SOFTWARE INTELIGENT PACKAGE FOR PHASE EQULIBRIA (PHEQ) IN SYSTEMS APPLIED IN CHEMISTRY AND CHEMICAL ENGINEERING

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Abstract

The importance and role of phase equilibria are related to plant design, safety, reliability, operation in chemical and biochemical engineering. For an effective and efficient utilization of large amounts of phase equilibrium data in chemical and biochemical engineering, an intelligent database program for phase equilibrium (PHEQ) data management and application was developed. Three modules of the PHEQ program were developed: (1) TERMOD1, for the pure component data base and applications, (2) VLE2, for the binary systems data base and applications, and (3) VLE3, for the ternary systems data base and applications. Furthermore, calculation programs of PVT and phase equilibrium properties of pure components (LVV1), calculation programs of vapour-liquid equilibria of binary systems (GEOSk2), and calculation programs of vapour-liquid equilibria of ternary systems (GEOS3) based on the most reliable models were implemented. Examples of application are given, including original data measured in our laboratory, using high pressure cells for isochoric PVT data and phase equilibria in binary and ternary mixtures. The PHEQ program enables the extraction of data and results so that the time-consuming data management, data processing and analysis are avoided. PHEQ Windows allow users to set up problems and to carry out calculations in a simple and rapid manner. It provides access to all PHEQ facilities and can produce output as text files, graphics or Excel worksheets.

INTRODUCTION

Phase equilibria software has been developed in our laboratory since long time. The first calculation programs were written in 1984, and used for pressure-volume-temperature (PVT) and phase equilibria calculations with the general cubic equation of state.[1] In 1985, calculation programs were written, and used for phase equilibria calculations in binary and ternary systems with the general cubic equation of state.

In 1995, the calculation programs, rewritten in FORTRAN 77, and running under Windows 95, were coupled with databases. The software for pure component equilibria and PVT calculations, called LVV1DT, the software for phase equilibria in binary systems, called GEOSK2, and the software for phase equilibria in ternary systems, called GEOS3, were used in our department and in other research groups, by doctorands and students both as learning and research tool. Special programs coupled with corresponding data bases were used for calculations.

This project (called PHEQ – Phase Equilibria Database and Calculation Programs) was started to develop software using modern features of the last Windows programs (2000, Me and XP), databases applications (MS Access, Visual Basics), and Fortran programming (Compaq Visual Fortran Compilator).

The first module of the PHEQ project, is a software package to manage a database for pure component (TERMOD1), and the application programs for correlation and/or prediction of PVT and phase behaviour of the pure component systems.

The second module of the PHEQ project, is a software package to manage a database for phase equilibria in binary systems (VLE2), and the application programs for correlation and/or prediction of phase behaviour of the binary systems.
The third module of the PHEQ project, is a software package to manage a database for phase equilibria in ternary systems (VLE3), and the application programs for calculation (prediction) of phase behaviour of the ternary systems.
Graphical output is integrated in the software, in order to provide plots of phase diagrams, and tools to export calculated and experimental information to other software like Word or Excel. The database software was programmed under Visual Basic 6.0. Special programs coupled with corresponding data bases were implemented for calculations of pure-component properties by equations of state[2,3] (LVV1 and LVV1DT), for calculations of phase equilibria in binary systems by equations of state[4,5] (GEOSK2 and GEOSHVID), and for calculations of phase equilibria in ternary/multicomponent systems by equations of state[6,7] (GEOSPH3, GEOSHVID, MHV2, UNIFAC). All calculation programs are Compaq Visual Fortran 6.6 compiled Windows versions.

DATABASE AND APPLICATION PROGRAM TERMOD1 IN PHEQ PACKAGE

Fig. 1 shows the main screen of intelligent database program developed in this project. An intelligent data base program written in Visual Basic 6.0 has been constructed under fully compatibility with Windows XP for the continuous upgrade version and the effective interface with users. The Pentium 4 PC was used to build and run the database program and applications. Fig. 2 shows the initial screen image for the pure component data base and applications (called TERMOD1) where we can pick up all the related information, applicable code and associated data management. A toolbar serves as a foundation for the higher levels convenient access to the database, interactive and automated data set selection and calculations.

This software may be used in relation to MS-Office (Word, Excel, PowerPoint and Access). Basically, the software MS Access is used for the implementation of the database as shown in the Fig. 3. Tables, queries and forms are the main parts of the database.

The data base contains five types of PVT and equilibrium data for 70 chemical compounds: saturation properties in two formats, isotherms, isobars and isochors. Data recommended in the literature (when available, IUPAC data), as well as data measured in our laboratory were introduced in the TERMOD1 data base.

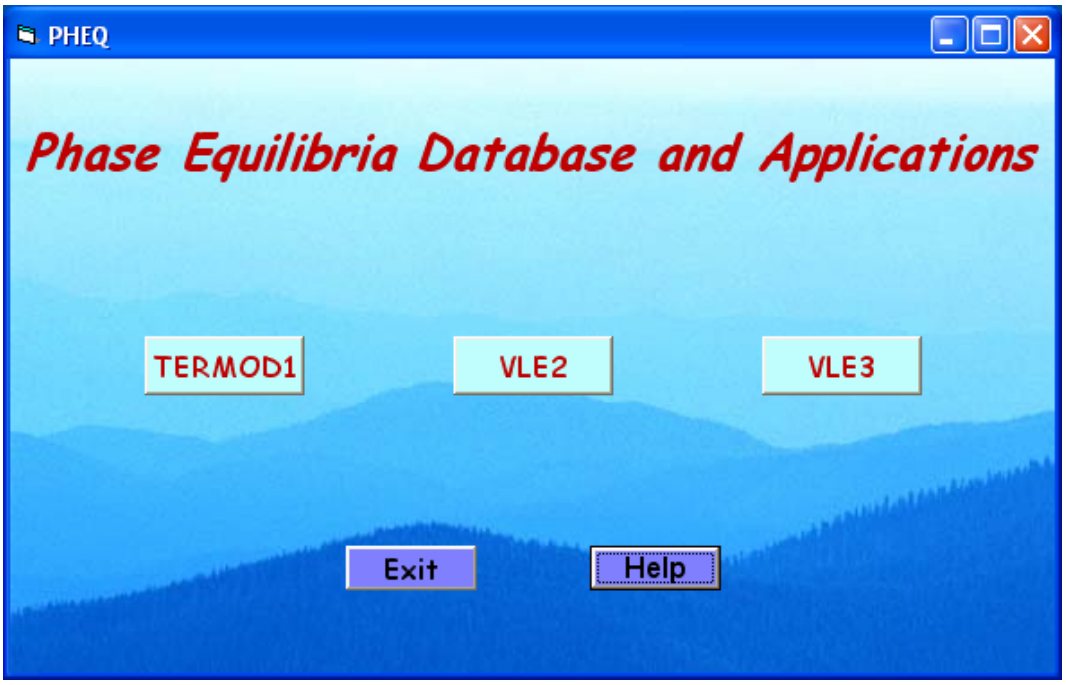
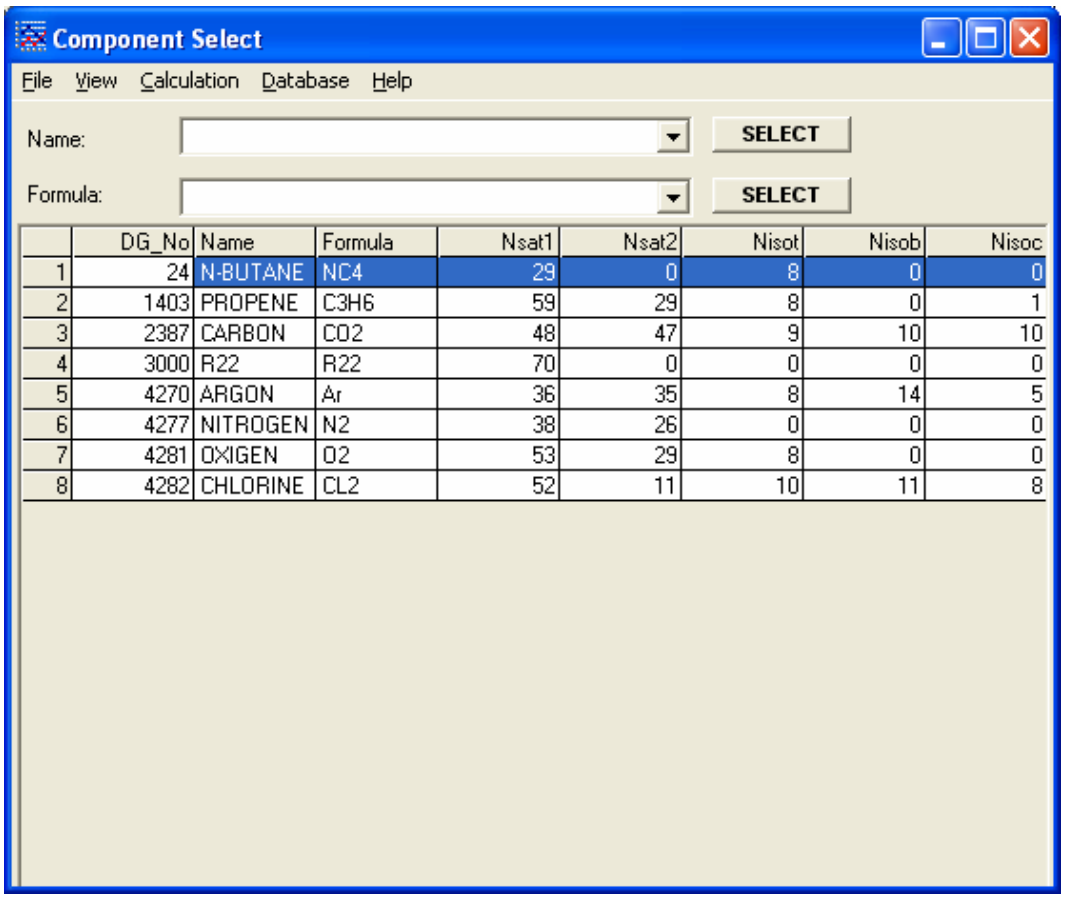


Fig.1. Main screen of PHEQ database program



	DG_No	Name	Formula	Nsat1	Nsat2	Nisot	Nisob	Nisoc
1	24	N-BUTANE	NC4	29	0	8	0	0
2	1403	PROPENE	C3H6	59	29	8	0	1
3	2387	CARBON	CO2	48	47	9	10	10
4	3000	R22	R22	70	0	0	0	0
5	4270	ARGON	Ar	36	35	8	14	5
6	4277	NITROGEN	N2	38	26	0	0	0
7	4281	OXIGEN	O2	53	29	8	0	0
8	4282	CHLORINE	CL2	52	11	10	11	8

Fig.2. Screen image for the pure component data base and applications (TERMOD1)

