

ProCAMD: Illustration with solvent selection or removal of phenol from water

Step1: Problem definition

We start by entering ProCamd from ICAS and then we need to fill-out the pages according to the instruction manual from section 1. The screens corresponding to the different pages of ProCamd are shown below.

General Problem Control | Non temperature depd. props.

Problem Title:
Title: solvent substitution (solvents for phenol) -SLE

Generate:
 Acyclic Compounds
 Aromatic Compounds
 Cyclic Compounds
 Generate Isomers
Autoslack in initial generation: ± 10%

Preselection:
 Generate Alcohols
 Generate Ketones
 Generate Aldehydes
 Generate Acids
 Generate Phenols
 Generate Compounds containing silicon
 Generate Compounds containing double bonds
 Generate Compounds containing triple bonds
 Generate Compounds containing flourine
 Generate Compounds containing chlorine
 Generate Compounds containing bromine
 Generate Compounds containing iodine
 Generate Compounds containing sulphur

Selected Groups:
CH3 CH2 CH C OH CH3CO
CH2CO CHO CH3O CH2O CH-O
Edit Groups

User specified compounds:
CH3 1 CH2 3 OH 1
CH3 2 CH2 1 CH 1 OH 1
CH3 2 CH 1 OH 1
Delete Define

	Min:	Max:	Goal:
Normal Boiling Point (K):	323	373	353.2
Normal Melting Point (K):	0	314	0
Total Solubility Param. (MPa ^{0.5}):	22	26	24.6
LogP (Octanol/Water):	1.5	2	2.13

Temperature depd. props. | Mixture Properties

General:
 Perform Mixture Calculations

Model:
 UNIPAR - Original UNIFAC (VLE)
 UNIPARL - Original UNIFAC (LLE)
 UNILIN - Original UNIFAC (2 parameter, linear, VLE)
 UNIMOD - Modified UNIFAC (3 parameter, MHV2, VLE)

Calculation Type:
 VLE - Calculations
 LLE - Calculations

Conditions:
Temperature (K): 298
Pressure (bar): 1

Selected Key Components:
Phenol
Edit...

Molefractions of Key Components:
Phenol 1.0000
1

Select Solute:
Phenol

Constraints:
Solvent Power: Min: 0.1 Max: 0 Goal: 0

Define as user-specified compounds, some of the solvents that appear in “common solv”

Problem specification pages from ProCamd for the solvent substitution exercise

Step 2: Run ProCAMD by clicking on the “run” button

Azeotrope/Miscibility Calculations Biodegradation Calculations

General:

Perform Azeotrope calculations
 Perform Miscibility calculations
 Perform SLE calculations

Azeotrope Specifications:

Phenol

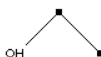
Don't calculate
 No azeotrope
 Form azeotrope

SLE Specifications:

Temperature K

Solid Phase must exist
 Solid Phase must not exist

Compound 1 :



Description :

No	Groupname
1	CH3
1	CH2
1	OH

Properties :

Property	Value	2. Value	Unit
Octanol/Water partition coef.	0.156	0.156	
Solubility parameter at 298 K	25.01	25.01	MPa ^{1/2}
Normal Melting point	164.57	164.57	K
Normal Boiling point	330.01	330.01	K
Solvent power	0.151	0.151	
NO AZEOTROP w. keycomp. no 1			
Solid phase of keycomp. 1 at X1	-	0.736	

⌂ << >> >E Sort Info ProPred Databank

Problem specification page from ProCamd. Results section from ProCamd. Note that “ProPred” and “Databank” are highlighted. This means that we can use these tools for this compound.

The solution statistics are shown in the figure below. This screen can also be obtained by clicking on “Info”.

Summary :

Number of compounds designed : 3071
 Number of compounds selected : 20
 Number of isomers designed : 37
 Number of isomer selected : 7
 Total time used to design : 1.70 s




'Screened Out' Statistics for Primary Calculations :

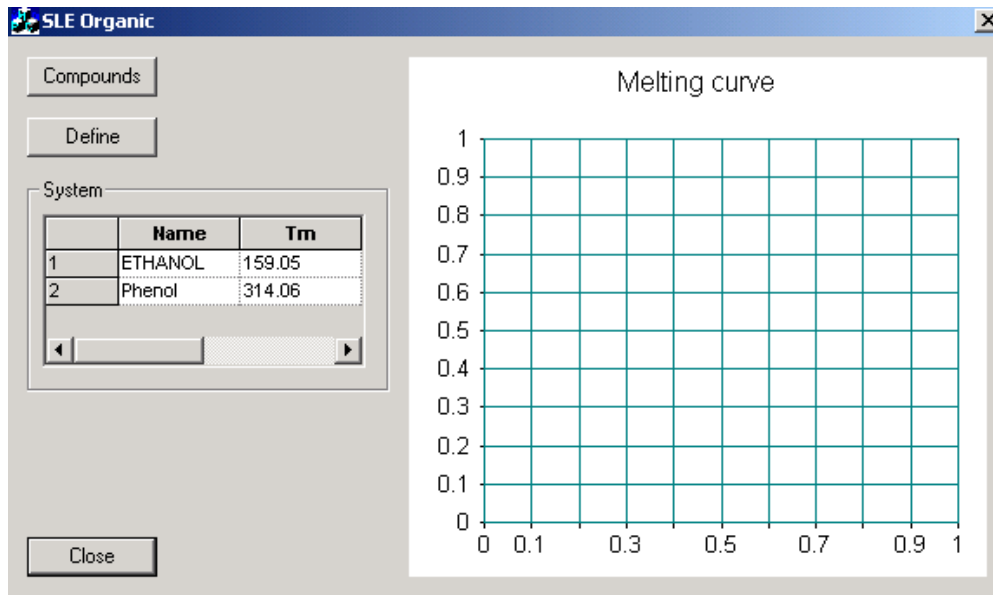
Functional group screening : 2816 of 3071
 Solubility parameter at 298 K : 232 of 255
 Normal Boiling point : 1 of 23
 Azeotrop Calculation : 2 of 22

