and substitution of greener solvent

Solvents can be toxic, volatile, highly flammable, non-biodegradable and non-renewable. Searching for a suitable green alternative for a nonbenign solvent can be an onerous task. Hannes Sels, Herwig De Smet and Dr Jeroen Geuens from Karel de Grote University of Applied Sciences and Arts, in close collaboration with their industrial partners, have developed a user-friendly software tool based on an AI algorithm, called SUSSOL (Sustainable Solvents Selection and Substitution Software). This tool enables a more efficient, objective and purposeful selection of the best-performing and most sustainable solvents for specific industrial applications.

A solvent is usually a liquid but can also be in solid or gas form. It is used to dissolve, suspend and extract other materials without chemical change to either the solvent or the other materials. Varied and versatile, solvents are used in the manufacture of a wide range of everyday products, including paint, pharmaceuticals, pesticides, cleaners, and inks. Numerous different solvents are used to meet specific requirements in order to make products with optimal performance attributes, such as inks that don't smudge, cleaning agents that remove grease and dirt effectively, and spray paints that dry quickly, last a long time, and don't clog the spray nozzle.

Traditional solvents can be toxic, volatile, highly flammable, non-biodegradable and non-renewable. Searching for a suitable solvent for a particular application can be difficult. Finding a green alternative for a nonbenign solvent can be even harder. Hannes Sels, Herwig De Smet and Dr Jeroen Geuens, from the Centre of Expertise on Sustainable Chemistry at Karel de Grote University of Applied Sciences and Arts in Antwerp, have developed a user-friendly software tool based on an Artificial Intelligence (AI) algorithm, called SUSSOL (Sustainable Solvents Selection and Substitution Software), that enables a more efficient, objective and purposeful selection of the best performing and most sustainable solvents for specific industrial applications.

CHEMICAL LEGISLATION

The Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH)

European regulation has been adopted to improve the protection of both human health and the environment from risks posed by chemicals. The REACH restriction list includes solvents such as cyclohexane, benzene, toluene, chloroform, and dichloromethane. ChemSec, an independent non-profit organisation, advocates for the substitution of toxic chemicals to safer alternatives and has consequently developed the SIN-list (Substitute It Now-list). Pressure from this legalisation is a main driver in steering industry towards greener alternatives to toxic solvents.

Moreover, the cost of disposing toxic solvents or recycling them can have a significant impact on production costs. Solvents typically contribute 56% of the materials used in the pharmaceutical industry. It is also estimated that solvents contribute 50% of the post-treatment greenhouse gas emissions of pharmaceutical manufacturing. Growing consumer awareness is also impelling manufacturers to look for alternative solvents for their products.

CHOOSING SUSTAINABLE SOLVENT ALTERNATIVES

While the pharmaceutical industry has put great efforts into solvent awareness and the substitution of toxic and hazardous solvents in their manufacturing processes, the researchers point out that the paints and coatings industry is a major user of solvents. Numerous solvent guides already exist; however, the research team believe that a data-driven, automated solvent selection/substitution



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guide would allow users, unfamiliar with the field of solvent selection, to search for greener solvents and thus creating more sustainable products and processes.

A variety of sustainable solvent alternatives are available but finding the most suitable for a particular manufacturing process is often time consuming, labour intensive, and requires specific expert knowledge. SME's (small and medium-sized enterprises) and small formulating companies where chemistry is not the core business may not have the means or knowledge to search for new and more sustainable solvents. A software-aided tool could be of great benefit to those companies that are unaware of the relevant physical solvent properties characterising their products and processes.

SUSSOL

Sels, De Smet and Dr Geuens have used AI to develop a user-friendly software tool named SUSSOL (Sustainable Solvents Selection and Substitution Software), which enables a more efficient, objective, and purposeful selection of solvents. SUSSOL provides support for businesses in their search for sustainable and viable alternatives for the nonbenign solvents they currently use in their products and processes. By providing a flexible tool that companies can use according to their own needs, SUSSOL is bridging the gap between academic research and applicability in industry.

The researchers explain how they consider a solvent selection/substitution tool to be an interactive data-centred catalogue, comprising both conventional and neoteric solvents, that directs the user towards the best possible

alternative. The process is effortless and transparent and offers the user flexibility in that they can use their own dataset, add new solvents, and add company-specific or confidential data. Solvent

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producers and distributors of green and neoteric solvents can also use the tool as a benchmark for the promotion of their solvents as an alternative for conventional nonbenign solvents.

This novel methodology for solvent selection and solvent substitution involves the application of AI software, in the form of Machine Learning algorithms,

to cluster a database of solvents based on their physical properties. An advantage of Machine Learning is its ability to cluster multidimensional data. The Machine Learning engine is given a matrix of solvents and their physical and chemical properties. This forms the training data for a knowledge model and provides a self-learning, extensible application for the future. Once the learning process has been carried out, the model can be queried.

