## User manual

for

# CAPEC Database Manager

Ravendra Singh and Rafiqul Gani June 2009

CAPEC, Department of Chemical and Biochemical Engineering Technical University of Denmark 2800 Kgs. Lyngby, Denmark

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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

Microsoft Excel
Procedure for Azeotropic data search: 1. Write full directory of azeotropic database file in text box (use browse option, if needed) 2. Press commond button, 'Select group' and Select group of compounds from the list (multiple groups can be selected) 3. Press commond button, 'Search azeotropic compounds' then a list of compounds will display 4. To view the azeotropic properties of compound, select the compound by clicking on its name and click on commond button, 'View azeotropic properties' 5. Click on commond button, 'Build report in MS Word', to see the report in MS Word
OK

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).

Select Dat	abase			
Available (	databases :	Capec		•
	Ok		Cancel	

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.

Search

C:\CAPEC\ICAS\DataBank\Accescano		chemname	formula	smiles
	000058-56-0	5-Hydroxy-6-methyl-3,4-pyridinedimethanol,Hydrochloride	C8H12CINO3	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
Compound Consultation 000076-84-6 000080-26-2		Benzenemethanol, alpha., alphadiphenyl-	C19H16O	OC(c(cccc1)c1)(c(cccc2)c2)c(cccc3)c3
		3-Cyclohexene-1-methanol, alpha. , alpha. ,4-trimethyl-,acetate	C12H20O2	0=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
Compound Properties	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, alpha1-(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, alphaphenyl-	C13H12O	OC(c(cccc1)c1)c(cccc2)c2
	000091-88-3	Ethanol,2ethyl(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,2bis(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	000(00001)01
	000100-55-0	3-Pyridinemethanol	C6H7NO	n(cccc1CO)c1
	000100-79-8	1,3-Dioxolane-4-methanol,2,2-dimethyl-	C6H12O3	0(CC(01)C0)C1(C)C
	000100-86-7	Benzeneethanol, alpha., alphadimethyl-	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	010(00)000100
	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	0(C(C)C)CCO
	000109-84-2	Ethanol,2-hydrazino-	C2H8N2O	OCCNN
	000110-49-6	Ethanol,2-methoxy-,acetate	C5H10O3	0=0(0000)0
	000110-73-6	Ethanol,2-(ethylamino)-	C4H11NO	OCCNCC
	000111-21-7	Ethanol,2,2'1,2-ethanediylbis(oxy)-bis-,diacetate	C10H1806	0=C(0CC0CC0CC(=0)C)C
	000111-45-5	Ethanol,2-(2-propenyloxy)-	C5H10O2	0(000)00=0
	1000111-75-1	Ethanol.2-(butylamino)-	C6H15NO	OCCNCCCC

Figure 5: Retrieval of compound properties (search result)

Chemname		ienyl-								
CasNo		000076-84-6								
Formula		C19H16O								
Smiles		OC(c(cccc1)	c1)(c(cccc2)	(cccc3)	:3					
Properties :										
Mw (g/mol)	260.34		Ptr(atm)			Epoint(K)			TMinA	
Omega			Vliq(m3/kn	nol)		Fpl(Vol%)			TMaxA	
Tc(K)			igHF(kJ/kn	nol)		Fpu(Vol%)			dens	1.199
Pc(atm)			igGF(kJ/kn	nol)		AIT(K)			Facdens	0
Vc(m3/kmol)			igS (kJ/(kn	nol*K)		NHYCIF			S-Dens	
Zc			RG(A)			IMCCIF			Nd	
Tm(K)	437.35		DM(Debye	)		MCC1			FacNd	
Tminfo			SolPar((MI	Pa)^.5)		MCC2			Comment	
Tb(K)	653.15		VdWV(m3/	kmol)		MCC3				
TbFac			VdWA(m2/	kmol)		IANCIE				
TbFacInfo			Hf(kJ/kmol	)		ANTOA				
Tbinfo			Hc(kJ/kmo	I)		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_Info	rmations						
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.

Advan	ced Search						
	Solvent:		Solvent Type:				
	Acetic Acid	▼	Soluble	•		Search Capeo	DB
	Classification 1:		Classification 2	:		Classification 3:	
◄	1. Normal Fluid	•	1. >C4	•	◄	1. Alkanes	•
	Property Select 1:		Property Value	1:			
Г	AIT (K)	Y	0			0	
			C less than	🖸 equals		C greater than	C between
	Property Select 2:		Property Value	2:			
	AIT (K)	-	0			0	
			C less than	🖸 equals		C greater than	C between
	Property Select 3:		Property Value	3:			
	AIT (K)	-	0			0	
			C less than	🖲 equals		C greater than	C between
	Property Select 4:		Property Value	4:			
	AIT (K)	-	0			0	
			C less than	🖲 equals		C greater than	C between
	Property Select 5:		Property Value	5:			
Γ	AIT (K)	-	0			0	
			${f C}$ less than	$\odot$ equals		C greater than	C between
Defa	ult location of ICA	S folder (cha	ange directo	ry if needed	d) 🔽	\CAPEC\ICAS	
			-				

Figure 7: Query sheet for advanced search

C	:\CAPEC\ICAS\DataBank\Acce	s Casno	Chemname	Mw
		001072-16-8	2,7-DIMETHYLOCTANE	142.28
				Ι
	Compound Consultation			
	Compound Properties			
	Compound Properties			

Figure 8: Search result

Chemname		2,7-DIMETH	LOCTANE							
CasNo		001072-16-8								
Formula		C10H22								
Smiles			U(U)U							
Properties :										
Mw (g/mol)	142.28		Ptr(atm)	2.6478E-06		Epoint(K)	306	TI	MinA	219.15
Omega	0.442		Vliq(m3/km	0.197594	1	Epl(Vol%)	0.7	TI	MaxA	604
Tc(K)	604		igHF(kJ/km	-264000	1	Epu(Vol%)	5.1	de	ens	0.7202
Pc(atm)	21.021		igGF(kJ/km	26090		AIT(K)	0	Fa	acdens	25
Vc(m3/kmol)	0.575		igS (kJ/(km	520.7	1	NHYCIF	0	S-	-Dens	
Zc	0.244		RG(A)	5.357	1	MCCIF	0	N	d	1.4086
Tm(K)	218.25		DM(Debye)	0	1	MCC1	0	Fa	acNd	20
Tminfo			SolPar((MP	15.0616	1	MCC2	0	C	omment	
Tb(K)	433.05		VdWV(m3/k	0.10916	1	MCC3	0			
TbFac			VdWA(m2/k	1502000000	1	IANCIE	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 Ed	quations	
Correlation Solid Density [kmol/m <sup>4</sup> 3	Value_A 6.39	Value_B 0	Value_C 0	Value_D O	Value_E V	Value_F O	TMin 219.15	TMax E 219.15 A	quations +B*T+C*T^2	+D*T^3+E*T^4
Correlation Solid Density [kmol/m <sup>43</sup> Liquid Density [kmol/m <sup>43</sup>	Value_A 6.39 0.46956	Value_B 0 0.27	Value_C 0 604	Value_D 0 0.29916	Value_E ' O O	Value_F O O	TMin 219.15 219.15	TMax E 219.15 A 604 A	<b>quations</b> +B*T+C*T^2 /B^(1+(1-T/C	+D*T^3+E*T^4 :)^D)
Correlation Solid Density [kmol/m <sup>43</sup> Liquid Density [kmol/m <sup>43</sup> Vapour Pressure [Pa]	Value_A 6.39 0.46956 99.878	Value_B 0 0.27 -8752.6	Value_C 0 604 -11.422	Value_D 0 0.29916 6.3915E-06	Value_E 0 0 2	Value_F O O O	TMin 219.15 219.15 219.15 219.15	TMax E 219.15 A 604 A 604 e	<b>quations</b> +B*T+C*T^2 /B^(1+(1-T/C «p(A+B/T+C	+D*T^3+E*T^4 :)^D) *In(T)+D*T^E)
Correlation Solid Density [kmol/m <sup>43</sup> Liquid Density [kmol/m <sup>43</sup> Vapour Pressure [Pa] Heat of Vaporization [J/k	Value_A 6.39 0.46956 99.878 61590000	Value_B 0 0.27 -8752.6 0.38785	Value_C 0 604 -11.422 0	Value_D 0 0.29916 6.3915E-06 0	Value_E ' 0 0 2 0	Value_F O O O O	TMin 219.15 219.15 219.15 219.15 219.15	TMax E ( 219.15 A 604 A 604 ex 604 A	<b>quations</b> +B*T+C*T^2 /B^(1+(1-T/C «p(A+B/T+C *(1-Tr)^(B+C	+D*Tr3+E*Tr4 )^D) *In(T)+D*TrE) *Tr+D*Tr2)
Correlation Solid Density [kmol/m <sup>43</sup> Liquid Density [kmol/m <sup>43</sup> Vapour Pressure [Pa] Heat of Vaporization [J/k Solid Heat Capacity [J/(]	Value_A 6.39 0.46956 99.878 61590000 0	Value_B 0 0.27 -8752.6 0.38785 0	Value_C 0 604 -11.422 0 0	Value_D 0 0.29916 6.3915E-06 0 0	Value_E 0 2 0 0	Value_F 0 0 0 0 0	TMin 219.15 219.15 219.15 219.15 219.15 0	TMax E ( 219.15 A 604 A 604 e 604 A 604 A 0 N	<b>quations</b> +B*T+C*T^2 /B^(1+(1-T/C «p(A+B/T+C *(1-Tr)^(B+C o Equation	+D*T^3+E*T^4 }^D) *In(T)+D*T^E) *Tr+D*Tr^2)
Correlation Solid Density [kmol/m <sup>43</sup> Liquid Density [kmol/m <sup>43</sup> Vapour Pressure [Pa] Heat of Vaporization [J/k Solid Heat Capacity [J/( Liquid Heat Capacity [J/	Value_A 6.39 0.46956 99.878 61590000 0 135780	Value_B 0.27 -8752.6 0.38785 0 826.48	Value_C 0 604 -11.422 0 0 -1.5309	Value_D 0.29916 6.3915E-06 0 0.0021941	Value_E 0 0 2 0 0 0 0	Value_F 0 0 0 0 0 0	TMin 219.15 219.15 219.15 219.15 0 219.15	TMax E ( 219.15 A 604 A 604 ex 604 A 604 A 0 N 570 A	<b>quations</b> +B*T+C*T^2 /B^(1+(1-T/C «p(A+B/T+C *(1-Tr)^(B+C o Equation +B*T+C*T^2	+D*T^3+E*T^4 )^D) "In(T)+D*T^E) *Tr+D*Tr^2) +D*T^3+E*T^4
Correlation Solid Density [kmol/m <sup>43</sup> Liquid Density [kmol/m <sup>43</sup> Vapour Pressure [Pa] Heat of Vaporization [J/ł Solid Heat Capacity [J/l Ideal Gas Heat Capacity] Ideal Gas Heat Capacity	Value A 6.39 0.46956 99.878 61590000 0 135780 135780 138420	Value_B 0.27 -8752.6 0.38785 0 826.48 592420	Value_C 0 604 -11.422 0 0 -1.5309 1522.2	Value_D 0.29916 6.3915E-06 0 0.0021941 400210	Value_E 0 0 2 0 0 0 0 664.94	Value_F 0 0 0 0 0 0 0 0 0	TMin 219.15 219.15 219.15 219.15 0 219.15 200	TMax E ( 219.15 A 604 A 604 A 604 A 604 A 0 N 570 A 1500 A	<b>quations</b> +B*T+C*T*2 /B*(1+(1-T/C «p(A+B/T+C *(1-Tr)*(B+C o Equation +B*T+C*T*2 +B*(C/T/sinł	+D*T^3+E*T^4 ;}D) *In(T)+D*T^E) *Tr+D*Tr*2) +D*T^3+E*T^4 n(C/T))*2+D*(E/T/cosh(E/T))*
Correlation Solid Density [kmol/m <sup>43</sup> Liquid Density [kmol/m <sup>43</sup> Vapour Pressure [Pa] Heat of Vaporization [J/k Solid Heat Capacity [J// Liquid Heat Capacity [J/ Ideal Gas Heat Capacity Second Virial Coefficient	Value_A 6.39 0.46956 99.878 61590000 0 135780 135780 138420 0.33706	Value_B 0 .27 -8752.6 0.38785 0 826.48 592420 -459.41	Value_C 0 604 -11.422 0 0 -1.5309 1522.2 -84779000	Value_D 0.29916 6.3915E-06 0 0.0021941 400210 -2.014E+20	Value_E 0 2 0 0 0 0 664.94 3.217E+22	Value_F 0 0 0 0 0 0 0 0 0 0 0 0 0 0	TMin 219.15 219.15 219.15 219.15 0 219.15 200 302	TMax E ( 219.15 A 604 A 604 ex 604 A <sup>*</sup> 0 N 570 A 1500 A 1500 A	quations   +B*T+C*T*2   /B*(1+(1-T/C   (#P(A+B/T+C))   *(1-Tr)*(B+C)   o Equation   +B*T+C*T*2   +B*T+C*T*2   +B*T+C*T*2   +B*T+C*T*2   +B*T+C*T*2	+D*T^3+E*T^4 )*D) *In(T)+D*T^E) *Tr+D*Tr*2) +D*T^3+E*T^4 (C/T)*2+D*(E/T/cosh(E/T))* +D/T*8+E/T*9
Correlation Solid Density [kmol/m <sup>43</sup> Liquid Density [kmol/m <sup>43</sup> Vapour Pressure [Pa] Heat of Vaporization [J/ Solid Heat Capacity [J/ Liquid Heat Capacity [J/ Ideal Gas Heat Capacity Second Virial Coefficient Liquid Viscosity [kg/(m <sup>*</sup>	Value_A 6.39 0.46956 99.878 61590000 0 135780 135780 138420 0.33706 -11.65	Value_B 0.27 -8752.6 0.38785 0 826.48 592420 -459.41 1318.5	Value_C 0 604 -11.422 0 0 -1.5309 1522.2 -84779000 0.012876	Value_D 0.29916 6.3915E-06 0 0.0021941 400210 -2.014E+20 0	Value_E ' 0 2 0 0 0 664.94 3.217E+22 0	Value_F 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	TMin 219.15 219.15 219.15 219.15 219.15 219.15 200 302 219.15	TMax Ed 219.15 A 604 A 604 A 604 A 0 N 570 A 1500 A 1500 A 433.02 ex	quations +B*T+C*T^2 /B^(1+(1-T/C «p(A+B/T+C (1-Tr)^(B+C o Equation +B*T+C*T^2 +B*(C/T/sinł +B/T+C/T^3: «p(A+B/T+C	+D*T^3+E*T^4 )*D) *In(T)+D*T^E) *Tr+D*Tr*2) +D*T^3+E*T^4 n(C/T))*2+D*(E/T/cosh(E/T))* +D/T*8+E/T*9 *In(T)+D*T^E)
Correlation Solid Density (kmol/m <sup>43</sup> Liquid Density (kmol/m <sup>43</sup> Vapour Pressure [Pa] Heat of Vaporization [J/ł Solid Heat Capacity [J/l Liquid Heat Capacity [J/l Ideal Gas Heat Capacity Second Virial Coefficient Liquid Viscosity [J/g/m <sup>4</sup> Vapour Viscosity [J/g/m <sup>4</sup>	Value_A 6.39 0.46956 99.878 61590000 0 135780 138420 0.33706 -11.65 6.0248E-08	Value_B 0 0.27 -8752.6 0.38785 0 826.48 592420 -459.41 1318.5 0.82735	Value_C 0 604 -11.422 0 -1.5309 1522.2 -84779000 0.012876 73.927	Value_D 0.29916 6.3915E-06 0 0.0021941 400210 -2.014E+20 0 0	Value E 0 0 2 0 0 664.94 3.217E+22 0 0	Value_F 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	TMin 219.15 219.15 219.15 219.15 219.15 219.15 200 302 219.15 2015 219.15	TMax Ec   219.15 A   604 A   604 A   604 A   604 A   604 A   500 A   1500 A   1500 A   433.02 ex   1000 A <sup>*</sup>	quations +B*T+C*T^2 /B^(1+(1-T/C «p(A+B/T+C *(1-Tr)^(B+C o Equation +B*T+C*T^2 +B*(C/T/sinł +B/T+C/T^3 «p(A+B/T+C *T^B/(1+C/T	+D*T^3+E*T^4 )^DD "h(T)+D*T^E) *Tr+D*Tr^2) +D*T^3+E*T^4 1(C/T)/v2+D*(E/T/cosh(E/T))* +D/T^8+E/T^9 +D/T^8+E/T^9 +D/T^8+E/T^9 +D/T^2)
Correlation Solid Density [kmol/m <sup>43</sup> Liquid Density [kmol/m <sup>43</sup> Vapour Pressure [Pa] Heat of Vaporization [J/ł Solid Heat Capacity [J/l Liquid Heat Capacity [J/l Ideal Gas Heat Capacity Second Virial Coefficient Liquid Viscosity [kg/(m <sup>*</sup> Vapour Viscosity [kg/(m <sup>*</sup> Liquid Thermal Conducti	Value_A 6.39 0.46956 99.878 61590000 135780 138420 0.33706 -11.65 6.0248E-08 0.15735	Value_B 0 .27 -8752.6 0.38785 0 826.48 592420 -459.41 1318.5 0.82735 -0.0001872	Value_C 0 604 -11.422 0 -1.5309 1522.2 -84779000 0.012876 73.927 0	Value 0 0.29916 6.3915E-06 0 0.0021941 400210 -2.014E+20 0 0 0	Value_E 0 0 2 0 0 0 0 664.94 3.217E+22 0 0 0 0	Value_F 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	TMin 219.15 219.15 219.15 219.15 219.15 200 219.15 200 302 219.15 219.15 219.15	TMax Ec   219.15 A:   604 A:   604 A:   604 A:   604 A:   604 A:   0 N:   570 A:   1500 A:   1500 A:   1000 A'   433.02 A:	quations +B*T+C*T^2 /B^(1+(1-T/C kp(A+B/T+C *(1-Tr)^(B+C o Equation +B*T+C*T^2 +B*(C/T/sin) +B/T+C/T^3 kp(A+B/T+C *T^B/(1+C/T +B*T+C*T^2	+D*T^3+E*T^4 )*D) th(T)+D*T^E) +D*T^3+E*T^4 ((C/T))*2+D*(E/T/cosh(E/T))* +D/T%+E/T*9 1n(T)+D*T^E) +D/T*2) +D*T^3+E*T^4
Correlation Solid Density [kmol/m <sup>43</sup> Liquid Density [kmol/m <sup>43</sup> Vapour Pressure [Pa] Heat of Vaporization [J/ Solid Heat Capacity [J/ Liquid Heat Capacity [J/ Ideal Gas Heat Capacity Second Virial Coefficient Liquid Viscosity [kg/(m <sup>2</sup> Vapour Viscosity [kg/(m Vapour Thermal Conducti Vapour Thermal Conducti	Value_A 6.39 0.46956 99.878 61590000 0 135780 138420 0.33706 -11.65 6.0248E-08 0.15735 0.000047724	Value_B 0 0.27 -8752.6 0.38785 0 826.48 592420 -459.41 1318.5 0.82735 -0.0001872 1.0923	Value_C 0 604 -11.422 0 -1.5309 1522.2 -84779000 0.012876 73.927 0 -108.07	Value_D 0.29916 6.3915E-06 0 0.0021941 400210 -2.014E+20 0 0 0 173490	Value_E 0 0 2 0 0 0 0 664.94 3.217E+22 0 0 0 0 0	Value_F 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	TMin 219.15 219.15 219.15 219.15 219.15 200 219.15 200 302 219.15 219.15 219.15 219.15	TMax EC   219.15 A:   604 A:   600 A:   1500 A:   1500 A:   433.02 A:   1000 A:	quations   +B*T+C*T^2   /B^(1+(1-T/C)   /pa(1+(1-T/C)   /pa(1+(1-T/C)   /pa(1+(1-T/C)   /pa(1+(1-T/C)   /pa(1+(1-T/C)   +B*T+C*T^2   +B*T+C*T^3   +pa(1+C/T)   +pa(1+C/T)   +T^AB/(1+C/T)   +B*T+C*T^2   *T^AB/(1+C/T)	+D*T^3+E*T^4 )*D) *In(T)+D*T^E) *Tr+D*Tr*2) +D*T^3+E*T^4 n(C/T))*2+D*(E/T/cosh(E/T))* +D/T*3+E*T^4 +D/T*2) +D/T*2) +D/T*2) +D/T*2) +D/T*2)
Correlation Solid Density [kmol/m <sup>43</sup> Liquid Density [kmol/m <sup>43</sup> Vapour Pressure [Pa] Heat of Vaporization [J/ł Solid Heat Capacity [J/l Liquid Heat Capacity [J/l Ideal Gas Heat Capacity Second Virial Coefficient Liquid Viscosity [kg/m <sup>4</sup> Vapour Viscosity [kg/m Liquid Thermal Conducti Vapour Internal Conducti Surface Tension [kg/s <sup>42</sup>	Value_A 6.39 0.46956 99.878 61590000 0 135780 0.33706 -11.65 6.0248E-08 0.15735 0.000047724 0.051203	Value_B 0 0.27 -8762.6 0.38785 0 826.48 592420 -459.41 1318.5 0.82735 -0.0001872 1.0923 1.2497	Value_C 0 604 -11.422 0 -1.5309 1522.2 -84779000 0.012876 7.3.927 0 -108.07 0	Value_D 0.29916 6.3915E-06 0 0.0021941 400210 -2.014E+20 0 0 173490 0	Value_E 0 0 2 0 0 0 0 664.94 3.217E+22 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Value_F 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	TMin 219.15 219.15 219.15 219.15 200 302 219.15 219.15 219.15 219.15 433.02 219.15	TMax E.   219.15 A:   604 A:   604 A:   604 A:   604 A:   500 A:   570 A:   1500 A:   1500 A:   1000 A'   433.02 A:   1000 A'   604 A'	quations +B*T+C*T^2 /B^(1+(1-T/C wp(A+B/T+C t^(1-Tr)^(B+C o Equation +B*T+C*T^2 +B*T+C*T^2 +B*T+C*T^3 wp(A+B/T+C *T^AB/(1+C/T *T^AB/(1+C/T *T^AB/(1+C/T *(1-Tr)^(B+C)	+D*T^3+E*T^4 )*D) *Tn(T)+D*T^E) *Tr+D*Tr*2) +D*TA3+E*T^4 1(C/T)*2+D*(E/T/cosh(E/T))* +D/TA3+E*T^4 +D/T*2) +D*T^2) +D*T^2) +D*T^2) +D*T^2) *Tr+D*Tr*2)
Correlation Solid Density [kmol/m <sup>43</sup> Liquid Density [kmol/m <sup>43</sup> Vapour Pressure [Pa] Heat of Vaporization [J/k Solid Heat Capacity [J// Liquid Heat Capacity [J// Ideal Gas Heat Capacity Second Virial Coefficient Liquid Viscosity [kg/(m <sup>1</sup> Vapour Viscosity [kg/(m Uqapour Viscosity [kg/(m Uqapour Thermal Conduct Surface Tension [kg/s <sup>4</sup> 2 Solvent table	Value_A 6.39 0.46956 99.878 61590000 0 135780 138420 0.33706 -11.65 6.0248E-08 0.15735 0.000047724 0.051203	Value_B 0 0.27 -8752.6 0.38785 0 826.48 592420 -459.41 1318.5 0.82735 -0.0001872 1.0923 1.2497	Value_C 0 604 -11.422 0 -1.5309 1522.2 -84779000 0.012876 73.927 0 -108.07 0	Value_0 0.29916 6.3915E-06 0 0.0021941 400210 -2.014E+20 0 0 173490 0	Value_E 0 0 2 0 664.94 3.217E+22 0 0 0 0 0 0	Value_F 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	TMin 219.15 219.15 219.15 219.15 219.15 219.15 200 302 219.15 219.15 219.15 219.15 433.02 219.15	TMax EC   219.15 A:   604 A:   1500 A:   1500 A:   1500 A:   1500 A:   1000 A:   433.02 A:   1000 A:   604 A:	quations   +B*T+C*T*2   H2(1-T/C)   (xp(A+B/T+C))   ('1-T)*(B+C)   o Equation   +B*T+C*T*2   +B*T+C*T*2   +B*T+C*T*2   +B*T+C*T*2   +B*T+C*T*2   +B*T+C*T*2   +B*T+C*T*2   +B*T+C*T*2   *T*B/(1+C/T)*   +B*T+C*T*2   *T*B/(1+C/T)*   *T*B/(1+C/T)*   *T*B/(1+C/T)*   *T*B/(1+C/T)*   *T*B/(1+C/T)*	+D*Tx3+E*Tx4 )*D) *In(T)+D*TxE) *Tr+D*Tr*2) +D*Tx3+E*Tx4 n(C/T))*2+D*(E/T/cosh(E/T))* +D/Tx3+E/Tx9 *In(T)+D*TxE) +D/Tx2 +D/Tx2 +D/Tx2 +Tx4 +D/Tx2) *Tr+D*Tr*2)
Correlation Solid Density [kmol/m <sup>43</sup> Liquid Density [kmol/m <sup>43</sup> Vapour Pressure [Pa] Heat of Vaporization [J/h Solid Heat Capacity [J/l Liquid Heat Capacity [J/l Ideal Gas Heat Capacity [J/l deal Gas Heat Capacity Second Virial Coefficient Liquid Viscosity [kg/m <sup>4</sup> Vapour Viscosity [kg/m <sup>4</sup> Vapour Thermal Conduct Vapour Thermal Conduct Solvent Cas_Number	Value_A 6.39 0.46956 99.878 6159000 0 135780 0.33706 -11.65 6.0248E-08 0.15735 0.000047724 0.051203 Solvent_Name	Value_B 0 0.27 -8752.6 0.38785 0 826.48 592420 -459.41 1318.5 0.82735 -0.0001872 1.0923 1.2497 Solubility	Value_C 0 604 -11.422 0 -1.5309 1522.2 -84779000 0.012876 73.927 -108.07 0 -108.07 0	Value_0 0.29916 6.3915E-06 0 0.0021941 400210 -2.014E+20 0 0 173490 0 173490 0	Value_E 0 0 2 0 664.94 3.217E+22 0 0 0 0 0 0	Value_F 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	TMin 219.15 219.15 219.15 219.15 200 302 219.15 219.15 219.15 219.15 219.15 219.15 219.15 219.15 219.15	TMax E.   219.15 A:   604 A:   604 A:   604 A:   604 A:   500 A:   570 A:   1500 A:   1500 A:   433.02 A:   1000 A:   433.02 A:   1000 A:   604 A:	quations   +B*T+C*T*2   H2(1-T/C)   KP(4(1-T/C)   xp(A+B/T+C)   q(1-T)*(1+C)   +B*T+C*T*2   +B*(C/T/Sin)   +B*(C/T/Sin)   +B*(C/T/Sin)   +B*(1+C)**   +B*(1+C)**   *PT+C*T*2   *T*AU(1+C/T)   *B*T+C*T*2   *T*AU(1+C/T)   *(1-Tr)*(B+C)	+D*T^3+E*T^4 )*D) *In(T)+D*T^E) *Tr+D*Tr*2) +D*T^3+E*T^4 n(C/T)*2+D*(E/T/cosh(E/T))* +D/T*3+E*T^4 +D/T*2) +D*T^2) +D*T^3+E*T^4 +D/T*2) *Tr+D*Tr*2) *Tr+D*Tr*2)
Correlation Solid Density [kmol/m <sup>4</sup> 3 Liquid Density [kmol/m <sup>4</sup> 3 Vapour Pressure [Pa] Heat of Vaporization [J/k Solid Heat Capacity [J/l Liquid Heat Capacity [J/l Ideal Gas Heat Capacity [J/l deal Gas Heat Capacity [J/l] deal Gas Heat C	Value_A 6.39 0.46956 99.878 61590000 0.135780 1.38420 0.33706 -11.65 6.0248E-08 0.15735 0.000047724 0.051203 Solvent_Name Ethyl ether	Value_B 0 0.27 -8752.6 0.38785 0 826.48 592420 -459.41 1318.5 0.82735 -0.0001872 1.0923 1.2497 Solubility Soluble	Value_C 0 604 -11.422 0 0 -1.5309 1522.2 -84779000 0.012876 73.927 0 -108.07 0 Extra_Inform	Value_0 0 0.29916 6.3915E-06 0 0 0.0021941 400210 -2.014E+20 0 0 173490 0 173490 0	Value_E 0 0 0 0 0 0 0 0 664.94 3.217E+22 0 0 0 0 0	Value_F 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	TMin 219.15 219.15 219.15 219.15 200 302 219.15 219.15 219.15 219.15 433.02 219.15	IMax Ec   219.15 A   604 A   604 A   604 A   604 A   604 A   604 A   500 A   1500 A   1500 A   1500 A   1500 A   1000 A'   433.02 A   1000 A'   604 A'	quations   +B*T+C*Tx2   Pb*(1+(1-T)C   pb*(1+(1-T)C   pb*(1-T)A   pb*(1-T)A	+D*Tr3+E*Tr4 )*D) +In(T)+D*TrAE) *Tr+D*Tr42) +D*Tr3+E*Tr4 ((C/T))*2+D*(E/T/cosh(E/T))* +D/T*0+E/T*9 *In(T)+D*TrAE) +D/T*2) +D*Tr3+E*Tr4 +D/T*2) *Tr+D*Tr*2)

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:

- 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)

100						
	CAPEC DB Manager Help		Ethanol			
	Basic Search	Help for Basic &	Azeotrope data from book			
	Basic Scarch	Advanced search	Component 1	Component 2		
	Advanced Search	Automoted boardin	Acrylonitrile	Ethanol		
	Advanced Search		Ethanol	1-Propene,1,2-dichloro-,(E)-		
		Help for azeotropic	1-Propene,3-bromo-	Ethanol		
	Change Database	data search	Propane,2,2-dichloro-	Ethanol		
			Ethanol	1-Propene,3-iodo-		
	Give the location of <i>k</i>	zeotronic data base	3-CHLOROPROPENE	Ethanol		
	onve the location of y	Teotropic data base	3-CHLOROPROPENE	Ethanol		
	D:\CAPEC DB Manager\Aze	eotropic_Database Browse	Ethanol	PROPIONITRILE		
		Benzoate	ACETONE	Ethanol		
	1. Select group	Phosphonic	ACETONE	Ethanol		
1		Methanol	ACETONE	Ethanol		
		Ethanol	METHYL-ACETATE	Ethanol		
		1-Propanol 🗾	METHYL-ACETATE	Ethanol		
ľ	2 Secreb erectropie	ampaunda	METHYL-ACETATE	Ethanol		
	2. Search azeotropic o	compounds	1,3-Dioxolane	Ethanol		
	3 View azeotropic pro	nerties	Ethanol	DIMETHYL-CARBONATE		
	o. view azeotropic pro	perces	1-BROMOPROPANE	Ethanol		
	Build report in MS	Nord	1-BROMOPROPANE	Ethanol		
			1-BROMOPROPANE	Ethanol		
			1-BROMOPROPANE	Ethanol		
	Component1 = Ethanol		2-BROMOPROPANE	Ethanol		
	Component? - DIMETH		n-PROPYL-CHLORIDE	Ethanol		
		INC.	ISOPROPYL-CHLORIDE	Ethanol		
	AZEOTROPE CONDIT	IUNS.	Ethanol	ISOPROPYL-IODIDE		
	Temperature (oC) = 34	6.65	n-PROPYL-MERCAPTAN	Ethanol		
	Pressure (KPa) = 101.3	32	Trimethyl-borate	Ethanol		
	Vapour phase compos	ition (v1) = 0.6154	Ethanol	THIOPHENE		
			Ethanol	THIOPHENE		
	Type - homPmax		Ethanol	THIOPHENE		
			Ethanol	THIOPHENE		
	Imethod = DS1		Ethanol	THIOPHENE		
			Ethanol	THIOPHENE		
			Ethanol	THIOPHENE		

Figure 10: Azeotropic database search

Azeotrope data					
Component1 = Ethanol					
Component2 = DIMETHYL-CARBONATE					
Reported Azeotrope d	ata				
Temperature	346.65				
Pressure	101.32				
Composition(y1)	0.6154				
Туре	homPmax				
Method	DST				
ICAS verification					
Temperature	N/A				
	DIMETHYL-CARBONATE can not be (or has not not been) descripted				
Pressure	with the existing UNIFAC groups				
Composition(y1)	N/A				
Туре	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_Binar					
γ	N/A				

Figure 11: Report in MS Word