

# **Process and Product Design Through ICAS**

*Product Design – Tutorial*

**By**

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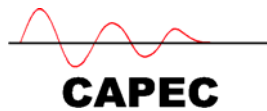
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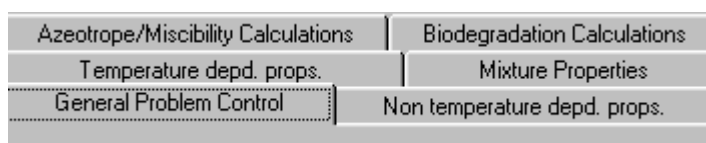



**CAPEC**

## *ProCamd Manual*

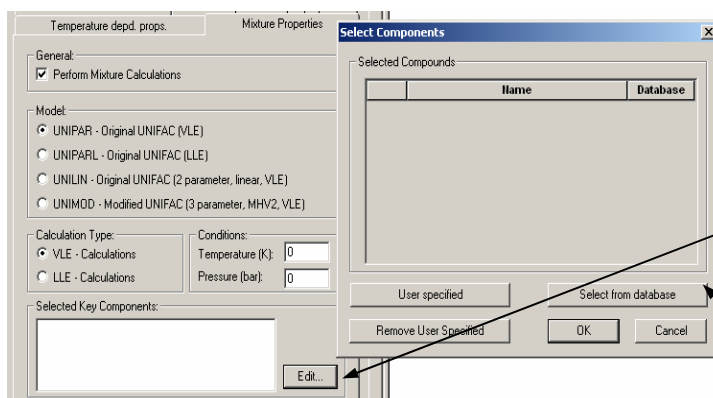
### 1. Introduction

To design a molecule, for example, a solvent, provide appropriate information on the following pages. In this problem, we are looking for a solvent that can replace benzene as the solvent for extraction of phenol from water by liquid-liquid extraction.



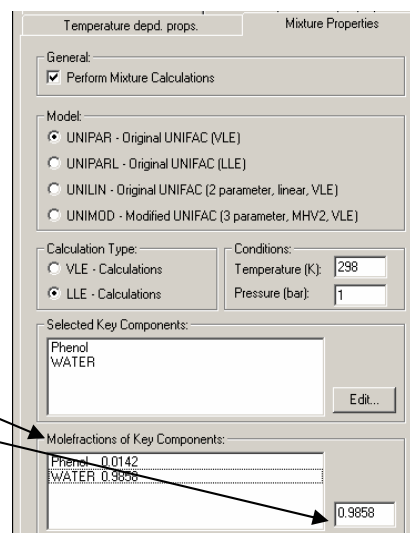
Click on  to start the calculations. In the screenshots below, the filled out pages for selection (design) of solvents for extraction of phenol from water is shown in sequential steps.

#### 1.1. *Components Selection*

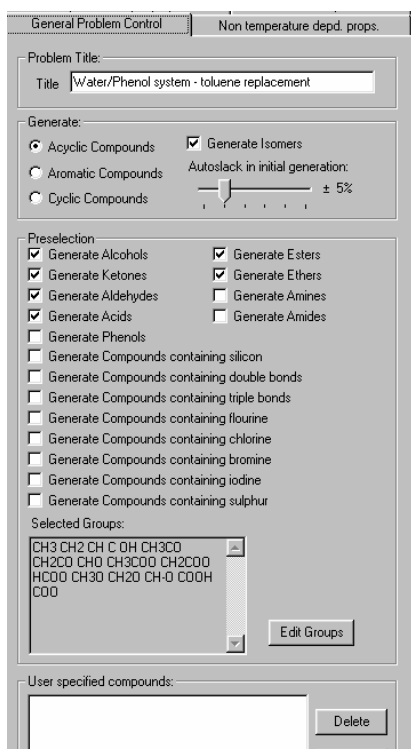
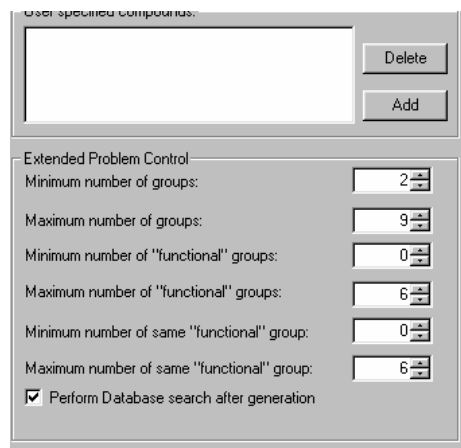


In the “Mixture Properties” tab check the “Perform Mixture Calculations” box. Click on “Edit...” in the “Selected Key Components” cage; in the displayed window click on “Select from database”, the “Component Selector” window will appear: select your compounds. Click “Ok”.

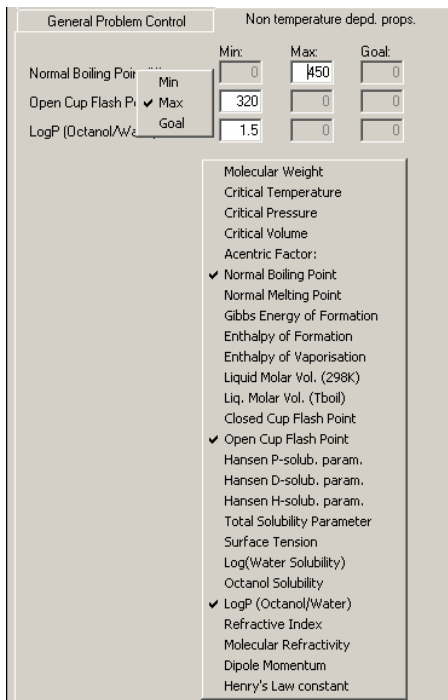
Enter the mole fractions. Click on the component (in the “Molefractions” cage) then type in the box the desired value and press “Enter”.



## 1.2. General Problem Control

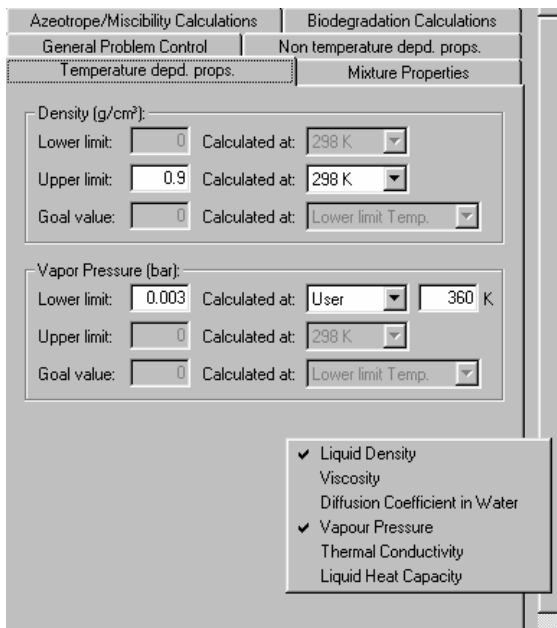



### 1.3. *Non-Temperature Dependent Properties*



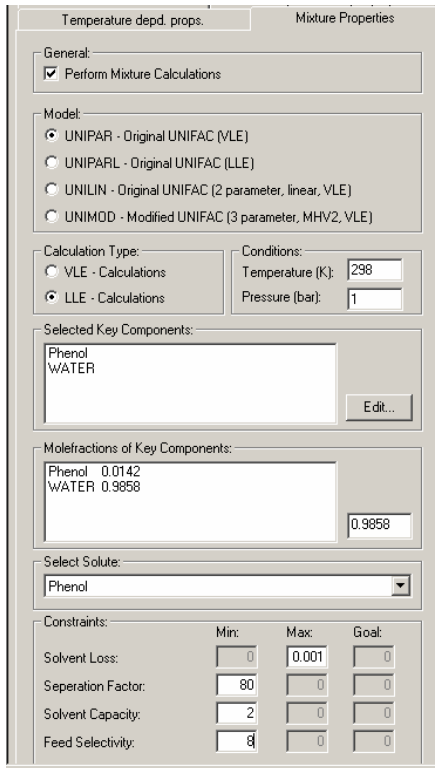
Right click on the left-hand side to obtain the list of properties. Left click on the property to select it and then fill out the data. In order to establish the limits the property can take, click on the property and uncheck the corresponding bounds.

### 1.4. *Temperature Dependent Properties*



Right click on the left-hand side to obtain the list of properties. Left click on the property to select it and then fill out the data.

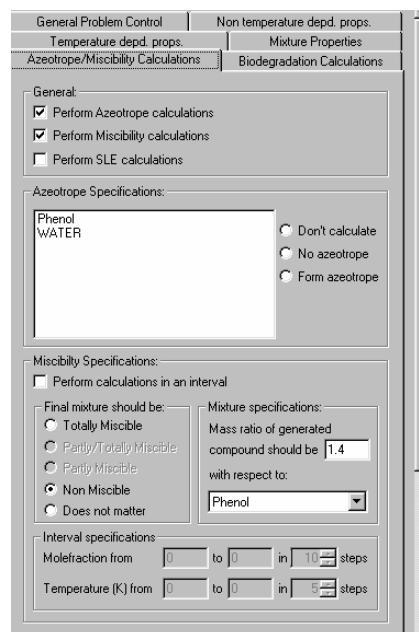
### 1.5. Mixture Properties.




