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The software tool to find greener solvent replacements, PARIS III

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Abstract

PARIS III (Program for Assisting the Replacement of Industrial Solvents III, Version 1.4.0) is a pollution prevention solvent substitution software tool used to find mixtures of solvents that are less harmful to the environment than the industrial solvents to be replaced. By searching extensively though hundreds of millions of possible solvent combinations, mixtures that perform the same as the original solvents may be found. Greener solvent substitutes may then be chosen from those mixtures that behave similarly but have less environmental impact. These extensive searches may be enhanced by fine-tuning impact weighting factors to better reflect regional environmental concerns; and by adjusting how close the properties of the replacement must be to those of the original solvent. Optimal replacements can then be compared again and selected for better performance, but less environmental impact. This method can be a very effective way of finding greener replacements for harmful solvents used by industry.

Keywords

green engineering; physicochemical characteristics; pollution prevention; risk assessment

1 INTRODUCTION

Since the industrial revolution, it has been found that the use of chemical mixtures during specific steps of industrial processes improves product development. However, in 1996, an estimated 19 million short tons of volatile organic compounds were emitted in the United States, of which 33% came from solvent utilization.¹ There are different ways industries uses solvents to improve product development. For example, solvents might be used to enhance the chemical reaction of contained solutes; they might be used to enable heat to be transferred to and from reactions; or, solvents might simply be used to clean up after processes. The number of ways solvents might be used to improve product development is only limited by the creativity of researchers and process engineers.

Unfortunately, many of the solvents used in these processes are simply disposed of as waste. For solvents assessed to be harmful to human health and the environment, there is no question of the need to find alternate solutions for their removal. However, even those

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solvents that are assessed to be not as harmful can have devastating effects when they are released as waste in very large quantities. Hence, it is important to understand what can be done to eliminate this harmful industrial solvent waste.

A first step is to identify industrial processes where the solvent waste appears. The U.S. EPA toxic release inventory (TRI) provides a list of the major industries that use and dispose of solvents.² Some of the TRI-Covered industry sectors are: mining; utilities; manufacturing; wholesale electronic markets; publishing; and hazardous waste. The sectors listed are made of specific industries with facilities that use solvents in their processes to enhance development.

Potential solutions to this problem have been explored ever since harmful industrial solvent waste came into existence. Many solutions to specific solvent problems have been presented over the years at numerous chemical conferences, symposiums, and in publications. Some of these solutions can be categorized as: preventing solvent waste by changing the industrial process^{3–5}; recycling the solvent, or atom economy^{6, 7}; designing chemicals at the molecular level that have similar solvent properties, but are not as harmful^{8, 9}; and identifying less harmful solvents and mixtures of solvents from databases of chemicals already available.^{10, 11}

The last category of searching chemical databases for appropriate solvent replacements is not an easy matter. For example, it must be determined which properties are the most important, or what negative impacts are the most significant for all solvents in the databases. Likewise, the metric used to compare one replacement with another must be determined. Obtaining this information is further complicated because different chemical databases may not contain the same level of information or may not contain the same chemicals. For example, information about newly developed solvents generated from biosources may not be contained in many databases. The challenge then is to aggregate these disparate pieces of information and process them collectively.

United States Environmental Protection Agency's (EPA's) first attempt to use chemical databases for solvent replacement, PARIS II, was developed to find replacements for solvents with a database generated by EPA's WAR (Waste Reduction) algorithm.¹² Like the current software, PARIS II used a database search method to find solvent mixtures with similar physical and chemical properties as the solvent to be replaced, but not as harmful to the environment.

EPA has developed the next generation of the software tool, PARIS III, along with advances in the PARIS III database. Like the previous version, the main purpose of this new tool is to find less harmful (i.e., greener) solvent replacements. The replacements have physical and chemical properties as close to the properties of original solvent as possible while still having less impact on the environment.

