United States Environmental Protection Agency

US EPA's Freely Downloaded Solvent Substitution Software Tool, 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.

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Solution

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

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PARIS III - EPA Solvent Substitution Software Tool

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

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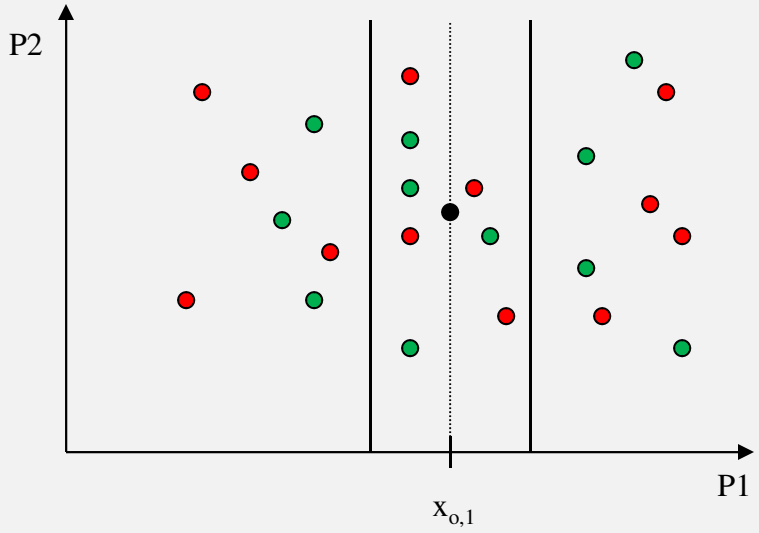
PARIS III Solvent Database

1) Over 5000 industrial solvents
2) Each solvent record contains values and source references for
   - 18 physical & chemical properties
   - 8 environmental indicators

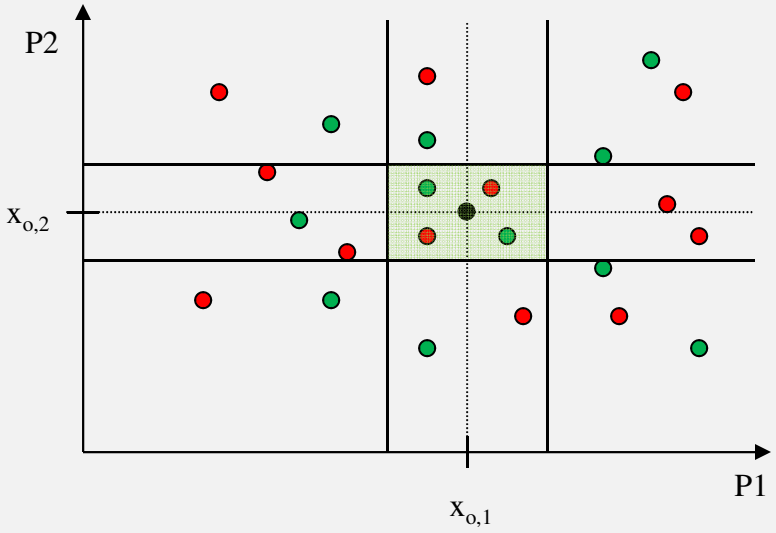
How to Find Similar Solvent Mixtures?

To find solvents with similar properties, consider one axis of a multi-dimensional property space.



How to Find Similar… (cont.)?

Now, consider a second axis of the property space. Note how the search is narrowed as more axes are considered.



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Eight Physical Properties

- Molecular Mass
- Liquid Density
- Boiling Temperature
- Vapor Pressure
- Surface Tension
- Viscosity
- Thermal Conductivity
- Flash Point

Solvent Interactions with Ten Chemical Families

Chemical Family	Solute
Alcohols:	ethanol
Ethers:	diethyl ether
Ketones:	acetone
Polar Inorganics:	water
Aromatics:	benzene
N-containing Organics:	n-propylamine
Unsaturated Organics:	cis-2-heptene
Halogenated Organics:	n-propyl chloride
Hydrocarbons:	n-heptadecane
S-containing Organics:	dimethyl disulfide

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Eight Categories of Human and Environmental Impact

- Human Health
  1) Toxicity: Ingestion
  2) Toxicity: Inhalation
- Ecological
  3) Aquatic Toxicity
  4) Terrestrial Toxicity
- Regional Effects
  5) Photochemical Oxidation
  6) Acid Rain
- Global Effects
  7) Ozone Depletion
  8) Global Warming

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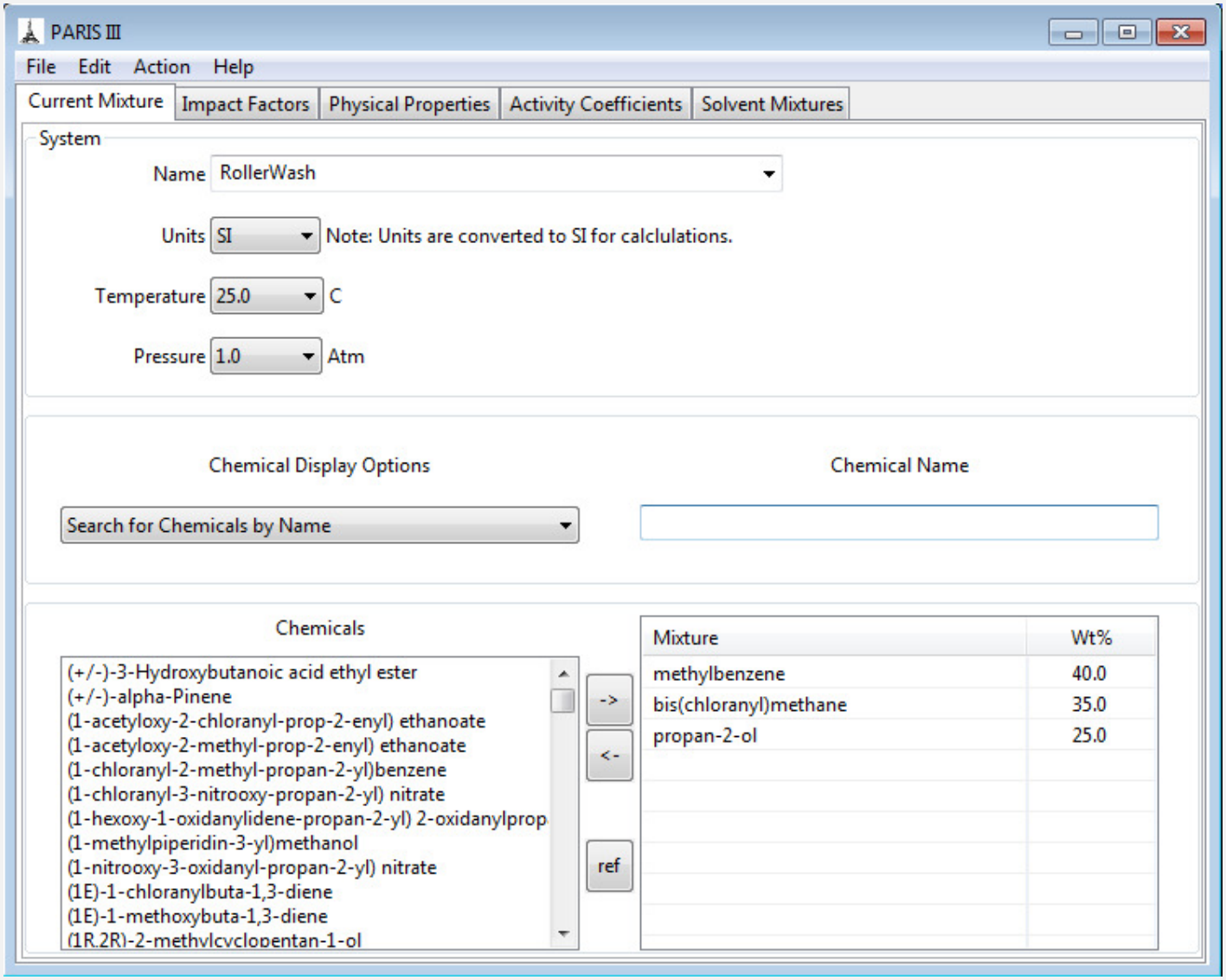
Replacement Example

After initial mixture of solvents is entered, similarly behaving mixtures are found that are less harmful to the environment.


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 calclulations.
Temperature 25.0 C
Pressure 1.0 Atm
Chemical Display Options
Search for Chemicals by Name
Chemical Name
Chemicals
(+/-)-3-Hydroxybutanoic acid ethyl ester
(+/-)-alpha-Pinene
(1-acetyloxy-2-chloranyl-prop-2-enyl) ethanoate
(1-acetyloxy-2-methyl-prop-2-enyl) ethanoate
(1-chloranyl-2-methyl-propan-2-yl)benzene
(1-chloranyl-3-nitrooxy-propan-2-yl) nitrate
(1-hexoxy-1-oxidanylidene-propan-2-yl) 2-oxidanylprop
(1-methylpiperidin-3-yl)methanol
(1-nitrooxy-3-oxidanyl-propan-2-yl) nitrate
(1E)-1-chloranylbuta-1,3-diene
(1E)-1-methoxybuta-1,3-diene
(1R,2R)-2-methylcyclopentan-1-ol
->
<-
ref
Mixture
Wt%
methylbenzene 40.0
bis(chloranyl)methane 35.0
propan-2-ol 25.0