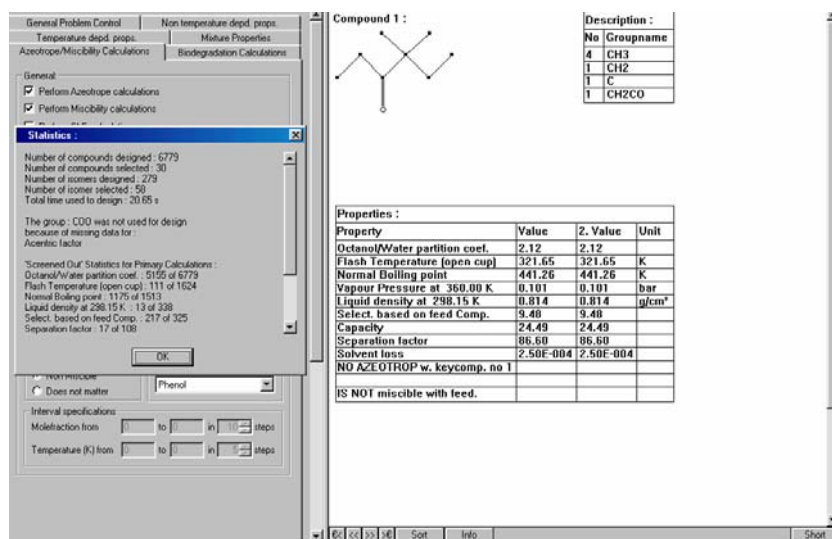
Constraints:	Min:	Max:	Goal:
Solvent Loss:	0	0.001	0
Separation Factor:	80	0	0
Solvent Capacity:	2	0	0
Feed Selectivity:	8	0	0

Right click on the left-hand side to obtain the list of constraints (solvent properties). Left click on “Constraints” to select it and then fill out the data.

### 1.6. Azeotrope/Miscibility Calculations.



- Click on  to start the calculations. On completion, the following screen is shown.



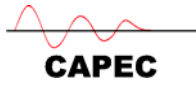
The screenshot displays the CAPEC software interface. On the left, a 'Statistics' window is open, showing the following data:

- Number of compounds designed: 6779
- Number of compounds selected: 30
- Number of isomers designed: 279
- Number of isomer selected: 58
- Total time used to design: 20.65 s

The 'Properties' window on the right shows the following data for Compound 1:

Property	Value	Z. Value	Unit
Octanol/Water partition coef.	2.12	2.12	
Flash Temperature (open cup)	321.65	321.65	K
Normal Boiling point	441.26	441.26	K
Vapour Pressure at 360.00 K	0.101	0.101	bar
Liquid density at 298.15 K	0.814	0.814	g/cm <sup>3</sup>
Select. based on lead Comp.	9.49	9.49	
Capacity	24.49	24.49	
Separation factor	86.60	86.60	
Solvent loss	2.50E-004	2.50E-004	
NO AZEOTROP w. keycomp. no 1			
IS NOT miscible with feed.			

- Click OK and then use the “>>” or “<<” buttons to move up or down to see the various feasible candidate solvents. If a candidate is available in the database, “database” will be highlighted on the lower menu-bar.




## 2. Exercises with ProCamd

### 2.1. Solvent Substitution

We have phenol deposits as a solid and we need to clean the equipment before our product can be produced. We already know that we can use benzene or toluene to dissolve the phenol. We would like to investigate if it is possible to use a more environmentally friendly anti-solvent to extract the phenol.

#### Step 1: Problem Formulation

We need to establish the needed properties for the replacement solvent. We can use the CAPEC database to search for the properties of phenol, benzene and toluene. In the screen shot below, the properties of phenol are highlighted (see appendix 1 on how to perform search in the CAPEC database .

Properties Page 1.		Properties Page 2.		Properties Page 3.		Solvent Properties Page.		Group Description.	
Name:	Phenol								
Synonym 1:	PHENOL								
Synonym 2:									
Synonym 3:	Phenol								
Cas-No:	000108-95-2	Mathias CC1	0.9723						
Formula:	C6H6O	Mathias CC2	1.5836						
Smiles:	Oc(cccc1)c1	Mathias CC3	-3.3395						
Classification 1:	3. Polar Associating Compounds	Antoine A:	6.93051						
Classification 2:	1. Organic	Antoine B:	1382.65						
Classification 3:	1. Alcohols	Antoine C:	159.493						
Date:	10-06-1999	Min Temp. (K):	314.06						
Notes:		Max Temp. (K):	694.25						

#### Other properties:

$$T_m = 314.06 \text{ K}$$

$$T_b = 454.99 \text{ K}$$

$$\delta_{SP} = 24.63 \text{ (MPa)}^{1/2}$$

$$H_{fus} = 11510 \text{ kJ/kmole}$$

$$T_c = 694.25 \text{ K}$$

$$P_c = 60.498 \text{ atm}$$

$$V_c = 0.229 \text{ m}^3/\text{kmole}$$

$$v = 0.889 \text{ m}^3/\text{kmole}$$

$$M_w = 94.113$$

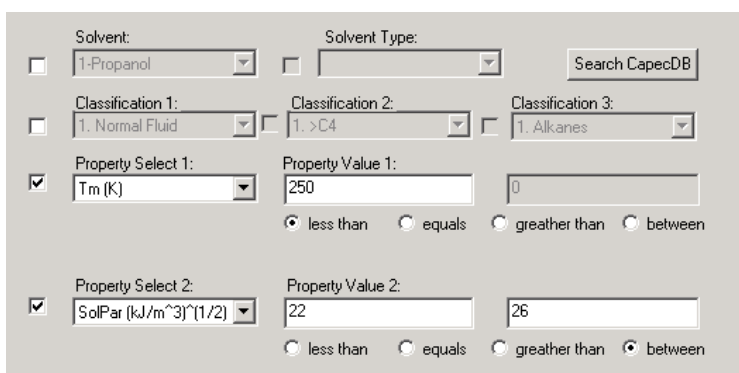
Pure component data for Phenol obtained by “basic search” in the CAPEC database

Based on the phenol data, we can formulate the solvent search problem as follows – The temperature of the operation is below 314 K (assume 300 K), at this condition, solvent

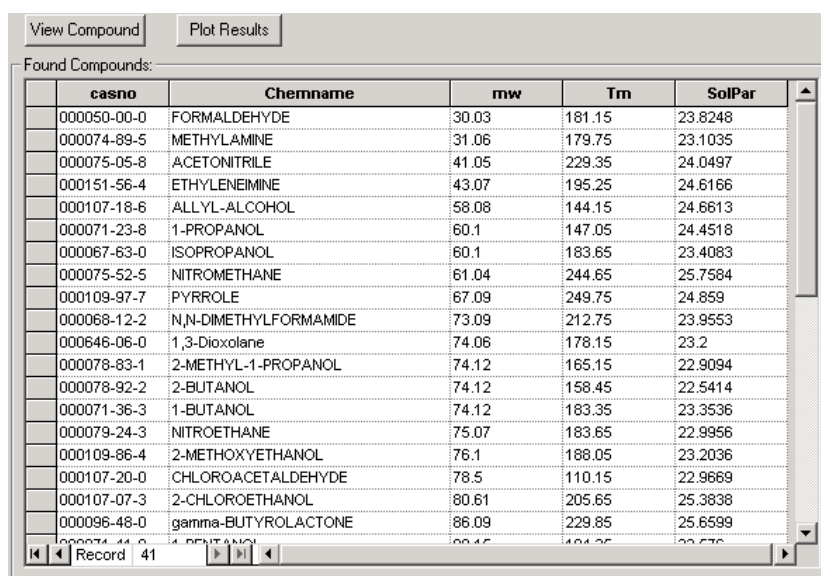
plus phenol must form a liquid solution and the composition of the phenol must be reasonably high. As a measure of solubility, initially, we can search for solvents having melting points below 250 K and having the Hildebrand solubility parameters  $22 < \delta_{SP} < 26$  (MPa)<sup>1/2</sup>. This problem can also be solved through the CAPEC database (using the “advanced search” option) or ProCamd.

## Step 2: Generation of candidates through CAPEC database search

To use the advanced search option in the CAPEC database, click on **M** and then click on “advanced search” in the CAPEC database. Then select the options for the search engine as shown below.



Now click on **Search CapecDB** to start the search engine. The search result is shown in the figure below. It can be noted that 41 candidates have been found.

