User manual

for

CAPEC Database Manager

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1. Introduction

Prerequisites

- CapecDB Manager.xls; user interface, as an excel file
- Azeotropic_Database.xls; database, as an excel file
- Installed ICAS in the computer

Precheck

Make sure that the macros are allowed in the excel file. If this is not the case, the following steps are needed to allow the use of macros in excel:

- On the Tools menu, click Options.
- Click the Security tab.
- Under Macro Security, click Macro Security.
- Click the Security Level tab, and then select the medium security level.

CAPEC Database

CAPEC Database contains mainly the, physiochemical properties of different compounds. It has the following data collections:

- Properties database
- Azeotropic database

2. User interface for data search

Open the file, CapecDB Manager.xls and allow the macros to run. The user interface is shown in figure 1. Two search options (basic search and advanced search) are created to retrieve the properties of compounds (see fig. 1, top, left). There is a separate option to retrieve the azeotropic properties of compounds (see fig. 1, bottom). Help options are also created to guide the user (see fig. 1, top, right) for data retrieval.

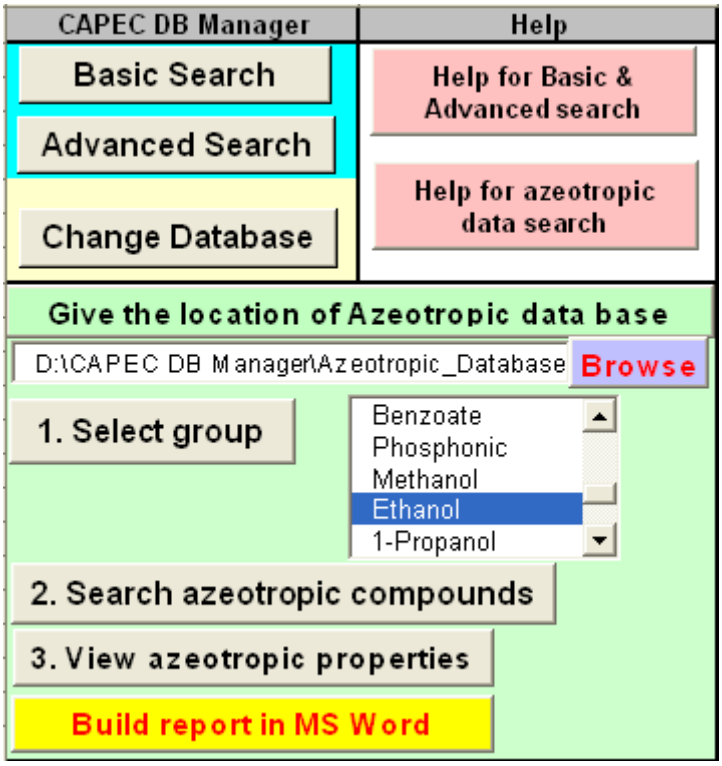

Figure 1: CAPEC Database Manager

2.1. Help options

To see the help for basic and advanced search click on command button, ***"Help for Basic & Advanced search".*** This action will open a help window as shown in figure 2a. Similarly, the help for azeotropic data search can be access by clicking on command button, ***"Help for azeotropic data search"*** (see fig. 2b)