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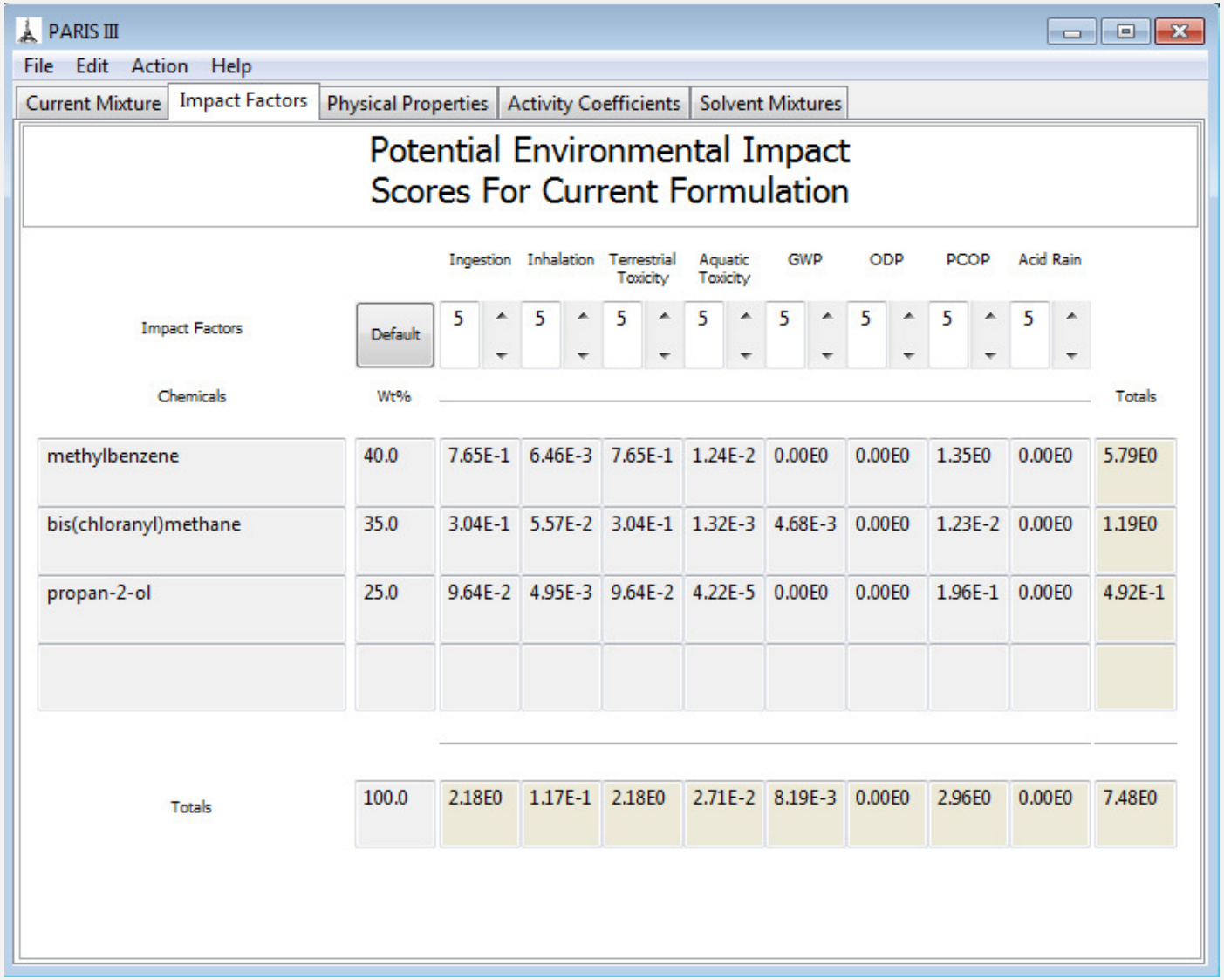
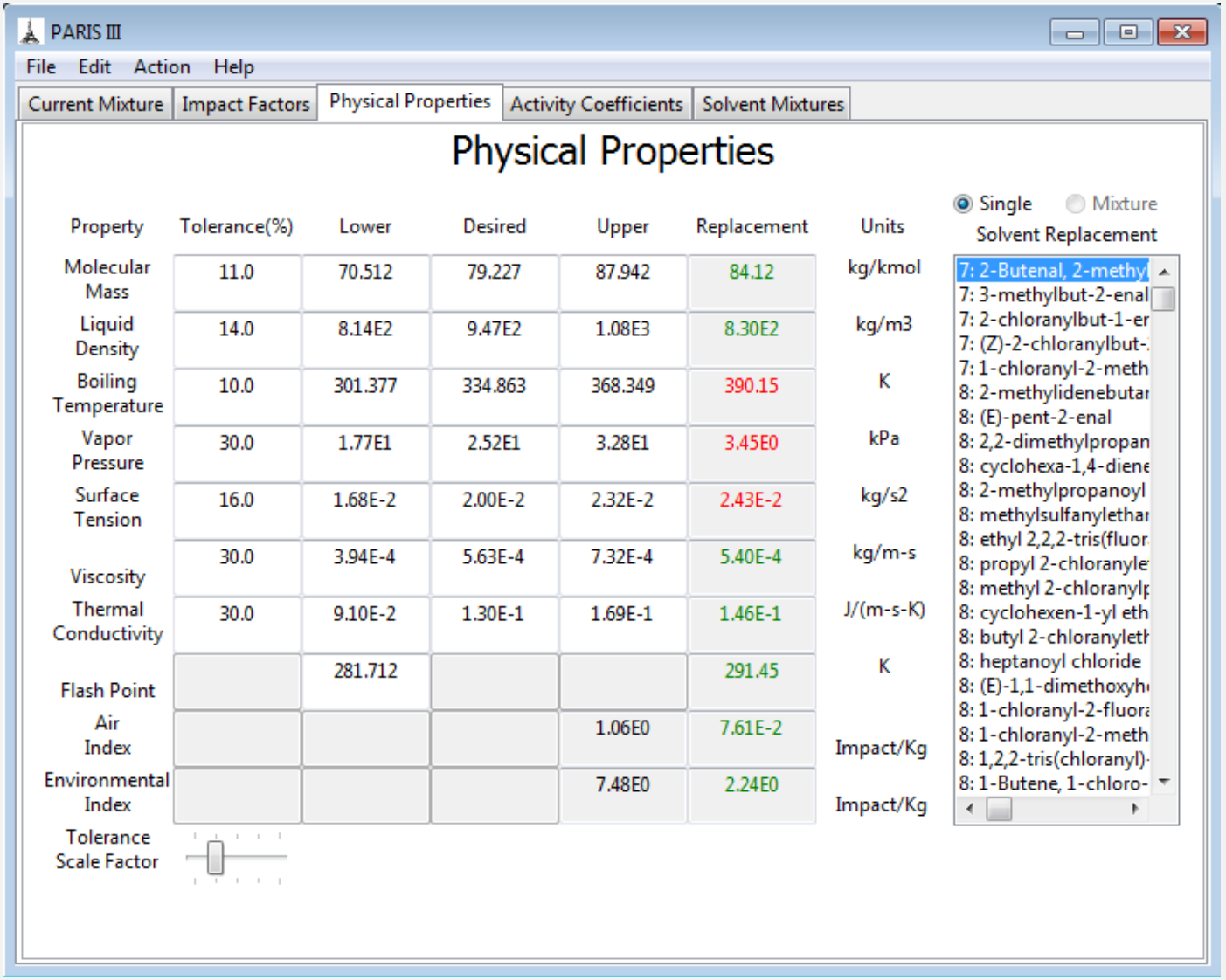
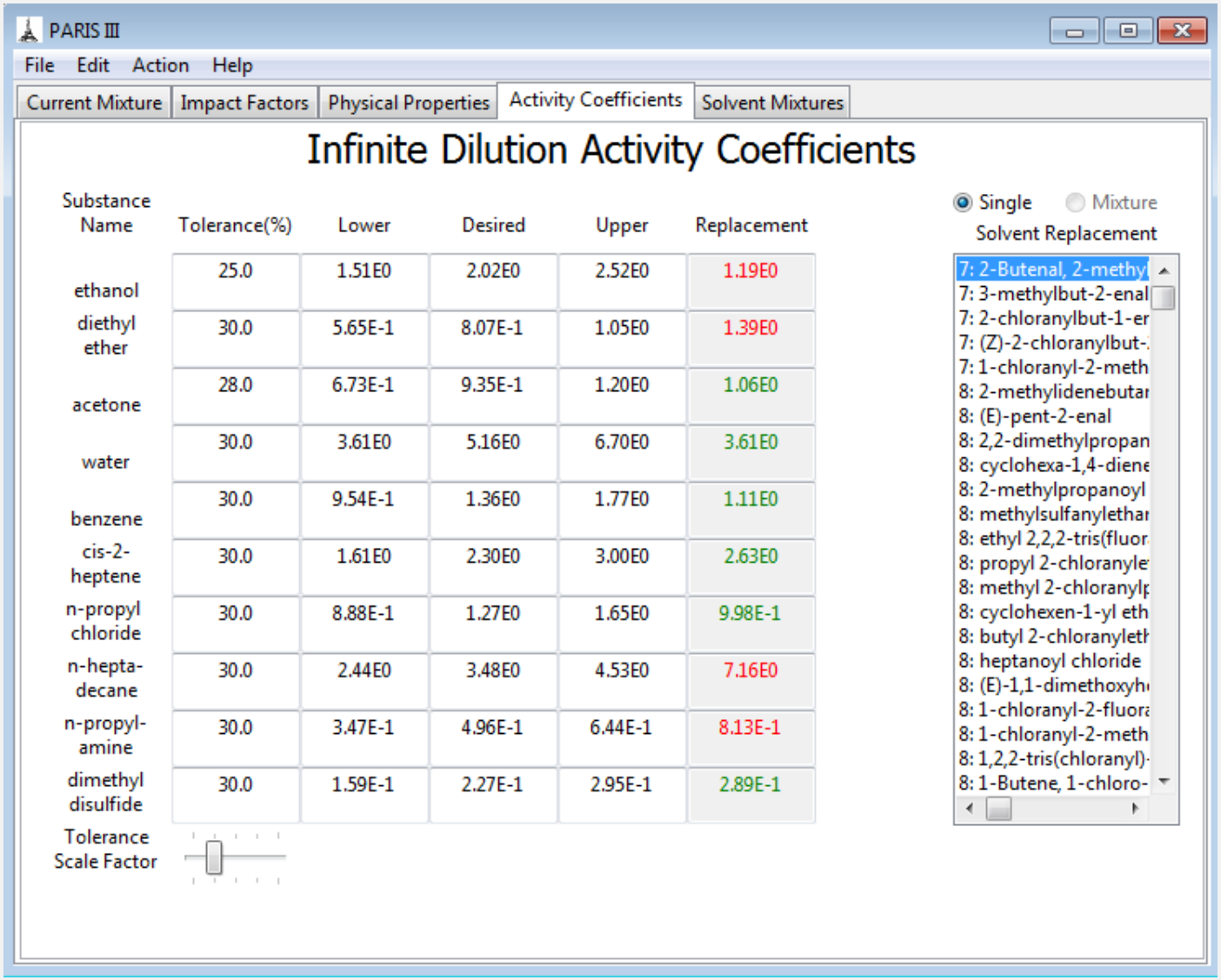



PARIS III
File Edit Action Help
Current Mixture
Impact Factors
Physical Properties
Activity Coefficients
Solvent Mixtures
Physical Properties
Single
Mixture
Solvent Replacement
Property
Tolerance(%)
Lower
Desired
Upper
Replacement
Units
Molecular Mass
11.0
70.512
79.227
87.942
84.12
kg/kmol
Liquid Density
14.0
8.14E2
9.47E2
1.08E3
8.30E2
kg/m3
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/s2
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
7: 2-Butenal, 2-methyl
7: 3-methylbut-2-enal
7: 2-chloranylbut-1-er
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-chloranylp
8: cyclohexen-1-yl eth
8: butyl 2-chloranyleth
8: heptanoyl chloride
8: (E)-1,1-dimethoxyh
8: 1-chloranyl-2-fluora
8: 1-chloranyl-2-meth
8: 1,2,2-tris(chloranyl)
8: 1-Butene, 1-chloro-


PARIS III
File Edit Action Help
Current Mixture
Impact Factors
Physical Properties
Activity Coefficients
Solvent Mixtures
Infinite Dilution Activity Coefficients
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-hepta-decane 30.0 2.44E0 3.48E0 4.53E0 7.16E0
n-propyl-amine 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
Single
Mixture
Solvent Replacement
7: 2-Butenal, 2-methyl
7: 3-methylbut-2-enal
7: 2-chloranylbut-1-er
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-chloranylp
8: cyclohexen-1-yl eth
8: butyl 2-chloranyleth
8: heptanoyl chloride
8: (E)-1,1-dimethoxyh
8: 1-chloranyl-2-fluora
8: 1-chloranyl-2-meth
8: 1,2,2-tris(chloranyl)
8: 1-Butene, 1-chloro-

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Modify Boundaries of the Replacement Search

- Change tolerance range percentages and re-calculate boundaries.
- Or, explicitly change desired property values and/or boundaries.
- Re-rank possible replacements

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Single Chemical Replacements Found

- Analyze properties of each replacement found.
- Pick replacements with properties closest to the original solvent and have lowest environmental indexes.

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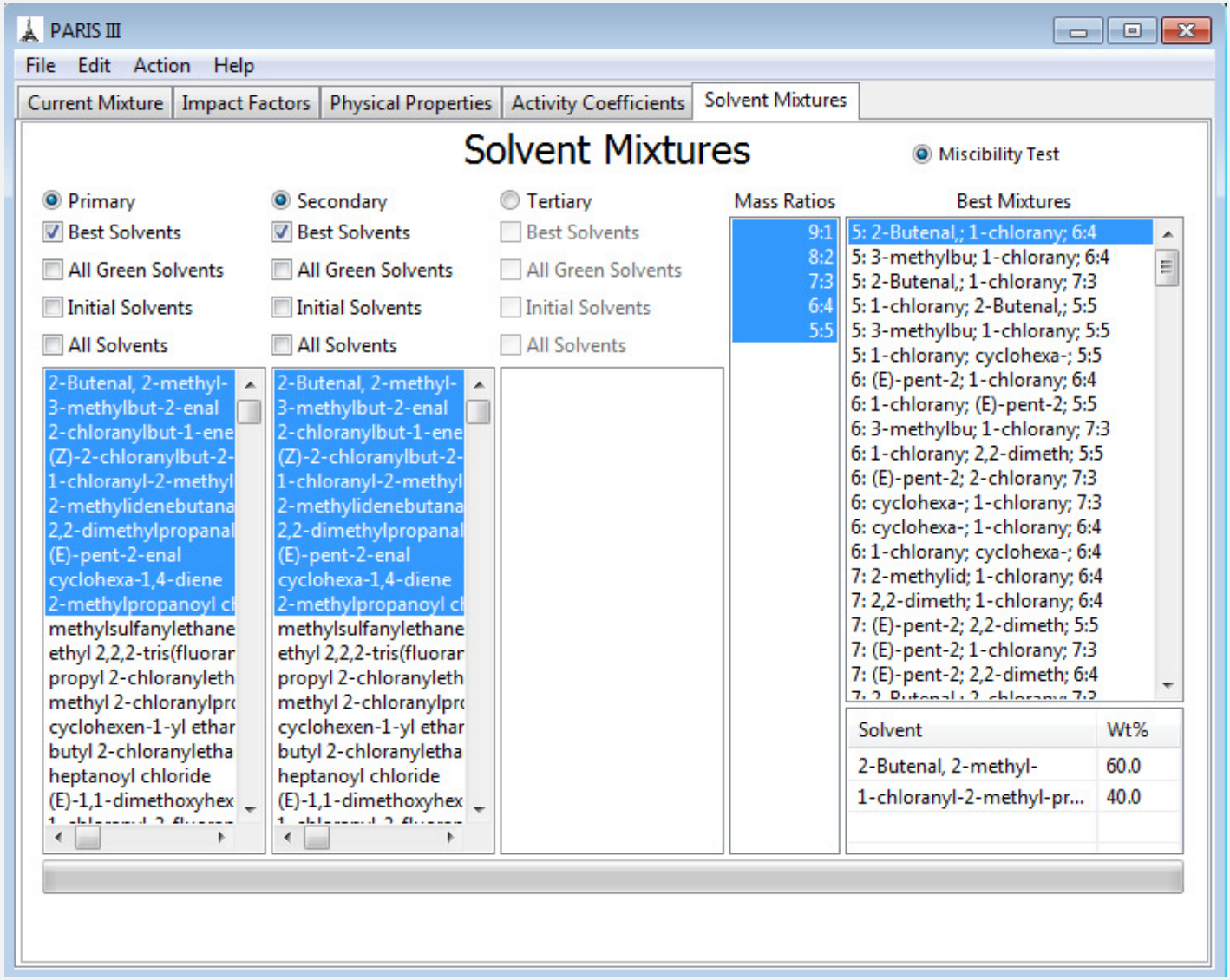
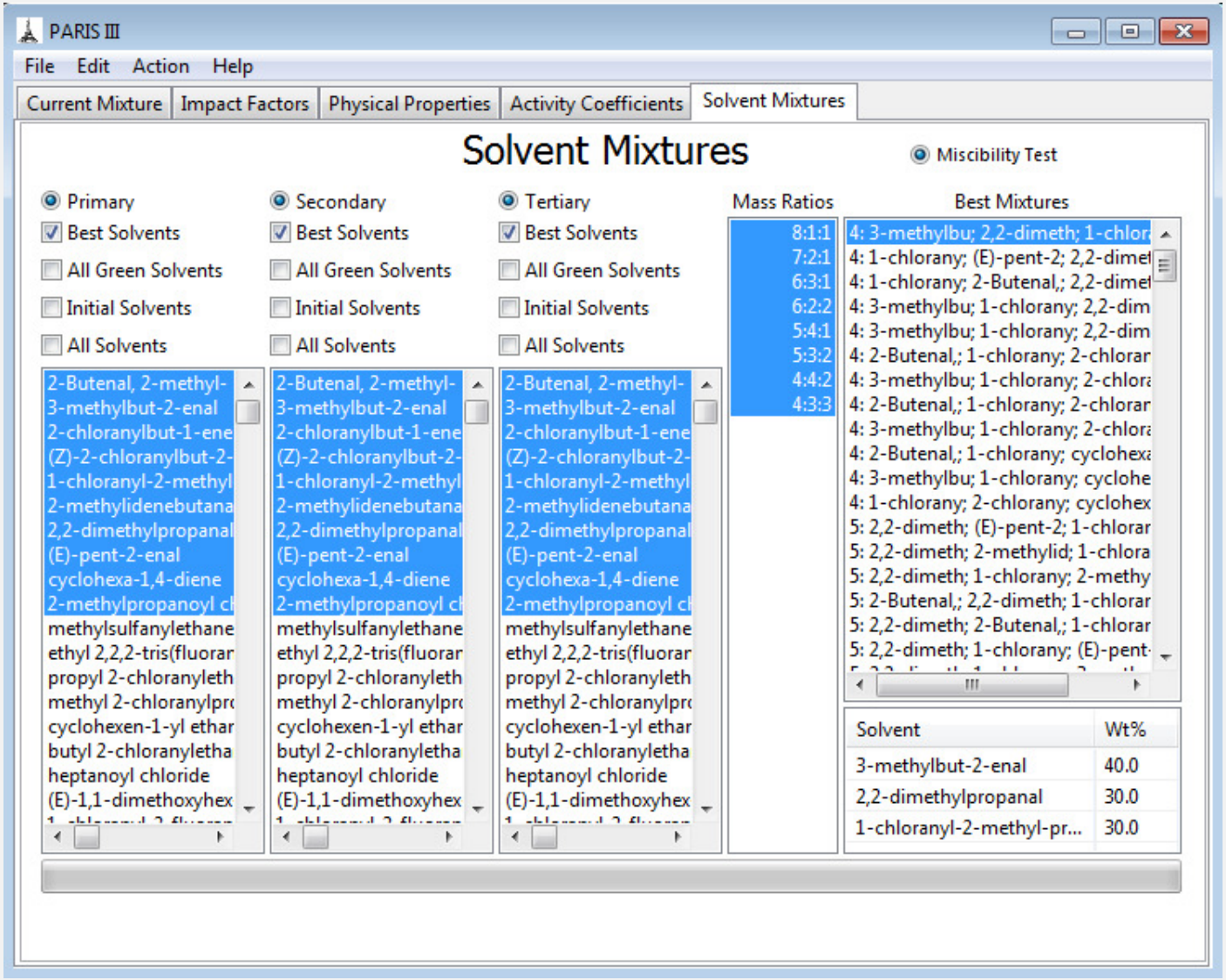
Replacement Mixtures

- What has been shown so far is single chemical replacement. This is only part of the solvent substitute solution.
- By calculating the properties of thousands of combinations of these ranked solvents, we can get even closer to finding greener replacements for the initial harmful solvent mixture.


PARIS III
File Edit Action Help
Current Mixture
Impact Factors
Physical Properties
Activity Coefficients
Solvent Mixtures
Solvent Mixtures
Miscibility Test
Primary
Secondary
Tertiary
Best Solvents
All Green Solvents
Initial Solvents
All Solvents
Mass Ratios
9:1
8:2
7:3
6:4
5:5
Best Mixtures
5: 2-Butenal,; 1-chlorany; 6:4
5: 3-methylbu; 1-chlorany; 6:4
5: 2-Butenal,; 1-chlorany; 7:3
5: 1-chlorany; 2-Butenal,; 5:5
5: 3-methylbu; 1-chlorany; 5:5
5: 1-chlorany; cyclohexa-; 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: 1-chlorany; 2,2-dimeth; 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: 2,2-dimeth; 1-chlorany; 6:4
7: (E)-pent-2; 2,2-dimeth; 5:5
7: (E)-pent-2; 1-chlorany; 7:3
7: (E)-pent-2; 2,2-dimeth; 6:4
2-Butenal, 2-methyl-
3-methylbut-2-enal
2-chloranylbut-1-ene
(Z)-2-chloranylbut-2-
1-chloranyl-2-methyl
2-methylidenebutana
2,2-dimethylpropanal
(E)-pent-2-enal
cyclohexa-1,4-diene
2-methylpropanoyl cl
methylsulfanylethane
ethyl 2,2,2-tris(fluorar
propyl 2-chloranyleth
methyl 2-chloranylpro
cyclohexen-1-yl ethar
butyl 2-chloranyletha
heptanoyl chloride
(E)-1,1-dimethoxyhex
Solvent
Wt%
2-Butenal, 2-methyl-
60.0
1-chloranyl-2-methyl-pr...
40.0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Activity Coefficients
Solvent Mixtures
Solvent Mixtures
Miscibility Test
Primary
Secondary
Tertiary
Best Solvents
All Green Solvents
Initial Solvents
All Solvents
Mass Ratios
Best Mixtures
8:1:1
7:2:1
6:3:1
6:2:2
5:4:1
5:3:2
4:4:2
4:3:3
Solvent
Wt%
3-methylbut-2-enal
40.0
2,2-dimethylpropanal
30.0
1-chloranyl-2-methyl-pr...
30.0

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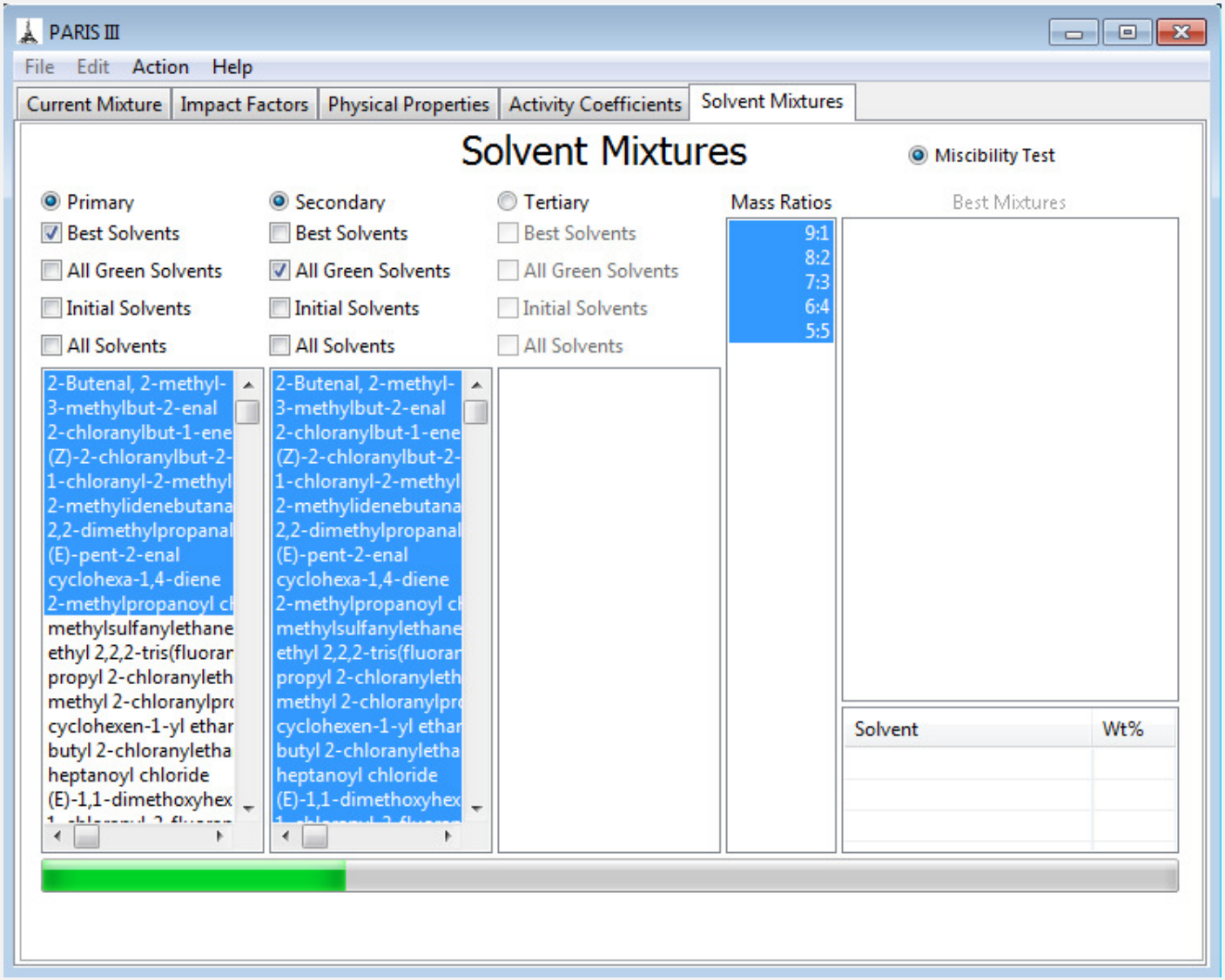