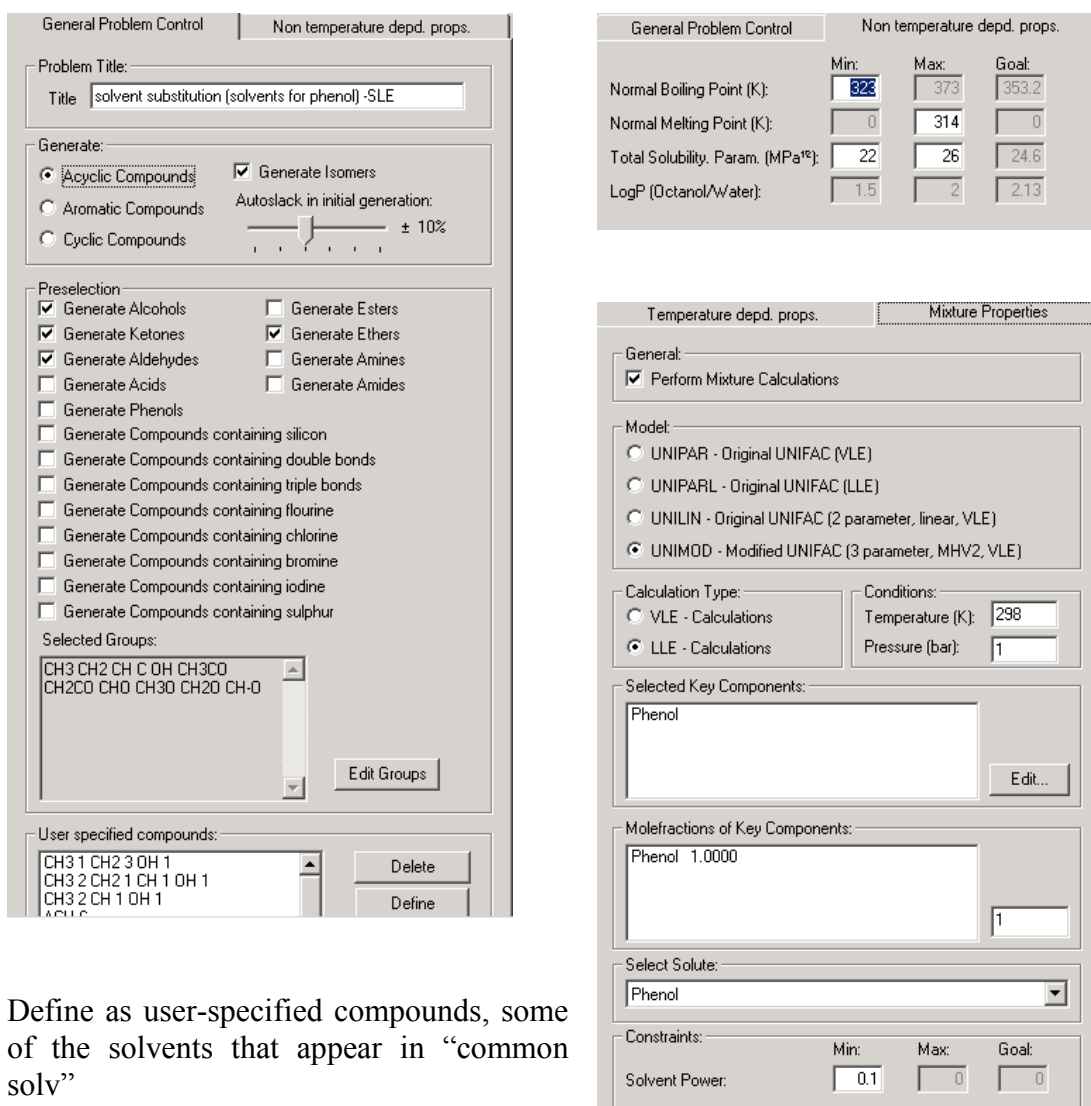


casno	Chemname	mw	Tm	SolPar
000050-00-0	FORMALDEHYDE	30.03	181.15	23.8248
000074-89-5	METHYLAMINE	31.06	179.75	23.1035
000075-05-8	ACETONITRILE	41.05	229.35	24.0497
000151-56-4	ETHYLENEIMINE	43.07	195.25	24.6166
000107-18-6	ALLYL-ALCOHOL	58.08	144.15	24.6613
000071-23-8	1-PROPANOL	60.1	147.05	24.4518
000067-63-0	ISOPROPANOL	60.1	183.65	23.4083
000075-52-5	NITROMETHANE	61.04	244.65	25.7584
000109-97-7	PYRROLE	67.09	249.75	24.859
000068-12-2	N,N-DIMETHYLFORMAMIDE	73.09	212.75	23.9553
000646-06-0	1,3-Dioxolane	74.06	178.15	23.2
000078-83-1	2-METHYL-1-PROPANOL	74.12	165.15	22.9094
000078-92-2	2-BUTANOL	74.12	158.45	22.5414
000071-36-3	1-BUTANOL	74.12	183.35	23.3536
000079-24-3	NITROETHANE	75.07	183.65	22.9956
000109-86-4	2-METHOXYETHANOL	76.1	188.05	23.2036
000107-20-0	CHLOROACETALDEHYDE	78.5	110.15	22.9669
000107-07-3	2-CHLOROETHANOL	80.61	205.65	25.3838
000096-48-0	gamma-BUTYROLACTONE	86.09	229.85	25.6599

Using the results from above, the next step would be to perform a search through ProCamd, which will generate new molecules as well as check known compounds.

### Step 3: Generation of candidates through ProCamd

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.



The image shows four screenshots of the ProCamd software interface, arranged in a 2x2 grid. The top-left screenshot shows the 'General Problem Control' tab with the problem title 'solvent substitution (solvents for phenol) -SLE'. The 'Generate' section has 'Acyclic Compounds' selected, and 'Generate Isomers' is checked. The 'Preselection' section has several options checked, including 'Generate Alcohols', 'Generate Ketones', and 'Generate Aldehydes'. The 'Selected Groups' list includes 'CH3 CH2 CH C OH CH3CO' and 'CH2CO CHO CH3O CH2O CH-O'. The 'User specified compounds' list includes 'CH3 1 CH2 3 OH 1', 'CH3 2 CH2 1 CH 1 OH 1', and 'CH3 2 CH 1 OH 1'. The top-right screenshot shows the 'Non temperature depd. props.' tab with a table of constraints:

	Min:	Max:	Goal:
Normal Boiling Point (K):	328	373	353.2
Normal Melting Point (K):	0	314	0
Total Solubility. Param. (MPa <sup>1/2</sup> ):	22	26	24.6
LogP (Octanol/Water):	1.5	2	2.13

The bottom-left screenshot shows the 'Temperature depd. props.' tab with 'Perform Mixture Calculations' checked. The 'Model' section has 'UNIMOD - Modified UNIFAC (3 parameter, MHV2, VLE)' selected. The 'Calculation Type' is 'LLE - Calculations'. The 'Conditions' are Temperature (K): 298 and Pressure (bar): 1. The 'Selected Key Components' list includes 'Phenol'. The 'Molefractions of Key Components' list includes 'Phenol 1.0000'. The 'Select Solute' dropdown is set to 'Phenol'. The bottom-right screenshot shows the 'Mixture Properties' tab with a table of constraints:

	Min:	Max:	Goal:
Solvent Power:	0.1	0	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

Azeotrope/Miscibility Calculations    Biodegradation Calculations

General:

Perform Azeotrope calculations  
 Perform Miscibility calculations  
 Perform SLE calculations

Azeotrope Specifications:

Phenol

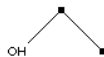
Don't calculate  
 No azeotrope  
 Form azeotrope

SLE Specifications:

Temperature: 298 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 <sup>1/2</sup>
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	

⏪ << >> ⏩ | Sort | Info | ProPred | Databank

Problem specification page from 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 :

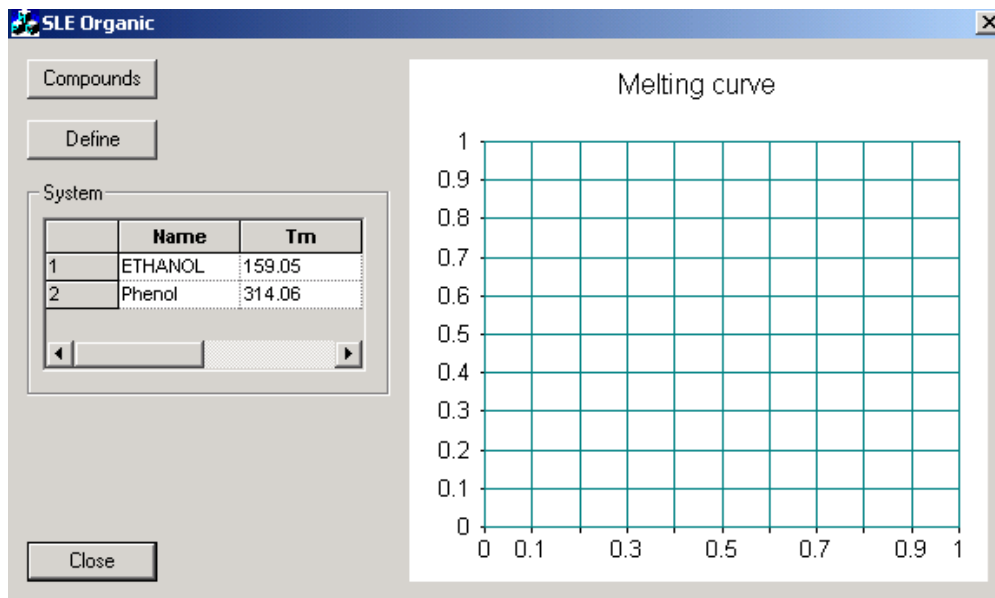
Functional group screening : 2816 of 3071  
 Solubility parameter at 298 K : 232 of 255  
 Normal Boiling point : 1 of 23  
 Azeotrop Calculation : 2 of 22

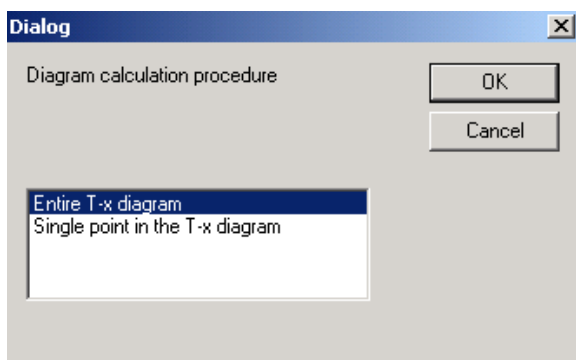
From the figures above, it can be noted that ethanol is also a feasible candidate as a solvent. We will verify the feasibility of ethanol in the next step.

#### Step 4: Verification of solvent through a solid-liquid equilibrium phase diagram

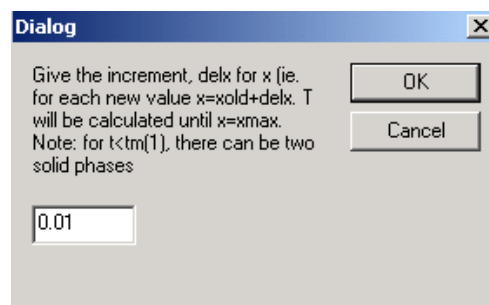
In order to obtain a solid-liquid equilibrium phase diagram, follow the steps given in appendix A3. The following steps are necessary:

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.

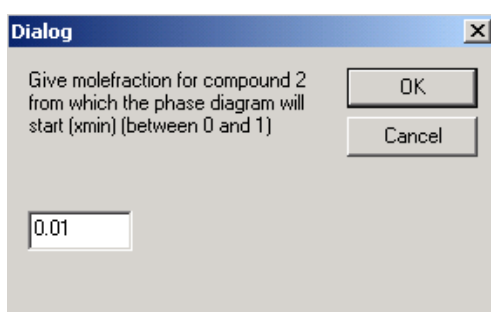




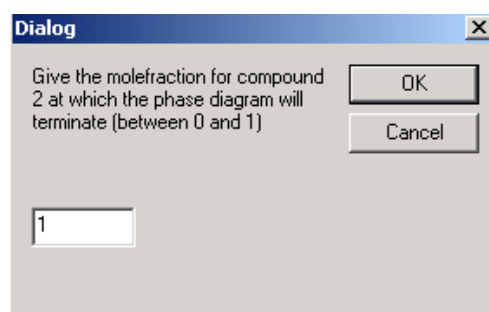
a



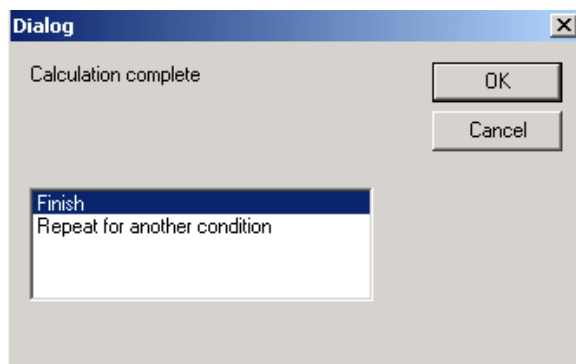
b



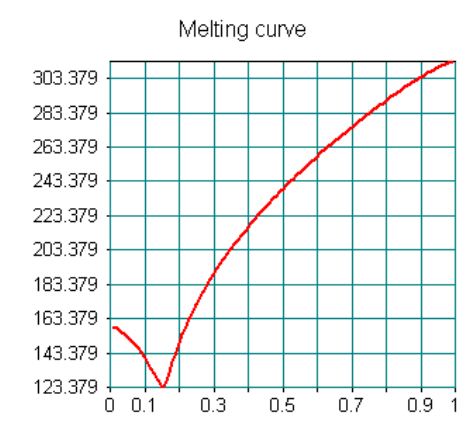
c



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.

Exercises related to solvent substitution

- A. Solve the problem in step 2 with ProCamd (note that only the “general problem control” and the “non-temperature depd. props” need to be specified).
- B. Verify another solvent through step 4
- C. If you change the solubility parameter bounds to less than 22 or more than 26, will the solvents be valid for phenol? Find solute products that will be valid for solvents with solubility parameter  $< 22$  and  $> 26$  (use both database search and ProCamd).
- D. Find solvents for Naphthalene.

## **2.2. Mixture Design**

In mixture design, we specify some mixture properties that a mixture of two or more compounds needs to satisfy. Consider the following problem –

Find all binary mixtures that form an azeotrope with ethanol at 1 atm pressure and where the second compound is a cyclic compound, with  $300\text{ K} < T_b < 500\text{ K}$ .

To solve this problem, we need to use ProCamd (“General problem control”, “non-temperature depd. props”, “mixture properties” and “azeotrope/miscibility” pages). A sample of the data specified is shown below.

<p>General Problem Control   Non temperature depd. props.</p> <p>Problem Title: Title: <input type="text" value="binary azeotrope with ethanol (totally miscible)"/></p> <p>Generate:</p> <p><input type="radio"/> Acyclic Compounds    <input type="checkbox"/> Generate Isomers  <input type="radio"/> Aromatic Compounds    Autoslack in initial generation:  <input checked="" type="radio"/> Cyclic Compounds    <input type="range" value="10"/> ± 10%</p> <p>Preselection:</p> <p><input checked="" type="checkbox"/> Generate Alcohols    <input checked="" type="checkbox"/> Generate Esters  <input checked="" type="checkbox"/> Generate Ketones    <input checked="" type="checkbox"/> Generate Ethers  <input checked="" type="checkbox"/> Generate Aldehydes    <input type="checkbox"/> Generate Amines  <input checked="" type="checkbox"/> Generate Acids    <input type="checkbox"/> Generate Amides  <input type="checkbox"/> Generate Phenols</p>	<p>Temperature depd. props.   Mixture Properties</p> <p>Azeotrope/Miscibility Calculations   Biodegradation Calculations</p> <p>General Problem Control   Non temperature depd. props.</p> <p>Normal Boiling Point (K):    Min: <input type="text" value="300"/>    Max: <input type="text" value="500"/>    Goal: <input type="text" value="0"/></p>
<p>Temperature depd. props.   Mixture Properties</p> <p>General:</p> <p><input checked="" type="checkbox"/> Perform Mixture Calculations</p> <p>Model:</p> <p><input checked="" type="radio"/> UNIPAR - Original UNIFAC (VLE)  <input type="radio"/> UNIPARL - Original UNIFAC (LLE)  <input type="radio"/> UNILIN - Original UNIFAC (2 parameter, linear, VLE)  <input type="radio"/> UNIMOD - Modified UNIFAC (3 parameter, MHV2, VLE)</p> <p>Calculation Type:    Conditions:</p> <p><input checked="" type="radio"/> VLE - Calculations    Temperature (K): <input type="text" value="300"/>  <input type="radio"/> LLE - Calculations    Pressure (bar): <input type="text" value="1"/></p> <p>Selected Key Components:</p> <p><input type="text" value="ETHANOL"/>    <input type="button" value="Edit..."/></p> <p>Molefractions of Key Components:</p> <p><input type="text" value="ETHANOL 1.0000"/>    <input type="text" value="0"/></p> <p>Select Solute:</p> <p><input type="text" value="ETHANOL"/></p>	<p>Azeotrope/Miscibility Calculations   Biodegradation Calculations</p> <p>General:</p> <p><input checked="" type="checkbox"/> Perform Azeotrope calculations  <input checked="" type="checkbox"/> Perform Miscibility calculations  <input type="checkbox"/> Perform SLE calculations</p> <p>Azeotrope Specifications:</p> <p><input type="text" value="ETHANOL"/>    <input type="radio"/> Don't calculate  <input type="radio"/> No azeotrope  <input checked="" type="radio"/> Form azeotrope</p> <p>Miscibility Specifications:</p> <p><input checked="" type="checkbox"/> Perform calculations in an interval</p> <p>Final mixture should be:</p> <p><input type="radio"/> Totally Miscible    Mixture specifications:  <input type="radio"/> Partly/Totally Miscible    Mass ratio of generated  <input checked="" type="radio"/> Partly Miscible    compound should be <input type="text" value="1.4"/>  <input type="radio"/> Non Miscible    with respect to:  <input type="radio"/> Does not matter    <input type="text"/></p> <p>Interval specifications</p> <p>Molefraction from <input type="text" value="0"/> to <input type="text" value="1"/> in <input type="text" value="10"/> steps  Temperature (K) from <input type="text" value="300"/> to <input type="text" value="400"/> in <input type="text" value="5"/> steps</p>

One of the feasible mixtures is shown below (note that what ProCamd provides is the information that the two compounds will form a single-phase solution. The exact compositions will need to be calculated separately, depending on the desired mixture property, for example, the bubble point temperature.

<b>Compound 37 :</b>		<b>Properties :</b>									
<b>Description :</b>		<b>Property</b>		<b>Value</b>					<b>Unit</b>		
<b>No</b>	<b>Groupname</b>	<b>Normal Boiling point</b>		<b>400.14</b>					<b>K</b>		
<b>4</b>	<b>CH2</b>	<b>AZEOTROP w. keycomp. 1 at Xgen/Taz:</b>		<b>0.60 / 341.53 K</b>							
<b>1</b>	<b>CH2COO</b>	<b>Miscibility :</b>									
<b>T \ x</b>	<b>0.00</b>	<b>0.11</b>	<b>0.22</b>	<b>0.33</b>	<b>0.45</b>	<b>0.56</b>	<b>0.67</b>	<b>0.78</b>	<b>0.89</b>	<b>1.00</b>	
<b>300.00</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	
<b>325.00</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	
<b>350.00</b>	<b>M</b>	<b>IM</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	
<b>375.00</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	
<b>400.00</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	<b>M</b>	

Exercises related to mixture design

- A. Repeat the above problem to find acyclic compounds that form azeotropes with ethanol
- B. Repeat the above problem where the cyclic compounds do not form azeotrope with ethanol

### 2.3. Design of Large Molecules

Design a large molecule having the following properties,

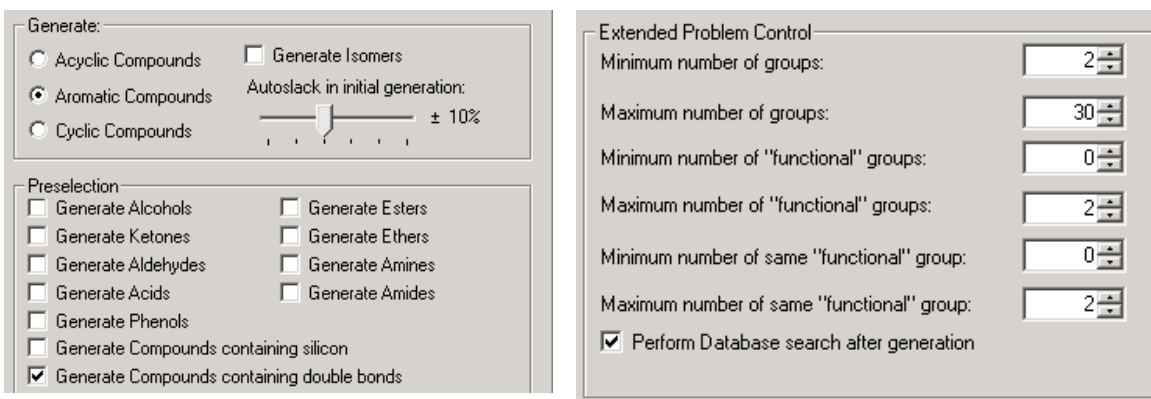
$$M_w > 300$$

$$T_b > 400 \text{ K}$$

$$T_m > 300 \text{ K}$$

Solve the problem with ProCamd and then switch to ProPred and further investigate the properties of the large molecule, including further increase of the size of the molecule.

Only the “general problem control” and the “non-temperature depd props” need to be specified. In the “general problem control”, select the following,



The screenshot shows two panels from the CAPEC software interface:

- Generate:**
  - Radio buttons:  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 Esters
  - Generate Ethers
  - Generate Amines
  - Generate Amides
- Extended Problem Control:**
  - Minimum number of groups:
  - Maximum number of groups:
  - Minimum number of "functional" groups:
  - Maximum number of "functional" groups:
  - Minimum number of same "functional" group:
  - Maximum number of same "functional" group:
  - Perform Database search after generation

Repeat the problem for acyclic compounds and cyclic compounds

## 2.4. Solvent Design

Find a solvent for the separation of acetone from chloroform. The problem definition is shown in the figures below. Use the same 4 steps as in solvent substitution problem.

- Define the problem with respect to pure component property targets and mixture property targets. Solvent needs to dissolve chloroform and not acetone (solubility parameter close to chloroform and not acetone. It must be liquid (boiling point higher than mixture temperature). It must be environmentally friendly (avoid aromatic compounds, chlorides, etc.)
- Use the advanced search engine of the database to find solvents (check the properties of acetone and chloroform and then use the values of the boiling point, the melting point and the Hildebrand solubility parameter for the advanced search)
- Use ProCamd to generate the list of feasible solvents (see figures below for the specifications)
- Verify the solvents (in this case, perform ternary VLE phase diagrams). If solvents that are totally miscible to the feed mixture are found, then the separation will be

based on vapour-liquid systems. Tools for verification of VLE systems will be used on day 2 of the workshop.

Azeotrope/Miscibility Calculations		Biodegradation Calculations	
Temperature depd. props.		Mixture Properties	
General Problem Control		Non temperature depd. props.	
Problem Title:			
Title: acetone-chloroform separation (solvent for chloroform)			
Generate:			
<input checked="" type="radio"/> Acyclic Compounds	<input checked="" type="checkbox"/> Generate Isomers	Autoslack in initial generation: ± 10%	
<input type="radio"/> Aromatic Compounds			
<input type="radio"/> Cyclic Compounds			
Preselection			
<input checked="" type="checkbox"/> Generate Alcohols	<input checked="" type="checkbox"/> Generate Esters		
<input checked="" type="checkbox"/> Generate Ketones	<input checked="" type="checkbox"/> Generate Ethers		
<input checked="" type="checkbox"/> Generate Aldehydes	<input type="checkbox"/> Generate Amines		
<input checked="" type="checkbox"/> Generate Acids	<input type="checkbox"/> Generate Amides		

Azeotrope/Miscibility Calculations		Biodegradation Calculations	
Temperature depd. props.		Mixture Properties	
General Problem Control		Non temperature depd. props.	
Molecular Weight (g/mol):	Min: 70	Max: 120	Goal: 0
Normal Boiling Point (K):	320	420	375

Calculation Type:		Conditions:	
<input checked="" type="radio"/> VLE - Calculations	Temperature (K): 345		
<input type="radio"/> LLE - Calculations	Pressure (bar): 1		
Selected Key Components:			
ACETONE CHLOROFORM			Edit...
Molefractions of Key Components:			
ACETONE	0.3440		
CHLOROFORM	0.6560		
		0.344	
Select Solute:			
CHLOROFORM			
Constraints:			
	Min:	Max:	Goal:
Selectivity:	1.7	0	0
Solvent Loss:	0	0.23	0

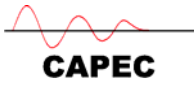
General:	
<input checked="" type="checkbox"/> Perform Azeotrope calculations	
<input checked="" type="checkbox"/> Perform Miscibility calculations	
<input type="checkbox"/> Perform SLE calculations	
Azeotrope Specifications:	
ACETONE	<input type="radio"/> Don't calculate
CHLOROFORM	<input checked="" type="radio"/> No azeotrope
	<input type="radio"/> Form azeotrope
Miscibility Specifications:	
<input type="checkbox"/> Perform calculations in an interval	
Final mixture should be:	
<input checked="" type="radio"/> Totally Miscible	
<input type="radio"/> Partly/Totally Miscible	
<input type="radio"/> Partly Miscible	
<input type="radio"/> Non Miscible	
<input type="radio"/> Does not matter	
Mixture specifications:	
Mass ratio of generated compound should be	3
with respect to:	CHLOROFORM

Related problems:

Find solvents to separate acetone from methanol separation (VLE separation)

Find solvents for methyl acetate from methanol separation (VLE separation)

Find solvents for hexane-benzene separation (LLE separation)



## 2.5. *Refrigerant Design*

A refrigerant needs to have the following properties.

Use ProCamd to generate the candidates and then use ProPred to verify the selection. Generate the P-H thermodynamic diagram through ProPred to validate the refrigeration cycle.

Related problem: Design of heat pump fluid.

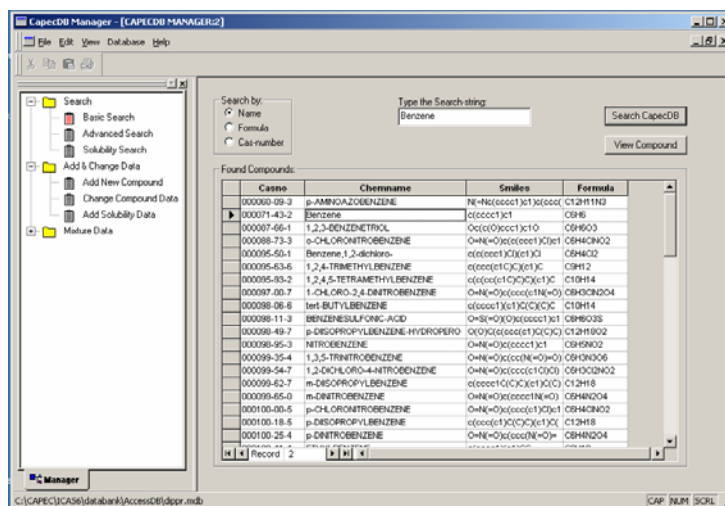
## Appendix A: CAPEC Database Manager

In this section the use of the Database Manager is briefly discussed.

Click on the "Database Manager" icon  in the task bar of ICAS main window.

### A1. Basic Search

Under the "Search" directory in the left panel you will find different options to perform the search of a compound. Select "Basic Search" → Type the name of your component → Click on "Search CapecDB" → Select your component from the displayed list → Click on "View Compound".



The Property pages will be displayed. Here you can find from Antoine Constants, Critical properties, property temperature dependent correlations, solvent properties and Group description. Click on "Back" button to return to the initial page.

CapecDB Manager - [CAPECDB MANAGER-3]

File Edit View Database Help

View Molecular Structure Make Report Back

Properties Page 1 | Properties Page 2 | Properties Page 3 | Solvent Properties Page | Group Description

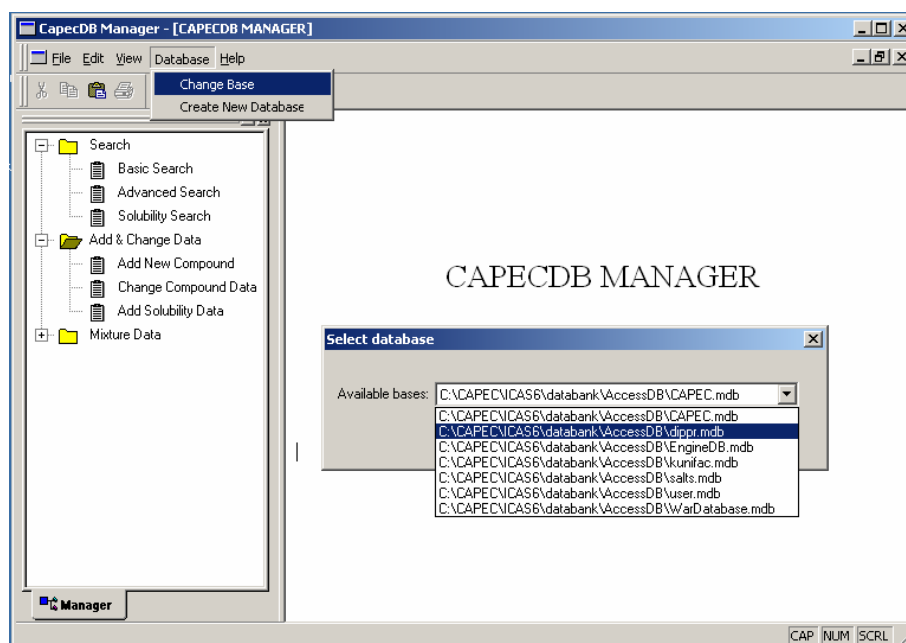
Mw (g/mol):	78.114	γ <sub>S</sub> (kJ/(mol·K)):	263.3
Omeg <sub>s</sub> :	0.21	RG (Å):	3.004
T <sub>c</sub> (K):	562.16	DM (Debye):	0
P <sub>c</sub> (atm):	48.339	Solpar (MPa <sup>-1</sup> ·S):	18.7296
V <sub>c</sub> (m <sup>3</sup> /mol):	0.259	VDW Vol (m <sup>3</sup> /mol):	0.0484
Z <sub>c</sub> :	0.271	VDW Area (m <sup>2</sup> /mol):	600000000
T <sub>m</sub> (K):	270.68	HFusion (kJ/mol):	9966
T <sub>b</sub> (K):	353.24	HCombus (kJ/mol):	-3136000
T <sub>v</sub> (K):	278.68	RI:	1.49782
P <sub>v</sub> (atm):	0.0469973	FPPoint (K):	262
V <sub>liq</sub> (m <sup>3</sup> /mol):	0.0894839	FP1 (vol %):	1.4
γ <sub>HF</sub> (kJ/mol):	62000	FPu (vol %):	7.1
γ <sub>GF</sub> (kJ/mol):	129600	AIT (K):	825

Manager

C:\CAPEC\ICASE\databank\AccessDB\dlppr.mdb CAP PALM SCRL

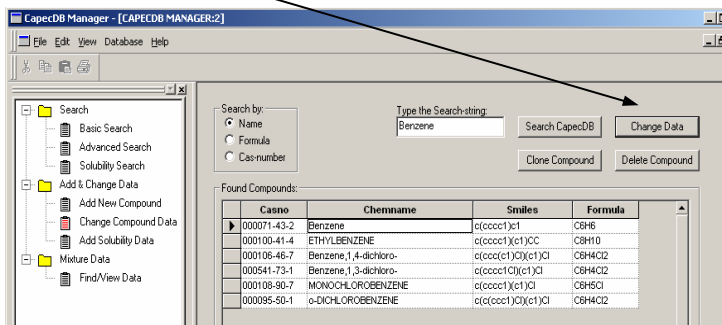
## A2. Add and Change of Data

1. Data can be changed only on the user-database. Go to the user-database where your compound exists (Database → Change to any of the user-databases)

