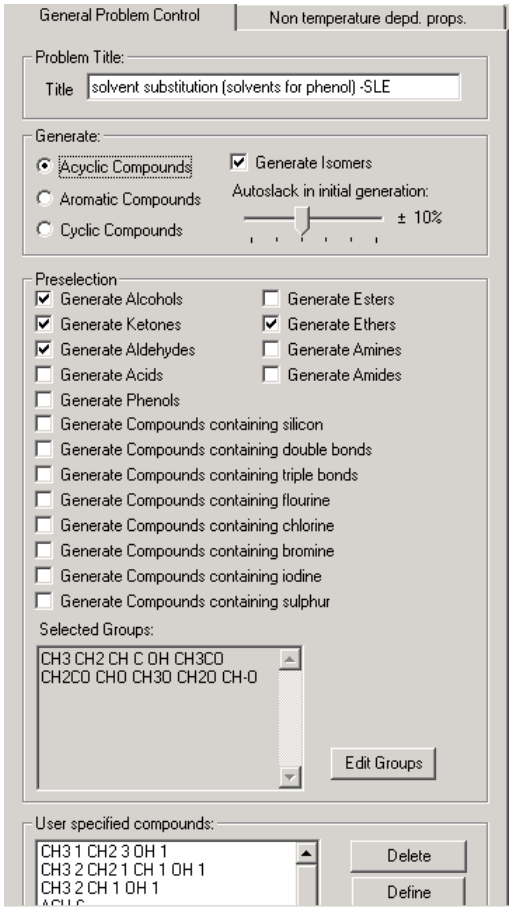
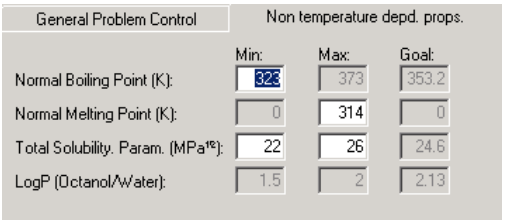
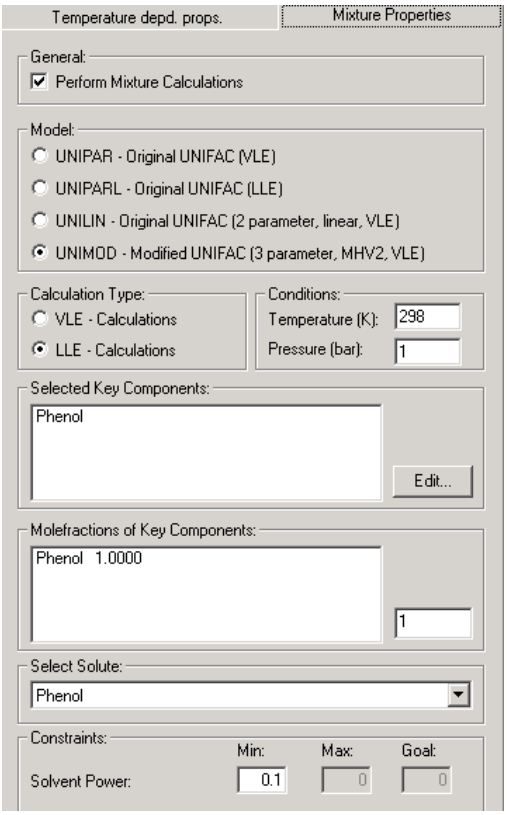
ProCAMD: Illustration with sovent selection or removal of phenol from water

**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.



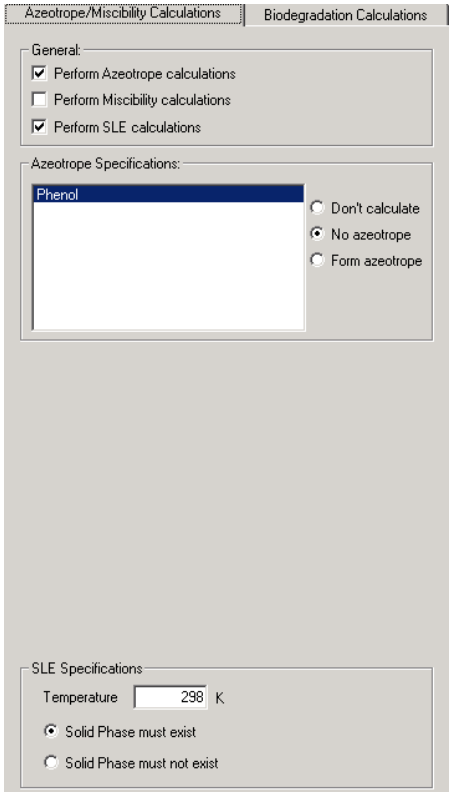




Define as user-specified compounds, some of the solvents that appear in “common solv”

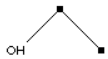
Problem specification pages from ProCamd for the solvent substitution exercise

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




Problem specification page from ProCamd.

**Compound 1 :**

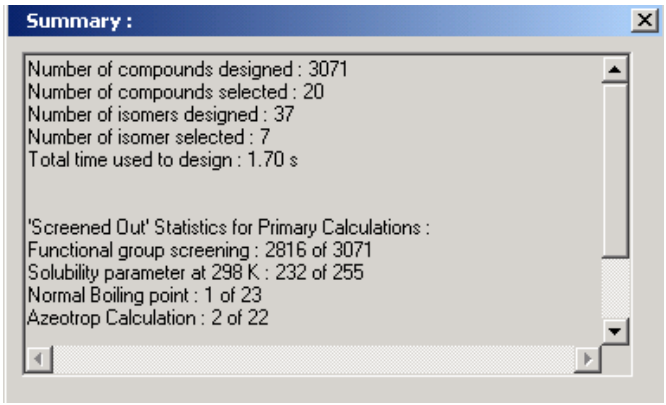



| Description : | |
|---|---|
| No | Groupname |
| 1 | CH3 |
| 1 | CH2 |
| 1 | OH |

| 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 | |


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".

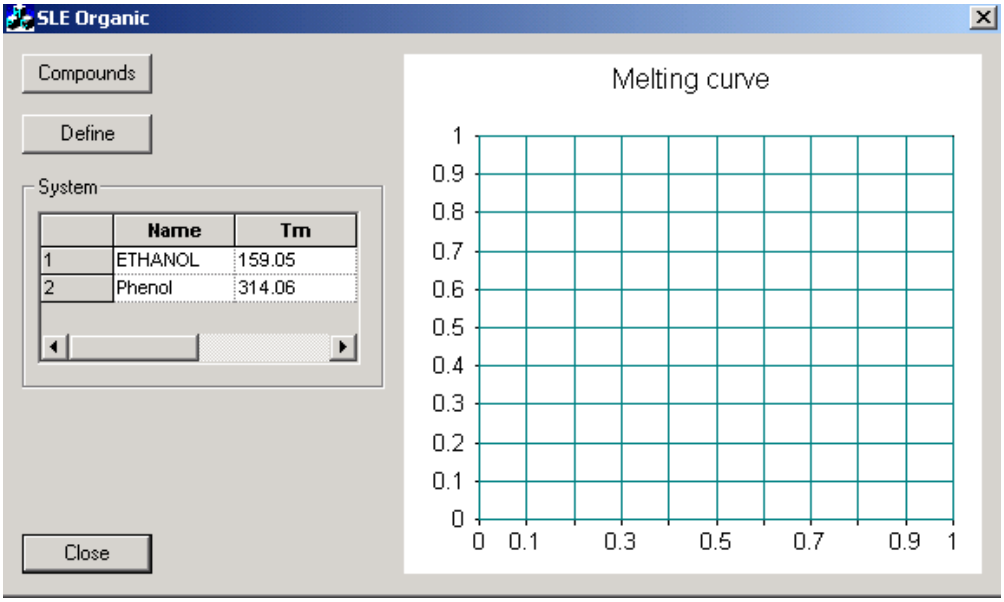


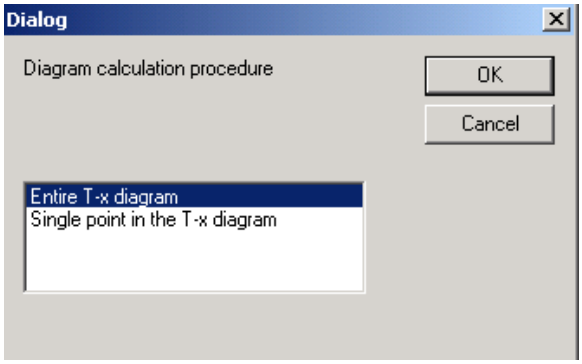

From the figures above, it can be noted that ethanol is also a feasible candidate as a solvent. We will verify the feasibility of ethanol in the next step.

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

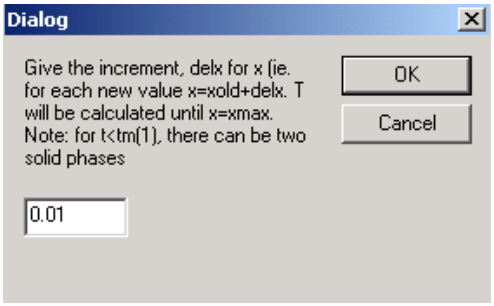
In order to obtain a solid-liquid equilibrium phase diagram, follow the steps given in appendix A3. The following steps are necessary:

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.

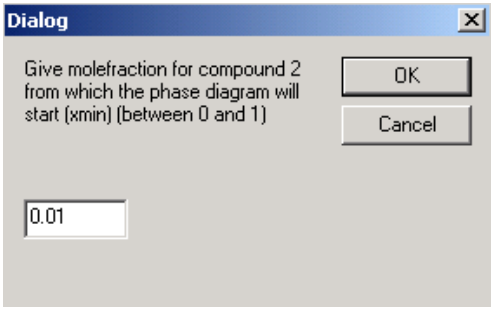




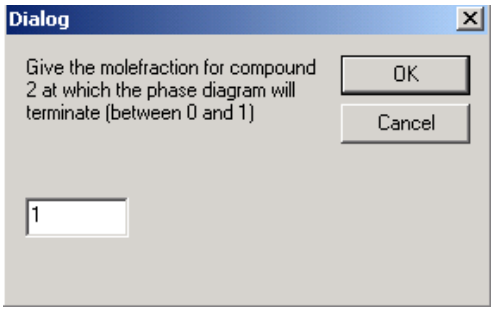

a



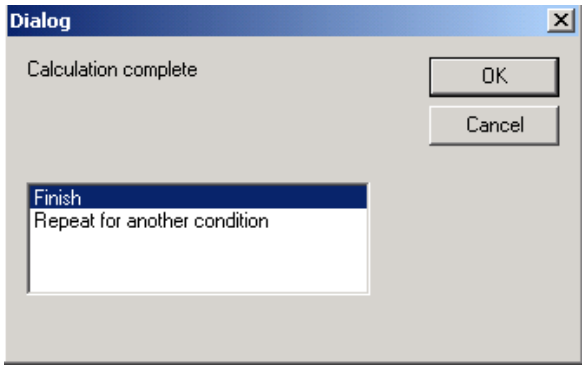

b



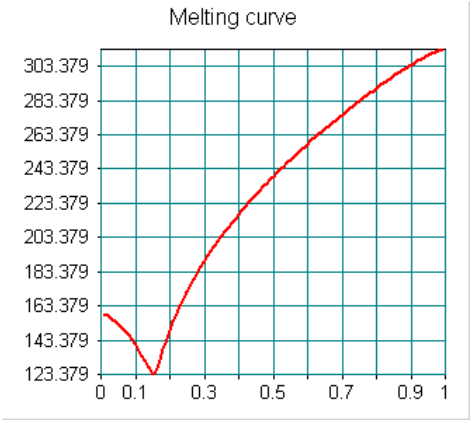

b




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.