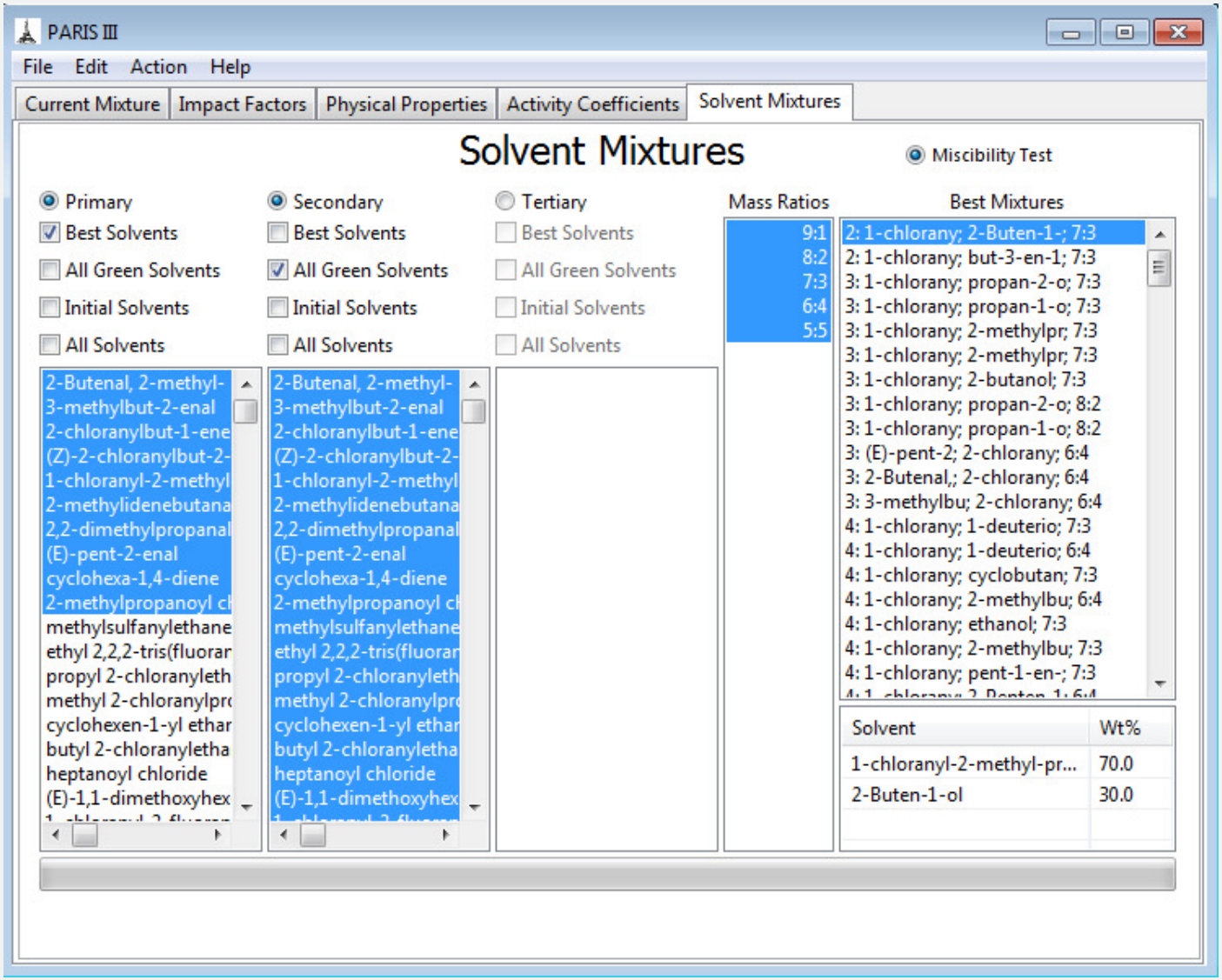
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Solvent Mixtures
Solvent Mixtures
Miscibility Test
Primary
Secondary
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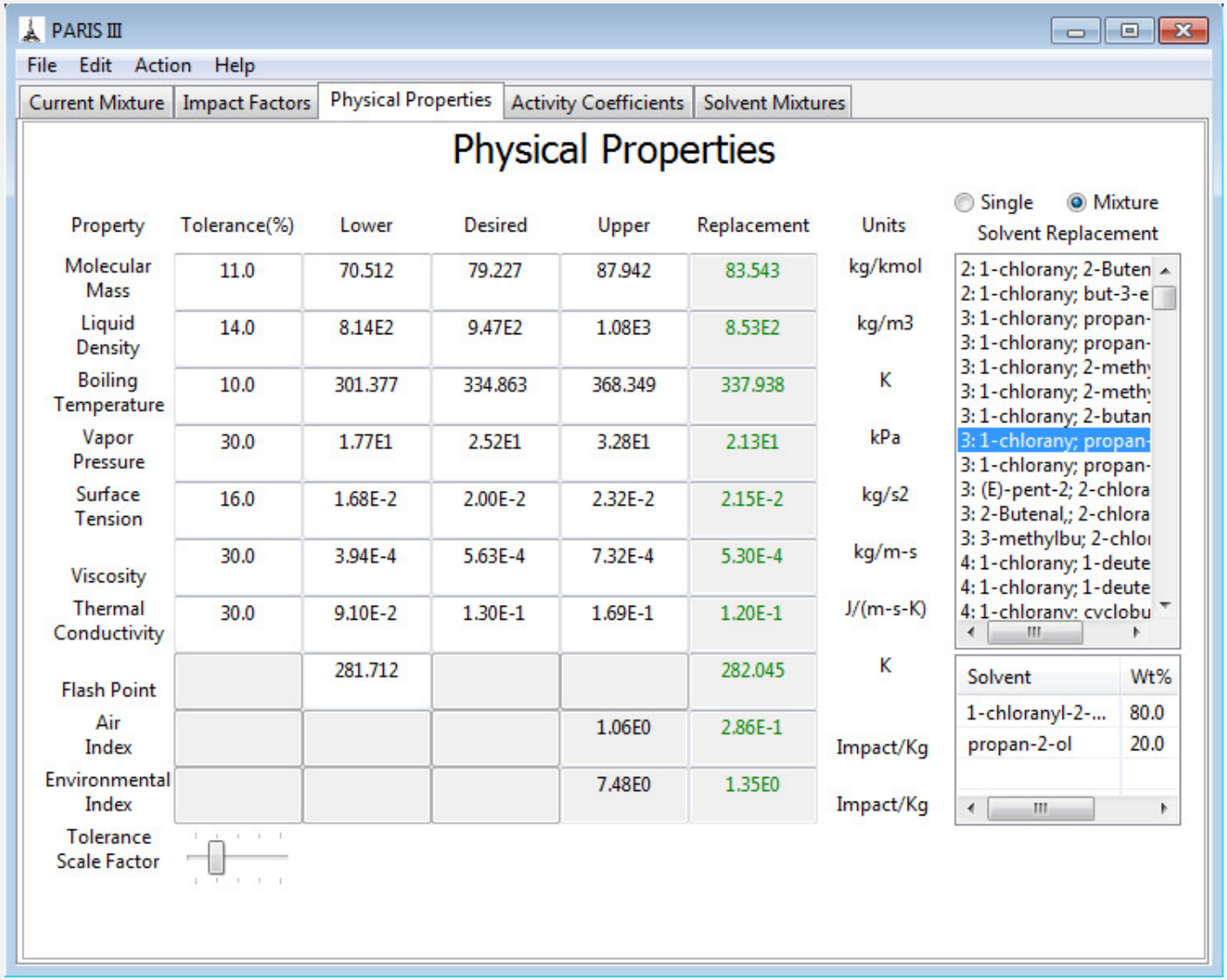
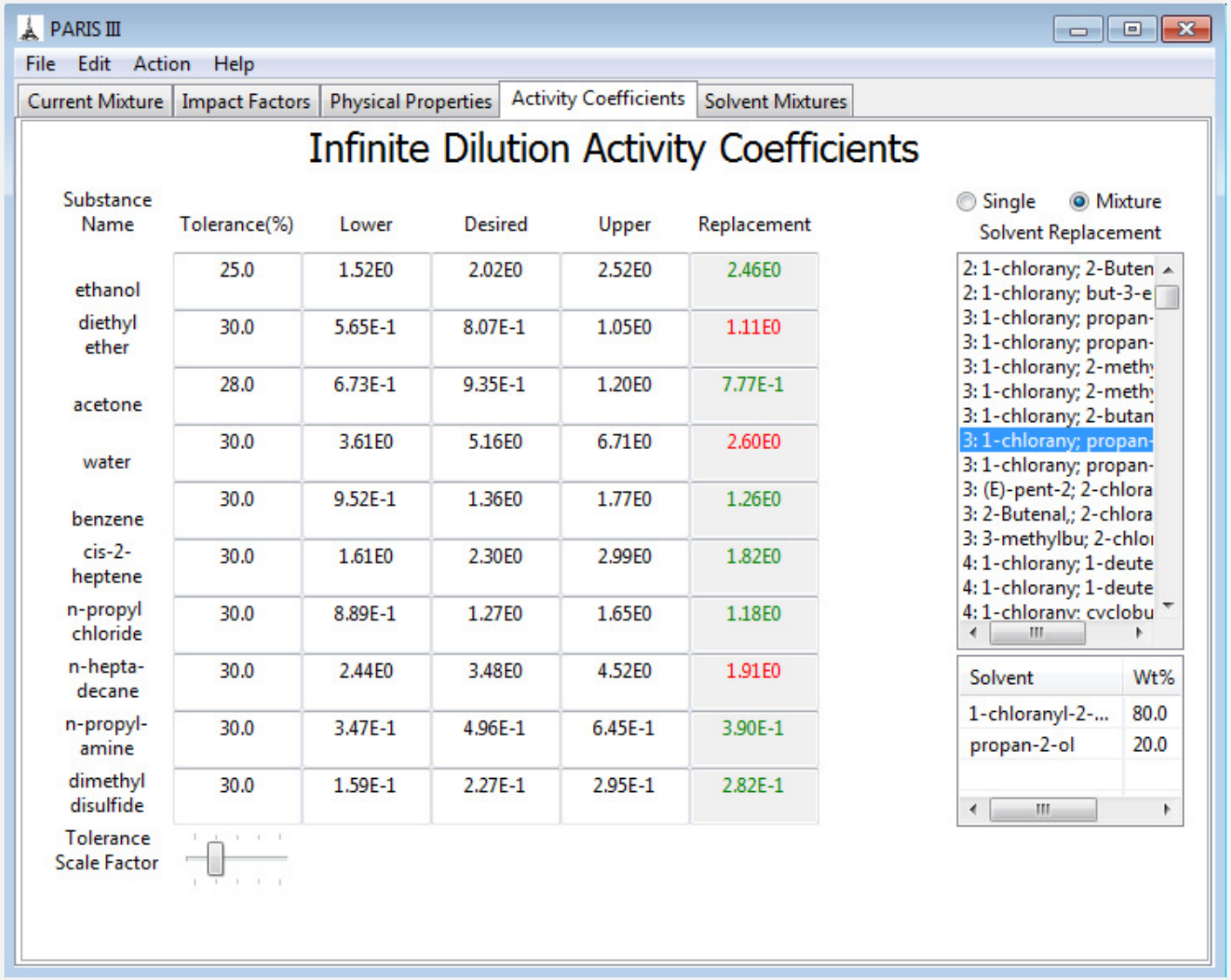
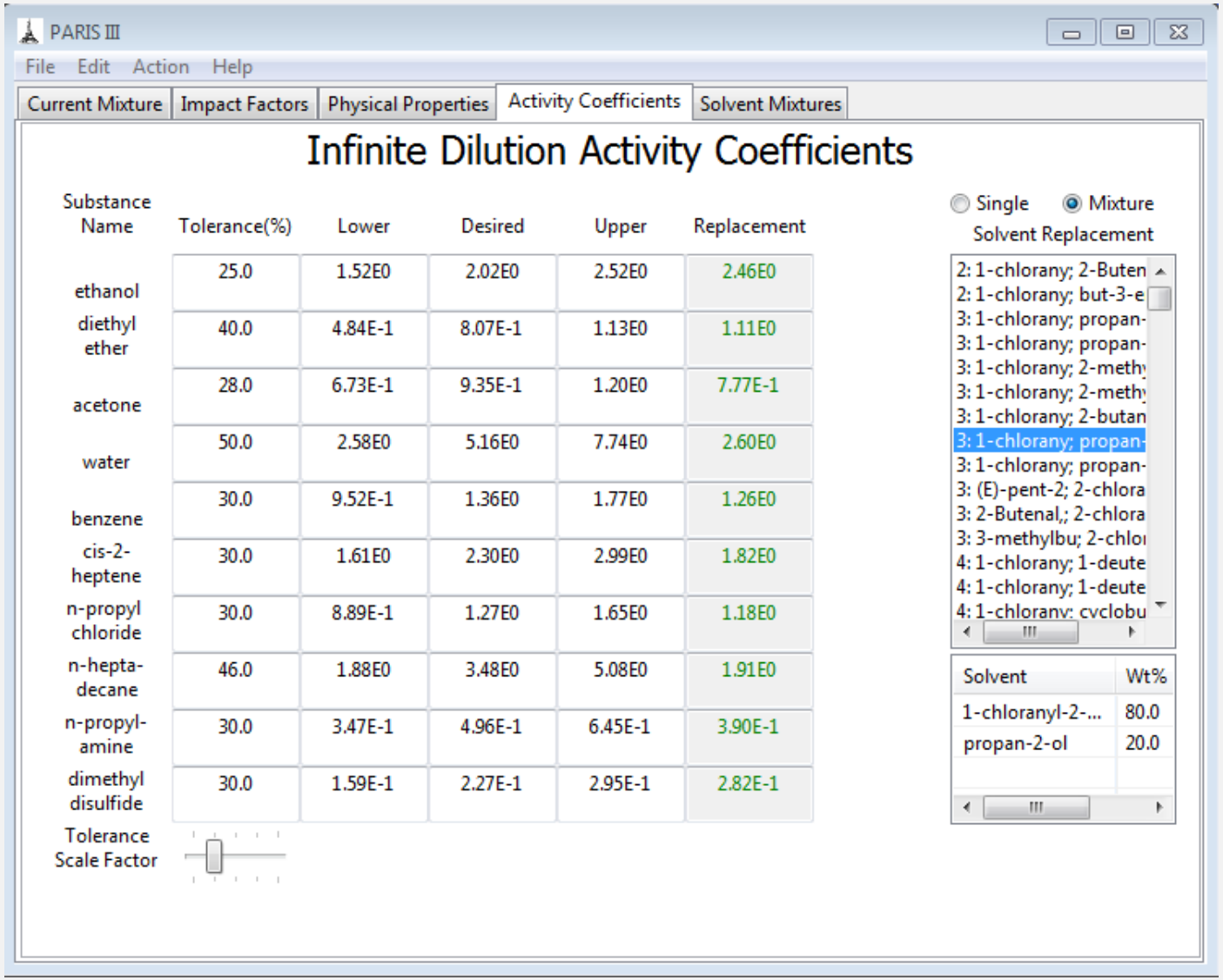
Best Solvents
All Green Solvents
Initial Solvents
All Solvents
Mass Ratios
Best Mixtures
9:1
8:2
7:3
6:4
5:5
2: 1-chlorany; 2-Buten-1-; 7:3
2: 1-chlorany; but-3-en-1; 7:3
3: 1-chlorany; propan-2-o; 7:3
3: 1-chlorany; propan-1-o; 7:3
3: 1-chlorany; 2-methylpr; 7:3
3: 1-chlorany; 2-methylpr; 7:3
3: 1-chlorany; 2-butanol; 7:3
3: 1-chlorany; propan-2-o; 8:2
3: 1-chlorany; propan-1-o; 8:2
3: (E)-pent-2; 2-chlorany; 6:4
3: 2-Butenal,; 2-chlorany; 6:4
3: 3-methylbu; 2-chlorany; 6:4
4: 1-chlorany; 1-deuterio; 7:3
4: 1-chlorany; 1-deuterio; 6:4
4: 1-chlorany; cyclobutan; 7:3
4: 1-chlorany; 2-methylbu; 6:4
4: 1-chlorany; ethanol; 7:3
4: 1-chlorany; 2-methylbu; 7:3
4: 1-chlorany; pent-1-en-; 7:3
2-Butenal, 2-methyl-
3-methylbut-2-enal
2-chloranylbut-1-ene
(Z)-2-chloranylbut-2-
1-chloranyl-2-methyl
2-methylidenebutana
2,2-dimethylpropanal
(E)-pent-2-enal
cyclohexa-1,4-diene
2-methylpropanoyl ch
methylsulfanylethane
ethyl 2,2,2-tris(fluorar
propyl 2-chloranyleth
methyl 2-chloranylpro
cyclohexen-1-yl ethar
butyl 2-chloranyletha
heptanoyl chloride
(E)-1,1-dimethoxyhex
Solvent
Wt%
1-chloranyl-2-methyl-pr...
70.0
2-Buten-1-ol
30.0