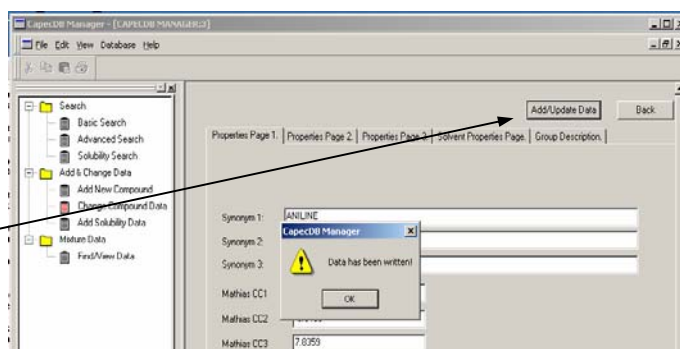


### 2. Change of Data:

- ✓ Go to “Change compound data” on the left panel.
- ✓ Type your component in the box → click on “Search CapecDB” → Select it.
- ✓ Click on the “Change Data” button

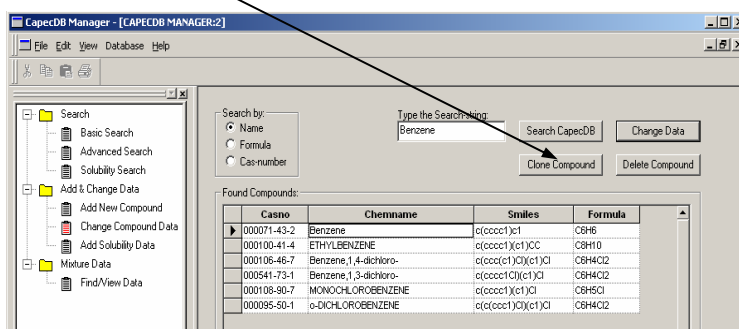


- ✓ Change the desired information in the corresponding fields. Once you finished click on “Add/Update Data” button. An updating message will appear.



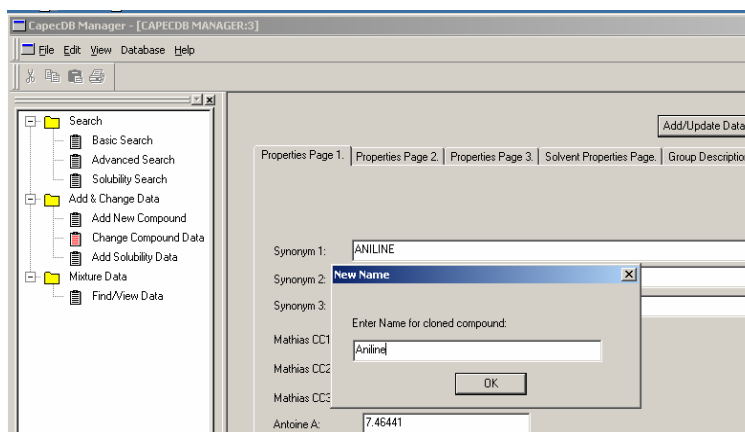
### 3. Clone of a Compound

- ✓ Go to “Change compound data” on the left panel.
- ✓ Type your component in the box → click on “Search CapecDB” → Select it.
- ✓ Click on “Clone Compound”.

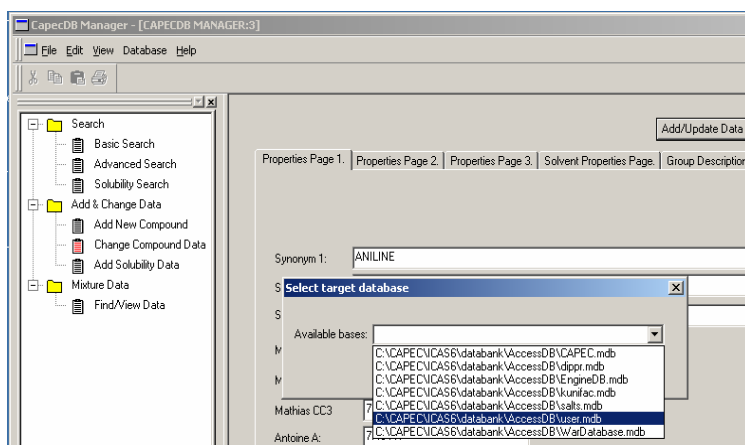


- ✓ If you change some information do it in the corresponding fields. Once you finished click on “Add/Update Data” button.

- ✓ Give a name in the “New Name” window → Click on “Ok”,



- ✓ Allocate the cloned component in a database (only to the “user” database”),



- ✓ Now there is a new compound in the selected database!

**A3. *How to Estimate Properties of a Chemical Product Not Found in the Database?***

- Launch the CAPEC database and then select the user-database.
- Click on “add/change” data
- Click on ProPred
- In ProPred, either draw the molecule or import the SMILES or import the mol.file corresponding to the chemical product. The database in ProPred can also be searched, if necessary.
- Check if all the necessary properties have been estimated by ProPred, if yes, exit from ProPred.
- Click on “update” data


Try the following exercise:

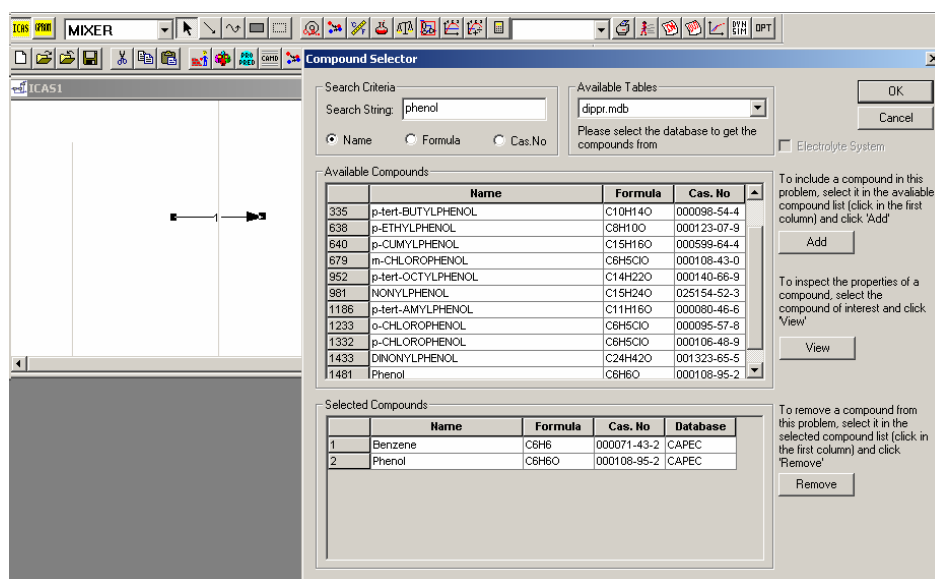
Try to put Morphine (Oc1ccc2CC3N(C)CCC45C3C=CC(O)C4Oc1c25) into the user-database. CAS number of morphine is 000057-27-2 (the database in ProPred has this compound).

## APPENDIX B. Manual for SLE

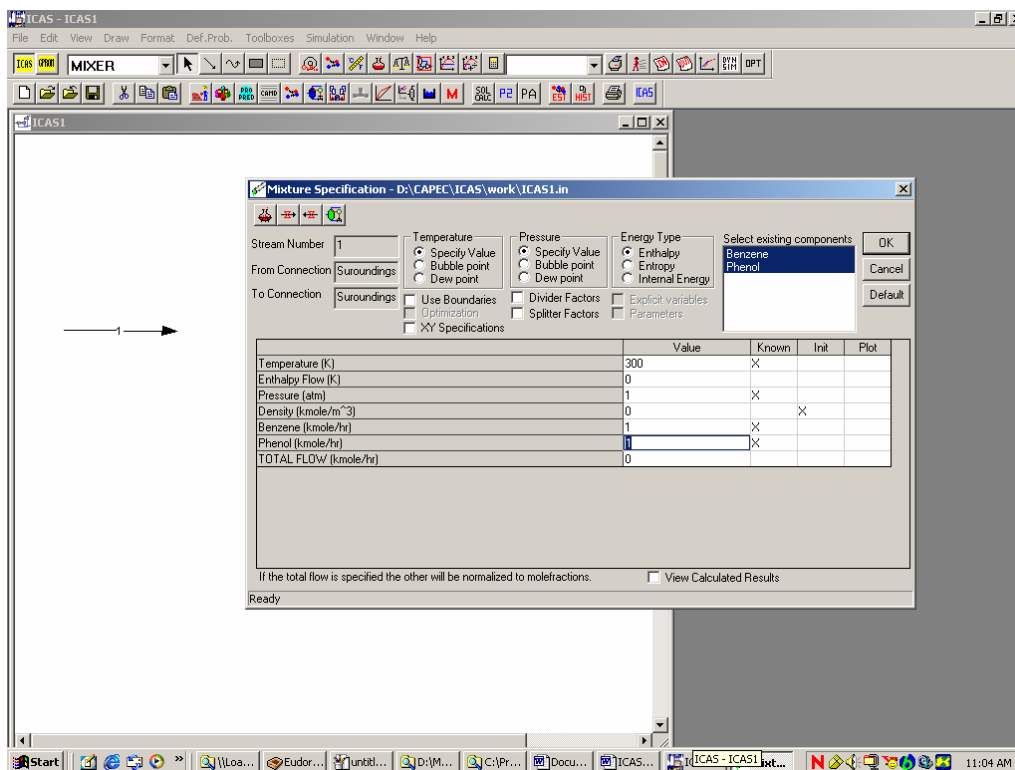
### B1. Use of Utility Toolbox



#### B1.1. Compound selection & property model selection

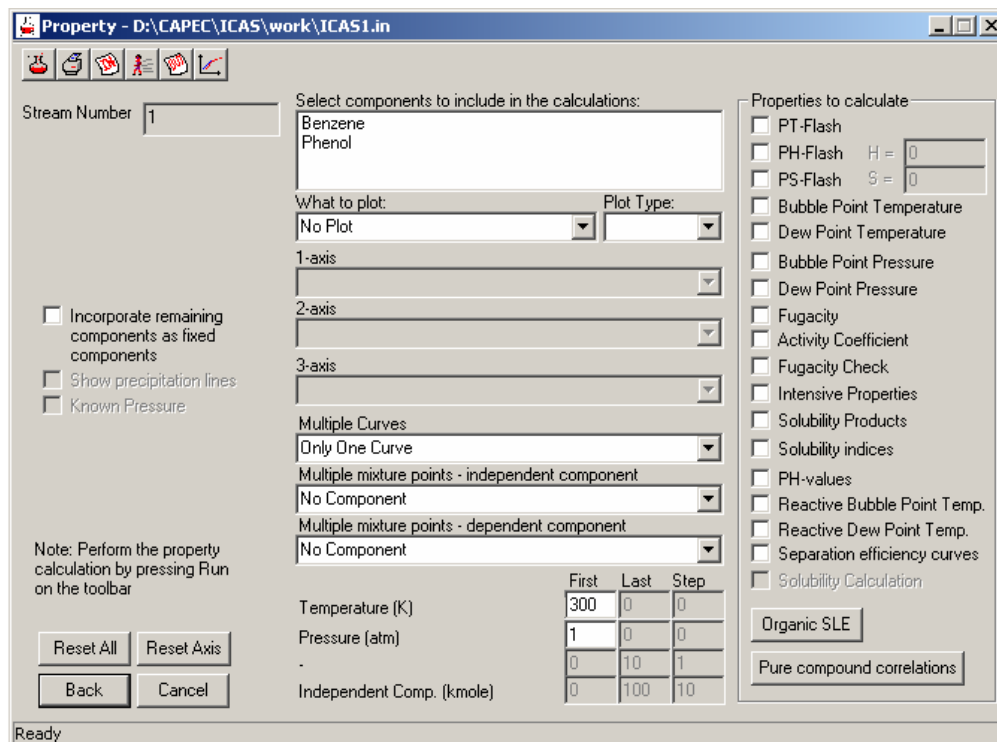
- I. Draw a stream and then select compounds by clicking on the “compounds”  button.



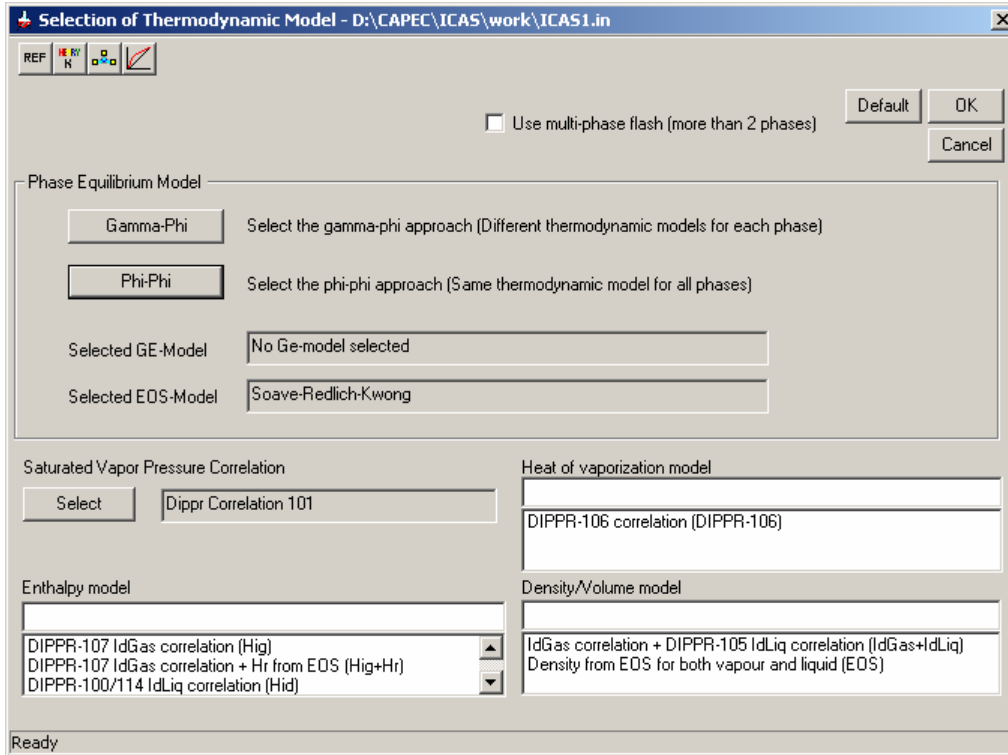
- II. Double click on the stream to enter the “mixture specification” window



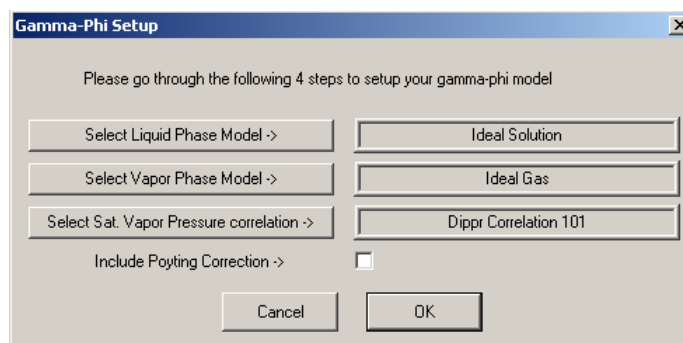
III. After specifying the temperature, pressure and component flows (as shown above) click on the top-left button  to enter the “property” window. Click on the top-left button  to go to the “property model” selection window.



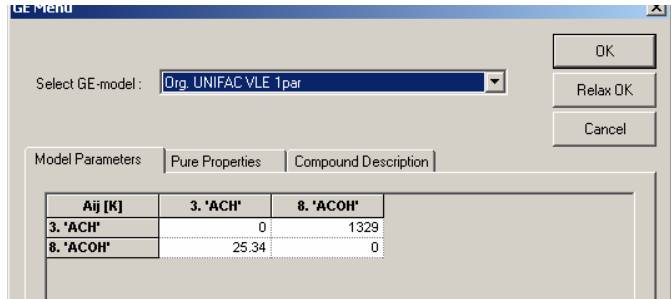
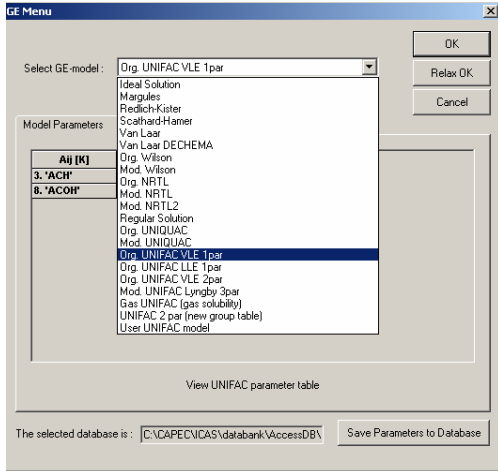
IV. Click on the “gamma-phi” option for this example



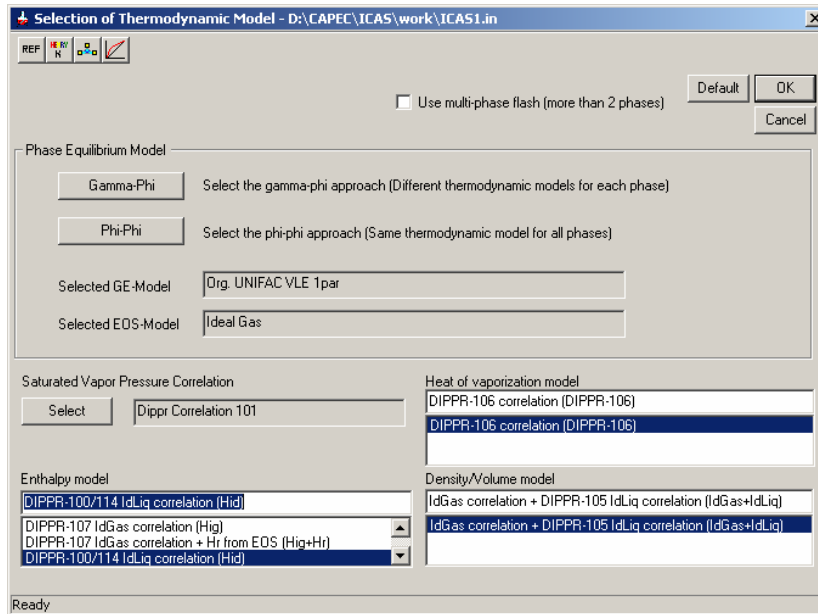
V. Click on the “select liquid phase model”



VI. Select the UNIFAC model as shown below. The UNIFAC model parameters are shown and if all parameters are available (as in this example), click OK

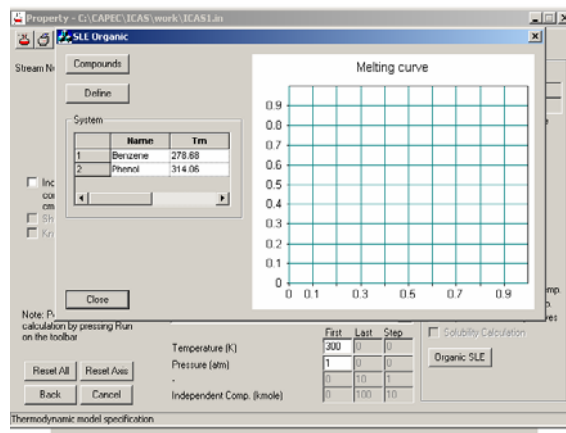


VII. On return to the main property model selection window click on default to select all the other model options (as shown below) and click OK.

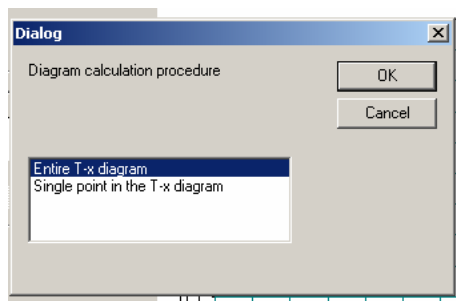


## B1.2 Utility calculation option (SLE)

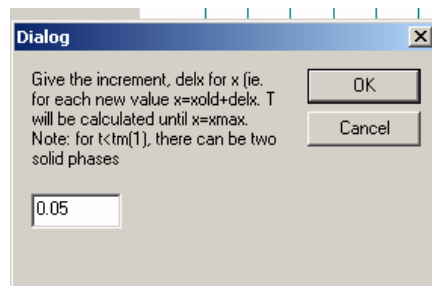
- I. On return to the Property “Utility” window, select the option(s) of choice for calculations. For this example, select the “SLE” option and follow the screens SLE-a to SLE-f.



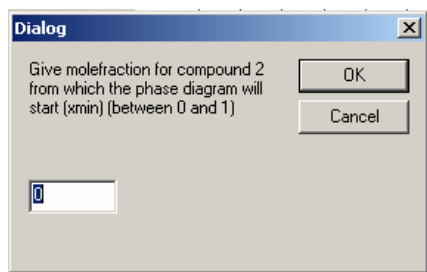
SLE-a



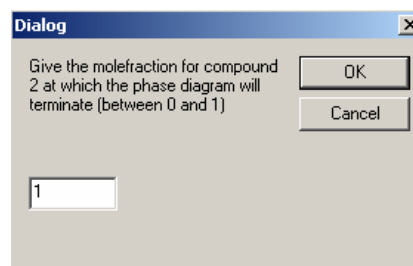
SLE-b



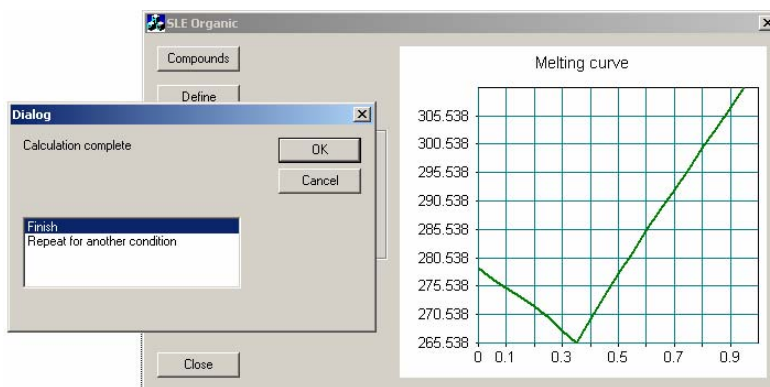
SLE-c



SLE-d



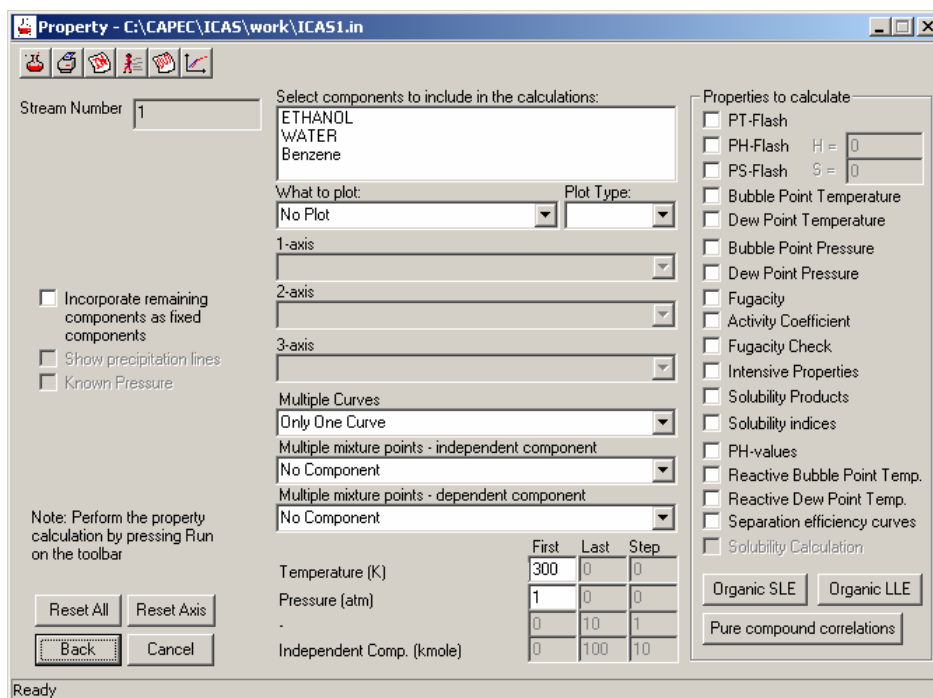
SLE-e



SLE-f

## B2. LLE Phase Diagram

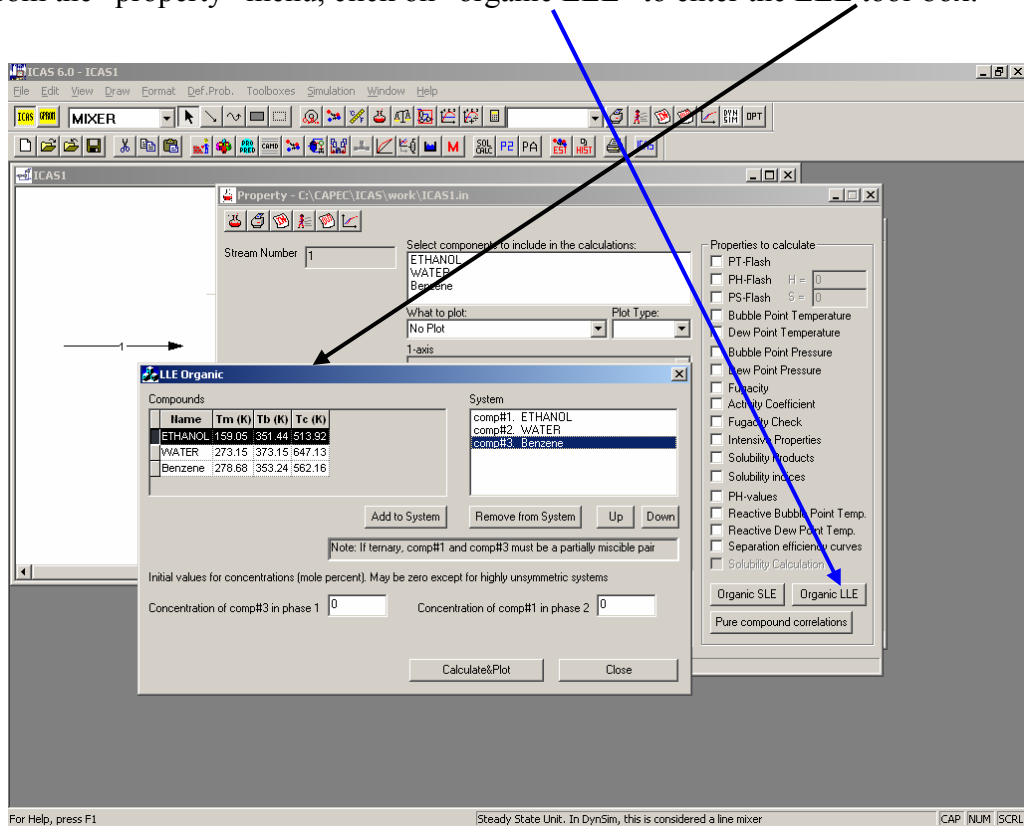
The mixture is changed to water-ethanol-benzene. The UNIFAC-LLE model is chosen and the LLE-phase diagram option is called from the ICAS-utility toolbox, as shown below.



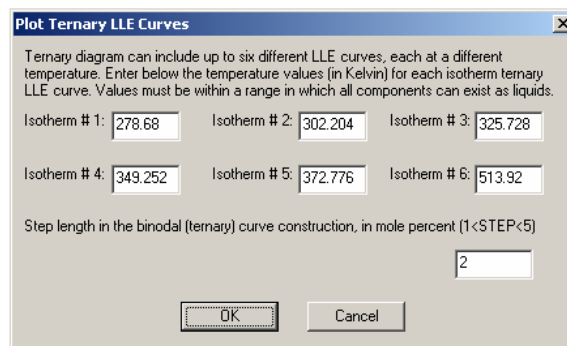
The screenshot shows the "Property" dialog box for the ICAS utility. The "Stream Number" is set to 1. The "Select components to include in the calculations:" list contains ETHANOL, WATER, and Benzene. The "What to plot:" dropdown is set to "No Plot". The "Properties to calculate" section has several options checked, including "Bubble Point Temperature", "Dew Point Temperature", "Bubble Point Pressure", "Dew Point Pressure", "Fugacity", "Activity Coefficient", "Fugacity Check", "Intensive Properties", "Solubility Products", "Solubility indices", "PH-values", "Reactive Bubble Point Temp.", "Reactive Dew Point Temp.", and "Separation efficiency curves". The "Organic SLE" and "Organic LLE" buttons are visible. A table at the bottom right shows the "First", "Last", and "Step" values for Temperature (K), Pressure (atm), and Independent Comp. (kmole).

	First	Last	Step
Temperature (K)	300	0	0
Pressure (atm)	1	0	0
Independent Comp. (kmole)	0	100	10

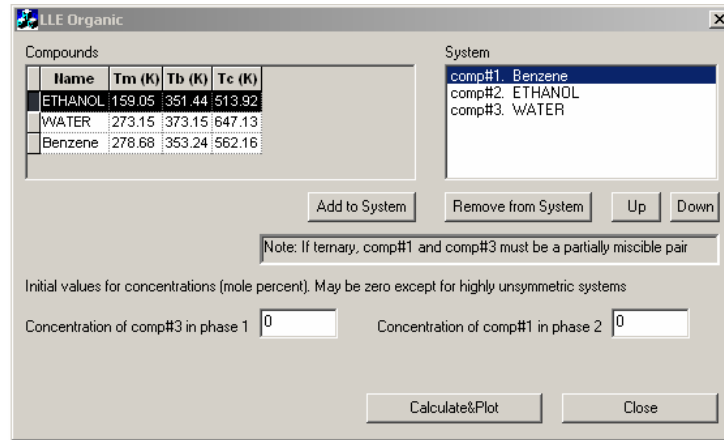
- From the “property” menu, click on “organic LLE” to enter the LLE tool-box:



- From the “LLE organic” window, click on “Calculate & Plot” to enter the “Plot Ternary LLE Curves”



- Click in OK in order to calculate a ternary LLE phase diagram:



- The calculated LLE phase diagram is shown:

