

Program for Assisting the Replacement of Industrial Solvents (PARIS III)

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Problem

- Solvents are used in industry because of their effective performance. Unfortunately, some of these solvents are particularly harmful to the environment

Solution

- Solvent replacements may be found with similar performance, but much less toxicity. Use of these replacements reduce harm to the environment without sacrificing performance.

PARIS III - EPA Solvent Substitution Software Tool

- PARIS III implements extensive searches for solvent mixtures with properties similar to solvent mixtures they replace, but with less impact to the environment.

PARIS III Solvent Database

1. Contains over 5000 Chemicals.
2. Each chemical record has values, numbers, and coefficients to get:
 - 8 physical properties.
 - 10 chemical properties.
 - 8 environmental indicators.

Replacement Example

- Mixture to be replaced is entered by its chemical make-up, or loaded from file.
“RollerWash” is a solvent mixture used to wash the ink from the rollers of a printing press.

Example: Screenshot 1

PARIS III

File Edit Action Help

Current Mixture Impact Factors Physical Properties Activity Coefficients Solvent Mixtures

System

Name RollerWash

Units SI Note: Units are converted to SI for calculations.

Temperature 25.0 C

Pressure 1.0 Atm

Chemical Display Options

Search for Chemicals by Name

Chemical Name

Chemicals

Mixture	Wt%
methylbenzene	40.0
bis(chloranyl)methane	35.0
propan-2-ol	25.0

Example: Screenshot 2

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Current Mixture Impact Factors Physical Properties Activity Coefficients Solvent Mixtures

Potential Environmental Impact Scores For Current Formulation

Impact Factors	Ingestion	Inhalation	Terrestrial Toxicity	Aquatic Toxicity	GWP	ODP	PCOP	Acid Rain	Totals	
Default	5	5	5	5	5	5	5	5		
Chemicals	Wt%									
methylbenzene	40.0	7.65E-1	6.46E-3	7.65E-1	1.24E-2	0.00E0	0.00E0	1.35E0	0.00E0	5.79E0
bis(chloranyl)methane	35.0	3.04E-1	5.57E-2	3.04E-1	1.32E-3	4.68E-3	0.00E0	1.23E-2	0.00E0	1.19E0
propan-2-ol	25.0	9.64E-2	4.95E-3	9.64E-2	4.22E-5	0.00E0	0.00E0	1.96E-1	0.00E0	4.92E-1
Totals	100.0	2.18E0	1.17E-1	2.18E0	2.71E-2	8.19E-3	0.00E0	2.96E0	0.00E0	7.48E0

Replacement Ex.. (cont.)

- The database is filtered to only use chemicals with lower environmental impact scores.
- Chemicals are then ranked by how close their properties are to those of the original mixture.

Example: Screenshot 3

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Current Mixture Impact Factors Physical Properties Activity Coefficients Solvent Mixtures

Physical Properties

Property Tolerance(%) Lower Desired Upper Replacement Units

Property	Tolerance(%)	Lower	Desired	Upper	Replacement	Units
Molecular Mass	11.0	70.512	79.227	87.942	84.12	kg/kmol
Liquid Density	14.0	8.14E2	9.47E2	1.08E3	8.30E2	kg/m ³
Boiling Temperature	10.0	301.377	334.863	368.349	390.15	K
Vapor Pressure	30.0	1.77E1	2.52E1	3.28E1	3.45E0	kPa
Surface Tension	16.0	1.68E-2	2.00E-2	2.32E-2	2.43E-2	kg/s ²
Viscosity	30.0	3.94E-4	5.63E-4	7.32E-4	5.40E-4	kg/m-s
Thermal Conductivity	30.0	9.10E-2	1.30E-1	1.69E-1	1.46E-1	J/(m-s-K)
Flash Point		281.712			291.45	K
Air Index				1.06E0	7.61E-2	Impact/Kg
Environmental Index				7.48E0	2.24E0	Impact/Kg