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
83.543
kg/kmol
Liquid Density
14.0
8.14E2
9.47E2
1.08E3
8.53E2
kg/m3
Boiling Temperature
10.0
301.377
334.863
368.349
337.938
K
Vapor Pressure
30.0
1.77E1
2.52E1
3.28E1
2.13E1
kPa
Surface Tension
16.0
1.68E-2
2.00E-2
2.32E-2
2.15E-2
kg/s2
Viscosity
30.0
3.94E-4
5.63E-4
7.32E-4
5.30E-4
kg/m-s
Thermal Conductivity
30.0
9.10E-2
1.30E-1
1.69E-1
1.20E-1
J/(m-s-K)
Flash Point
281.712
282.045
K
Air Index
1.06E0
2.86E-1
Impact/Kg
Environmental Index
7.48E0
1.35E0
Impact/Kg
Tolerance Scale Factor
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-meth
3: 1-chlorany; 2-butan
3: 1-chlorany; propan-
3: 1-chlorany; propan-
3: (E)-pent-2; 2-chlora
3: 2-Butenal,; 2-chlora
3: 3-methylbu; 2-chlo
4: 1-chlorany; 1-deute
4: 1-chlorany; 1-deute
4: 1-chloranv: cvclobu
Solvent
Wt%
1-chloranyl-2-...
80.0
propan-2-ol
20.0


PARIS III
File Edit Action Help
Current Mixture
Impact Factors
Physical Properties
Activity Coefficients
Solvent Mixtures
Infinite Dilution Activity Coefficients
Substance Name
Tolerance(%)
Lower
Desired
Upper
Replacement
ethanol 25.0 1.52E0 2.02E0 2.52E0 2.46E0
diethyl ether 30.0 5.65E-1 8.07E-1 1.05E0 1.11E0
acetone 28.0 6.73E-1 9.35E-1 1.20E0 7.77E-1
water 30.0 3.61E0 5.16E0 6.71E0 2.60E0
benzene 30.0 9.52E-1 1.36E0 1.77E0 1.26E0
cis-2-heptene 30.0 1.61E0 2.30E0 2.99E0 1.82E0
n-propyl chloride 30.0 8.89E-1 1.27E0 1.65E0 1.18E0
n-hepta-decane 30.0 2.44E0 3.48E0 4.52E0 1.91E0
n-propyl-amine 30.0 3.47E-1 4.96E-1 6.45E-1 3.90E-1
dimethyl disulfide 30.0 1.59E-1 2.27E-1 2.95E-1 2.82E-1
Tolerance Scale Factor
Single
Mixture
Solvent Replacement
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-meth
3: 1-chlorany; 2-butan
3: 1-chlorany; propan-
3: 1-chlorany; propan-
3: (E)-pent-2; 2-chlora
3: 2-Butenal,; 2-chlora
3: 3-methylbu; 2-chlo
4: 1-chlorany; 1-deute
4: 1-chlorany; 1-deute
4: 1-chloranv: cvclobu
Solvent
Wt%
1-chloranyl-2-... 80.0
propan-2-ol 20.0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Current Mixture
Impact Factors
Physical Properties
Activity Coefficients
Solvent Mixtures
Infinite Dilution Activity Coefficients
Substance Name
Tolerance(%)
Lower
Desired
Upper
Replacement
ethanol 25.0 1.52E0 2.02E0 2.52E0 2.46E0
diethyl ether 40.0 4.84E-1 8.07E-1 1.13E0 1.11E0
acetone 28.0 6.73E-1 9.35E-1 1.20E0 7.77E-1
water 50.0 2.58E0 5.16E0 7.74E0 2.60E0
benzene 30.0 9.52E-1 1.36E0 1.77E0 1.26E0
cis-2-heptene 30.0 1.61E0 2.30E0 2.99E0 1.82E0
n-propyl chloride 30.0 8.89E-1 1.27E0 1.65E0 1.18E0
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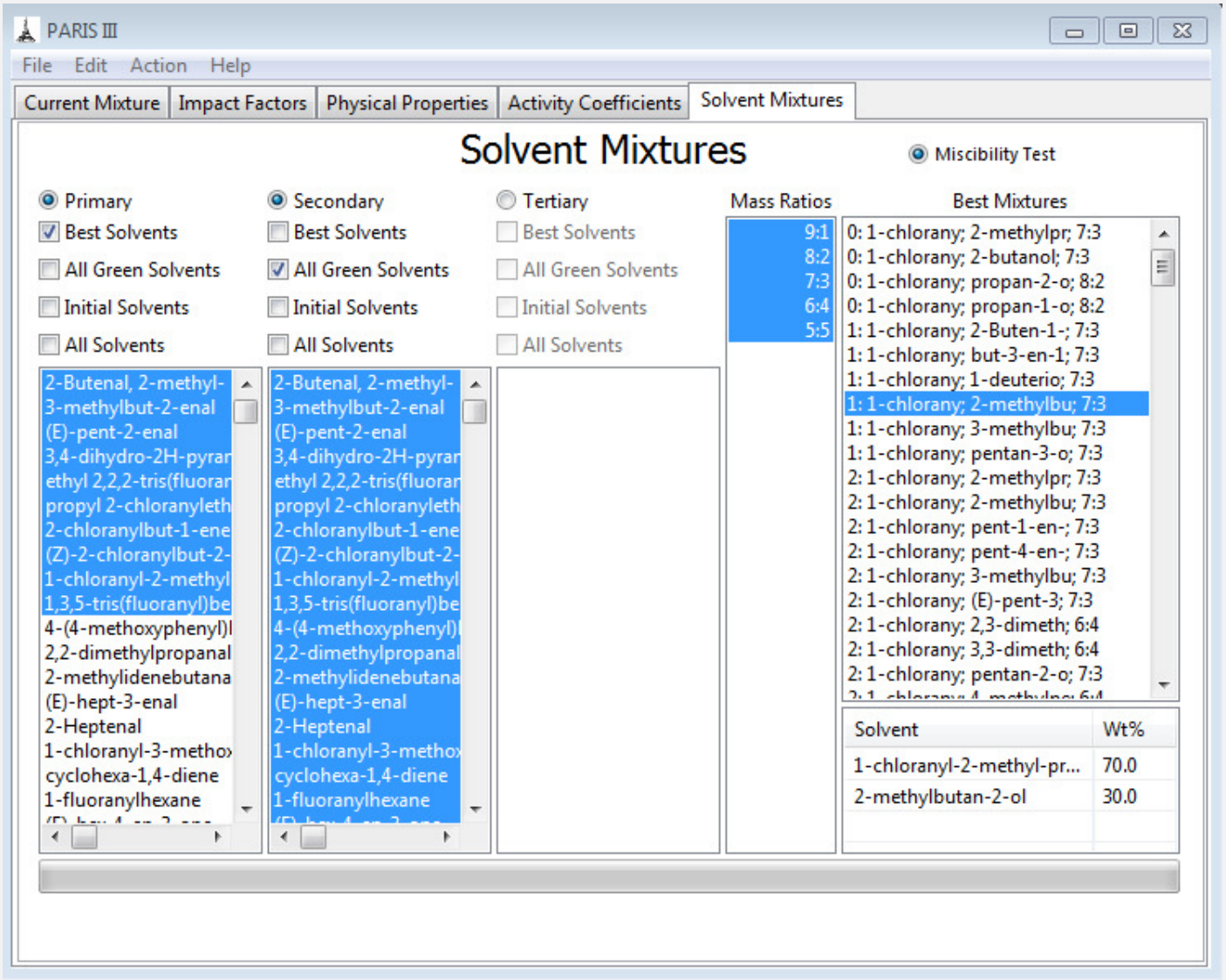
n-propyl-amine 30.0 3.47E-1 4.96E-1 6.45E-1 3.90E-1
dimethyl disulfide 30.0 1.59E-1 2.27E-1 2.95E-1 2.82E-1
Tolerance Scale Factor
Single
Mixture
Solvent Replacement
2: 1-chlorany; 2-Buten
2: 1-chlorany; but-3-e
3: 1-chlorany; propan-
3: 1-chlorany; propan-
3: 1-chlorany; 2-meth
3: 1-chlorany; 2-meth
3: 1-chlorany; 2-butan
3: 1-chlorany; propan-
3: 1-chlorany; propan-
3: (E)-pent-2; 2-chlora
3: 2-Butenal,; 2-chlora
3: 3-methylbu; 2-chlo
4: 1-chlorany; 1-deute
4: 1-chlorany; 1-deute
4: 1-chloranv: cvclobu
Solvent
Wt%
1-chloranyl-2-...
80.0
propan-2-ol
20.0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Current Mixture
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Physical Properties
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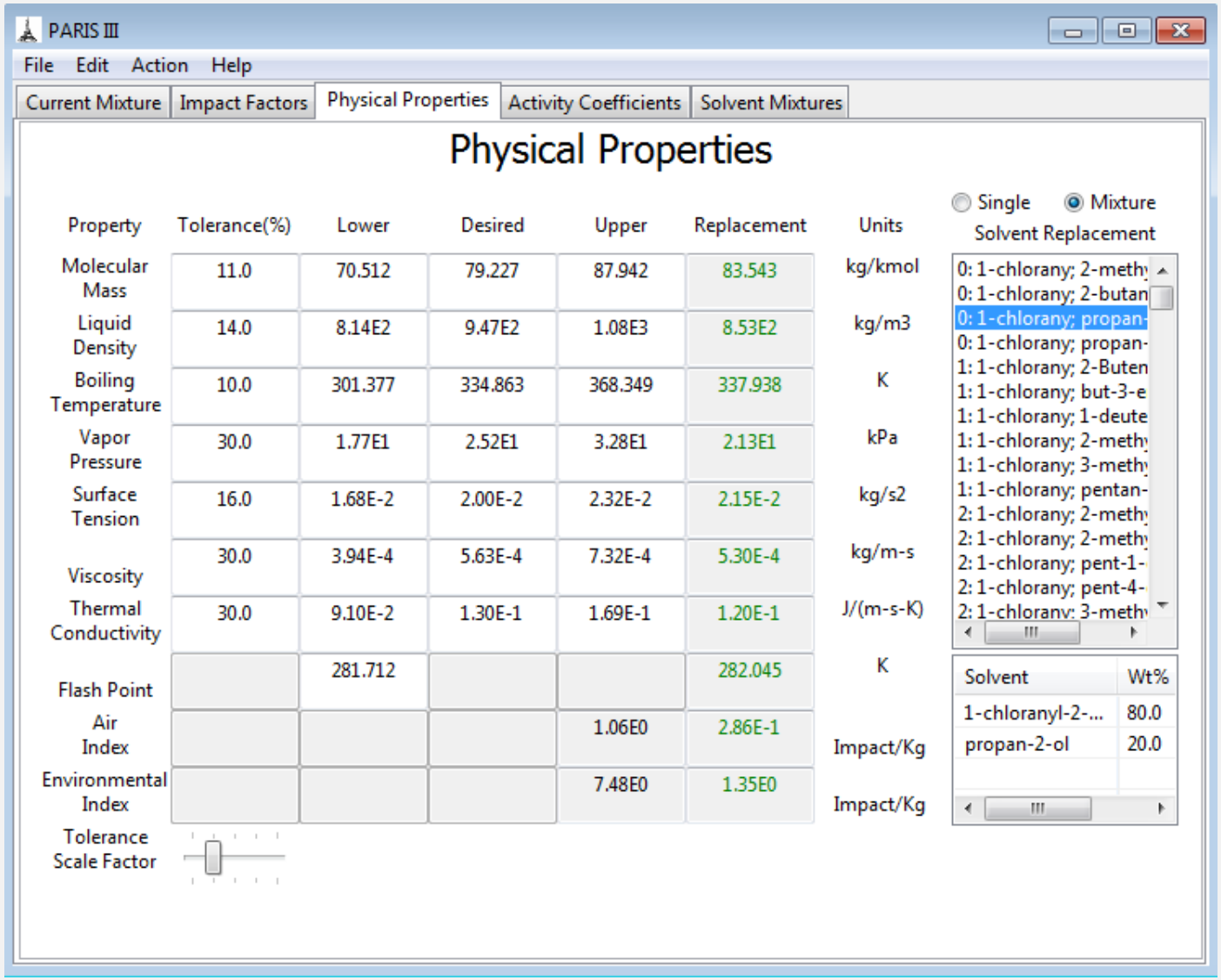
Solvent Mixtures
Solvent Mixtures
Miscibility Test
Primary
Secondary
Tertiary
Best Solvents
All Green Solvents
Initial Solvents
All Solvents
Mass Ratios
9:1
8:2
7:3
6:4
5:5
Best Mixtures
0: 1-chlorany; 2-methylpr; 7:3
0: 1-chlorany; 2-butanol; 7:3
0: 1-chlorany; propan-2-o; 8:2
0: 1-chlorany; propan-1-o; 8:2
1: 1-chlorany; 2-Buten-1-; 7:3
1: 1-chlorany; but-3-en-1; 7:3
1: 1-chlorany; 1-deuterio; 7:3
1: 1-chlorany; 2-methylbu; 7:3
1: 1-chlorany; 3-methylbu; 7:3
1: 1-chlorany; pentan-3-o; 7:3
2: 1-chlorany; 2-methylpr; 7:3
2: 1-chlorany; 2-methylbu; 7:3
2: 1-chlorany; pent-1-en-; 7:3
2: 1-chlorany; pent-4-en-; 7:3
2: 1-chlorany; 3-methylbu; 7:3
2: 1-chlorany; (E)-pent-3; 7:3
2: 1-chlorany; 2,3-dimeth; 6:4
2: 1-chlorany; 3,3-dimeth; 6:4
2: 1-chlorany; pentan-2-o; 7:3
2-Butenal, 2-methyl-
3-methylbut-2-enal
(E)-pent-2-enal
3,4-dihydro-2H-pyran
ethyl 2,2,2-tris(fluoran
propyl 2-chloranyleth
2-chloranylbut-1-ene
(Z)-2-chloranylbut-2-
1-chloranyl-2-methyl
1,3,5-tris(fluoranyl)be
4-(4-methoxyphenyl)
2,2-dimethylpropanal
2-methylidenebutana
(E)-hept-3-enal
2-Heptenal
1-chloranyl-3-metho
cyclohexa-1,4-diene
1-fluoranylhexane
Solvent
Wt%
1-chloranyl-2-methyl-pr...
70.0
2-methylbutan-2-ol
30.0