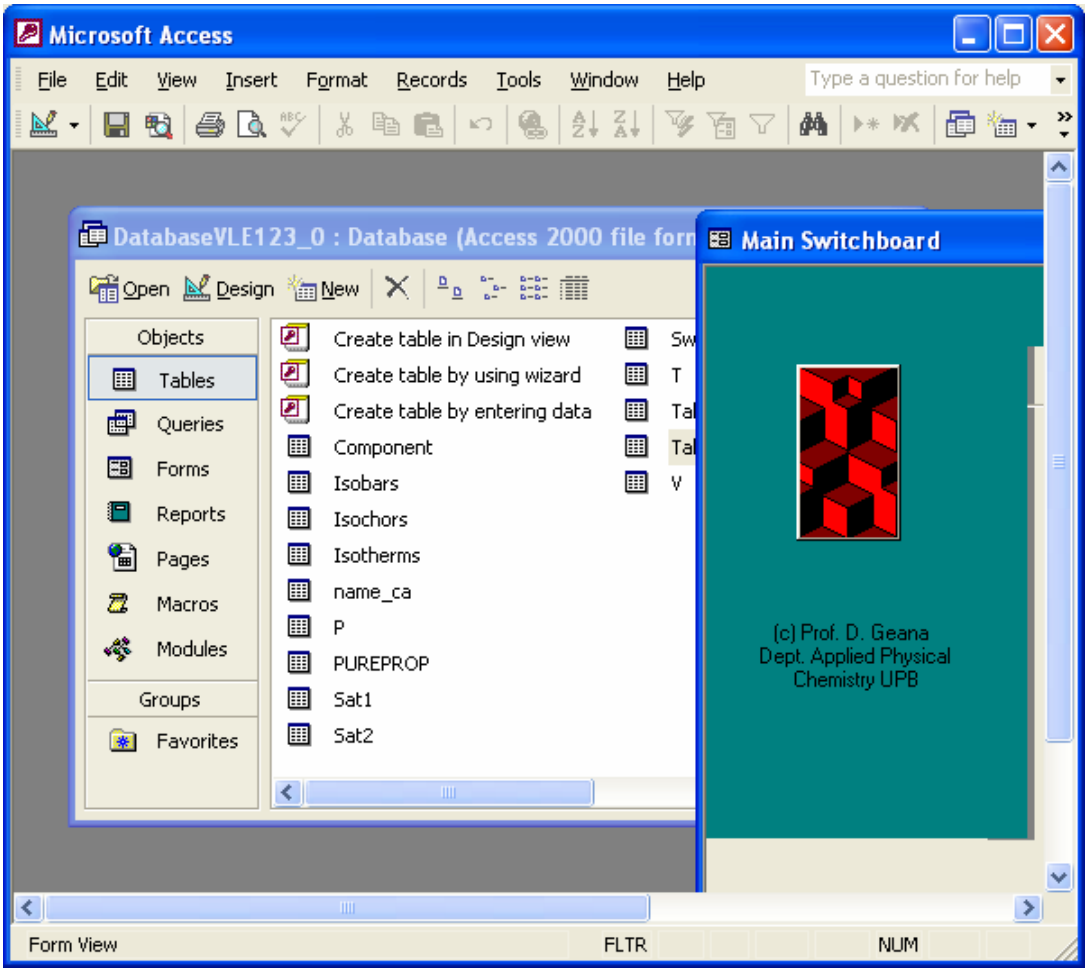


Fig. 3. Access database used by the PHEQ program in TERMOD1 section

Measurements of isochoric data were made with a high pressure apparatus for argon, nitrogen and carbon dioxide in the temperature range (5-80 C) and pressure (5-120 bar). A schematic diagram of the experimental setup for isochoric high pressure measurements is shown in Fig. 4. As an example, in Fig. 5 the measured isochors for carbon dioxide are reported. A comparison of measured data with the calculated values from the equation of state of Span and Wagner is presented in Fig. 5. As can be seen the agreement of measured and calculated data is very good. The calculations were made with the TERMOD1 module of the PHEQ program.

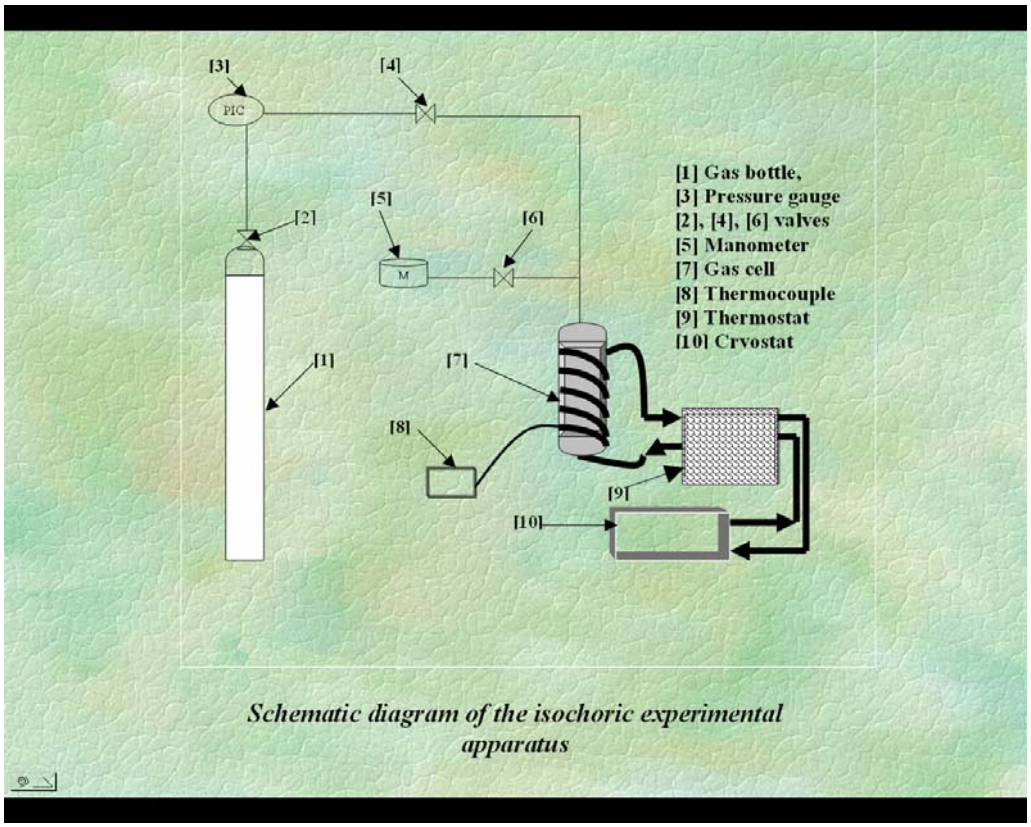


Fig.4. Schematic diagram of the isochoric high pressure experimental setup.

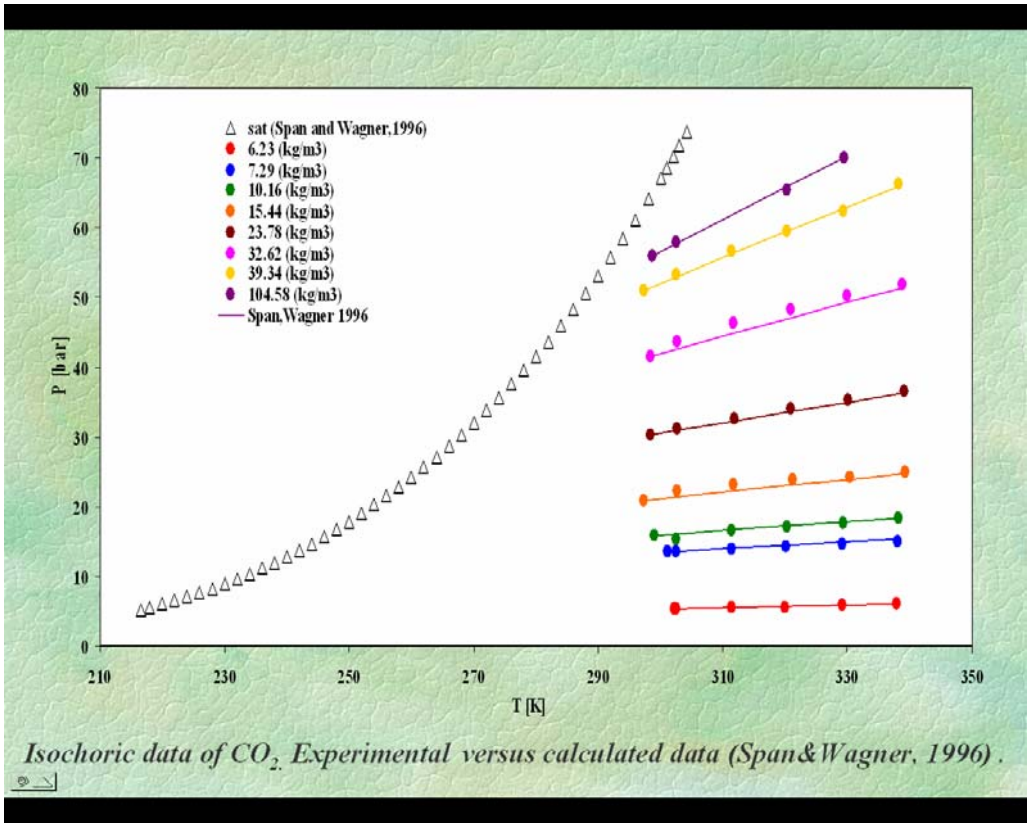


Fig.5. The measured isochors for carbon dioxide. A comparison of measured data with the calculated values from the equation of state of Span and Wagner.[8]

TERMOD1 module of the PHEQ program was used to store the PVT and equilibrium data for carbon dioxide from the compilation of Span and Wagner[8]. Calculation can be made with different equations of state implemented in the THERMOD program. Results can be analysed from the table outputs of the program, or from different kinds of diagrams. An example of the results analysis is shown in Fig. 6, for the enthalpy-pressure diagram of CO_2. The literature recommended data[8], compiled from the best experimental available data, are compared with the predictions of the GEOS3C equation of state[9], developed in our laboratory. As can be seen, GEOS3C predictions for carbon dioxide are reasonable good on a wide range of temperatures and pressures.

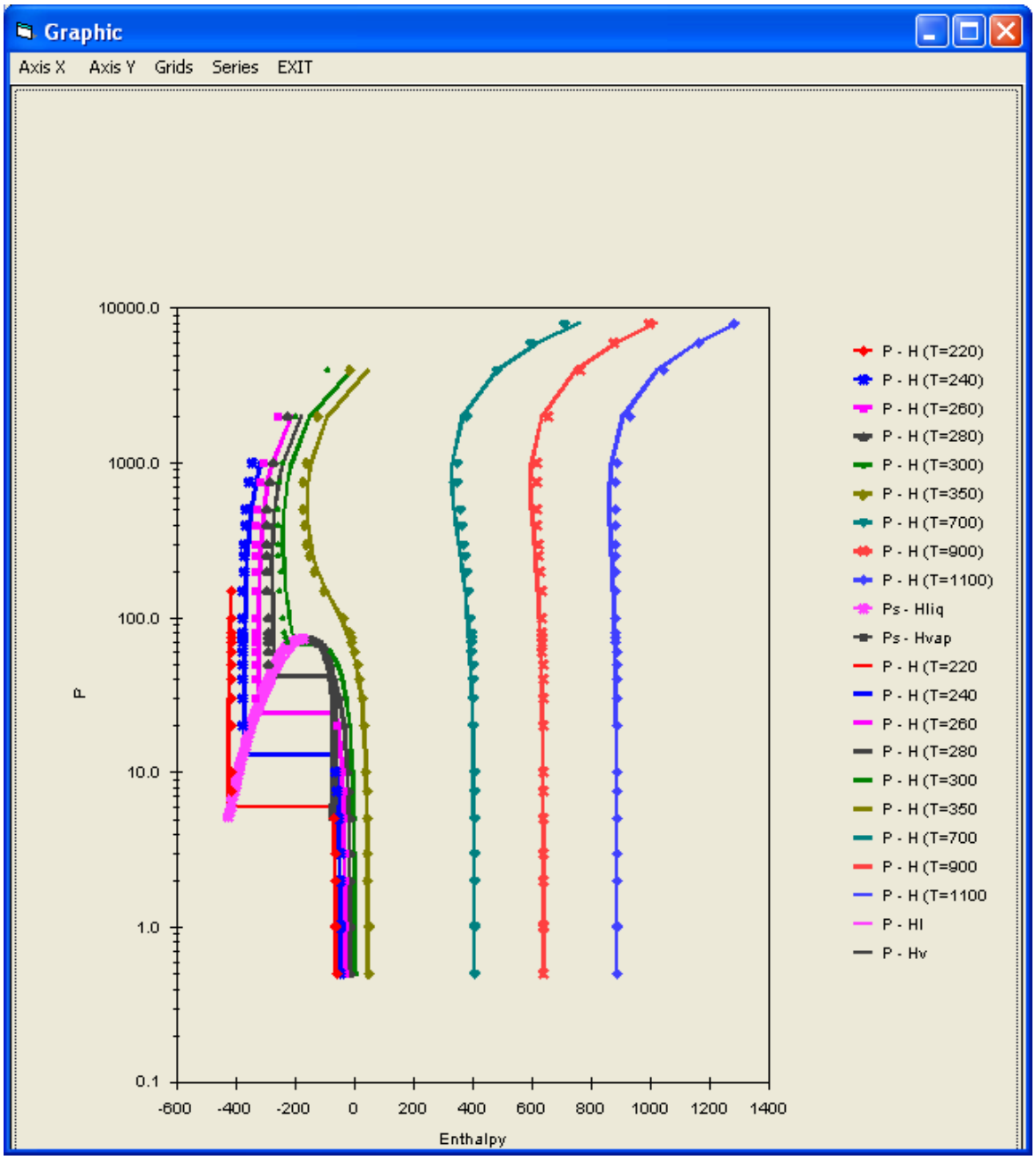
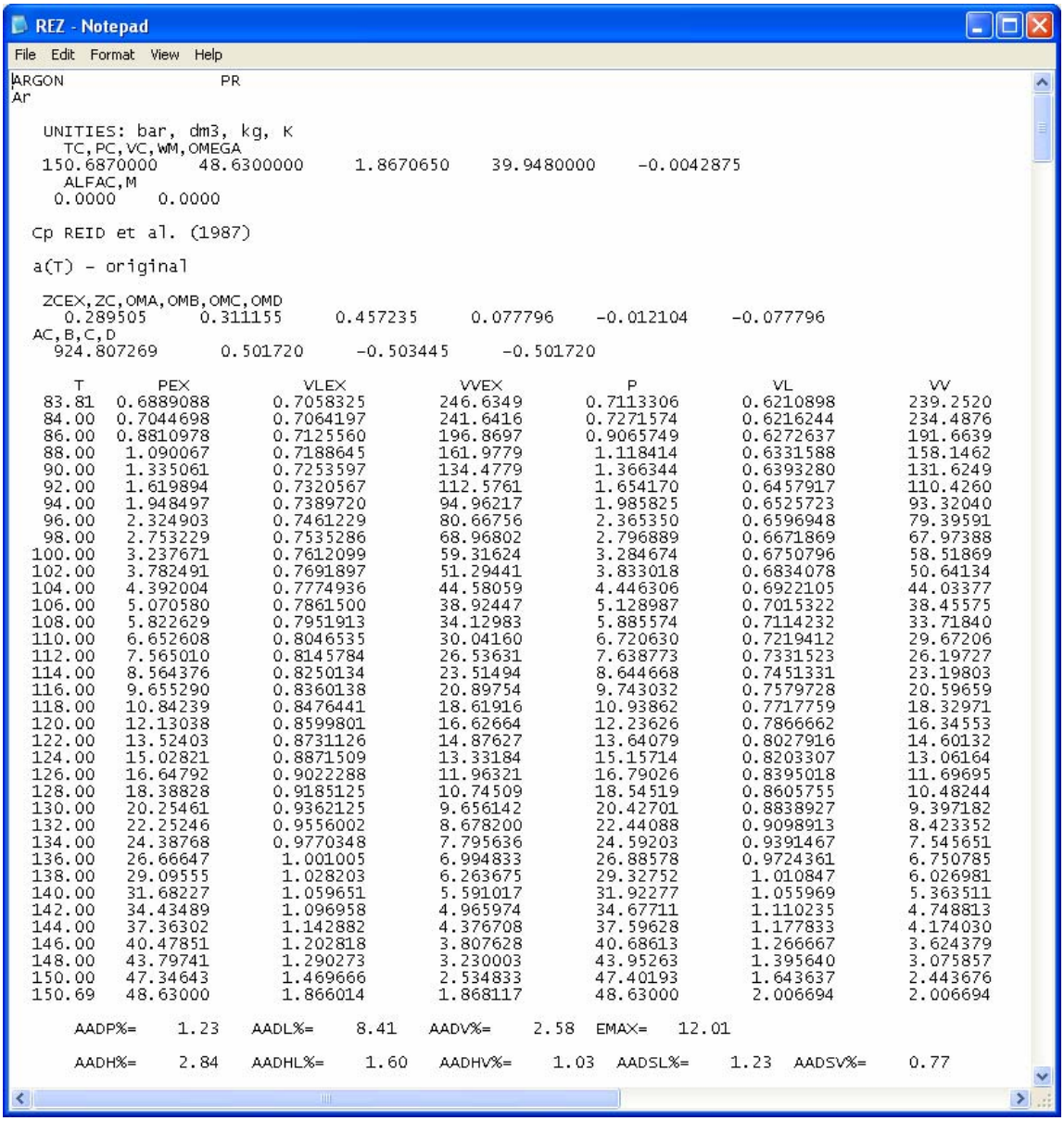


Fig. 6. Enthalpy-pressure diagram of carbon dioxide in PHEQ program. Points are literature data,[8] and lines are calculations with GEOS3C EOS.

Fig. 7 shows another example of the output of THERMOD1 module of PHEQ program, for argon. Calculations are made with Peng-Robinson equation of state[10], and compared in the table of results with recommended data of the literature[11]. The Fig. 8 presents a graphic output of the saturation and isotherm data for argon, in a pressure-density diagram. Experimental data[11] are compared with the predicted results of the Peng-Robinson equation of state. As can be seen, the Peng-Robinson equation of state can not predict satisfactory the saturated liquid densities.

Another example of graphic output is shown in Fig. 9 for argon in a pressure-entropy diagram. Points are recommended data of the literature and lines are calculated values with the Peng-Robinson equation of state. The equation predicts reasonably good the pressure-entropy diagram of argon.


REZ - Notepad

File Edit Format View Help

ARGON PR
Ar

UNITIES: bar, dm3, kg, K
TC,PC,VC,WM,OMEGA
150.6870000 48.6300000 1.8670650 39.9480000 -0.0042875
ALFAC,M
0.0000 0.0000

Cp REID et al. (1987)

a(T) - original

ZCEX,ZC,OMA,OMB,OMC,OMD
0.289505 0.311155 0.457235 0.077796 -0.012104 -0.077796
AC,B,C,D
924.807269 0.501720 -0.503445 -0.501720

T	PEX	VLEX	VVEX	P	VL	VV
83.81	0.6889088	0.7058325	246.6349	0.7113306	0.6210898	239.2520
84.00	0.7044698	0.7064197	241.6416	0.7271574	0.6216244	234.4876
86.00	0.8810978	0.7125560	196.8697	0.9065749	0.6272637	191.6639
88.00	1.090067	0.7188645	161.9779	1.118414	0.6331588	158.1462
90.00	1.335061	0.7253597	134.4779	1.366344	0.6393280	131.6249
92.00	1.619894	0.7320567	112.5761	1.654170	0.6457917	110.4260
94.00	1.948497	0.7389720	94.96217	1.985825	0.6525723	93.32040
96.00	2.324903	0.7461229	80.66756	2.365350	0.6596948	79.39591
98.00	2.753229	0.7535286	68.96802	2.796889	0.6671869	67.97388
100.00	3.237671	0.7612099	59.31624	3.284674	0.6750796	58.51869
102.00	3.782491	0.7691897	51.29441	3.833018	0.6834078	50.64134
104.00	4.392004	0.7774936	44.58059	4.446306	0.6922105	44.03377
106.00	5.070580	0.7861500	38.92447	5.128987	0.7015322	38.45575
108.00	5.822629	0.7951913	34.12983	5.885574	0.7114232	33.71840
110.00	6.652608	0.8046535	30.04160	6.720630	0.7219412	29.67206
112.00	7.565010	0.8145784	26.53631	7.638773	0.7331523	26.19727
114.00	8.564376	0.8250134	23.51494	8.644668	0.7451331	23.19803
116.00	9.655290	0.8360138	20.89754	9.743032	0.7579728	20.59659
118.00	10.84239	0.8476441	18.61916	10.93862	0.7717759	18.32971
120.00	12.13038	0.8599801	16.62664	12.23626	0.7866662	16.34553
122.00	13.52403	0.8731126	14.87627	13.64079	0.8027916	14.60132
124.00	15.02821	0.8871509	13.33184	15.15714	0.8203307	13.06164
126.00	16.64792	0.9022288	11.96321	16.79026	0.8395018	11.69695
128.00	18.38828	0.9185125	10.74509	18.54519	0.8605755	10.48244
130.00	20.25461	0.9362125	9.656142	20.42701	0.8838927	9.397182
132.00	22.25246	0.9556002	8.678200	22.44088	0.9098913	8.423352
134.00	24.38768	0.9770348	7.795636	24.59203	0.9391467	7.545651
136.00	26.66647	1.001005	6.994833	26.88578	0.9724361	6.750785
138.00	29.09555	1.028203	6.263675	29.32752	1.010847	6.026981
140.00	31.68227	1.059651	5.591017	31.92277	1.055969	5.363511
142.00	34.43489	1.096958	4.965974	34.67711	1.110235	4.748813
144.00	37.36302	1.142882	4.376708	37.59628	1.177833	4.174030
146.00	40.47851	1.202818	3.807628	40.68613	1.266667	3.624379
148.00	43.79741	1.290273	3.230003	43.95263	1.395640	3.075857
150.00	47.34643	1.469666	2.534833	47.40193	1.643637	2.443676
150.69	48.63000	1.866014	1.868117	48.63000	2.006694	2.006694

AADP%= 1.23 AADL%= 8.41 AADV%= 2.58 EMAX= 12.01

AADH%= 2.84 AADHL%= 1.60 AADHV%= 1.03 AADSL%= 1.23 AADSV%= 0.77

Fig. 7. Result Output of THERMOD1 module of PHEQ program, for argon. Calculations are made with Peng-Robinson (PR) equation of state, and compared in the table of results with recommended data of the literature.[11]

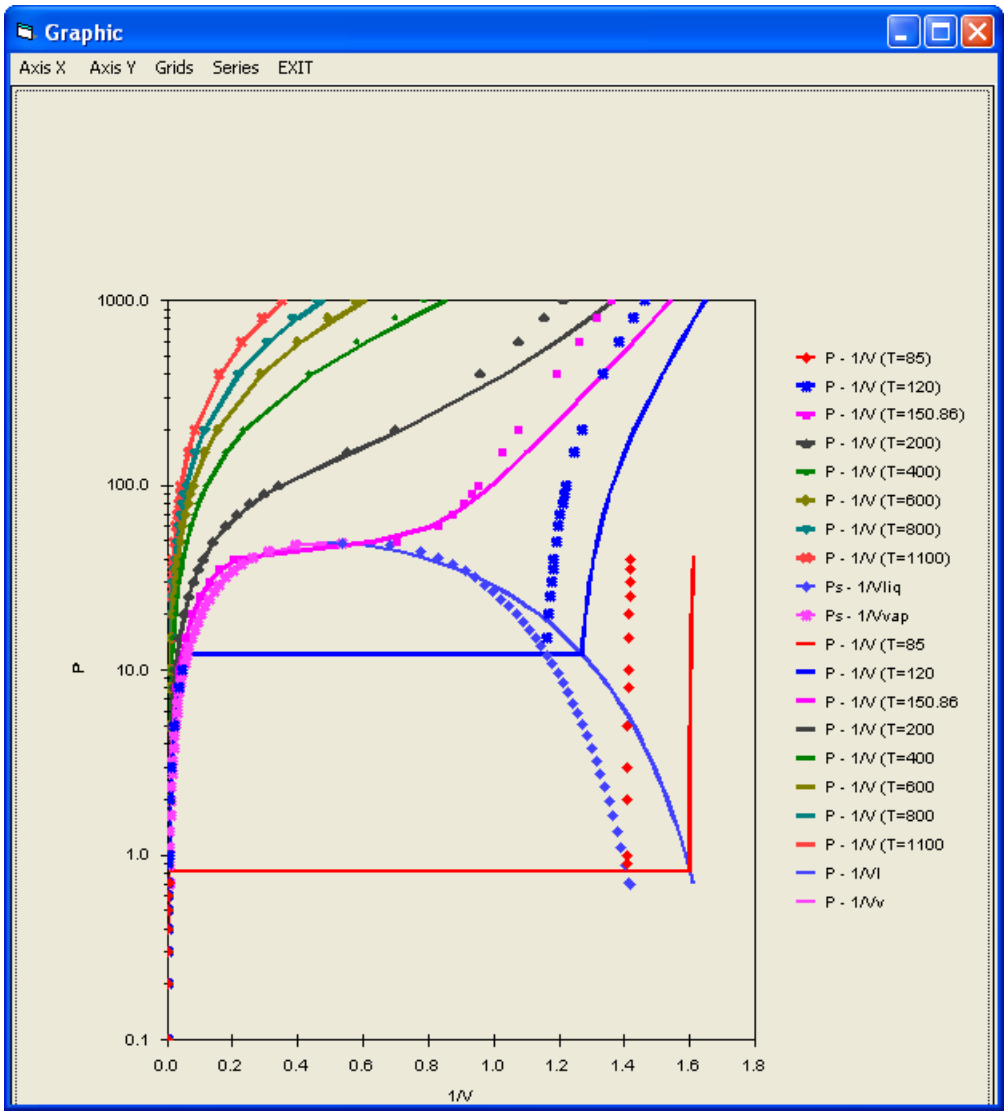


Fig. 8. Pressure-density diagram of argon in PHEQ program. Points are literature data,[11] and lines are calculations with Peng-Robinson equation of state.

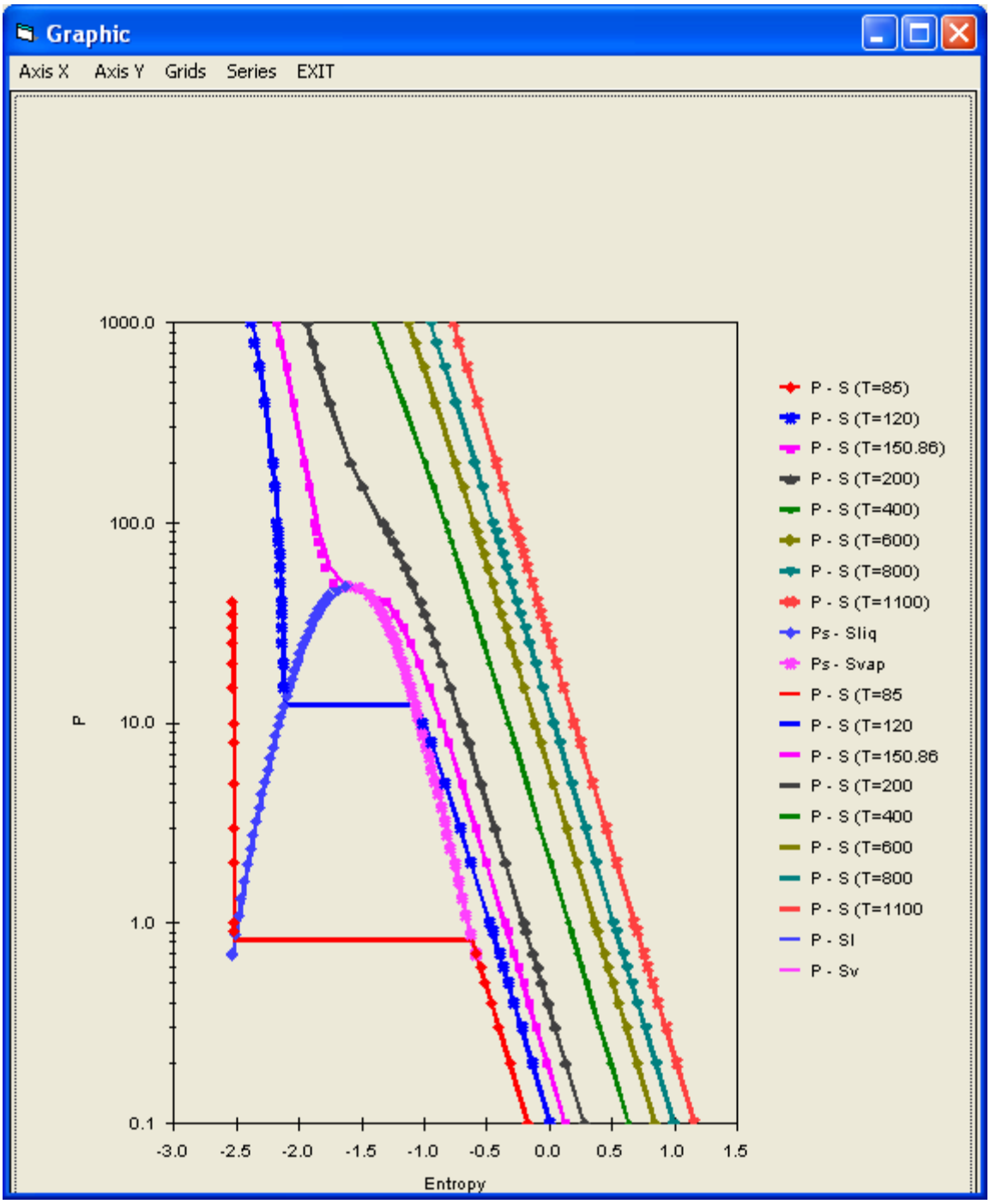


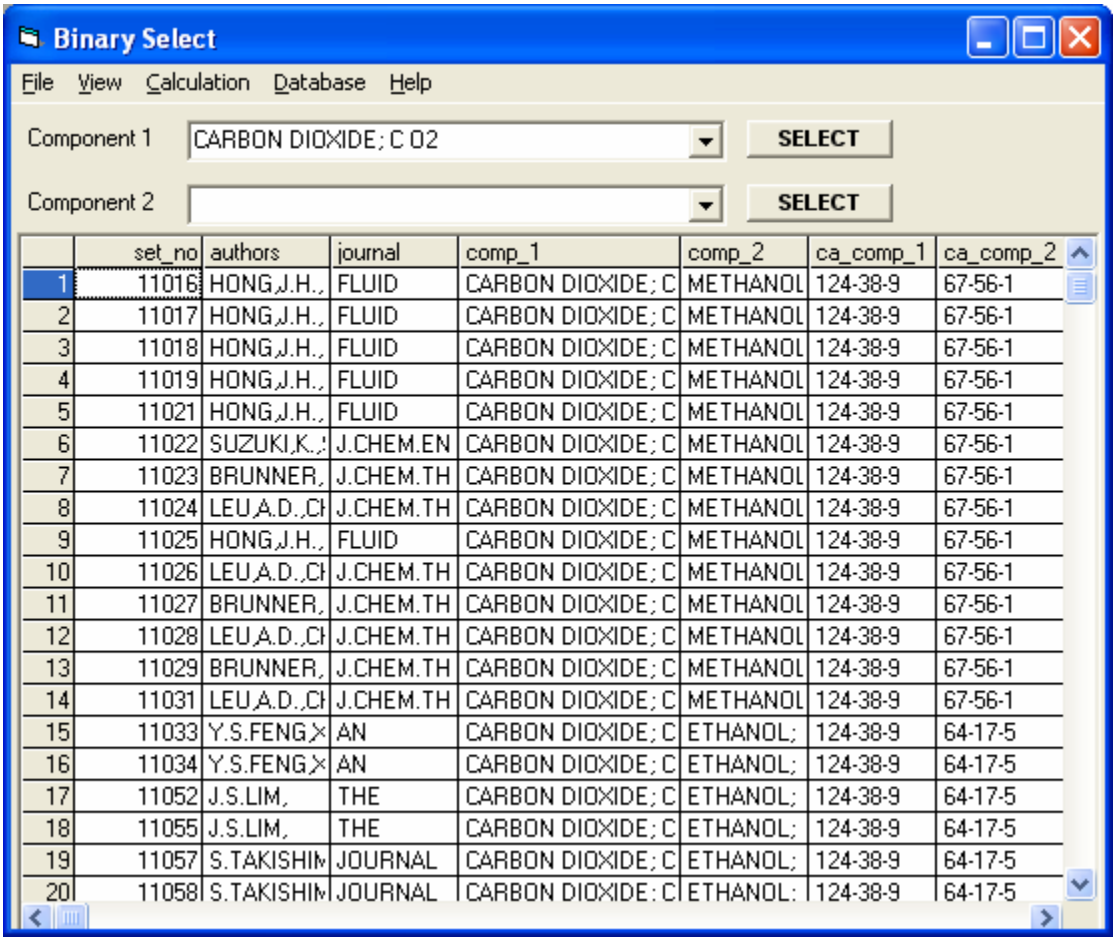
Fig. 9. Entropy-pressure diagram of argon in PHEQ program. Points are literature data,[11] and lines are calculations with Peng-Robinson equation of state.

The calculation of different problems of PVT and phase equilibria properties is the main task in applications of the TERMOD1 module in the PHEQ package. Several equations of state have been evaluated to determine their accuracy in predicting and correlation of the data. GEOS, as a general cubic equation of state was used in computer programs, allowing the particular specification of many popular cubic forms like Soave-Redlich-Kwong EOS (SRK), Peng-Robinson EOS (PR). Non-cubic

equations of state are also implemented in computer codes, like PHSGEOS a perturbed hard-sphere mode[12].

DATABASE AND APPLICATION PROGRAM VLE2 IN PHEQ PACKAGE

Fig. 10 shows the initial screen image for the pure component data base and applications (called TERMOD1) where we can pick up all the related information, applicable code and associated data management. A toolbar serves as a foundation for the higher levels convenient access to the database, interactive and automated data set selection and calculations.



	set_no	authors	journal	comp_1	comp_2	ca_comp_1	ca_comp_2
1	11016	HONG,J.H.,	FLUID	CARBON DIOXIDE; C	METHANOL	124-38-9	67-56-1
2	11017	HONG,J.H.,	FLUID	CARBON DIOXIDE; C	METHANOL	124-38-9	67-56-1
3	11018	HONG,J.H.,	FLUID	CARBON DIOXIDE; C	METHANOL	124-38-9	67-56-1
4	11019	HONG,J.H.,	FLUID	CARBON DIOXIDE; C	METHANOL	124-38-9	67-56-1
5	11021	HONG,J.H.,	FLUID	CARBON DIOXIDE; C	METHANOL	124-38-9	67-56-1
6	11022	SUZUKI,K.,	J.CHEM.EN	CARBON DIOXIDE; C	METHANOL	124-38-9	67-56-1
7	11023	BRUNNER,	J.CHEM.TH	CARBON DIOXIDE; C	METHANOL	124-38-9	67-56-1
8	11024	LEU,A.D.,CI	J.CHEM.TH	CARBON DIOXIDE; C	METHANOL	124-38-9	67-56-1
9	11025	HONG,J.H.,	FLUID	CARBON DIOXIDE; C	METHANOL	124-38-9	67-56-1
10	11026	LEU,A.D.,CI	J.CHEM.TH	CARBON DIOXIDE; C	METHANOL	124-38-9	67-56-1
11	11027	BRUNNER,	J.CHEM.TH	CARBON DIOXIDE; C	METHANOL	124-38-9	67-56-1
12	11028	LEU,A.D.,CI	J.CHEM.TH	CARBON DIOXIDE; C	METHANOL	124-38-9	67-56-1
13	11029	BRUNNER,	J.CHEM.TH	CARBON DIOXIDE; C	METHANOL	124-38-9	67-56-1
14	11031	LEU,A.D.,CI	J.CHEM.TH	CARBON DIOXIDE; C	METHANOL	124-38-9	67-56-1
15	11033	Y.S.FENG,X	AN	CARBON DIOXIDE; C	ETHANOL;	124-38-9	64-17-5
16	11034	Y.S.FENG,X	AN	CARBON DIOXIDE; C	ETHANOL;	124-38-9	64-17-5
17	11052	J.S.LIM,	THE	CARBON DIOXIDE; C	ETHANOL;	124-38-9	64-17-5
18	11055	J.S.LIM,	THE	CARBON DIOXIDE; C	ETHANOL;	124-38-9	64-17-5
19	11057	S.TAKISHIM	JOURNAL	CARBON DIOXIDE; C	ETHANOL;	124-38-9	64-17-5
20	11058	S.TAKISHIM	JOURNAL	CARBON DIOXIDE; C	ETHANOL;	124-38-9	64-17-5

Fig.10. Screen image for the phase equilibria in binary systems data base and applications (VLE2)

This software may be used in relation to MS-Office (Word, Excel, PowerPoint and Access). Basically, the software MS Access is used for the implementation of the database. Tables, queries and forms are the main parts of the database.

The data base contains different types of phase equilibrium data for 1000 binary systems: compositions of phases (x1, y1) temperature and pressure. Data published in the literature, as well as data measured in our laboratory were introduced in the VLE2 data base. Measurements of isothermal VLE data were made with a high pressure apparatus, essentially a visual cell with variable volume. Phase equilibrium data were measured for carbon dioxide–1-heptanol[13] and carbon dioxide–1-nonanol in the temperature range (10-80 C) and pressure (5-120 bar). A schematic diagram of the experimental setup for phase equilibria measurements is shown in Fig. 11. As an example, in Fig. 12 the measured isotherm for carbon dioxide–1-heptanol at T=353.15 K is reported.

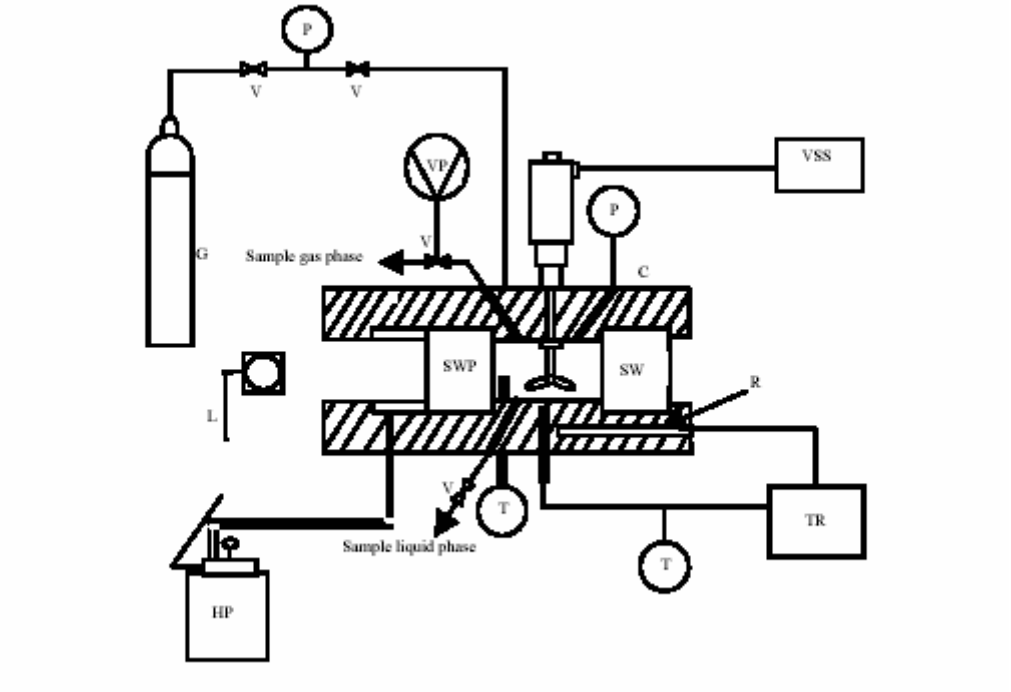


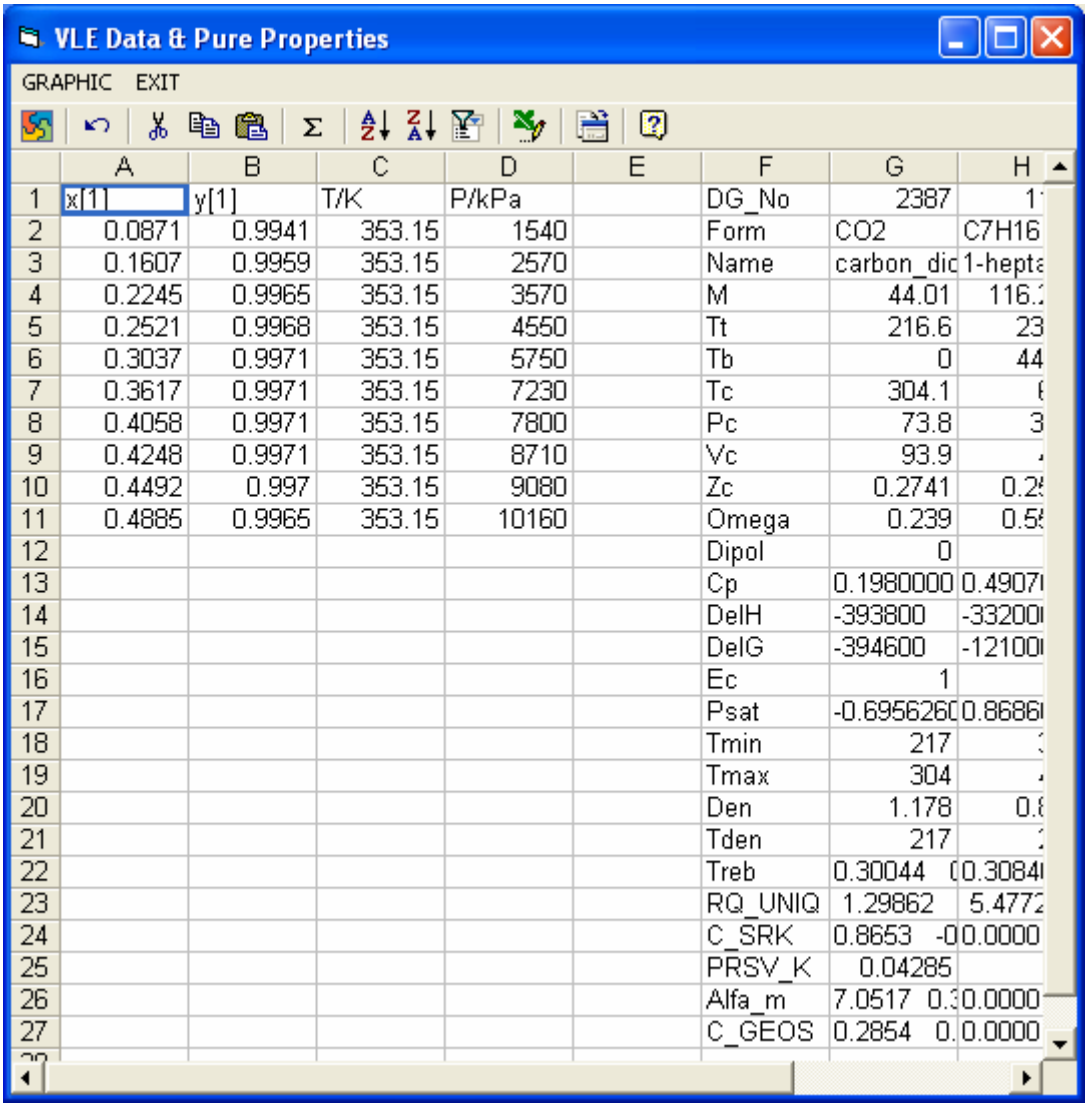
Fig.11. Schematic diagram of experimental apparatus: (C) variable volume cell; (G) carbon dioxide reservoir; (HP) hand pump; (P) pressure gauge; (R) resistance for electric heating; (SW) sapphire window; (T) thermocouple; (TR) temperature regulator; (V) valve; (VP) vacuum pump; (VSS) variable speed stirring assembly; (L) lamp..

VLE2 module of the PHEQ program was used to store the phase equilibrium data for carbon dioxide–1-heptanol, both our measurements and literature data. Calculation can be made with different equations of state and mixing rules[9] implemented in the VLE2 program. Results can be analysed from the table outputs of the program, or from different kinds of diagrams. An example of the results analysis is shown in Fig. 13, for the pressure-phase compositions diagram of CO_2–1-heptanol system. As can be seen, GEOSHVID predictions for carbon dioxide–1-heptanol system are reasonable good on a wide range of pressures.

Fig. 14 shows a table output of VLE2 module of PHEQ program, for CO_2–1-heptanol system. Calculations are made with Soave-Redlich-Kwong equation of state,[14] and compared in the table of results with our measured data[13]. The Fig. 15 presents a graphic output of the pressure-composition diagram for carbon dioxide–methanol system, at T-313.4 K. Experimental data[15] are compared with

the predicted results of the Soave-Redlich-Kwong(SRK) equation of state with 1PCMR mixing rule. As can be seen, the equation of state can predict satisfactory the phase behaviour of the system.

An example of input in VLE2 calculation is shown in Fig. 16. The different options for the calculation are selected by user: the equation of state, mixing rule, correlation procedure, and initial parameter values.



	A	B	C	D	E	F	G	H
1	x[1]	y[1]	T/K	P/kPa		DG_No	2387	1
2	0.0871	0.9941	353.15	1540		Form	CO2	C7H16
3	0.1607	0.9959	353.15	2570		Name	carbon_dic	1-hepta
4	0.2245	0.9965	353.15	3570		M	44.01	116.
5	0.2521	0.9968	353.15	4550		Tt	216.6	23
6	0.3037	0.9971	353.15	5750		Tb	0	44
7	0.3617	0.9971	353.15	7230		Tc	304.1	
8	0.4058	0.9971	353.15	7800		Pc	73.8	3
9	0.4248	0.9971	353.15	8710		Vc	93.9	
10	0.4492	0.997	353.15	9080		Zc	0.2741	0.2
11	0.4885	0.9965	353.15	10160		Omega	0.239	0.5
12						Dipol	0	
13						Cp	0.1980000	0.4907
14						DelH	-393800	-33200
15						DelG	-394600	-12100
16						Ec	1	
17						Psat	-0.6956260	0.8686
18						Tmin	217	
19						Tmax	304	
20						Den	1.178	0.8
21						Tden	217	
22						Treb	0.30044	0.3084
23						RQ_UNIQ	1.29862	5.4772
24						C_SRK	0.8653	-0.0000
25						PRSV_K	0.04285	
26						Alfa_m	7.0517	0.3 0.0000
27						C_GEOS	0.2854	0. 0.0000

Fig.12. The measured VLE isotherm for carbon dioxide–1-heptanol system at T=353.15 K in our laboratory.

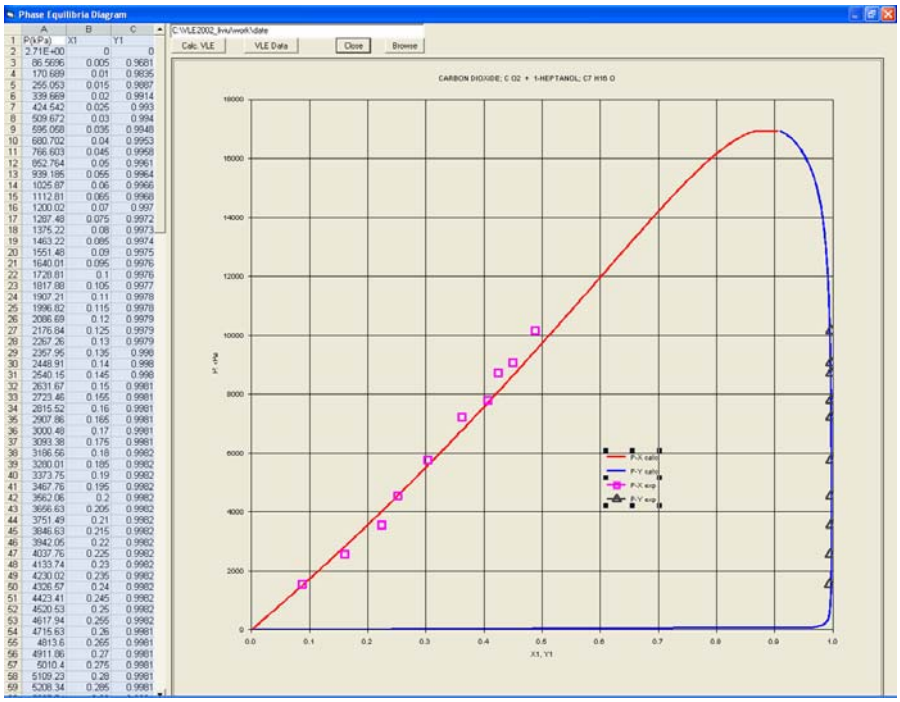


Fig. 13. Pressure-composition diagram of carbon dioxide–1-heptanol in PHEQ program. Points are our measured data,[13] and lines are calculations with GEOSHVID program in VLE2.

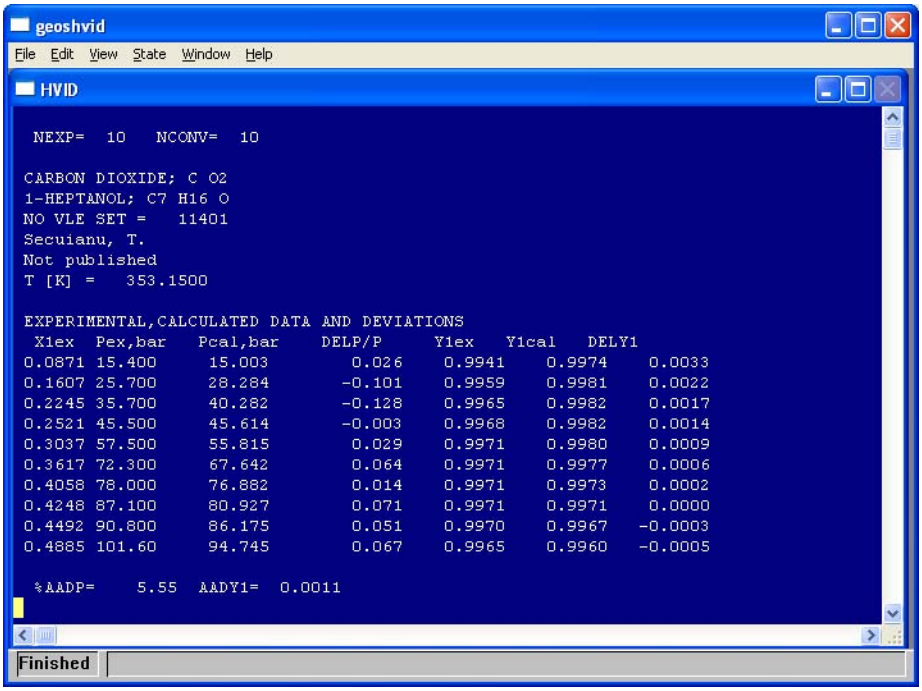
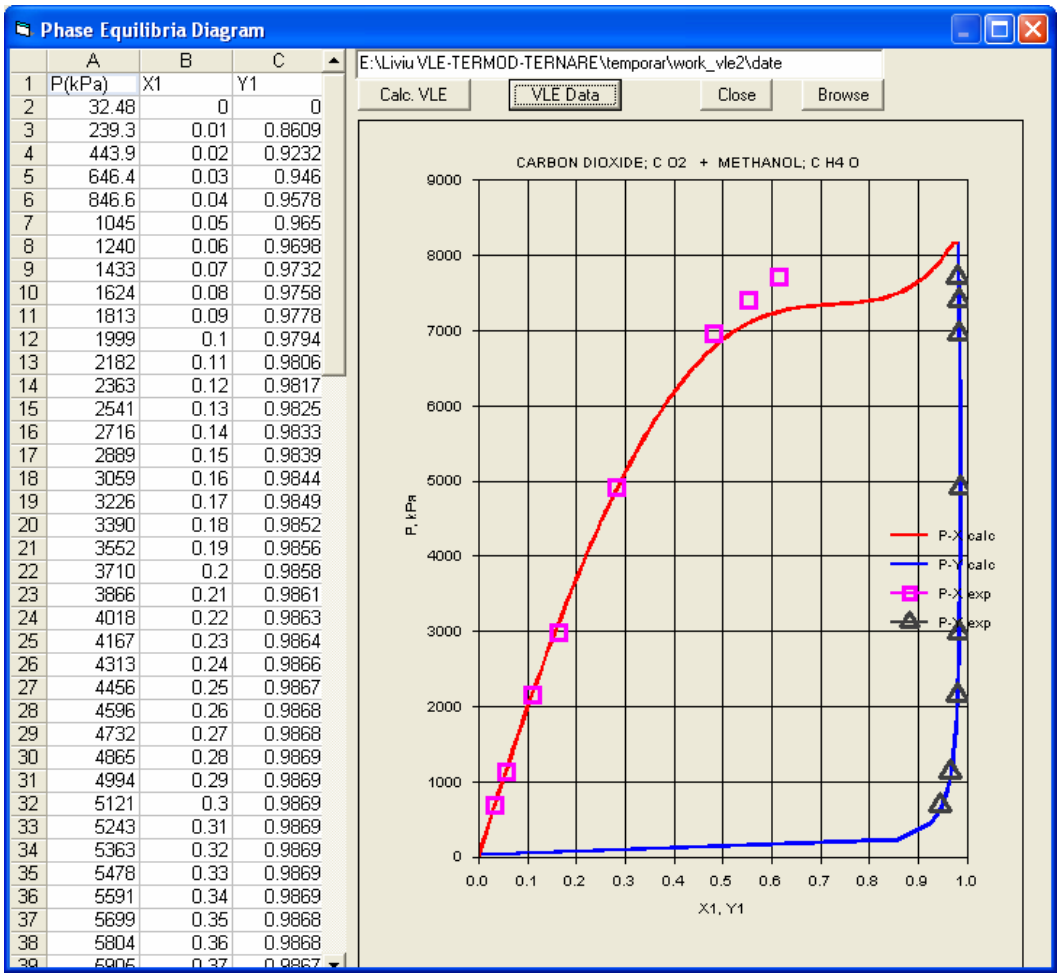


Fig. 14. Result output of VLE2 module of PHEQ program, for carbon dioxide–1-heptanol system.[13] Calculations are made with Soave-Redlich-Kwong (SRK) equation of state, and compared in the experimental results.



	A	B	C
1	P(kPa)	X1	Y1
2	32.48	0	0
3	239.3	0.01	0.8609
4	443.9	0.02	0.9232
5	646.4	0.03	0.946
6	846.6	0.04	0.9578
7	1045	0.05	0.965
8	1240	0.06	0.9698
9	1433	0.07	0.9732
10	1624	0.08	0.9758
11	1813	0.09	0.9778
12	1999	0.1	0.9794
13	2182	0.11	0.9806
14	2363	0.12	0.9817
15	2541	0.13	0.9825
16	2716	0.14	0.9833
17	2889	0.15	0.9839
18	3059	0.16	0.9844
19	3226	0.17	0.9849
20	3390	0.18	0.9852
21	3552	0.19	0.9856
22	3710	0.2	0.9858
23	3866	0.21	0.9861
24	4018	0.22	0.9863
25	4167	0.23	0.9864
26	4313	0.24	0.9866
27	4456	0.25	0.9867
28	4596	0.26	0.9868
29	4732	0.27	0.9868
30	4865	0.28	0.9869
31	4994	0.29	0.9869
32	5121	0.3	0.9869
33	5243	0.31	0.9869
34	5363	0.32	0.9869
35	5478	0.33	0.9869
36	5591	0.34	0.9869
37	5699	0.35	0.9868
38	5804	0.36	0.9868
39	5906	0.37	0.9867

Fig. 15. Pressure-phase compositions of carbon dioxide–methanol system at 313.4 K in PHEQ program. Points are literature data,[15] and lines are calculations with Soave-Redlich-Kwong equation of state.

The calculation of different problems of phase equilibria properties is the main task in applications of the VLE2 module in the PHEQ package. Several equations of state have been evaluated to determine their accuracy in predicting and correlation of the data. GEOS, as a general cubic equation of state was used in computer programs, allowing the particular specification of many popular cubic forms like Soave-Redlich-Kwong EOS (SRK), Peng-Robinson EOS (PR). Non-cubic equations of state are also implemented in computer codes, like PHSGEOS a perturbed hard-sphere model.[16]

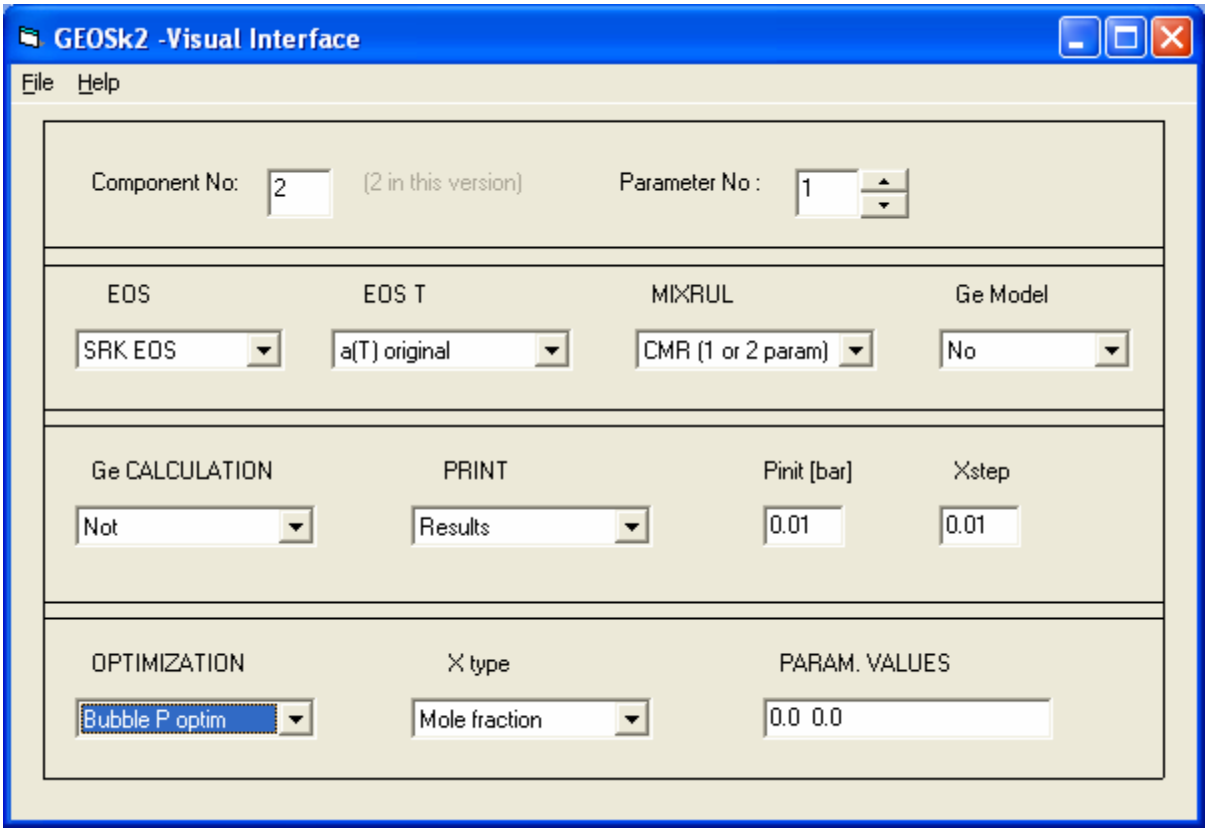
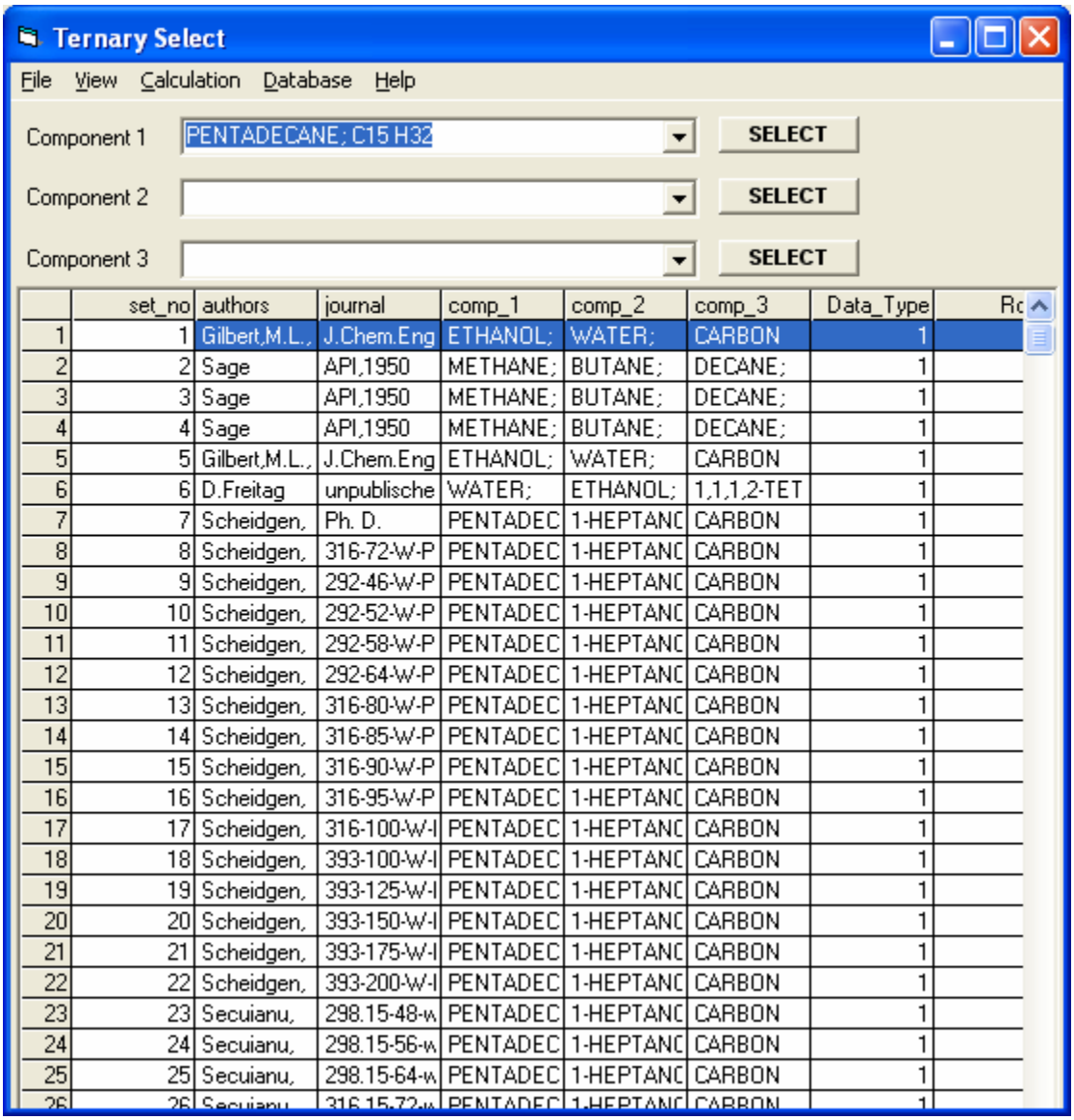


Fig. 16. Visual interface in calculations with VLE2 module in PHEQ program. GEOSK2 application program.

DATABASE AND APPLICATION PROGRAM VLE3 IN PHEQ PACKAGE

Fig. 17 shows the initial screen image for the pure component data base and applications (called VLE3) where we can pick up all the related information, applicable code and associated data management. A toolbar serves as a foundation for the higher levels convenient access to the database, interactive and automated data set selection and calculations.
This software may be used in relation to MS-Office (Word, Excel, PowerPoint and Access). Basically, the software MS Access is used for the implementation of the database. Tables, queries and forms are the main parts of the database.

The data base contains different types of phase equilibrium data for 10 ternary systems: compositions of phases (x1, x2, x3, y1, y2, y3) temperature and pressure. Data published in the literature, as well as data measured in our laboratory were introduced in the VLE3 data base.



	set_no	authors	journal	comp_1	comp_2	comp_3	Data_Type	Rc
1	1	Gilbert,M.L.,	J.Chem.Eng	ETHANOL;	WATER;	CARBON	1	
2	2	Sage	API,1950	METHANE;	BUTANE;	DECANE;	1	
3	3	Sage	API,1950	METHANE;	BUTANE;	DECANE;	1	
4	4	Sage	API,1950	METHANE;	BUTANE;	DECANE;	1	
5	5	Gilbert,M.L.,	J.Chem.Eng	ETHANOL;	WATER;	CARBON	1	
6	6	D.Freitag	unpublische	WATER;	ETHANOL;	1,1,1,2-TET	1	
7	7	Scheidgen,	Ph. D.	PENTADEC	1-HEPTANC	CARBON	1	
8	8	Scheidgen,	316-72-W-P	PENTADEC	1-HEPTANC	CARBON	1	
9	9	Scheidgen,	292-46-W-P	PENTADEC	1-HEPTANC	CARBON	1	
10	10	Scheidgen,	292-52-W-P	PENTADEC	1-HEPTANC	CARBON	1	
11	11	Scheidgen,	292-58-W-P	PENTADEC	1-HEPTANC	CARBON	1	
12	12	Scheidgen,	292-64-W-P	PENTADEC	1-HEPTANC	CARBON	1	
13	13	Scheidgen,	316-80-W-P	PENTADEC	1-HEPTANC	CARBON	1	
14	14	Scheidgen,	316-85-W-P	PENTADEC	1-HEPTANC	CARBON	1	
15	15	Scheidgen,	316-90-W-P	PENTADEC	1-HEPTANC	CARBON	1	
16	16	Scheidgen,	316-95-W-P	PENTADEC	1-HEPTANC	CARBON	1	
17	17	Scheidgen,	316-100-W-I	PENTADEC	1-HEPTANC	CARBON	1	
18	18	Scheidgen,	393-100-W-I	PENTADEC	1-HEPTANC	CARBON	1	
19	19	Scheidgen,	393-125-W-I	PENTADEC	1-HEPTANC	CARBON	1	
20	20	Scheidgen,	393-150-W-I	PENTADEC	1-HEPTANC	CARBON	1	
21	21	Scheidgen,	393-175-W-I	PENTADEC	1-HEPTANC	CARBON	1	
22	22	Scheidgen,	393-200-W-I	PENTADEC	1-HEPTANC	CARBON	1	
23	23	Secuianu,	298.15-48-w	PENTADEC	1-HEPTANC	CARBON	1	
24	24	Secuianu,	298.15-56-w	PENTADEC	1-HEPTANC	CARBON	1	
25	25	Secuianu,	298.15-64-w	PENTADEC	1-HEPTANC	CARBON	1	
26	26	Secuianu,	316.15-72-w	PENTADEC	1-HEPTANC	CARBON	1	

Fig.17. Screen image for the phase equilibria in ternary systems data base and applications (VLE3)

Measurements of isothermal–isobaric VLE data were made with a high pressure apparatus, essentially a visual cell with variable volume. Phase equilibrium data (conodes) were measured for carbon dioxide–1-heptanol–pentadecane [17,18] in the temperature range (10-80 C) and pressure (5-120 bar). The experimental setup for phase equilibria measurements was presented in the Fig. 11.

VLE3 module of the PHEQ program was used to store the phase equilibrium data for carbon dioxide–1-heptanol– pentadecane, both our measurements and literature data. An example of input/modifying data in VLE3 module is shown in Fig. 18. After insertion of the data, these are available for analysis both as table and graphically. As an example, in Fig. 19 the conodes measured in our laboratory, for carbon dioxide–1-heptanol–pentadecane system at T=316.15 K and 72 bar, are presented.

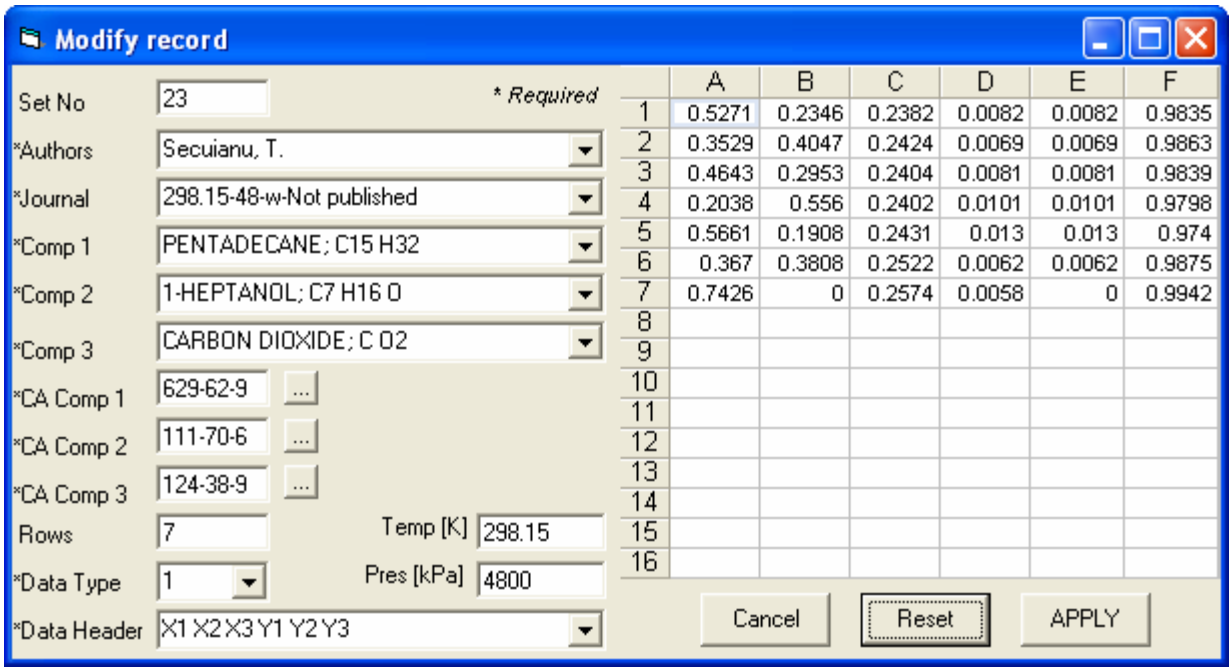


Fig. 18. Visual interface in VLE3 module in PHEQ program. Input/modifying experimental data.

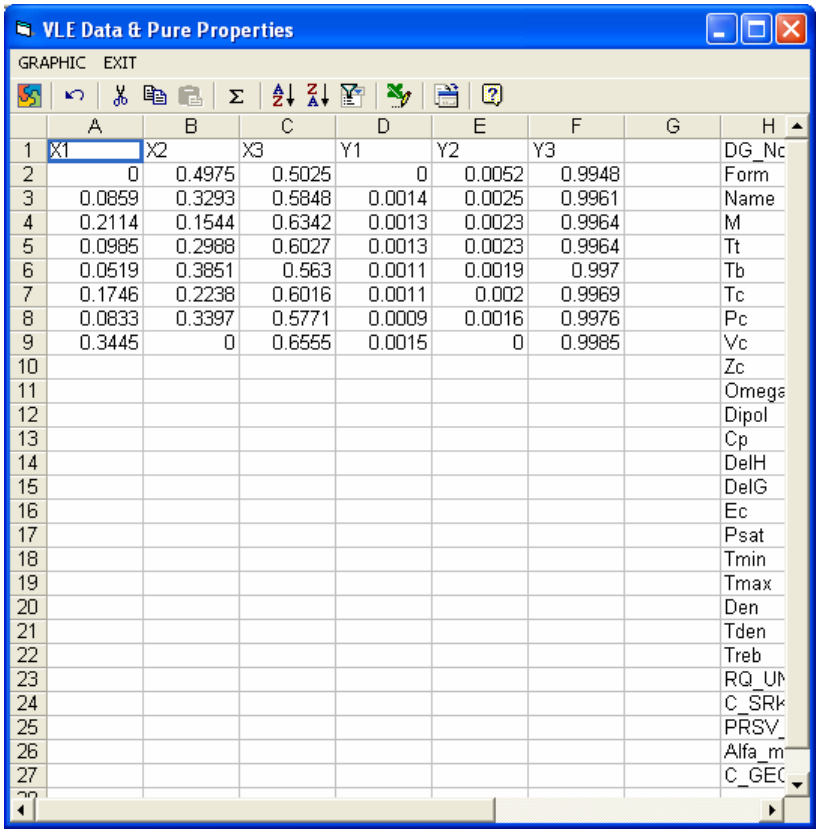


Fig.19. The measured VLE conodes for carbon dioxide–1-heptanol–pentadecane system at T=316.15 K and P= 72 bar in our laboratory.

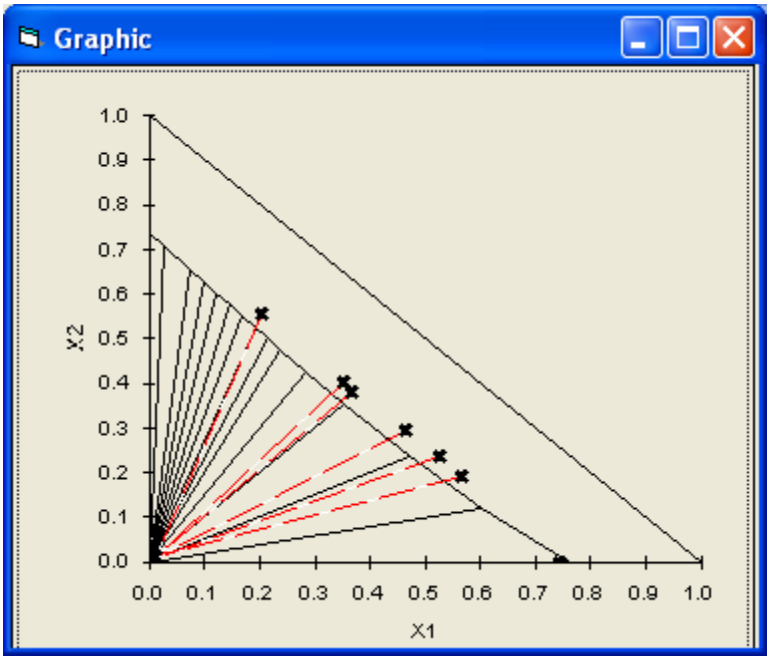


Fig. 20. Phase diagram of ternary system carbon dioxide–1-heptanol–pentadecane in PHEQ program. Points are our measured data,[17] and lines are calculations with GEOS3 program in VLE3 module.

Phase Equilibria Diagram

Graphics Exit

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	A	B	C	D	E	F
1	X1	X2	X3	Y1	Y2	Y3
2	0.5271	0.2346	0.2382	0.0082	0.0082	0.9835
3	0.3529	0.4047	0.2424	0.0069	0.0069	0.9863
4	0.4643	0.2953	0.2404	0.0081	0.0081	0.9839
5	0.2038	0.556	0.2402	0.0101	0.0101	0.9798
6	0.5661	0.1908	0.2431	0.013	0.013	0.974
7	0.367	0.3808	0.2522	0.0062	0.0062	0.9875
8	0.7426	0	0.2574	0.0058	0	0.9942
9						
10	X1	X2	X3	Y1	Y2	Y3
11	0	0.736	0.264	0	1.36E-03	0.9986
12	2.44E-02	0.7087	0.2669	4.51E-05	4.01E-04	0.9996
13	7.29E-02	0.6551	0.2721	9.37E-07	3.83E-04	0.9996
14	9.68E-02	0.6287	0.2745	1.35E-06	3.73E-04	0.9996
15	0.1206	0.6025	0.2769	1.81E-06	3.63E-04	0.9996
16	0.1443	0.5766	0.2792	2.33E-06	3.52E-04	0.9996
17	0.1678	0.5508	0.2814	2.92E-06	3.40E-04	0.9997
18	0.1912	0.5254	0.2834	3.57E-06	3.28E-04	0.9997
19	0.2145	0.5001	0.2853	4.30E-06	3.15E-04	0.9997
20	0.2378	0.4751	0.2871	5.10E-06	3.01E-04	0.9997
21	0.2841	0.4258	0.2902	6.95E-06	2.73E-04	0.9997
22	0.3536	0.3533	0.2931	1.04E-05	2.28E-04	0.9998
23	0.4722	0.2359	0.2918	1.80E-05	1.49E-04	0.9998
24	0.602	0.1203	0.2776	2.76E-05	7.20E-05	0.9999
25	0.7613	0	0.2387	3.84E-05	0	1
26						

Fig. 21. Result output of VLE3 module of PHEQ program, for carbon dioxide–1-heptanol–pentadecane system. Calculations (second set of data) are made with Soave-Redlich-Kwong (SRK) equation of state coupled with HVID mixing rules, and compared to our experimental results (first set of data).

Calculation can be made with different equations of state and mixing rules[9] implemented in the GEOS3 program. Results can be analysed from the table outputs of the program, or from different kinds of diagrams. An example of the results analysis is shown in Fig. 20, for the CO_2–1-heptanol–pentadecane system. As can be seen, GEOS3 predictions, using SRK equation of state coupled with HVID mixing rules, for carbon dioxide–1-heptanol–pentadecane system are reasonable good.
Fig. 21 shows a table output of VLE3 module of PHEQ program, for CO_2–1-heptanol–pentadecane system. Calculations are made with Soave-Redlich-Kwong (SRK) equation of state[14] coupled with HVID mixing rules,[19,20] and compared in the table of results with our measured data.[17,18]

The calculation of the flash problem of phase equilibria is the main task in applications of the VLE3 module in the PHEQ package. Several equations of state have been implemented. GEOS, as a general cubic equation of state was used in computer programs, allowing the particular specification of many popular cubic forms like Soave-Redlich-Kwong EOS (SRK), Peng-Robinson EOS (PR). Non-cubic equations of state are also implemented in computer codes, like PHSGEOS a perturbed hard-sphere model.[16]

CONCLUDING REMARKS

The PHEQ software is an intelligent Windows-based package for the management of large amounts of PVT and phase equilibrium data, and calculation programs for the correlation and/or prediction of many thermodynamic properties and phase behavior of chemical compounds and mixtures with applications in chemistry, biochemistry, chemical and biochemical engineering.

The TERMOD1 module in the PHEQ software is a package for the management of large amounts of PVT and phase equilibrium data, and calculation programs for the correlation and/or prediction of many thermodynamic properties and phase behavior of pure chemical compounds.

The VLE2 module in the PHEQ software is a package for the management of large amounts of phase equilibrium data of binary systems, and calculation programs for the correlation and/or prediction of phase behavior of binary systems.

The VLE3 module in the PHEQ software is a package for the management of large amounts of phase equilibrium data of ternary systems, and calculation programs of phase behavior of ternary/multicomponent systems.

The project involves programs at three software levels: the intelligent user friendly interface, calculation programs for PVT and phase equilibria problems, implementing the new models (our and from the literature), and the data base.

PHEQ program enables the prompt extraction of data and facilities for analysis of calculation results. Data and applications can be easily added for subsequent operation of PHEQ program.[21] A short presentation of the PHEQ program is posted in Internet on the site of the Applied Physical Chemistry and Electrochemistry Department, University Politehnica of Bucharest.[22]

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