Tolerance Scale Factor

Single Mixture Solvent Replacement

7: 2-Butenal, 2-methylbut-2-enal
7: 2-chloranylbut-1-enal
7: (Z)-2-chloranylbut-1-enal
7: 1-chloranyl-2-methyl-2-butene
8: 2-methylidenebutanal
8: (E)-pent-2-enal
8: 2,2-dimethylpropanal
8: cyclohexa-1,4-diene
8: 2-methylpropanoal
8: methylsulfanylethanol
8: ethyl 2,2,2-tris(fluoro)acetate
8: propyl 2-chloranylacetate
8: methyl 2-chloranylacetate
8: cyclohexen-1-yl ethyl ether
8: heptanoyl chloride
8: butyl 2-chloranylacetate
8: (E)-1,1-dimethoxybutane
8: 1-chloranyl-2-fluorobutane
8: 1-chloranyl-2-methylbutane
8: 1,2,2-tris(chloranyl)butane
8: 1-Butene, 1-chloro-

Example: Screenshot 4

PARIS III

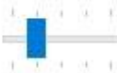
File Edit Action Help



Current Mixture Impact Factors Physical Properties Activity Coefficients Solvent Mixtures

Infinite Dilution Activity Coefficients

☒ Single ☐ Mixture
Solvent Replacement

Substance Name	Tolerance(%)	Lower	Desired	Upper	Replacement
ethanol	25.0	1.51E0	2.02E0	2.52E0	1.19E0
diethyl ether	30.0	5.65E-1	8.07E-1	1.05E0	1.39E0
acetone	28.0	6.73E-1	9.35E-1	1.20E0	1.06E0
water	30.0	3.61E0	5.16E0	6.70E0	3.61E0
benzene	30.0	9.54E-1	1.36E0	1.77E0	1.11E0
cis-2-heptene	30.0	1.61E0	2.30E0	3.00E0	2.63E0
n-propyl chloride	30.0	8.88E-1	1.27E0	1.65E0	9.98E-1
n-heptadecane	30.0	2.44E0	3.48E0	4.53E0	7.16E0
n-propylamine	30.0	3.47E-1	4.96E-1	6.44E-1	8.13E-1
dimethyl disulfide	30.0	1.59E-1	2.27E-1	2.95E-1	2.89E-1

Tolerance Scale Factor 

7: 2-Butenal, 2-methyl 
 7: 3-methylbut-2-enal
 7: 2-chloranylbut-1-en
 7: (Z)-2-chloranylbut-
 7: 1-chloranyl-2-meth
 8: 2-methylidenebutar
 8: (E)-pent-2-enal
 8: 2,2-dimethylpropan
 8: cyclohexa-1,4-diene
 8: 2-methylpropanoyl
 8: methylsulfanylethar
 8: ethyl 2,2,2-tris(fluor
 8: propyl 2-chloranyle
 8: methyl 2-chloranyle
 8: cyclohexen-1-yl eth
 8: heptanoyl chloride
 8: butyl 2-chloranyleth
 8: (E)-1,1-dimethoxyhy
 8: 1-chloranyl-2-fluor
 8: 1-chloranyl-2-meth
 8: 1,2,2-tris(chloranyl)-
 8: 1-Butene, 1-chloro- 

Replacement Mixtures

- Single chemical replacements are only part of the solvent substitute solution.
- Even better replacements for the initial solvent mixture may be found by examining thousands/millions of combinations of these ranked solvents.

Example: Screenshot 5

PARIS III

File Edit Action Help

Current Mixture Impact Factors Physical Properties Activity Coefficients Solvent Mixtures

Solvent Mixtures

☒ Primary ☒ Secondary ☐ Tertiary

☒ Best Solvents ☒ Best Solvents ☐ Best Solvents

☐ All Green Solvents ☐ All Green Solvents ☐ All Green Solvents

☐ Initial Solvents ☐ Initial Solvents ☐ Initial Solvents

☐ All Solvents ☐ All Solvents ☐ All Solvents

Mass Ratio

Best Mixtures

9:1 4: 2-Butenal; 1-chlorany; 6:4
8:2 5: 3-methylbu; 1-chlorany; 6:4
7:3 5: 2-Butenal; 1-chlorany; 7:3
6:4 5: 1-chlorany; 2-Butenal; 5:5
5:5 5: 1-chlorany; 3-methylbu; 5:5
5: cyclohexa-; 1-chlorany; 5:5
6: (E)-pent-2; 1-chlorany; 6:4
6: 1-chlorany; (E)-pent-2; 5:5
6: 3-methylbu; 1-chlorany; 7:3
6: 2,2-dimeth; 1-chlorany; 5:5
6: (E)-pent-2; 2-chlorany; 7:3
6: cyclohexa-; 1-chlorany; 7:3
6: cyclohexa-; 1-chlorany; 6:4
6: 1-chlorany; cyclohexa-; 6:4
7: 2-methylid; 1-chlorany; 6:4
7: 2-methylid; 1-chlorany; 5:5
7: 2,2-dimeth; 1-chlorany; 6:4
7: 2,2-dimeth; (E)-pent-2; 5:5
7: (E)-pent-2; 1-chlorany; 7:3
7: (E)-pent-2; 2,2-dimeth; 6:4

Solvent **Wt%**

2-Butenal, 2-methyl- 60.0
1-chloranyl-2-methyl-pr... 40.0

Example: Screenshot 6

PARIS III

File Edit Action Help

Current Mixture Impact Factors Physical Properties Activity Coefficients Solvent Mixtures

Solvent Mixtures

☒ Miscibility Test

☒ Primary
☒ Best Solvents
☐ All Green Solvents
☐ Initial Solvents
☐ All Solvents

☒ Secondary
☒ Best Solvents
☐ All Green Solvents
☐ Initial Solvents
☐ All Solvents

☒ Tertiary
☒ Best Solvents
☐ All Green Solvents
☐ Initial Solvents
☐ All Solvents

Mass Ratios	Best Mixtures
8:1:1	4: 3-methylbu; 1-chlorany; 2,2-dim
7:2:1	4: 2-Butenal; 1-chlorany; 2-chlorar
6:3:1	4: 3-methylbu; 1-chlorany; (Z)-2-ch
6:2:2	4: 3-methylbu; 1-chlorany; 2-chlorar
5:4:1	4: 2-Butenal; 1-chlorany; 2-chlorar
5:3:2	4: 3-methylbu; 1-chlorany; 2-chlorar
4:4:2	4: 2-Butenal; 1-chlorany; cyclohexa
4:3:3	4: 3-methylbu; 1-chlorany; cyclohexa
	4: 1-chlorany; 2-chlorany; cyclohexa
	5: 2,2-dimeth; (E)-pent-2; 1-chlorar
	5: 2,2-dimeth; 1-chlorany; 2-methyl
	5: 2-Butenal; 1-chlorany; 2,2-dimeth
	5: 2,2-dimeth; 1-chlorany; 2-methyl
	5: 3-methylbu; 1-chlorany; 2,2-dim
	5: 2,2-dimeth; 2-Butenal; 1-chlorar
	5: 1-chlorany; (E)-pent-2; 2,2-dimeth
	5: 2,2-dimeth; 3-methylbu; 1-chlorar
	5: (E)-pent-2; 1-chlorany; 2,2-dimeth

Solvent	Wt%
3-methylbut-2-enal	50.0
1-chloranyl-2-methyl-pr...	40.0
2,2-dimethylpropanal	10.0

Example: Screenshot 7

PARIS III

File Edit Action Help

Current Mixture Impact Factors Physical Properties Activity Coefficients Solvent Mixtures

Solvent Mixtures

☒ Primary ☒ Secondary ☐ Tertiary

☒ Best Solvents ☐ Best Solvents ☐ Best Solvents

☐ All Green Solvents ☒ All Green Solvents ☐ All Green Solvents

☐ Initial Solvents ☐ Initial Solvents ☐ Initial Solvents

☐ All Solvents ☐ All Solvents ☐ All Solvents

2-Butenal, 2-methyl-3-methylbut-2-enal 2-chloranylbut-1-ene (Z)-2-chloranylbut-2-1-chloranyl-2-methyl-2-methylidenebutana (E)-pent-2-enal 2,2-dimethylpropanal cyclohexa-1,4-diene 2-methylpropanoyl cl methylsulfanylethane ethyl 2,2,2-tris(fluorapropyl 2-chloranyleth methyl 2-chloranylpro cyclohexen-1-yl ethar heptanoyl chloride butyl 2-chloranyletha (E)-1,1-dimethoxyhex 1-chloranyl-2-fluor...

2-Butenal, 2-methyl-3-methylbut-2-enal 2-chloranylbut-1-ene (Z)-2-chloranylbut-2-1-chloranyl-2-methyl-2-methylidenebutana (E)-pent-2-enal 2,2-dimethylpropanal cyclohexa-1,4-diene 2-methylpropanoyl cl methylsulfanylethane ethyl 2,2,2-tris(fluorapropyl 2-chloranyleth methyl 2-chloranylpro cyclohexen-1-yl ethar heptanoyl chloride butyl 2-chloranyletha (E)-1,1-dimethoxyhex 1-chloranyl-2-fluor...

Mass Ratios: 9:1 8:2 7:3 6:4 5:5

Best Mixtures

☒ Miscibility Test

2: 1-chloranyl; 2-methylpr; 7:3
2: 1-chloranyl; 2-Buten-1-; 7:3
2: 1-chloranyl; but-3-en-1; 7:3
1-chloranyl; propan-2-o; 7:3
3: 1-chloranyl; propan-1-o; 7:3
3: 1-chloranyl; 2-methylpr; 7:3
3: 1-chloranyl; 2-butanol; 7:3
3: 1-chloranyl; propan-2-o; 8:2
3: 1-chloranyl; propan-1-o; 8:2
3: 1-chloranyl; 3-methylpe; 6:4
3: 1-chloranyl; hexa-1,5-d; 7:3
3: (E)-pent-2; 2-chloranyl; 6:4
3: 1-chloranyl; 5-methylhe; 5:5
3: 2-Butenal; 2-chloranyl; 6:4
3: 3-methylbu; 2-chloranyl; 6:4
4: 1-chloranyl; 1-deuterio; 7:3
4: 1-chloranyl; 1-deuterio; 6:4
4: 1-chloranyl; cyclobutan; 7:3
4: 1-chloranyl; 2-methylbu; 6:4
4: 1-chloranyl; ethanol; 7:3

Solvent	Wt%
1-chloranyl-2-methyl-pr...	70.0
2-methylprop-2-en-1-ol	30.0

Replacement Mixtures (cont.)

- Mixtures may be examined on the Physical Properties screen to find those that significantly reduce the air and environmental impact, but still have properties close to those of the original solvent mixture.

Example: Screenshot 8

PARIS III


File Edit Action Help

Current Mixture Impact Factors Physical Properties Activity Coefficients Solvent Mixtures

Physical Properties

☐ Single ☒ Mixture
Solvent Replacement

Property	Tolerance(%)	Lower	Desired	Upper	Replacement	Units
Molecular Mass	11.0	70.512	79.227	87.942	108.217	kg/kmol
Liquid Density	14.0	8.14E2	9.47E2	1.08E3	8.44E2	kg/m ³
Boiling Temperature	10.0	301.377	334.863	368.349	354.504	K
Vapor Pressure	30.0	1.77E1	2.52E1	3.28E1	1.49E1	kPa
Surface Tension	16.0	1.68E-2	2.00E-2	2.32E-2	2.32E-2	kg/s ²
Viscosity	30.0	3.94E-4	5.63E-4	7.32E-4	6.61E-4	kg/m-s
Thermal Conductivity	30.0	9.10E-2	1.30E-1	1.69E-1	1.27E-1	J/(m-s-K)
Flash Point		281.712			300.011	K
Air Index				1.06E0	1.55E-1	Impact/Kg
Environmental Index				7.48E0	1.25E0	Impact/Kg

Tolerance Scale Factor 

2: 1-chlorany; 2-meth...
2: 1-chlorany; 2-Buten...
2: 1-chlorany; but-3-e...
3: 1-chlorany; propan...
3: 1-chlorany; propan...
3: 1-chlorany; 2-meth...
3: 1-chlorany; 2-butan...
3: 1-chlorany; propan...
3: 1-chlorany; propan...
3: 1-chlorany; 3-meth...
3: 1-chlorany; hexa-1,...
3: (E)-pent-2; 2-chlor...
3: 1-chlorany; 5-meth...
3: 2-Butenal; 2-chlor...
3: 3-methylbu; 2-chlor...

Solvent	Wt%
1-chloranyl-2-...	50.0
5-methylhepta...	50.0

Example: Screenshot 9

PARIS III


File Edit Action Help

Current Mixture Impact Factors Physical Properties Activity Coefficients Solvent Mixtures

Physical Properties

☐ Single ☒ Mixture
Solvent Replacement

Property	Tolerance(%)	Lower	Desired	Upper	Replacement	Units
Molecular Mass	38.0	49.121	79.227	109.333	108.217	kg/kmol
Liquid Density	14.0	8.14E2	9.47E2	1.08E3	8.44E2	kg/m ³
Boiling Temperature	10.0	301.377	334.863	368.349	354.504	K
Vapor Pressure	42.0	1.46E1	2.52E1	3.58E1	1.49E1	kPa
Surface Tension	16.0	1.68E-2	2.00E-2	2.32E-2	2.32E-2	kg/s ²
Viscosity	30.0	3.94E-4	5.63E-4	7.32E-4	6.61E-4	kg/m-s
Thermal Conductivity	30.0	9.10E-2	1.30E-1	1.69E-1	1.27E-1	J/(m-s-K)
Flash Point		281.712			300.014	K
Air Index				1.06E0	1.55E-1	Impact/Kg
Environmental Index				7.48E0	1.25E0	Impact/Kg

Tolerance Scale Factor 

2: 1-chlorany; 2-meth... ^

2: 1-chlorany; 2-Buten

2: 1-chlorany; but-3-e

3: 1-chlorany; propan-

3: 1-chlorany; propan-

3: 1-chlorany; 2-meth

3: 1-chlorany; 2-butan

3: 1-chlorany; propan-

3: 1-chlorany; propan-

3: 1-chlorany; 3-meth

3: 1-chlorany; hexa-1,1

3: (E)-pent-2; 2-chlor

3: 1-chlorany; 5-meth

3: 2-Butenal; 2-chlor

3: 3-methylbu; 2-chlor

Solvent	Wt%
1-chloranyl-2-...	50.0
5-methylhepta...	50.0

Example: Screenshot 10

PARIS III

File Edit Action Help

Current Mixture Impact Factors Physical Properties Activity Coefficients Solvent Mixtures

Solvent Mixtures

☒ Miscibility Test

☒ Primary
☒ Best Solvents
☐ All Green Solvents
☐ Initial Solvents
☐ All Solvents

☒ Secondary
☐ Best Solvents
☒ All Green Solvents
☐ Initial Solvents
☐ All Solvents

☐ Tertiary
☐ Best Solvents
☐ All Green Solvents
☐ Initial Solvents
☐ All Solvents

2-chloranylbut-1-ene
(Z)-2-chloranylbut-2-ene
1-chloranyl-2-methyl-2-Butenal, 2-methyl-3-methylbut-2-enal
2-methylpropanoyl chloride
1-chloranyl-2-methyl-1-Butene, 1-chloro-3-2-methylidenebutanal
(E)-pent-2-enal
2,2-dimethylpropanal
1-chloranyl-3-methoxypropan-2-yl ethanoate
2,3-dihydrofuran
cyclohexa-1,4-diene
ethyl 2,2,2-tris(fluoro)propyl 2-chloranylethylmethylsulfanylethane

2-chloranylbut-1-ene
(Z)-2-chloranylbut-2-ene
1-chloranyl-2-methyl-2-Butenal, 2-methyl-3-methylbut-2-enal
2-methylpropanoyl chloride
1-chloranyl-2-methyl-1-Butene, 1-chloro-3-2-methylidenebutanal
(E)-pent-2-enal
2,2-dimethylpropanal
1-chloranyl-3-methoxypropan-2-yl ethanoate
2,3-dihydrofuran
cyclohexa-1,4-diene
ethyl 2,2,2-tris(fluoro)propyl 2-chloranylethylmethylsulfanylethane

Mass Ratios

9:1
8:2
7:3
6:4
5:5

Best Mixtures

0: 1-chloranyl; 5-methylhe; 5:5
1: 1-chloranyl; 3-methylpe; 6:4
1: 1-chloranyl; 4-methylhe; 5:5
1: 1-chloranyl; 6-methylhe; 5:5
1: 1-chloranyl; 3-methylhe; 5:5
1: 1-chloranyl; 2,5-dimeth; 5:5
1: 1-chloranyl; 3,4-dimeth; 5:5
1: 1-chloranyl; 2-methylhe; 5:5
2: 1-chloranyl; 2-methylpr; 7:3
2: 1-chloranyl; 2-Buten-1-; 7:3
2: 1-chloranyl; but-3-en-1; 7:3
2: 1-chloranyl; 2-methylpe; 6:4
2: 1-chloranyl; 2-Penten-1; 6:4
2: 1-chloranyl; 2,3-dimeth; 6:4
2: 1-chloranyl; 3,3-dimeth; 6:4
2: 1-chloranyl; 4-methylpe; 6:4
2: 1-chloranyl; (E)-2-meth; 6:4
2: 1-chloranyl; 4-methylpe; 6:4
2: 1-chloranyl; 3-methylpe; 6:4
2: 1-chloranyl; 5-methylhe; 5:5

Solvent	Wt%
1-chloranyl-2-methyl-pr...	50.0
5-methylheptan-3-ol	50.0

Replacement Mixture (cont.)

A replacement mixture for RollerWash was found with all properties within bounds; and it reduces impact to the:

- air by a factor of 6.84.
- environment by a factor of 5.98.

Toxic Substance Control Act (TSCA) Chemical Replacements

- Using this same process, mixture replacements may be found for industrial solvents containing TSCA chemicals, and significantly reduce impact to the air and the environment.

Impact Reduction for TSCA Chemical Replacements

TSCA Chemical	CAS#	Air Impact Reduction	Env. Impact Reduction
Benzene	71-43-2	8.04	3.58
Toluene	108-88-3	8.90	9.08
PCE	127-18-4	7.64	2.76
TCE	70-01-6	9.56	2.98
nPB	106-94-5	9.95	12.74

Verify Replacements

- The final step of finding greener solvent replacements is to verify they serve as good substitutes in original industrial processes.

Conclusions

- PARIS III is a very strong and versatile solvent substitution software tool that can find significantly less harmful replacements for solvents currently used by industry.

Acknowledgements

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Free Public Domain Software at EPA Website



<https://www.epa.gov/chemical-research/program-assisting-replacement-industrial-solvents-paris-iii>