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
83.543
kg/kmol
Liquid Density
14.0
8.14E2
9.47E2
1.08E3
8.53E2
kg/m3
Boiling Temperature
10.0
301.377
334.863
368.349
337.938
K
Vapor Pressure
30.0
1.77E1
2.52E1
3.28E1
2.13E1
kPa
Surface Tension
16.0
1.68E-2
2.00E-2
2.32E-2
2.15E-2
kg/s2
Viscosity
30.0
3.94E-4
5.63E-4
7.32E-4
5.30E-4
kg/m-s
Thermal Conductivity
30.0
9.10E-2
1.30E-1
1.69E-1
1.20E-1
J/(m-s-K)
Flash Point
281.712
282.045
K
Air Index
1.06E0
2.86E-1
Impact/Kg
Environmental Index
7.48E0
1.35E0
Impact/Kg
Tolerance Scale Factor
0: 1-chlorany; 2-methy
0: 1-chlorany; 2-butan
0: 1-chlorany; propan-
0: 1-chlorany; propan-
1: 1-chlorany; 2-Buten
1: 1-chlorany; but-3-e
1: 1-chlorany; 1-deute
1: 1-chlorany; 2-methy
1: 1-chlorany; 3-methy
1: 1-chlorany; pentan-
2: 1-chlorany; 2-methy
2: 1-chlorany; 2-methy
2: 1-chlorany; pent-1-
2: 1-chlorany; pent-4-
2: 1-chloranv; 3-methy
Solvent
Wt%
1-chloranyl-2-...
80.0
propan-2-ol
20.0

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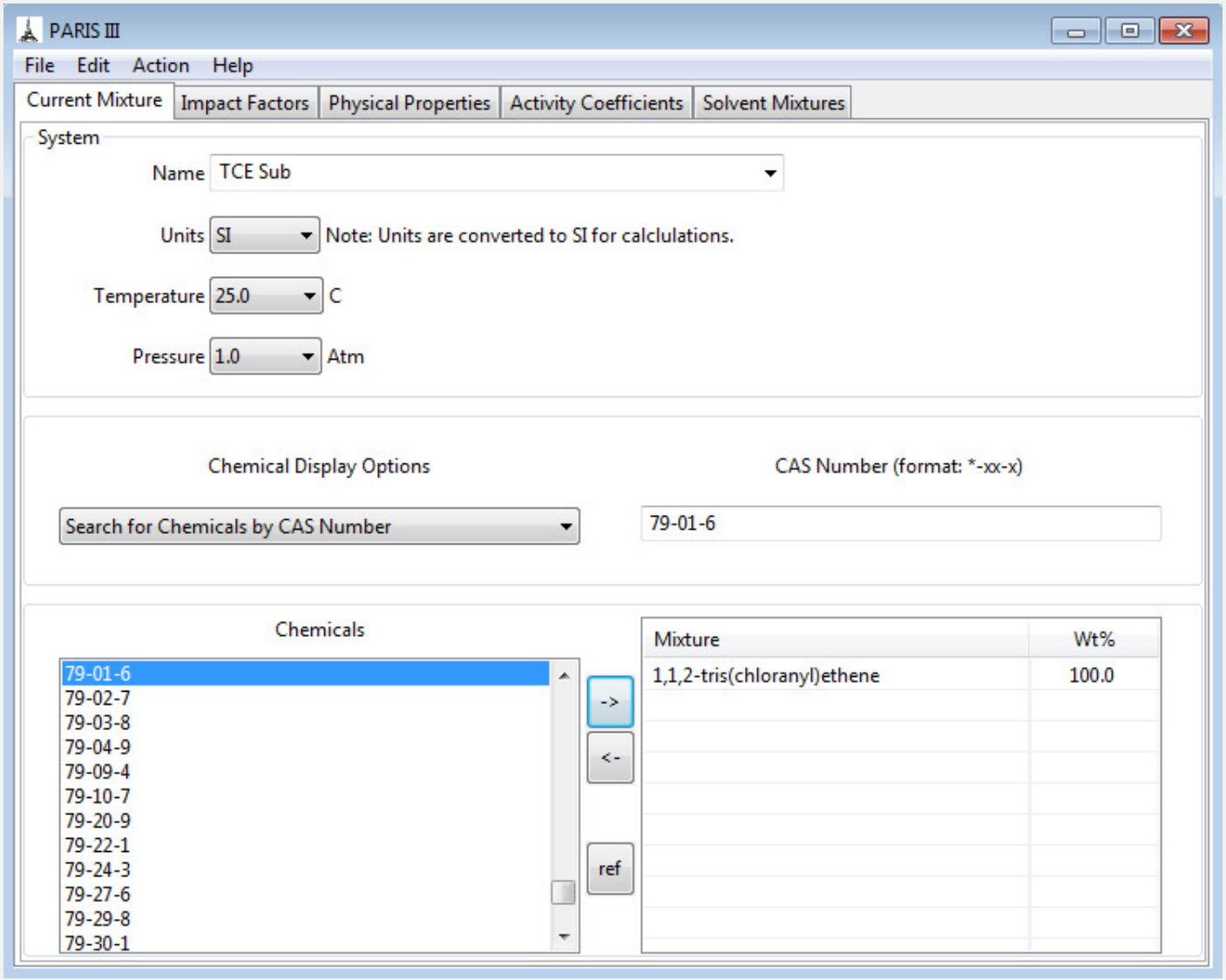
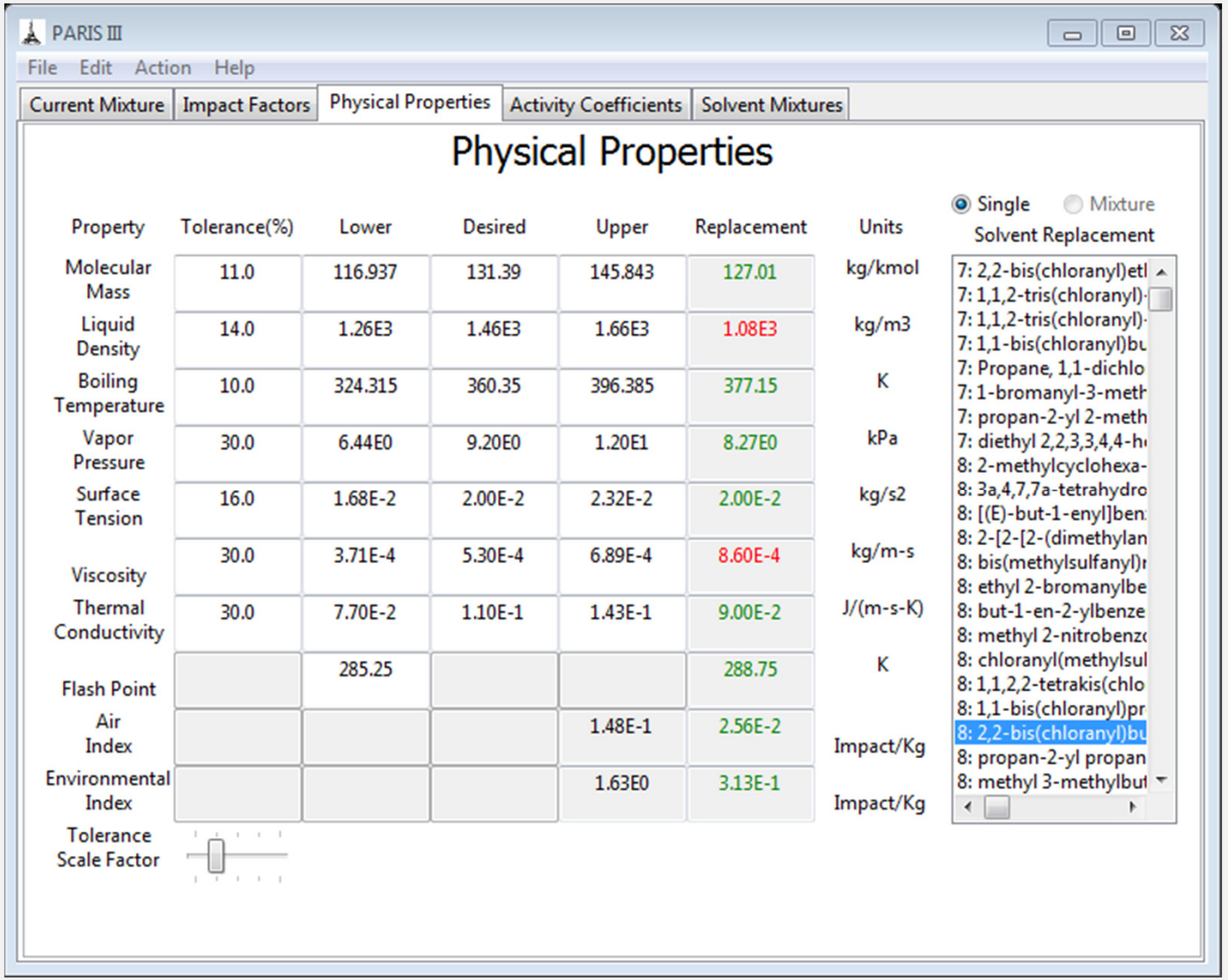
Another Replacement Example

A replacement search can be performed using a different set of priorities. For example, we can look for a replacement for TCE that has similar vapor degreasing properties, but a very low air index.