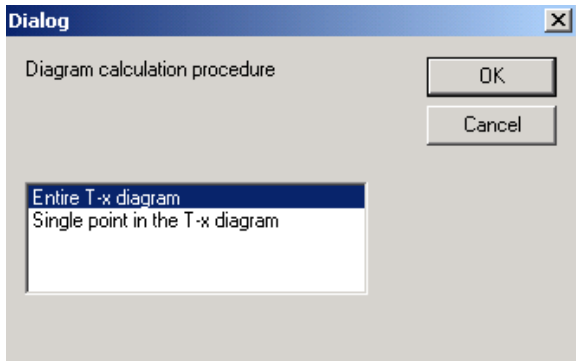
From the figures above, it can be noted that ethanol is also a feasible candidate as a solvent. We will verify the feasibility of ethanol in the next step.

Step 3: Verification of solvent through a solid-liquid equilibrium phase diagram

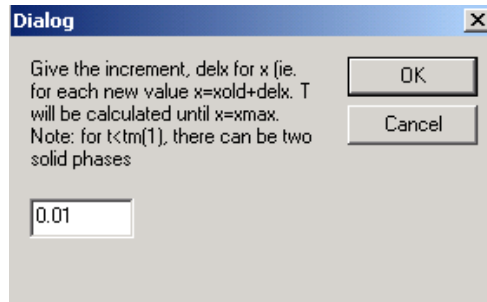
In order to obtain a solid-liquid equilibrium phase diagram, follow the steps given in appendix A3. The following steps are necessary:

1. Draw a stream in the ICAS-main window
2. Select  the compounds phenol and ethanol
3. Select  the property models (select UNIFAC-VLE model for liquid phase activity coefficients)
4. Double click on the stream, specify the pressure (1 atm) and any values for temperature (for example, 300 K) and composition (for example, 1 and 1). Click on  located on the top left hand corner.
5. Click on "Organic SLE" and then specify the data as shown below.

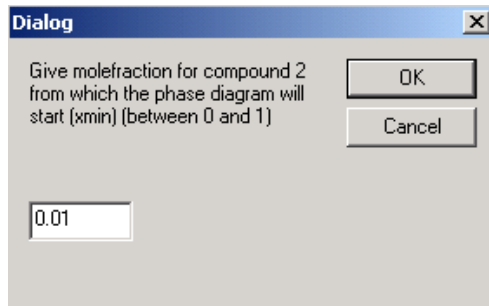




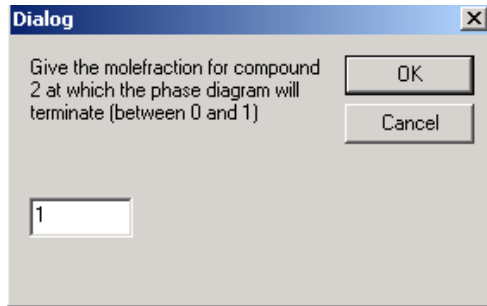
a



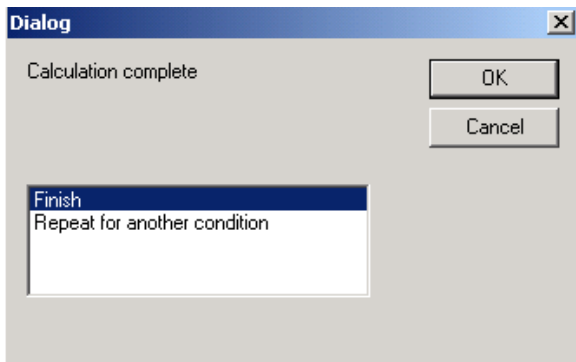
b



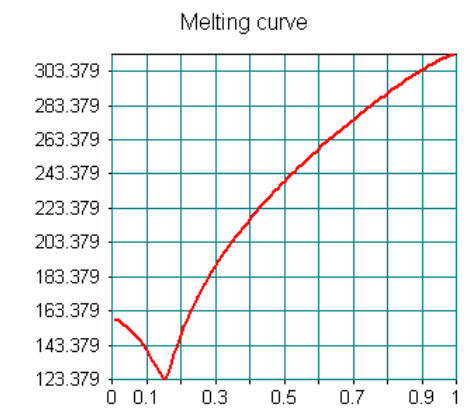
b



d



e



f

The specifications to generate the “entire T-X” diagram with the organic SLE toolbox of ICAS. Figure f shows the generated diagram. Clearly, at 300 K, a large amount of phenol can be dissolved.