SELECTION AND SUBSTITUTION MODES

The SUSSOL software accepts a solvent dataset in the form of a .csv file. SUSSOL can operate in two modes: the selection mode and the substitution mode. The solvent selection mode involves a Multidimensional Scaling plot of all solvents in the dataset, while the solvent substitution mode forms clusters, or

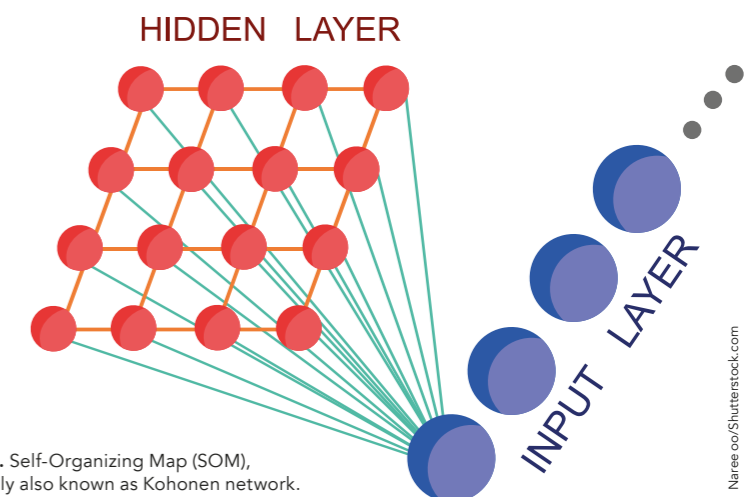
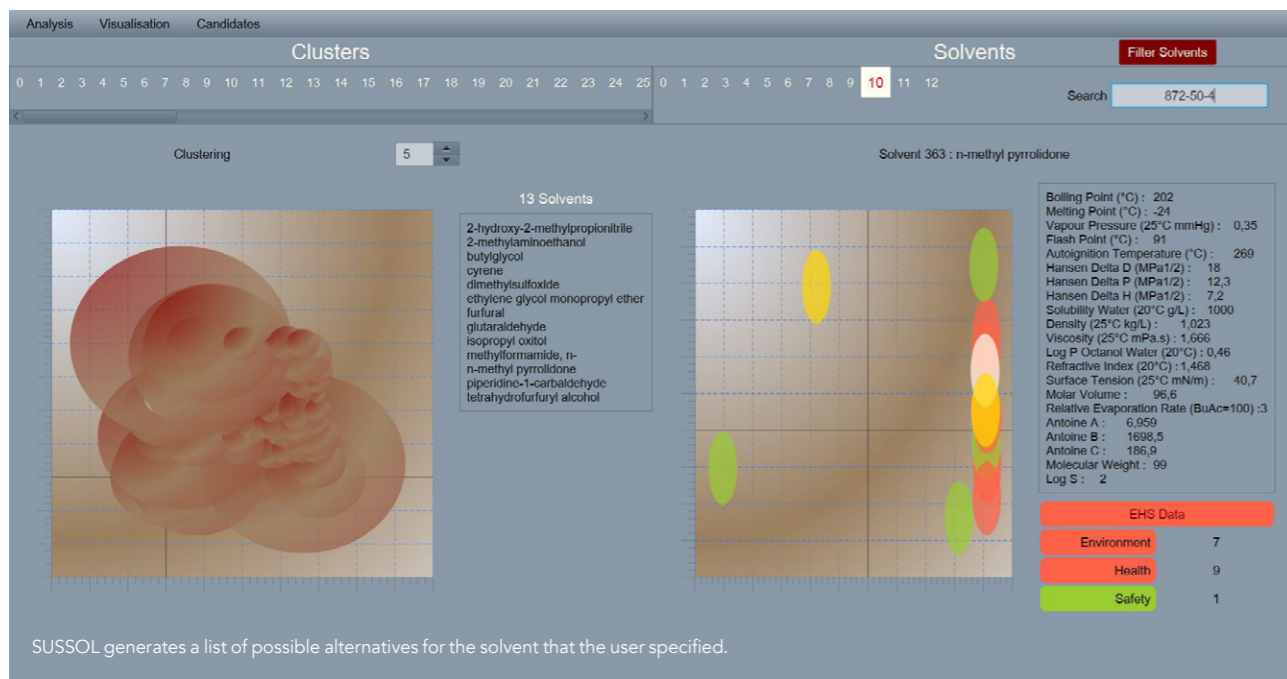


Figure 1. Self-Organizing Map (SOM), commonly also known as Kohonen network.



specific chemical knowledge. The user can specify the solvent they want to replace. Once the cluster analysis has taken place, SUSSOL generates a candidate list of similar solvents. The user can then select the most sustainable candidates and laboratory testing can be initiated.

Multidimensional Scaling is employed to visualise the clustering process. The user then selects a cluster and explores the cluster contents. Each solvent is colour-coded, using the CHEM 21 methodology (CHEM 21 is a European public-private partnership which promotes sustainable biological and chemical methodologies). SUSSOL helps the user explore the solvent space and generates and evaluates a list of possible alternatives for the solvent that the user specified. The alternatives are ranked based on their SH&E (safety, health, and environment) scores.

SOFTWARE VALIDATION

The research team used case studies to demonstrate their SUSSOL approach and establish how it can help in the search for more sustainable and

greener solvents. To validate both the Multidimensional Scaling plot and the clustering approach via the Self-organising Map algorithm, they selected a number of case studies to display a variety of industrial applications.

The researchers demonstrate the use of SUSSOL in finding a greener alternative for cellulose thinners as a cleaning agent for ink in screen printing, for toluene in a contact adhesive and for selecting a greener and more efficient reaction medium for an active pharmaceutical

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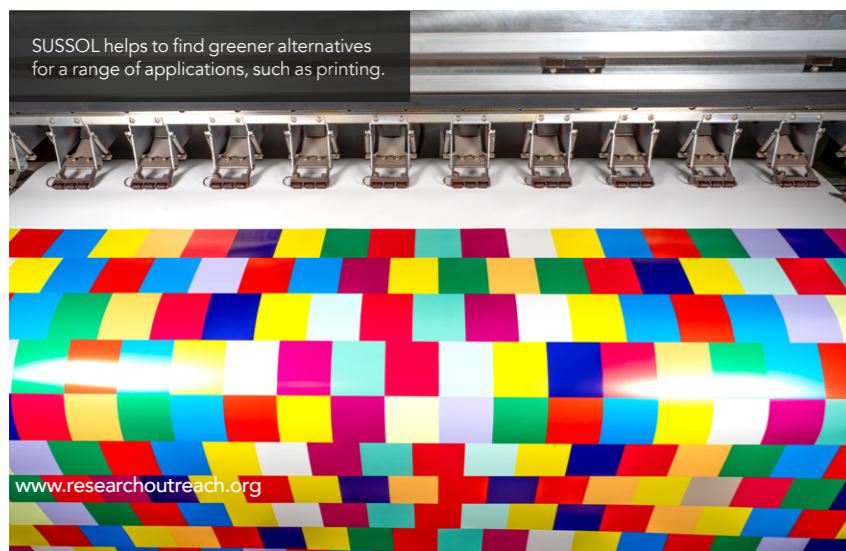
ingredient synthesis. For each case, SUSSOL was employed to generate a shortlist of possible solvents and display the normalised values of a selection of physicochemical properties of each solvents. In all applications, lab tests showed promising results with good

similarities being observed overall. SUSSOL software makes intuitive sense. In the majority of cases, the software confirms the findings in literature, confirming that SUSSOL provides a sound platform for the selection of the most sustainable solvent candidate.

COLLABORATION WITH INDUSTRIAL PARTNERS

SUSSOL was developed in close collaboration with the researchers' industrial partners. This consortium covered the whole value chain

and included solvent producers, distributors, and end-users. After three years of intensive development, testing and statistical validation, the SUSSOL software tool was ready for use. The initial results were promising: SUSSOL has already been utilised to successfully determine suitable alternative solvents for toluene in a contact adhesive, industrial cleaners and a chromatographic application. The collaborating companies, among others Soudal, eco-point, Caldic, Janssen Pharmaceuticals and Boss Paints, have identified sustainable solvents (sometimes as part of a mixture) that meet their specific requests, either for substitution in existing or for use in new applications.



SUSSOL helps to find greener alternatives for a range of applications, such as printing.

Behind the Research



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Research Objectives

The researchers describe a new methodology for solvent selection and substitution by applying Artificial Intelligence software to a database of solvents.

Detail

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Bio

Since 2015, the Centre of Expertise on Sustainable Chemistry works on employing AI models for optimising chemical processes and making them more sustainable. The main goal is to make this technology available for SME's and non-research-intensive companies.

Funding

This research was supported by the Karel de Grote University of Applied Sciences and Arts (KdG) through funding by the Flemish government specifically allocated to practice-based research at universities of applied sciences.

Collaborators

Agfa, Boss paints, Caldic, Chemstream, eco-point, Janssen pharmaceutical companies, mcu coatings, Provion, Q Frame, Soudal

"Surprisingly, SUSSOL can give you suggestions that you would not expect based on common knowledge and experience, but that are certainly functional."

Jacco Quist – Product Manager Eco-Point

"A key feature of SUSSOL is that non-experts can readily get a good idea of likely safer solvents, just from the default smart clustering based on solubility and a few other general characteristics. Yet those who wish to go deeper can refine the clustering according to their specific requirements. I like this balance of simplicity and power."

Prof Steven Abbot – Steven Abbott TCNF Ltd

References

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Personal Response

What initially motivated you to develop SUSSOL?

// As a research group focusing on extraction of natural compounds, we used a lot of solvents such as hexane and THF for extractions and chromatographic applications. We wanted to go greener. At the same time, we saw some companies in our network struggling with solvent-related issues. We realised that often there are greener alternatives available, but it is hard to find the best alternative if you are not a solvent expert. Together with colleagues from the Applied Informatics research group at KdG and a consortium of industrial partners, we started the SUSSOL project. //