Unfortunately, the PARIS III software is limited to include only the impact of a solvent's direct release to the environment. It does not perform a full life cycle assessment (LCA) of the total impact of the solvent to the environment. However, there are LCA resources

available in literature and software to help better compare the total impact of using one solvent in a process to another.^{13, 14}

Still, the new search algorithm of PARIS III allows for a much wider selection of replacement mixtures examined in a shorter time. It allows better control of which solvents are included as components in the search, and it allows better control of the fractional proportions considered. Once the search has been performed, a list of most similar solvents and mixtures may be inspected to find the greenest, most functional replacements.

PARIS III gives industry a way of finding solvent mixtures that require very little change to industrial processes yet may greatly reduce harmful impacts to the environment. This solvent substitution software tool can be freely downloaded from EPA's PARIS III website¹⁵ (<https://www.epa.gov/chemical-research/program-assisting-replacement-industrial-solvents-paris-iii>), along with a user manual and tutorial.

2 THEORY

Industrial solvents can be characterized by specific physical and chemical properties that are particularly relevant to the various industrial processes they improve. Solvent mixtures with physical and chemical properties very similar to those properties of the original industrial solvents can improve industrial processes in much the same way. A straightforward solution is to find solvents with very similar properties as the original but generate less harmful waste when released to the environment. Then, the processes improved by the industrial solvents would change very little, but the amount of harmful waste generated and released to the environment would be significantly reduced.

The PARIS III database contains chemicals that are included in many of the solvents currently used by industry as well as many less harmful solvents. Not only are the physical and chemical properties of the solvent included in the database, but indicators are included that govern the solvent's impact on human health and the environment. Many of these properties and indicators have been determined experimentally; some are calculated from empirically determined equations; some have been approximated using semi-empirical UNIFAC methods; while others have been approximated using linearly regressive quantitative structure–activity relationship (QSAR) calculations.¹⁶

Finding solvents with properties like those of the original solvent to be replaced is an extensive process. This process can be described in a more simplified process (Figure 1). The first axis, P1, represents one property of the solvents and the second axis, P2, represents another property of the solvents. All solvents with property values along P1 and P2 may be represented as marks in this two-dimensional property space.

The original solvent to be replaced is represented by a black dot, with a property value of $x_{0,1}$ on the first axis, and a property value of $x_{0,2}$ on the second axis. The lower and upper bounds of the original solvent's property values are shown as the solid lines parallel to the dashed lines starting at the original solvent's property values. Note how the total number of solvents within bounds of the original solvent's property values decreases as the number of axes with bound constraints increases. Just for illustration, solvents more harmful to human

health and the environment than the original solvent are displayed as red dots, and those less harmful are displayed as green dots.

The PARIS III software performs extensive searches through an 18-dimensional property space with 18 axes; eight of these axes are physical properties, and 10 are chemical properties. The eight physical properties represent the behavior of solvents in various industrial processes (Table 1). For example, the physical property of thermal conductivity may accurately represent how solvents carry heat away from industrial processes that involve exothermic chemical reactions.

The 10 chemical properties used to characterize the behavior of solvents in industrial processes are the infinite dilution activity coefficients of solvent mixtures containing solutes from the 10 different chemical families chosen (Table 2). For example, solvent mixtures with infinite dilution activity coefficients of acetone within bounds of the original solvent to be replaced may accurately represent how possible solvent replacements might affect chemical reactions involving ketones.

The replacement of harmful chemicals used in industrial processes with less harmful chemicals of very similar properties can show a significant reduction of environmental costs with very little additional costs of implementation. A weighted measure of a solvent's total environmental impact can be calculated for every chemical in the PARIS III database using eight categories of environmental impact (Table 3). The categories covered include human exposure, local impacts, regional impacts, and global impacts.

This amount of environmental impact of a solvent is represented by two different indexes, the environment index and the air index. The environment index is a measure of the impact of solvent waste released to the environment, and the air index is a measure of the impact of solvent waste released to the environment and then evaporated into the air. These indexes can show how environmentally benign or harmful one solvent is relative to another. For example, if the environment index of a possible replacement is one-fourth the environment index of the original, it has one-fourth of the environmental impact.

The environmental impact $\varphi_{i,j}$ for chemical i in the PARIS III database is normalized by the average of all chemicals in that database with nonzero impact in category j . This becomes

$$\overline{\varphi_{i,j}} = \frac{\varphi_{i,j}}{\frac{1}{n_j} \sum_{k=1}^{n_j} \varphi_{k,j}} \quad (1)$$

Note that regardless of the initial dimensions, the environmental impact in category j for each chemical is described relative to the average impact in category j . After the user assigns important factors α_j for each category of impact to accurately reflect their environment, the environment index ψ_i^{env} for chemical i may then be calculated as:

$$\psi_i^{env} = \sum_{j=1}^8 \alpha_j \overline{\varphi_{i,j}} \quad (2)$$

where the summation is taken over the eight categories of impact, and $\bar{\varphi}_{i,j}$ is the normalized environmental impact score as defined in Equation 1 for chemical i and impact category j . The importance factors α_j for each impact category can be set by the user to any integer value from 0 to 10. They are all initially set to default values of 5, which implies all impact categories are equivalent. However, the importance factors should be set in a way appropriate to the user. For any impact categories considered irrelevant, their importance factors can be set to 0 to eliminate these categories from consideration. The total environment index ψ^{env} of a solvent mixture of chemicals in the database is finally determined by summing contributions from each chemical of the m -components in the solvent mixture:

$$\psi^{env} = \sum_{i=1}^m W_i \psi_i^{env} \quad (3)$$

where W_i is the weight fraction of the i th component in the solvent mixture.

The air index ψ_i^{air} for chemical i can be calculated in much the same way from its environment index based on the amount of chemical released to the environment and then evaporated into the air.¹¹ That is:

$$\psi_i^{air} = \gamma_i \left(\frac{P_i^v}{P} \right) \psi_i^{env} \quad (4)$$

where γ_i is the activity coefficient for component i of the solvent mixture, P_i^v is the vapor pressure for component i , and P is the pressure at which the solvent is being used. The total air index ψ^{air} is arrived at by summing contributions from each chemical of the m -components in the solvent mixture:

$$\psi^{air} = \sum_{i=1}^m W_i \psi_i^{air} \quad (5)$$

where as in Equation 3, W_i is the weight fraction of the i th component in the solvent mixture.

3 PARIS III DATABASE

A fundamental resource used by the PARIS III software is its database. The PARIS III database was initially constructed by querying the database of almost 24,000 validated structures used by the Toxicity Estimation Software Tool (TEST)¹⁷ (<https://www.epa.gov/chemical-research/toxicity-estimation-software-tool-test>) for chemicals that are liquid at 25°C. The assumption is that most industrial solvents are liquid at standard conditions. Chemicals were defined to be liquids if the normal boiling point is greater than 25°C and the melting point was less than 25°C. Approximately 6,390 chemicals in the TEST structure

database were determined to be liquids. Chemicals contained in the database are included in many of the solvents currently used by industry as well as many less harmful solvents.

The PARIS III database holds property values, toxicity values, Antoine constants, critical constants, environmental indexes, and UNIFAC infinite dilution activity coefficients. Thus, not only are the physical and chemical properties of the solvent available, but also indicators that govern the solvent's impact to human health and the environment. After removing chemicals that lack necessary information, the PARIS III database contains more than 5,200 chemicals. The PARIS III database is periodically updated.^{18, 19}

The four toxicity indicators in Table 3 are based upon toxicity databases, predictive methods and standards of the National Institutes of Health (NIH), the National Institute for Occupational Safety and Health (NIOSH), the Environmental Protection Agency (EPA), and the Occupational Safety and Health Administration (OSHA). More details on the toxicity values included are given in the PARIS III User Manual found at EPA's PARIS III website.¹⁵ The four environmental indicators in Table 3 are global warming potential, photochemical oxidation potential (smog formation), ozone depletion potential, and acidification potential (acid rain). All eight indicators are generated by and taken from the WAR Algorithm²⁰ (<https://www.epa.gov/chemical-research/waste-reduction-algorithm-chemical-process-simulation-waste-reduction>).

4 SOLVENT REPLACEMENT AND DESIGN

Industrial solvents can be characterized by specific physical and chemical properties that are relevant to the various industrial processes they improve. Solvent mixtures with physical and chemical properties very similar to those properties of the original industrial solvents can improve industrial processes in much the same way. A straightforward solution is to find solvents with very similar properties as the original solvent but generate much less harmful waste when released to the environment. Then, the industrial processes that are improved by the solvents would not be changed at all, but the amount of harmful waste released to the environment because of the industrial processes can be substantially reduced.

The challenge is to implement such a solution when possible and replace solvent mixtures that are harmful to the environment with solvent mixtures that have very similar properties but reduce harm to the environment. PARIS III is a pollution prevention solvent substitution software tool explicitly designed for this purpose. It is a user-friendly environmental software tool that can be freely downloaded from EPA's PARIS III website¹⁵ and installed on personal computers or workstations.

Within PARIS III, the user enters: (a) the temperature and pressure of typical industrial processes, (b) the chemical makeup of the solvent mixture to be replaced, and (c) the importance factors for each of the environmental impact categories. The environment index and the air index of each chemical in the PARIS III database and of the original solvent mixture to be replaced are calculated. All chemicals in the database are filtered to use only those chemicals that have the environment index and air index less than or equal to the

respective indexes of the original solvent mixture. This insures that replacements found will have lower environmental impact.

The physical and chemicals properties of the original solvent mixture and the chemicals in the filtered database are calculated. The filtered chemicals are then (d) ranked by how close the physical and chemical properties are to those of the original solvent. This distance from the original solvent can be measured by a normalized metric in an 18-dimensional property space given by:

$$d(\vec{x}_0, \vec{x}) = \sum_{i=1}^{18} \left| \frac{(x_{0,i} - x_i)}{tol(x_{0,i})} \right| \quad (6)$$

where $\vec{x}_0$ is a vector of the 18 properties of the original solvent mixture, $\vec{x}$ is a vector of 18 properties of a possible replacement mixture, and $tol(x_{0,i})$ is the width of the tolerance boundaries of the original solvent on the i th property axis.

After steps (a) through (d) are taken as described above, the remaining steps to find less harmful replacements for solvents used by industry are: (e) examine the ranked list of single chemical replacements and save those with the most important properties very close to those of the original solvent mixture but have less environmental impact. If no appropriate single chemical replacements are found in the PARIS III database, then: (f) calculate the properties of many simple mixtures of chemicals chosen by the user from the large number of chemicals in the filtered database, and create a ranked list of the 500 closest mixtures; (g) examine mixtures from the ranked list and save those with the most important properties very close to those of the original solvent, but significantly reduce impact to human health and the environment.

5 RESULTS

Using this search method, many less harmful replacements have been found for industrial solvents containing chemicals listed in the Toxic Substance Control Act (TSCA) Chemical Substance Inventory as of 04/2018 and designated by the EPA as “active” in U.S. commerce. Solvent mixtures have been found for the replacement of benzene and toluene; and for the replacement of the common solvent degreasers PCE, TCE, and nPB. These replacements do not get rid of all the harmful environmental impacts of each solvent, but they do provide very good reductions of the harmful impacts. These reductions may be approximated by comparing indexes of the original solvent mixture and the replacement mixtures. For example, when the environmental index of the original solvent mixture is 10.0 times larger than the environmental index of a replacement, the replacement reduces harm to the environment by a factor of 10.0.

Solvent mixtures replacements for benzene (CAS# 71-43-2) found using PARIS III are the top two greener replacements (Table 4). The first replacement mixture contains fluorobenzene and 2-methylhex-3-yne. Only two out of 18 properties of the mixture are outside the tolerance bounds of benzene. The molecular mass of this mixture is heavier than the upper bound of the molecular mass of benzene; and the infinite dilution activity

coefficient of this mixture with solute water is less than the lower bound of the infinite dilution activity coefficient of benzene with solute water. However, as shown in the next two columns, this substitution would reduce harmful impact to the air by a factor of 10.6, and harmful impact to the environment by 6.65. If the two properties are not vital for the industrial process under consideration, then use of the replacement can significantly reduce harm to human health and the environment.

Another replacement mixture for benzene (Table 4) is made from 3,3-dimethyloxetane and *N*'-ethylethane-1,2-diamine. Two properties of the mixture are outside the tolerance bounds of the original solvent. Both infinite dilution activity coefficients of the mixture are less than those of benzene; one is for solute ethanol and the other is for solute water. This substitution would reduce harmful impact to the air by a factor of 8.04, and harmful impact to the environment by 3.58. Again, use of this replacement can significantly reduce harm to human health and the environment.

For toluene (Table 4), the first replacement mixture has only one property outside of toluene's tolerance bounds. Like the prior replacement mixtures described for benzene, this replacement mixture has an infinite dilution activity coefficient for solute water less than toluene's. This replacement can reduce harmful impact to the air by a factor of 8.90, and harmful impact to the environment by 9.08.

Hot vapor degreasers are used by industry to remove contaminants from manufactured items. The vaporized solvent condenses on the impurities, dissolves them, and removes them by dripping off the part. Unfortunately, the vaporized solvent degreasers spread through the surrounding air in the manufacturing environment and can create unhealthy working conditions. As it is necessary to vaporize the solvent in the manufacturing process, only replacements that have vapor pressures and boiling temperatures within bounds of the original vapor degreasers were considered. In addition, single component solvent substitutes were included in the search to increase the likelihood of being used by industry as less harmful replacements.

There are three solvent greasers commonly used by industry that appear in the TSCA Inventory. Replacements for these solvents are needed that reduce harm considerably to human health and the environment. A general rule exists that the more components used in a mixture, the wider the selection of replacements (Table 5). For PCE (tetrachloroethylene, CAS# 127-18-4) and TCE (trichloroethylene, CAS# 79-01-6), two single solvent replacements are shown initially, and two 2-component mixtures are shown afterward. The single component replacements have more properties outside of the tolerance bound of the original vapor degreaser, while the 2-component mixtures can be selected to have fewer properties outside the tolerance bounds. Likewise, the 2-component mixtures can be selected to better reduce impact to the air and the environment.

The solvent degreaser nPB (*n*-propyl bromide, CAS# 106-94-5; Table 5) has a low flashpoint of 298.75 K. It is hard to find single chemical replacements with similar vapor degreasing properties that have higher flashpoints. Two single chemical replacements listed for nPB that are significantly less harmful to human health and the environment have

slightly lower flashpoints. The first single solvent replacement has a flashpoint of 291.15 K, and the second single solvent replacement has a flashpoint of 294.25 K. If the degreasing process is not affected by this, these single solvent replacements might be worth the significantly reduced impacts.

Both 2-component replacements for nPB have 17 properties within the tolerance bounds and the flashpoint is above that of the solvent degreaser nPB. Again, this reflects the facts that the replacements behave in ways very similar to nPB. Yet, use of the first 2-component replacement can reduce harmful impact to the air by a factor of 9.95, and harmful impacts to the environment by 12.64. Likewise, use of the second 2-component replacement can reduce harmful impact to the air and the environment in similar ways.

6 CONCLUSION

As shown above, the PARIS III environmental software tool can be effectively used to find many less harmful replacements for various types of solvents used by industry. This is accomplished by calculating properties of millions of combinations of less harmful chemicals included in the PARIS III database. This environmental software tool provides a unique method for finding alternate industrial solvents that are less harmful to human health and the environment. In addition, the software and database are updated periodically, enhancing its capabilities and enabling a wider selection of chemicals.^{21, 22}

With PARIS III, finding alternate greener solvents can be accomplished by process technicians, chemical and environmental engineers, environmental consultants, and environmental health and safety managers. As shown, this tool can be used to find significantly less harmful alternatives for chemicals listed in the TSCA Inventory, and other harmful solvents encountered in EPA Regions. Increased use of this software tool greatly improves the possibility of finding alternate industrial solvents that significantly reduce harm to human health and the environment.

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Table 1.

The eight physical properties used in the PARIS III search for similar solvents

Physical properties			
Molecular mass	Liquid density	Boiling temperature	Vapor pressure
Surface tension	Viscosity	Thermal conductivity	Flash point

Table 2.

The ten chemical properties used in the PARIS III search for similar solvents

Chemical family	Representative solute
Alcohols	Ethanol
Ethers	Diethyl ether
Ketones	Acetone
Polar inorganics	Water
Aromatics	Benzene
<i>N</i> -containing organics	<i>n</i> -propylamine
Unsaturated organics	Cis-2-heptene
Halogenated organics	<i>n</i> -propyl chloride
Hydrocarbons	<i>n</i> -heptadecane
<i>S</i> -containing organics	Dimethyl disulfide

- *Note* : Each solvent in the Paris III database is characterized by the solvent's interaction with representative solutes from each of the ten chemical families shown above. These interactions are measured by the infinite dilution activity coefficients between the solvent and the solute.

Table 3.

The eight environmental impact categories summed to compare total potential impact of solvents

Human health	Ecological	Regional impacts	Global impacts
Human toxicity potential by ingestion	Aquatic toxicity potential	Photochemical oxidation potential	Ozone depletion potential
Human toxicity potential by inhalation	Terrestrial toxicity potential	Acidification potential	Global warming potential

Table 4.

Several replacements for TSCA solvents benzene and toluene

TSCA solvents	Greener replacement mixtures	CAS#	wt%	No. of properties out-of-bounds	Air impact reduction	Environmental impact reduction
Benzene 71-43-2	Fluorobenzene	462-06-6	60.0	2	10.60	6.65
	2-methylhex-3-yne	36566-80-0	40.0			
	3,3-dimethyloxetane	6921-35-3	80.0	2	8.04	3.58
Toluene 108-88-3	<i>N'</i> -ethylethane-1,2-diamine	110-72-5	20.0			
	Hept-1-en-3-yne	2384-73-8	80.0	1	8.90	9.08
	N,N-diethylbutanimide	114-76-7	20.0			
	2-methylhex-3-yne	36566-80-0	50.0	2	16.70	8.53
	2-methylpyrazine	109-08-0	50.0			

Table 5.

Several replacements for the TSCA vapor degreasers PCE, TCE, and nPB

TSCA vapor degreaser	Greener replacement mixtures	CAS#	wt%	No. of properties out-of-bounds	Air impact reduction	Environmental impact reduction
PCE 127-18-4	Methyl 2-ethylbutanoate	816-11-5	100.0	7	3.95	3.30
	Methyl pentanoate	624-24-8	100.0	8	3.47	3.60
	Methyl pentanoate	624-24-8	50.0	6	7.11	3.47
	Dihexyl benzene-1,2-dicarboxylate	84-75-3	50.0			
	Hexyl butanoate	2693-63-6	80.0	6	7.64	2.76
	1-ethenyl-2-methylpropane	109-53-5	20.0			
TCE 79-01-6	2,2-dichlorobutane	4279-22-5	100.0	8	4.65	4.19
	1-methylpropane-1-thiol	513-44-0	100.0	9	3.22	3.27
	Propan-2-yl 2-methylpropanoate	617-50-5	80.0	6	9.56	2.98
	3-ethyl-2,2-dimethyl-oxiran	1192-22-9	20.0			
	Bis(methylsulfonyl)methane	1618-26-4	80.0	5	6.69	2.35
	2-chloro-1-(difluoromethoxy)-1,1,2-trifluoro-	13838-16-9	20.0			
nPB 106-94-5	2-bromo-2-methylpropane	507-19-7	100.0	3	4.66	4.28
	1-chloro-2-methylpropane	513-36-0	100.0	6	8.69	8.87
	2-bromopropane	75-26-3	80.0	0	9.95	12.64
	3-methyl-oxolan-2-one	106-03-9	20.0			
	1-bromo-3-methylbutane	107-82-4	80.0	0	5.38	5.37
	Dichloromethane	75-09-2	20.0			