PARIS III
File Edit Action Help
Current Mixture
Impact Factors
Physical Properties
Activity Coefficients
Solvent Mixtures
System
Name TCE Sub
Units SI
Note: Units are converted to SI for calclulations.
Temperature 25.0 C
Pressure 1.0 Atm
Chemical Display Options
CAS Number (format: *-xx-x)
Search for Chemicals by CAS Number
79-01-6
Chemicals
79-01-6
79-02-7
79-03-8
79-04-9
79-09-4
79-10-7
79-20-9
79-22-1
79-24-3
79-27-6
79-29-8
79-30-1
->
<-
ref
Mixture
Wt%
1,1,2-tris(chloranyl)ethene
100.0


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
116.937
131.39
145.843
127.01
kg/kmol
Liquid Density
14.0
1.26E3
1.46E3
1.66E3
1.08E3
kg/m3
Boiling Temperature
10.0
324.315
360.35
396.385
377.15
K
Vapor Pressure
30.0
6.44E0
9.20E0
1.20E1
8.27E0
kPa
Surface Tension
16.0
1.68E-2
2.00E-2
2.32E-2
2.00E-2
kg/s2
Viscosity
30.0
3.71E-4
5.30E-4
6.89E-4
8.60E-4
kg/m-s
Thermal Conductivity
30.0
7.70E-2
1.10E-1
1.43E-1
9.00E-2
J/(m-s-K)
Flash Point
285.25
288.75
K
Air Index
1.48E-1
2.56E-2
Impact/Kg
Environmental Index
1.63E0
3.13E-1
Impact/Kg
Tolerance Scale Factor
7: 2,2-bis(chloranyl)etl
7: 1,1,2-tris(chloranyl)
7: 1,1,2-tris(chloranyl)
7: 1,1-bis(chloranyl)bu
7: Propane, 1,1-dichlo
7: 1-bromanyl-3-meth
7: propan-2-yl 2-meth
7: diethyl 2,2,3,3,4,4-h
8: 2-methylcyclohexa-
8: 3a,4,7,7a-tetrahydro
8: [(E)-but-1-enyl]ben
8: 2-[2-[2-(dimethylan
8: bis(methylsulfanyl)
8: ethyl 2-bromanylbe
8: but-1-en-2-ylbenze
8: methyl 2-nitrobenz
8: chloranyl(methylsul
8: 1,1,2,2-tetrakis(chlo
8: 1,1-bis(chloranyl)pr
8: 2,2-bis(chloranyl)bu
8: propan-2-yl propan
8: methyl 3-methylbut

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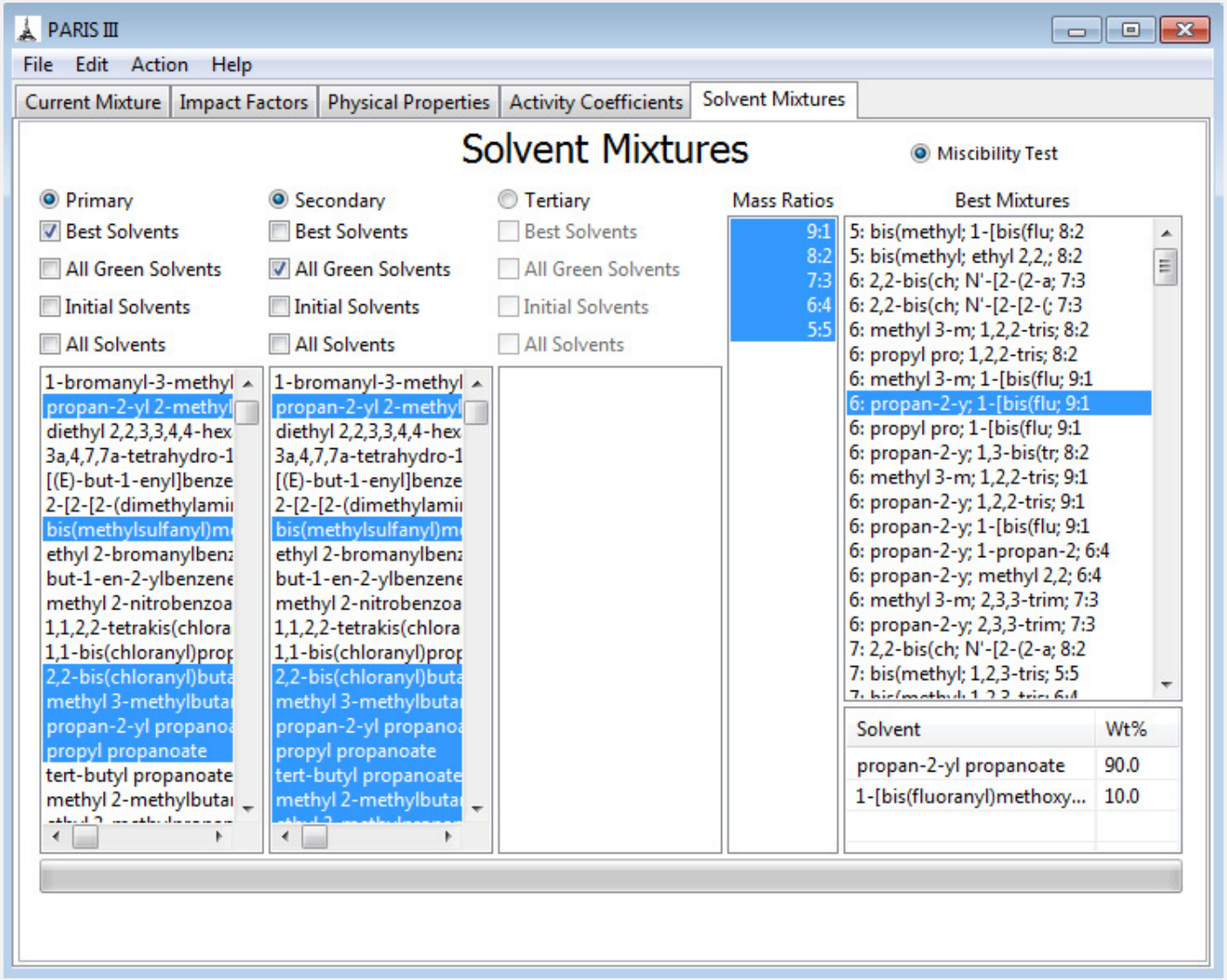
Single Solvent Replacements for Trichloroethylene (TCE)

1) propan-2-yl 2-methylpropanoate reduces harmful impact to the air by a factor of 15.67, and to the environment by a factor of 3.62.
2) 2,2-bis(chloranyl)butane reduces harmful impact to the air by a factor of 4.65, and to the environment by a factor of 4.19.


PARIS III
File Edit Action Help
Current Mixture
Impact Factors
Physical Properties
Activity Coefficients
Solvent Mixtures
Solvent Mixtures
Miscibility Test
Primary
Secondary
Tertiary
Best Solvents
All Green Solvents
Initial Solvents
All Solvents
Mass Ratios
9:1
8:2
7:3
6:4
5:5
Best Mixtures
5: bis(methyl; 1-[bis(flu; 8:2
5: bis(methyl; ethyl 2,2,; 8:2
6: 2,2-bis(ch; N'-[2-(2-a; 7:3
6: 2,2-bis(ch; N'-[2-[2-(; 7:3
6: methyl 3-m; 1,2,2-tris; 8:2
6: propyl pro; 1,2,2-tris; 8:2
6: methyl 3-m; 1-[bis(flu; 9:1
6: propan-2-y; 1-[bis(flu; 9:1
6: propyl pro; 1-[bis(flu; 9:1
6: propan-2-y; 1,3-bis(tr; 8:2
6: methyl 3-m; 1,2,2-tris; 9:1
6: propan-2-y; 1,2,2-tris; 9:1
6: propan-2-y; 1-[bis(flu; 9:1
6: propan-2-y; 1-propan-2; 6:4
6: propan-2-y; methyl 2,2; 6:4
6: methyl 3-m; 2,3,3-trim; 7:3
6: propan-2-y; 2,3,3-trim; 7:3
7: 2,2-bis(ch; N'-[2-(2-a; 8:2
7: bis(methyl; 1,2,3-tris; 5:5
1-bromanyl-3-methyl
propan-2-yl 2-methyl
diethyl 2,2,3,3,4,4-hex
3a,4,7,7a-tetrahydro-1
[(E)-but-1-enyl]benze
2-[2-[2-(dimethylamii
bis(methylsulfanyl)m
ethyl 2-bromanylbenz
but-1-en-2-ylbenzene
methyl 2-nitrobenzoa
1,1,2,2-tetrakis(chlora
1,1-bis(chloranyl)prop
2,2-bis(chloranyl)buta
methyl 3-methylbutar
propan-2-yl propanoa
propyl propanoate
tert-butyl propanoate
methyl 2-methylbutar
Solvent
Wt%
propan-2-yl propanoate
90.0
1-[bis(fluoranyl)methoxy...
10.0

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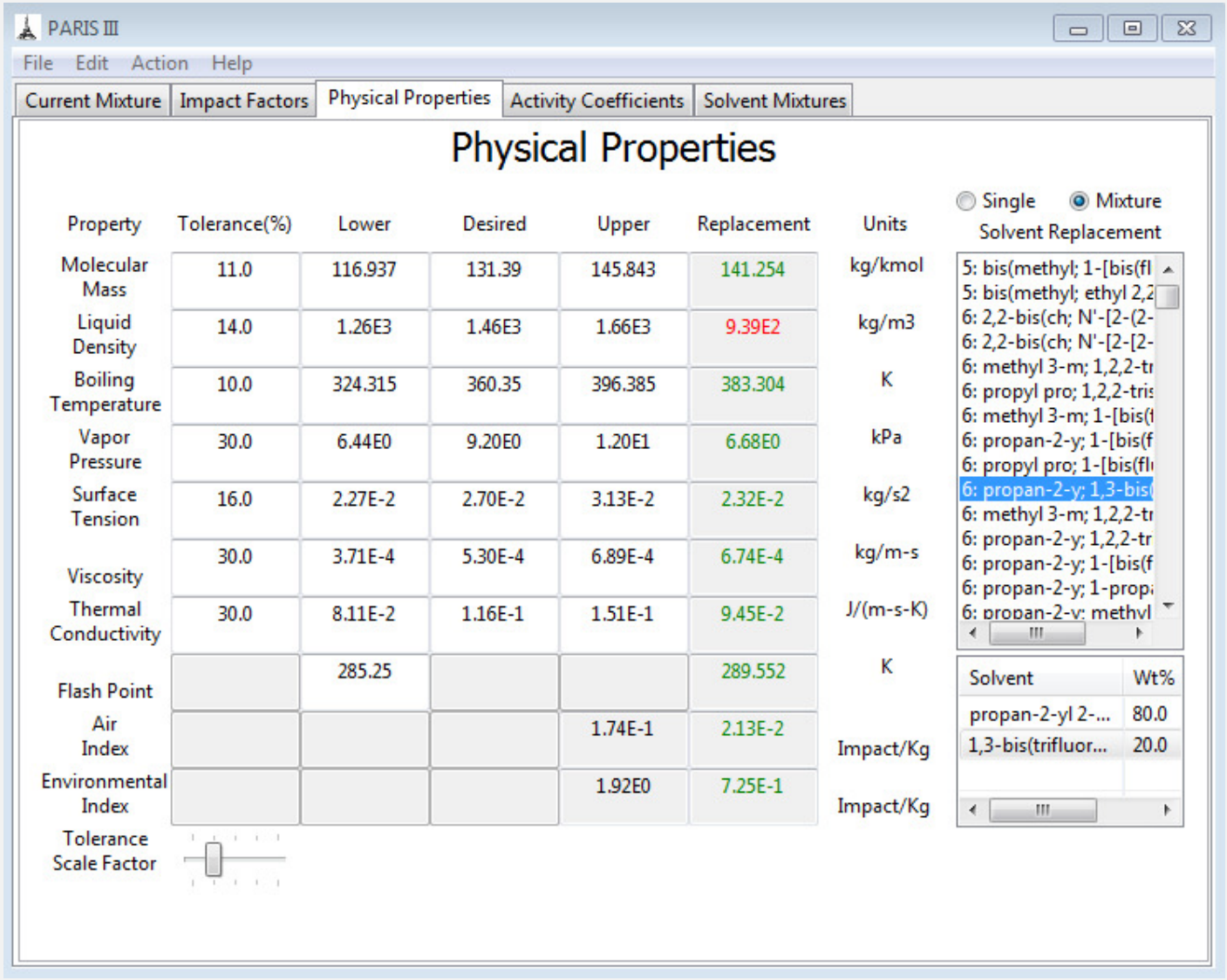

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Solvent Mixture Replacements for TCE

1) 80% propan-2-yl 2-methylpropanoate
   20% 1,3-bis(trifluromethyl)benzene
   Reduces air impact by 8.17, and environmental impact by 2.64.
2) 80% bis(methylsulfanyl)methane
   20% 1-[bis(flouranyl)methoxy]-2…
   Reduces air impact by 6.69, and environmental impact by 2.34.

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Final Step

The final step of all searches for greener solvent mixtures is to verify they serve as good replacements in the original industrial processes.

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Conclusions

PARIS III is a very strong and versatile tool to find greener solvent replacements for those currently used by industry.

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Acknowledgements

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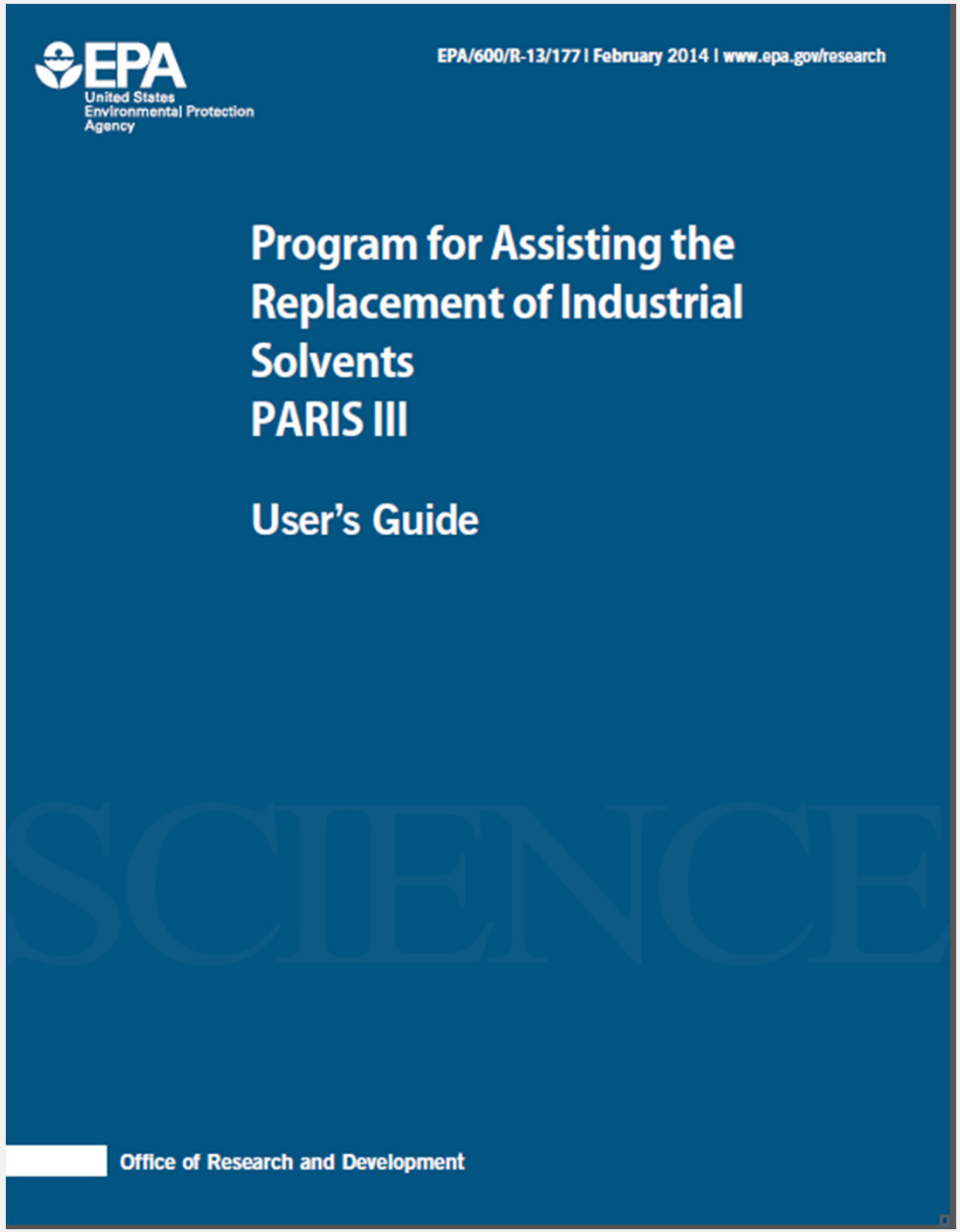
- Dr. Douglas Young, Chemical Engineer
- Dr. Heriberto Cabezas, Chemical Engineer

Free Public Domain Software at EPA Website

https://www.epa.gov/chemical-research/program-assisting-replacement-industrial-solvents-paris-iii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United States
Environmental Protection
Agency
EPA/600/R-13/177 | February 2014 | www.epa.gov/research
Program for Assisting the Replacement of Industrial Solvents PARIS III
User's Guide
SCIENCE
Office of Research and Development

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EPA Solvent Substitution Software Tool

- PARIS III -

Download Website:

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


Program for Assisting the
www.epa.gov/chemical-research/program-assisting-replacement-industrial-solvents-paris-iii
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Program for Assisting the Replacement of Industrial Solvents (PARIS III)
You will need Adobe Reader to view some of the files on this page. See EPA's About PDF page to learn more.
Solvent Substitution Software Tool, PARIS III, is a desktop/laptop application that allows users to find mixtures of solvents with specific physical and chemical properties, that also have relatively low environmental impacts. The software helps users find replacements for solvent mixtures that are currently being used in industrial processes, but have dangerous environmental side effects. The software can also be used to find solvents with lower environmental impact when designing new industrial processes, as well as more benign solvents that can be added to harmful solvents favored by industry to help reduce the harmful environmental impact of their processes.
These replacement solvent mixtures may be used by companies interested in reducing the environmental impact of their industrial processes. Interested individuals may include:
• solvent technicians
• solvent engineers
• environmental engineers
• environmental consultants
Install PARIS III
1. Download the latest version of PARIS III to your computer
o Windows OS PARIS III (Version 1.3.0) (EXE) (69 MB)
o Unix OS PARIS III (Version 1.3.0) (Unix OS) (80 MB)
o MacOS PARIS III (ZIP) (77 MB)
2. If your browser offers the option to run the setup program then do so.
3. Otherwise have your browser display its list of recent downloads and select the setup file to run it.
4. If you have problems installing the calculator contact your system administrator.
The theoretical basis for the PARIS III program is the observation that the properties governing solvent behavior are universal, and that the performance of each solvent is quantified by coefficients representing various physical and chemical properties (e.g., viscosity, diffusivity, activity coefficients, etc.). The solvent's features used by PARIS III include dynamic and equilibrium properties, environmental behavior (air index and environmental index), and performance and safety requirements.
By applying this representation to solvent design, PARIS III can rank alternative solvents by choosing those that come as close as possible to the coefficients of the original solvent. A ranked list of replacement solvents can be created within minutes. PARIS III provides a cost-effective approach to pollution prevention because users do not have to change equipment or modify their chemical processes in order to adopt safer, "greener" solvents.

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Distance Between Solvent Mixtures

How close mixtures are to an original solvent may be calculated by a normalized metric in 18 dimensional property space…

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

Here $tol(x_{o,i})$ is the width between the boundaries on the ith property axis.

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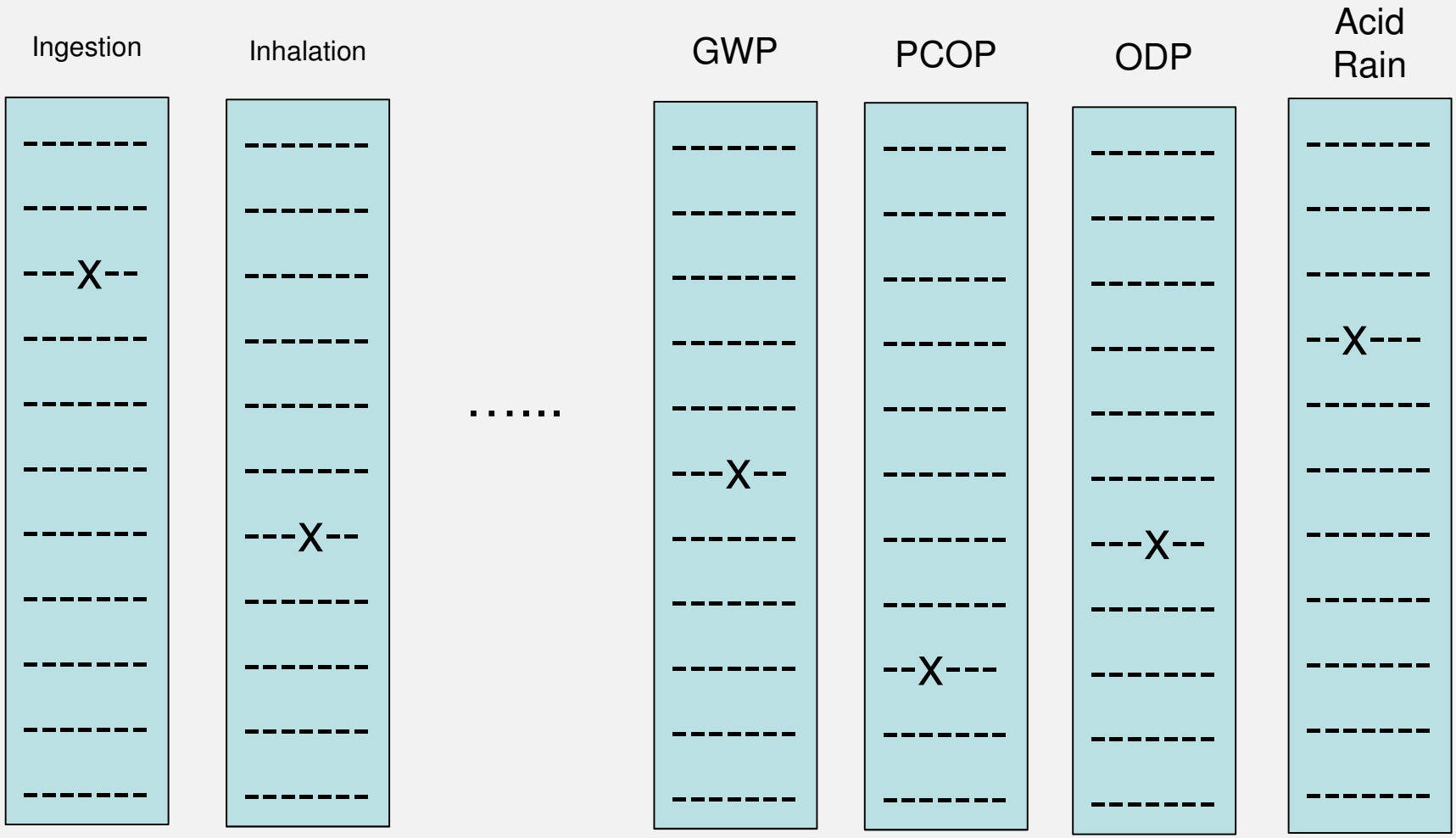
Impact of the Average Solvent



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Normalized Potential 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.

$$\overline{\varphi}_{i,j} = \frac{\varphi_{i,j}}{\left(\frac{1}{n_j}\right)\sum_{k=1}^{n_j} \varphi_{k,j}}$$

Notice that, regardless of the initial dimensions, this process describes each environmental impact relative to an average impact in category j.

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Environmental Index

The user assigns importance factors α_j for each category of impact to accurately reflect their environment. The Environmental Index ψ_i^{env} for solvent *i* may then be calculated as:

$$\psi_i^{env} = \sum_{j=1}^{8} \alpha_j \overline{\varphi}_{i,j}$$

where the summation is taken over the 8 categories of impact, and $\overline{\varphi}_{i,j}$ is the normalized environmental impact score from the PARIS III database for chemical *i* and impact category *j*.

Environmental Index (cont.)

The total Environmental Index ψ^{env} of a solvent mixture is determined by summing contributions from each of the n-components of the solvent mixture:

$$\psi^{env} = \sum_{i=1}^{n} W_i \psi_i^{env}$$

Where W_i is the weight fraction of the i^{th} solvent.

Air Index

The Air Index ψ_i^{air} for solvent i, can be calculate from the Environmental Index based on the amount of solvent released to the air:

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

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.

Air Index (cont.)

As before, the total Air Index ψ^{air} is arrived at by summing contributions from each of the n-components of the solvent mixture:

$$\psi^{air} = \sum_{i=1}^{n} W_i \psi_i^{air}$$

Where W_i is the weight fraction of the i^{th} solvent.

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Importance factors - α_i

- Impact factors range from 0 to 10. They are initially set to 5, which implies all impact categories are equivalent.
- Importance factors should be set in a way appropriate to the user.
- For any impact categories felt to be irrelevant, their importance factors can be set to 0.

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The views expressed in this presentation are those of the author and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency.