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PARIS II: Computer Aided Solvent Design for Pollution Prevention

Background

Chemicals are essential to modern life. However, due to increasing awareness of the potential human health and environmental risks of solvent use, some industrial users may wish to switch to more benign solvents. This can be a difficult task because many parameters of different solvents need to be evaluated before a new solvent or solvent mixture is selected.

Project Overview and Purpose

To support the use of benign solvents, U.S. EPA researchers developed the solvent substitution software tool PARIS II (Program for Assisting the Replacement of Industrial Solvents, version 2.0). PARIS II finds less toxic solvents or solvent mixtures to replace more toxic solvents commonly used by industry. The greener solvents formulated by PARIS II have improved environmental properties, and perform as well as the solvents they replace.

PARIS II is a cost-effective approach to pollution prevention because users do not have to change equipment in order to adopt safer, greener solvents. Designed to be user-friendly, the user need only know what solvents they are using to administer the application.

Some of the industries that could benefit from using PARIS include pharmaceuticals, paints, cleaners, chemical manufacture, plastics, degreasers, electronic component manufacture, and petrochemicals.

Theory and Features

The theoretical basis for the PARIS II program is the observation that the mathematical expressions governing solvent behavior are universal, and that the performance of solvent mixtures may be quantified by a number of coefficients representing various physical and chemical properties (e.g., viscosity, thermal conductivity, activity, etc.). Likewise, the environmental toxicity of solvent mixtures may be quantified by values taken from several different categories of environmental impact (e.g. aquatic toxicity, terrestrial toxicity, acid rain, ozone depletion, etc.).

The replacement process identifies a toxic industrial solvent or solvent mixture to be replaced, calculates its physical and chemical property coefficients, and calculates its total potential environmental impact. Then, the same property coefficients and the total potential environmental impact of various solvent mixtures are calculated.

Within minutes, PARIS II can create a ranked list of replacement solvent mixtures that minimize the difference of coefficients with the original solvent and reduce the total potential environmental impact.

Results and Discussion

PARIS II was used to develop solvent substitutes for pure chemicals and mixtures involving components from a wide range of chemical families, including normal hydrocarbons, ketones, alcohols, aromatics, ethers and organic and aqueous mixtures. In several cases, PARIS II was used to identify substitutes for solvents that appear on the Agency's Resource Conservation and Recovery Act chemicals list.

Case studies demonstrate that PARIS II can suggest replacement solvents with consistently lower potential environmental impact while likely maintaining similar levels of technical performance. Researchers have identified replacement solvents with a fifth or a sixth of the environmental effects of the commonly used solvent.

Future Work

U.S. EPA researchers are working on the next version of this software tool, PARIS III. This next version will have many significant changes, including:
1) a new Graphical User Interface,
2) a new database of solvent properties referenced,
3) and a new search mechanism to find solvent mixture replacements.
The final version of this software will be available for scientists to download and use free of charge, with a beta version of this software available on October 1, 2013.

Collaborators

The development of PARIS II has been implemented by the work of researchers from the following entities:
U.S. EPA Office of Research and Development
Technical University of Denmark
Research Triangle Institute
University of Cincinnati

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Reference

Harten, P.F., and G. Salama, "PARIS II, the Search for Cleaner Solvent Replacements for RCRA Chemicals," *Clean Tech.*, Vol. 4, Number 11, p. 20 (2004).

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