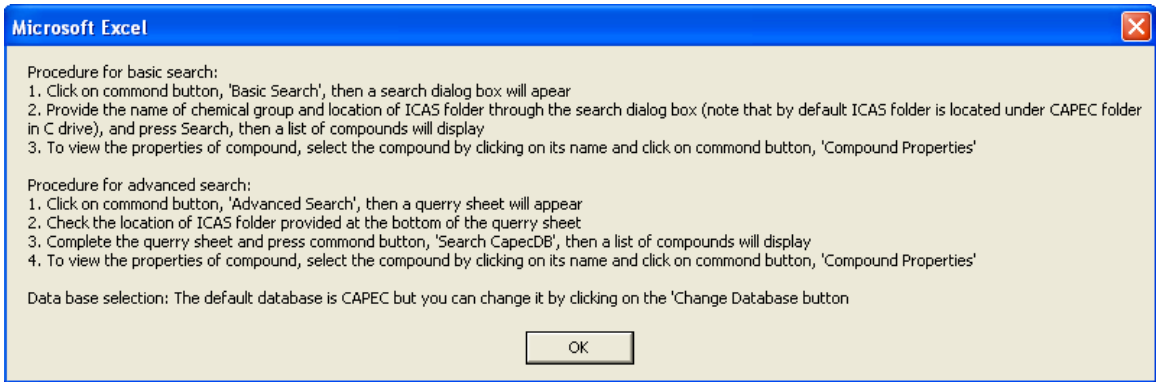

Figure 2a: Help for Basic & Advanced search

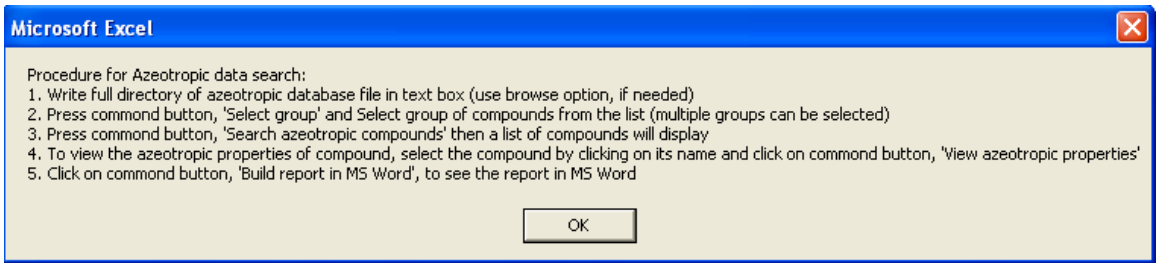

Figure 2b: Help for azeotropic data search

2.2. Change Database

'Capec' is the default data base for both basic & advanced search. However the user can change the data base by Clicking on command button, ***"Change Database"*** and selecting the name of database from the dropdown list (see fig. 3).

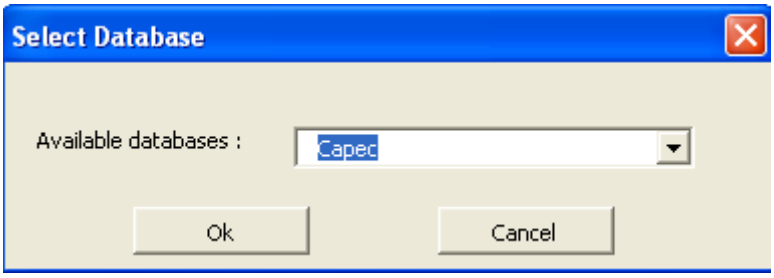

Figure 3: Select data base

2.3. Basic search

The following steps are need to be taken for basic search:

1. Click on the command button ***"Basic search"***, then a search dialog box will appear as shown in figure 4.
2. Provide the search string (e.g. name of chemical group/compound) in the allocated place
3. Check whether the provided location of ICAS folder (C:\CAPEC\ICAS) is right, if not then provide the right directory of ICAS folder
4. Click on the command button, ***"Search",*** to retrieve the compounds related to the search string. Note that, if no search string will be provided then all the compounds will be retrieved. This action will direct to a new sheet ("SearchResult") as shown in

figure 5. Figure shows the some of compounds related to Ethanol group (due to space limit, all compounds are not shown).

5. To retrieve the properties of an individual compound, first select the compound then click on command button, ***"Compound Properties"***. Figure 5 shows a selected compound and command button (fig. 5, left). This action will open a new sheet containing the properties of the selected compound. Properties of a selected compound (Benzenemethanol,.alpha.,.alpha.-diphenyl-) is shown in figure 6.

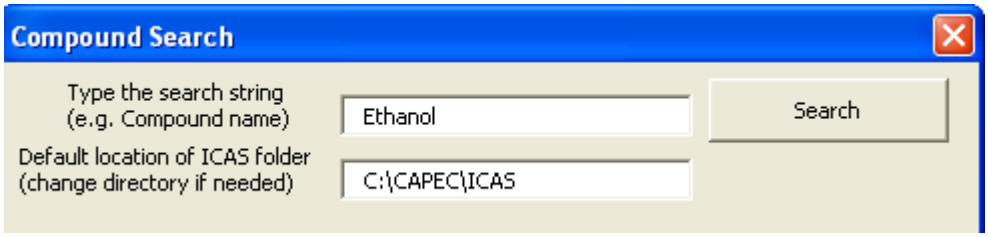

Figure 4: Search dialog box for basic search

C:\CAPEC\ICAS\DataBank\Acces

Compound Consultation

Compound Properties

casno	chemname	formula	smiles
000058-56-0	5-Hydroxy-6-methyl-3,4-pyridinedimethanol,Hydrochloride	C8H12ClNO3	Hn(Cl)(cc(c1CO)CO)c(c1O)C
000075-80-9	Ethanol,2,2,2-tribromo-	C2H3Br3O	OCC(Br)(Br)Br
000075-89-8	Ethanol,2,2,2-trifluoro-	C2H3F3O	FC(F)(F)CO
000076-84-6	Benzenemethanol,.alpha.,.alpha.-diphenyl-	C19H16O	OC(c(cccc1)c1)(c(cccc2)c2)c(cccc3)c3
000080-26-2	3-Cyclohexene-1-methanol,.alpha.,.alpha.,4-trimethyl-,acetate	C12H20O2	O=C(OC(C(CCC(=C1)C)C1)(C)C)C
000081-92-5	Benzenemethanol,2-[bis(4-hydroxyphenyl)methyl]-	C20H18O3	c1cc(O)ccc1C(c2ccc(O)cc2)c3ccccc3CO
000089-95-2	BENZENEMETHANOL,2-METHYL-	C8H10O	c(ccc1CO)cc1C
000090-01-7	Benzenemethanol,2-hydroxy-	C7H8O2	OCc(c(O)ccc1)c1
000090-81-3	Benzenemethanol,.alpha.--1-(methylamino)ethyl--,(R*,S*)-(.+-.)-	C10H15NO	OC(c(cccc1)c1)C(NC)C
000090-86-8	Benzenemethanol,alpha-(1-(methyl(3-phenyl-2-propenyl)amino)ethyl)-	C19H23NO	OC(c(cccc1)c1)C(N(CC=Cc(cccc2)c2)C)C
000091-01-0	Benzenemethanol,.alpha.-phenyl-	C13H12O	OC(c(cccc1)c1)c(cccc2)c2
000091-88-3	Ethanol,2--ethyl(3-methylphenyl)amino--	C11H17NO	OCCN(c(cccc1C)c1)CC
000092-35-3	5H-Thiachromine-8-ethanol,2,7-dimethyl-	C12H14N4OS	n(cc(c(n1)N=C(N2C(=C3CCO)C)S3)C2)c1C
000093-03-8	Benzenemethanol,3,4-dimethoxy-	C9H12O3	O(c(c(OC)cc(c1)CO)c1)C
000093-90-3	Ethanol,2-(methylphenylamino)-	C9H13NO	OCCN(c(cccc1)c1)C
000096-80-0	Ethanol,2--bis(1-methylethyl)amino--	C8H19NO	OCCN(C(C)C)C(C)C
000100-37-8	Ethanol,2-(diethylamino)-	C6H15NO	OCCN(CC)CC
000100-49-2	Cyclohexanemethanol	C7H14O	OCC(CCCC1)C1
000100-55-0	3-Pyridinemethanol	C6H7NO	n(cccc1CO)c1
000100-79-8	1,3-Dioxolane-4-methanol,2,2-dimethyl-	C6H12O3	O(CC(O1)CO)C1(C)C
000100-86-7	Benzeneethanol,.alpha.,.alpha.-dimethyl-	C10H14O	OC(Cc(cccc1)c1)(C)C
000102-79-4	Ethanol,2,2'-(butylimino)bis-	C8H19NO2	OCCN(CCCC)CCO
000102-81-8	Ethanol,2-(dibutylamino)-	C10H23NO	OCCN(CCCC)CCCC
000103-74-2	2-Pyridineethanol	C7H9NO	n(c(ccc1)CCO)c1
000103-76-4	1-Piperazineethanol	C6H14N2O	OCCN(CCNC1)C1
000104-21-2	Benzenemethanol,4-methoxy-,acetate	C10H12O3	O=C(OCc(ccc(OC)c1)c1)C
000104-63-2	Ethanol,2--(phenylmethyl)amino--	C9H13NO	OCCNCc(cccc1)c1
000104-80-3	Furan,tetrahydro-,2,5-diyldimethanol	C6H12O3	O1C(CO)CCC1CO
000105-13-5	Benzenemethanol,4-methoxy-	C8H10O2	O(c(ccc(c1)CO)c1)C
000109-56-8	Ethanol,2--(1-methylethyl)amino--	C5H13NO	OCCNC(C)C
000109-59-1	Ethanol,2-(1-methylethoxy)-	C5H12O2	O(C(C)C)CCO
000109-84-2	Ethanol,2-hydrazino-	C2H8N2O	OCCNN
000110-49-6	Ethanol,2-methoxy-,acetate	C5H10O3	O=C(OCCOC)C
000110-73-6	Ethanol,2-(ethylamino)-	C4H11NO	OCCNCC
000111-21-7	Ethanol,2,2'-1,2-ethanediylbis(oxy)-bis-,diacetate	C10H18O6	O=C(OCCOCCOCCOC(=O)C)C
000111-45-5	Ethanol,2-(2-propenyloxy)-	C5H10O2	O(CCO)CC=C
000111-75-1	Ethanol,2-(butylamino)-	C6H15NO	OCCNCCCC

Figure 5: Retrieval of compound properties (search result)

Chemname	Benzenemethanol,.alpha.,.alpha.-diphenyl-
CasNo	000076-84-6
Formula	C19H16O
Smiles	OC(c(cccc1)c1)(c(cccc2)c2)c(cccc3)c3

Properties :

Mw (g/mol)	260.34	**Ptr(atm)**	**Fpoint(K)**	**TMinA**	
Omega		**Vliq(m3/kmol)**	**Fpl(Vol%)**	**TMaxA**	
Tc(K)		**igHF(kJ/kmol)**	**Fpu(Vol%)**	**dens**	1.199
Pc(atm)		**igGF(kJ/kmol)**	**AIT(K)**	**Facdens**	0
Vc(m3/kmol)		**igS (kJ/(kmol*K)**	**NHYCIF**	**S-Dens**	
Zc		**RG(A)**	**IMCCIF**	**Nd**	
Tm(K)	437.35	**DM(Debye)**	**MCC1**	**FacNd**	
TmInfo		**SolPar((MPa)^.5)**	**MCC2**	**Comment**	
Tb(K)	653.15	**VdWV(m3/kmol)**	**MCC3**		
TbFac		**VdWA(m2/kmol)**	**IANCIF**		
TbFacInfo		**Hf(kJ/kmol)**	**ANTOA**		
TbInfo		**Hc(kJ/kmol)**	**ANTOB**		
Ttr(K)		**RI**	**ANTOC**		

Correlations table

Correlation	Value_A	Value_B	Value_C	Value_D	Value_E	Value_F	TMin	TMax	Equations

Solvent table

Solvent_Cas_Number	Solvent_Name	Solubility	Extra_Informations
007732-18-5	Water	Insoluble	
000064-17-5	Ethanol	Very Soluble	
000060-29-7	Ethyl ether	Very Soluble	
000067-64-1	Acetone	Soluble	

Figure 6: Retrieved properties of selected compound (Benzenemethanol,.alpha.,.alpha.-diphenyl-)

2.4. Advanced search

The following steps need to be taken for advanced search:

1. Click on the command button ***"Advanced search"***, then a query sheet will appear as shown in figure 7.
2. Check whether the provided location of ICAS folder (C:\CAPEC\ICAS) is right (a default location of ICAS folder is given at the bottom of the query sheet), if not then provide the right directory of ICAS folder
3. Complete the query sheet
4. Click on the command button, ***"Search CapecDB"*,** to retrieve the compounds that satisfied the constraints imposed by user. Note that, if no constraints will be provided then all the compounds will be retrieved. This action will direct to a new sheet ("SearchResult") as shown in figure 8, where relevant compounds will be listed
5. To retrieve the properties of an individual compound, first select the compound then click on command button, ***"Compound Properties"***. Figure 8 shows a selected compound and command button (fig. 8, left). This action will open a new sheet containing the properties of the selected compound. The retrieved properties of the selected compound is shown in figure 9.

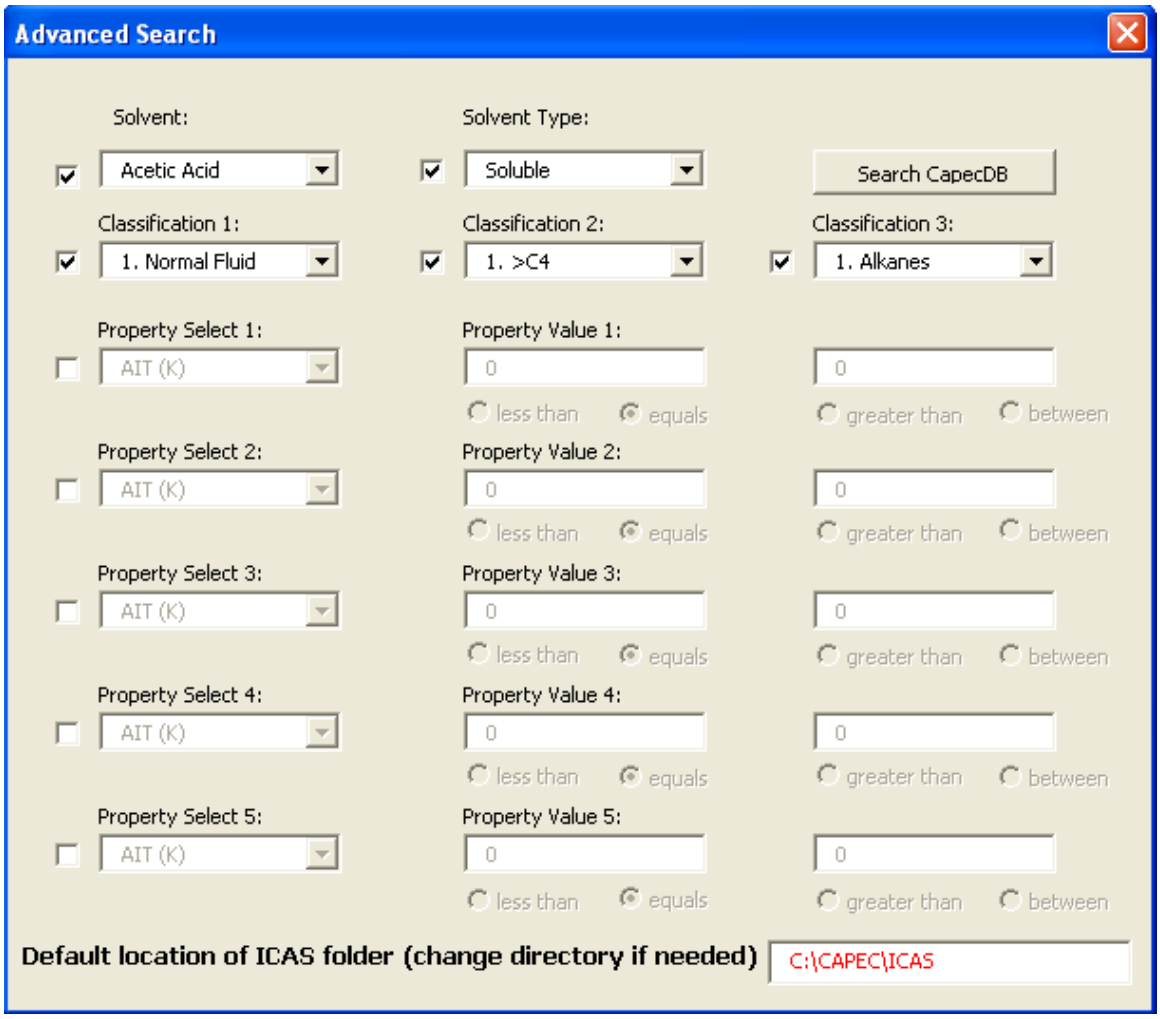

Figure 7: Query sheet for advanced search

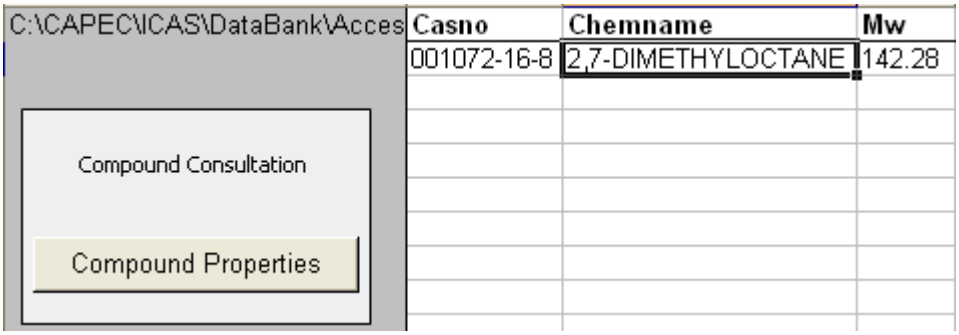

Figure 8: Search result

Chemname	2,7-DIMETHYLOCTANE
CasNo	001072-16-8
Formula	C10H22
Smiles	CC(C)CCCCC(C)C

Properties :

Mw (g/mol)	142.28	**Ptr(atm)**	2.6478E-06	**Fpoint(K)**	306	**TMinA**	219.15
Omega	0.442	**Vliq(m3/km**	0.197594	**Fpl(Vol%)**	0.7	**TMaxA**	604
Tc(K)	604	**igHF(kJ/km**	-264000	**Fpu(Vol%)**	5.1	**dens**	0.7202
Pc(atm)	21.021	**igGF(kJ/km**	26090	**AIT(K)**	0	**Facdens**	25
Vc(m3/kmol)	0.575	**igS (kJ/(km**	520.7	**NHYCIF**	0	**S-Dens**	
Zc	0.244	**RG(A)**	5.357	**IMCCIF**	0	**Nd**	1.4086
Tm(K)	218.25	**DM(Debye)**	0	**MCC1**	0	**FacNd**	20
TmInfo		**SolPar((MP**	15.0616	**MCC2**	0	**Comment**	
Tb(K)	433.05	**VdWV(m3/k**	0.10916	**MCC3**	0		
TbFac		**VdWA(m2/k**	1502000000	**IANCIF**	1		
TbFacInfo		**Hf(kJ/kmol)**	17300	**ANTOA**	7.14408		
TbInfo		**Hc(kJ/kmol)**	-6283400	**ANTOB**	1609.589		
Ttr(K)	219.15	**RI**	1.4062	**ANTOC**	217.005		

Correlations table

Correlation	Value_A	Value_B	Value_C	Value_D	Value_E	Value_F	TMin	TMax	Equations
Solid Density [kmol/m^3	6.39	0	0	0	0	0	219.15	219.15	A+B*T+C*T^2+D*T^3+E*T^4
Liquid Density [kmol/m^	0.46956	0.27	604	0.29916	0	0	219.15	604	A/B^(1+(1-T/C)^D)
Vapour Pressure [Pa]	99.878	-8752.6	-11.422	6.3915E-06	2	0	219.15	604	exp(A+B/T+C*ln(T)+D*T^E)
Heat of Vaporization [J/k	61590000	0.38785	0	0	0	0	219.15	604	A*(1-Tr)^(B+C*Tr+D*Tr^2)
Solid Heat Capacity [J/(l	0	0	0	0	0	0	0	0	No Equation
Liquid Heat Capacity [J/	135780	826.48	-1.5309	0.0021941	0	0	219.15	570	A+B*T+C*T^2+D*T^3+E*T^4
Ideal Gas Heat Capacity	138420	592420	1522.2	400210	664.94	0	200	1500	A+B*(C/T/sinh(C/T))^2+D*(E/T/cosh(E/T))^2
Second Virial Coefficient	0.33706	-459.41	-84779000	-2.014E+20	3.217E+22	0	302	1500	A+B/T+C/T^3+D/T^8+E/T^9
Liquid Viscosity [kg/(m*s	-11.65	1318.5	0.012876	0	0	0	219.15	433.02	exp(A+B/T+C*ln(T)+D*T^E)
Vapour Viscosity [kg/(m	6.0248E-08	0.82735	73.927	0	0	0	219.15	1000	A*T^B/(1+C/T+D/T^2)
Liquid Thermal Conductiv	0.15735	-0.0001872	0	0	0	0	219.15	433.02	A+B*T+C*T^2+D*T^3+E*T^4
Vapour Thermal Conduc	0.000047724	1.0923	-108.07	173490	0	0	433.02	1000	A*T^B/(1+C/T+D/T^2)
Surface Tension [kg/s^2	0.051203	1.2497	0	0	0	0	219.15	604	A*(1-Tr)^(B+C*Tr+D*Tr^2)

Solvent table

Solvent_Cas_Number	Solvent_Name	Solubility	Extra_Informations
000060-29-7	Ethyl ether	Soluble	
000064-19-7	Acetic acid	Soluble	

Figure 9: Retrieved properties of selected compound (2,7-DIMETHYLOCTANE)

2.5. Azeotropic data search

The user interface for azeotropic data search is shown in figure 1 (see at buttom). The following steps need to be taken for azeotropic data search:

1. Specify the directory of azeotropic database. Click on command button ***"Browse"*** to browse the file, if needed. Once the file will be selected, the program automatically write the correct director to the right place
2. Click on the command button, ***"1. Select group",*** to list the available chemical groups in the list box and select the group. Note that multi group can be selected at a time
3. Click on the command button, ***"2. Search azeotropic compounds",*** to retrieve the compounds related to the selected group. Figure 10 (see right) shows the some of compounds related to Ethanol group (due to space limit, all compounds are not shown).
4. To retrieve the azeotropic properties of pair of compounds, first select the compounds then click on command button, ***"2. View azeotropic properties"***. This action will display a short summary of the azeotropic properties in the same window (see fig. 10

button, left) and the detailed azeotropic properties of the selected pair of compounds will be listed in a separate file (not shown here)

5. Click on the command button, ***"Build report in MS Word",*** to make a report of azeotropic properties in a word file (see fig. 11 for report of selected compounds)

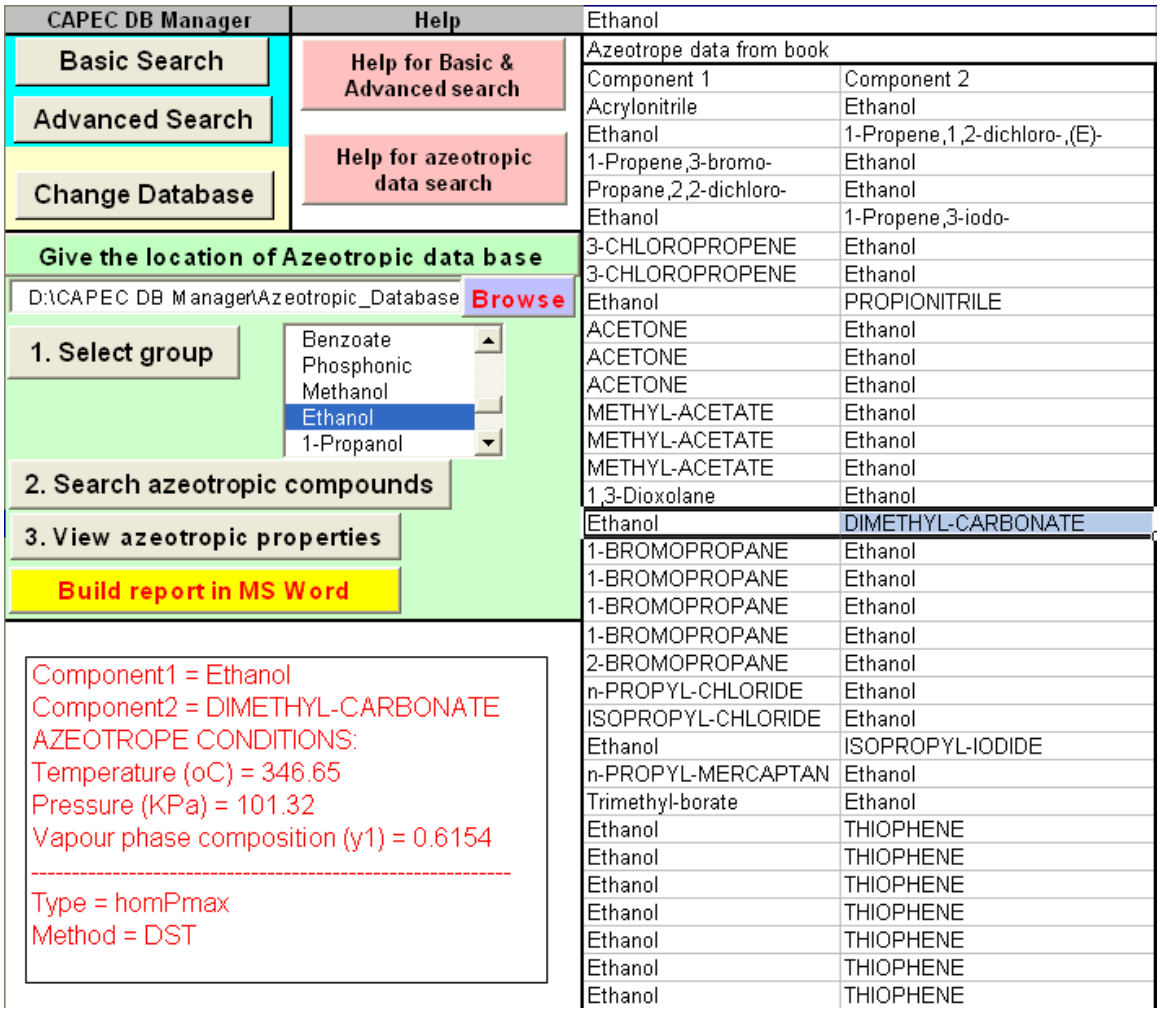

Figure 10: Azeotropic database search

Azeotrope data	
Component1 = Ethanol	
Component2 = DIMETHYL-CARBONATE	
Reported Azeotrope data	
Temperature	346.65
Pressure	101.32
Composition(y1)	0.6154
Type	homPmax
Method	DST
ICAS verification	
Temperature	N/A
Pressure	DIMETHYL-CARBONATE can not be (or has not not been) descripted with the existing UNIFAC groups
Composition(y1)	N/A
Type	N/A
ProCAMD	
Composition (y1)	N/A
Temperature (K)	N/A
Missibility	N/A
Extraction solvent	
Solvent for Ethanol	water, acetone
Solvent for other component	-
Ternary	N/A
Medium	N/A
Heterogeneous_Binary	N/A

Figure 11: Report in MS Word