Phase Equilibria Database and Calculation Program for Pure Component Systems and Mixtures

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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. PHEQ program enables the extraction of data and results so that the time-consuming data management, data processing and analysis are avoided. Furthermore, calculation programs of phase equilibrium based on the most reliable models were implemented. PHEQ Windows allows 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 1995, the calculation programs, rewritten in FORTRAN 77, and running under Windows 95, were coupled with databases. The software for binary vapor-liquid equilibria calculations, called VLE 95, was 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.

A 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),

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databases applications (MS Access, Visual Basics), and Fortran programming (Compaq Visual Fortran Compilator).

The first product of the PHEQ project, is a software package to manage a database for pure component, binary and ternary/multicomponent VLE experimental data which can be supplied by the user, and the application programs for correlation and/or prediction of phase behaviour of the three types of 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 binary phase equilibria systems a series of programs were developed, based on G^E models (GAMMA, UNIFAC) for low pressures or on EOS at high-pressures[4,5] (GEOSK2, HVID). Other programs were developed for calculations of ternary systems and three-phase equilibria[6] (GEOSPH3), as well as for critical lines calculation of mixtures (CRIMIX). All calculation programs are Compaq Visual Fortran 6.6 compiled Windows versions.

Database and application program PHEQ

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 managment. 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.

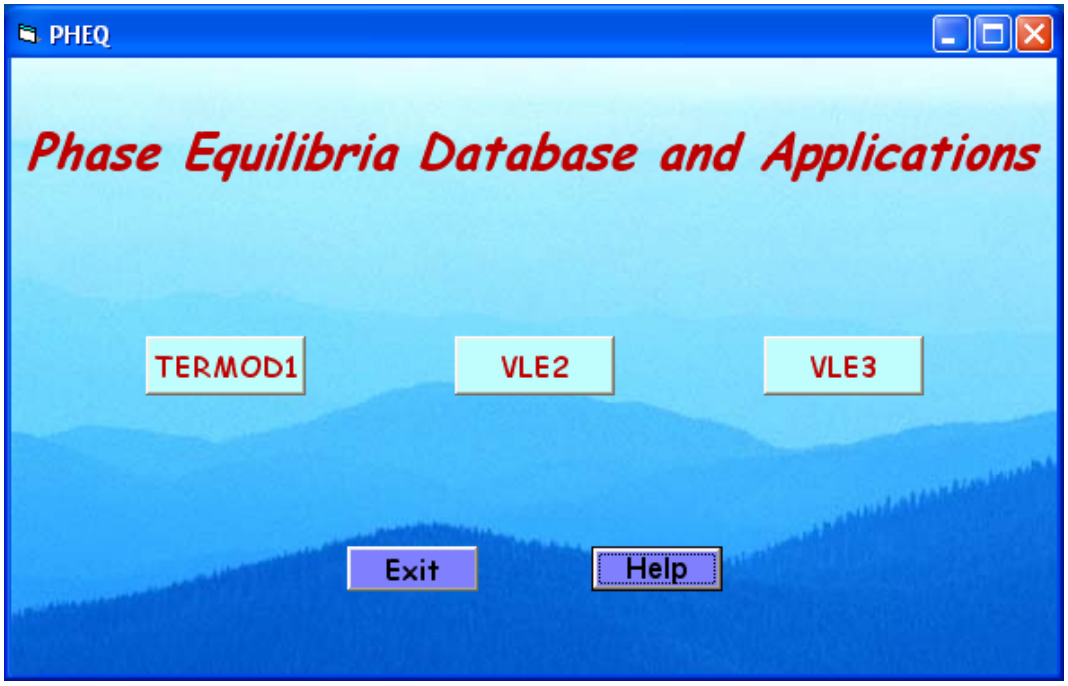
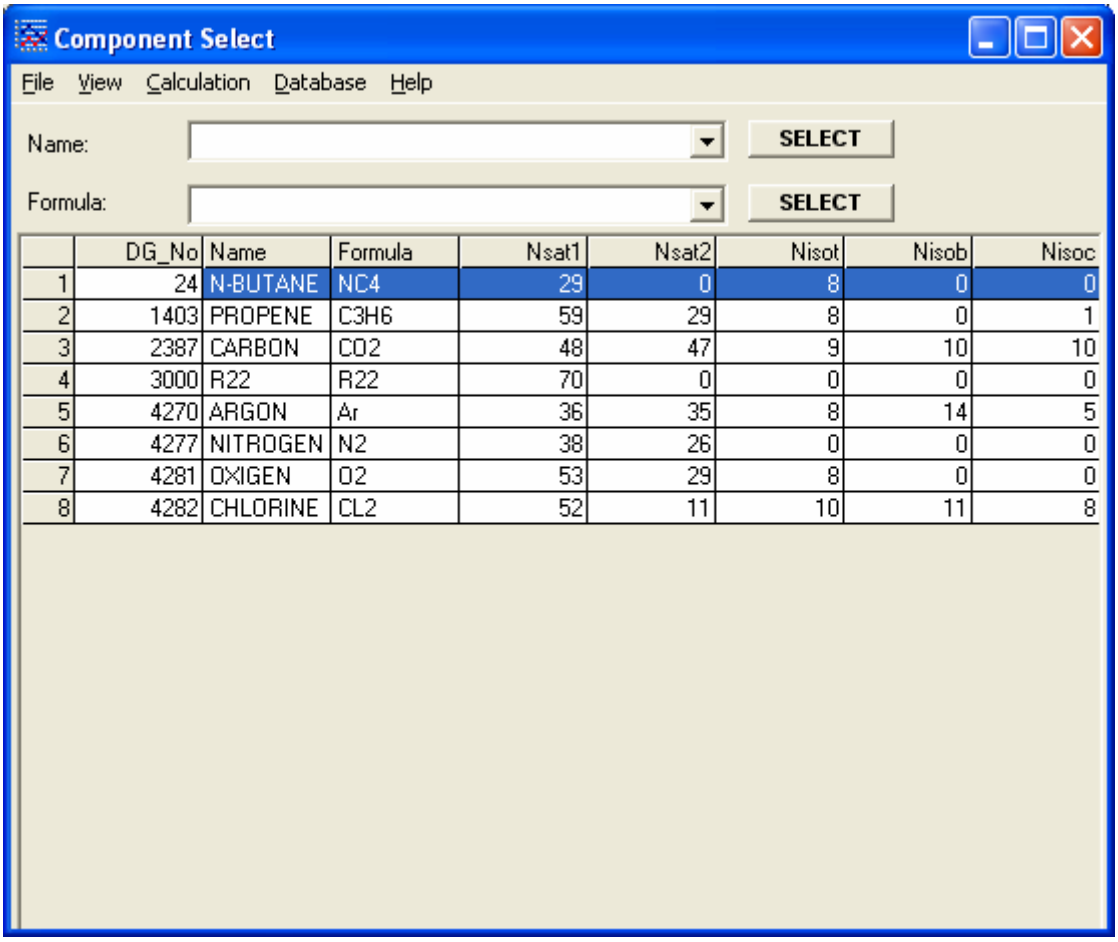


Fig.1. Main screen of PHEQ database program



	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)

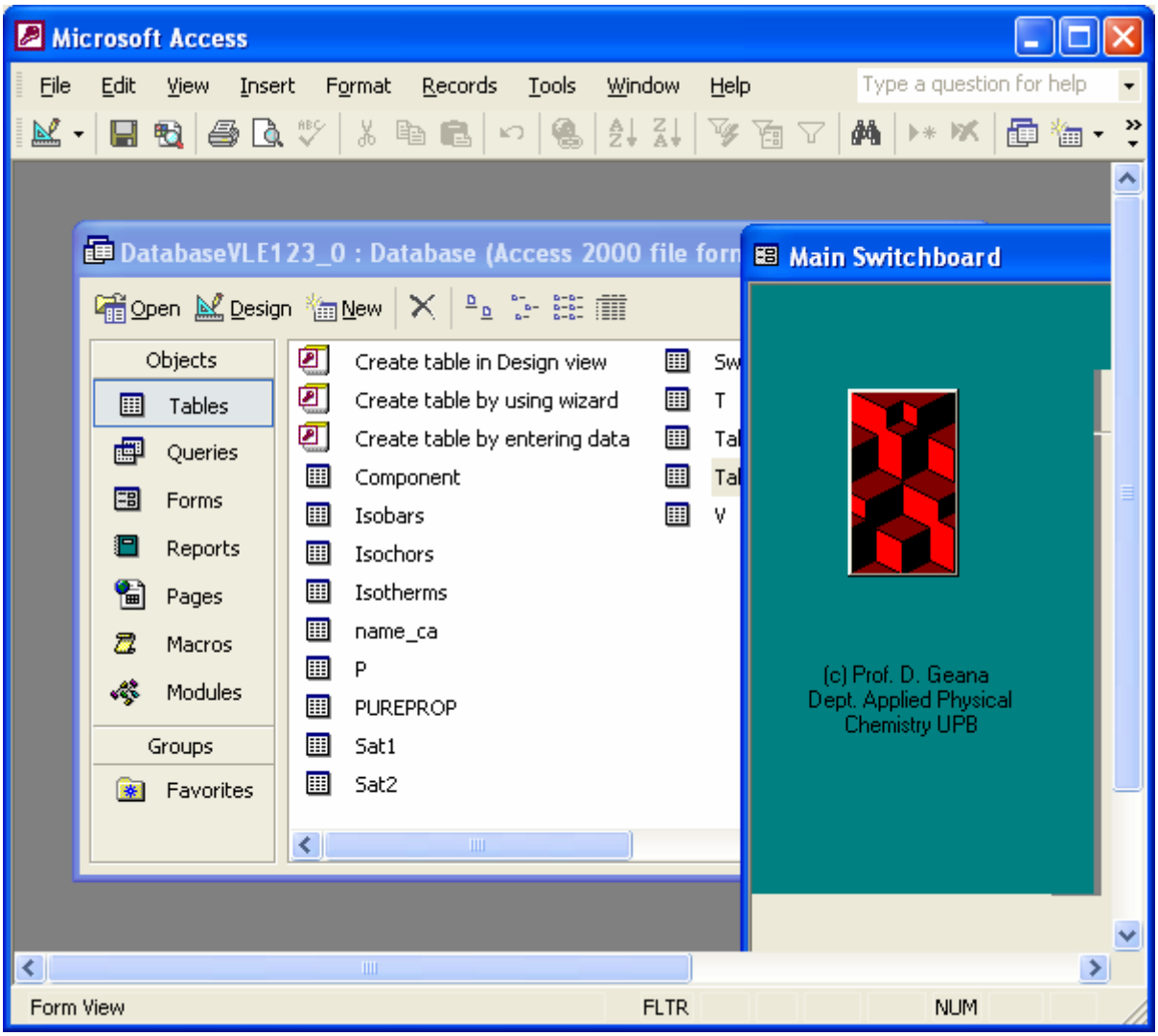
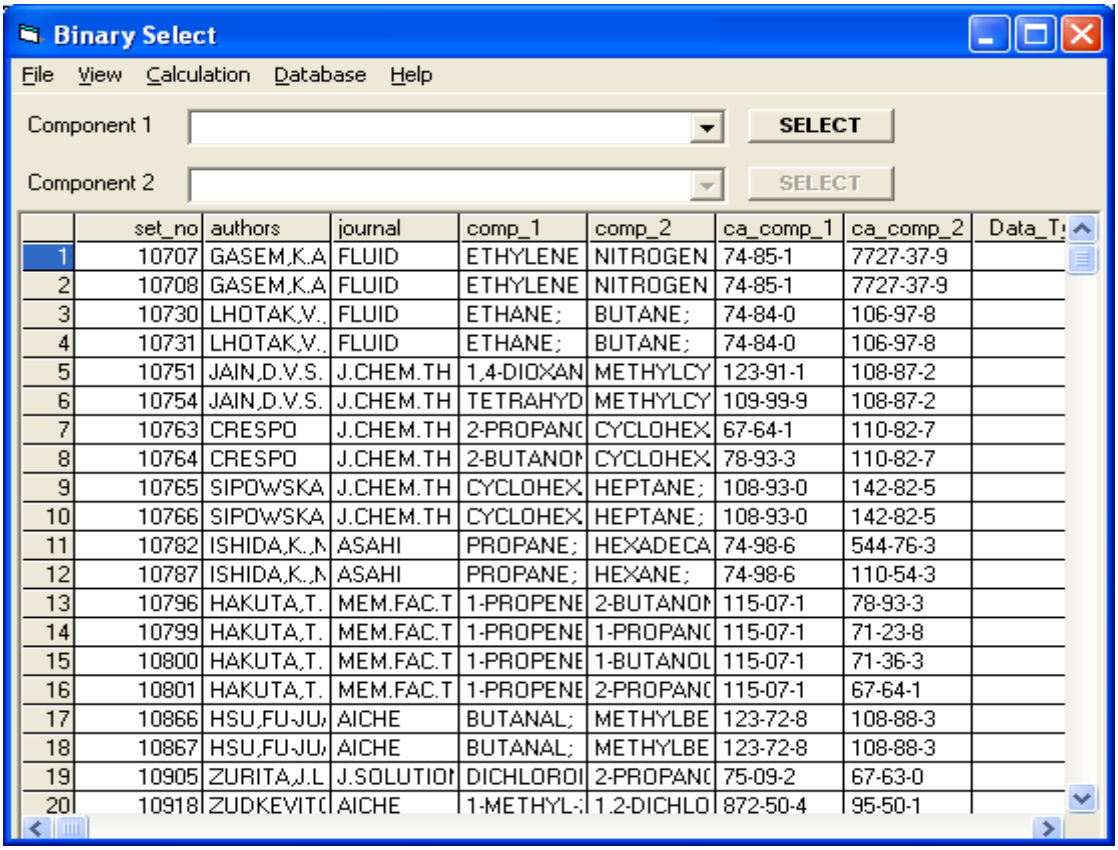


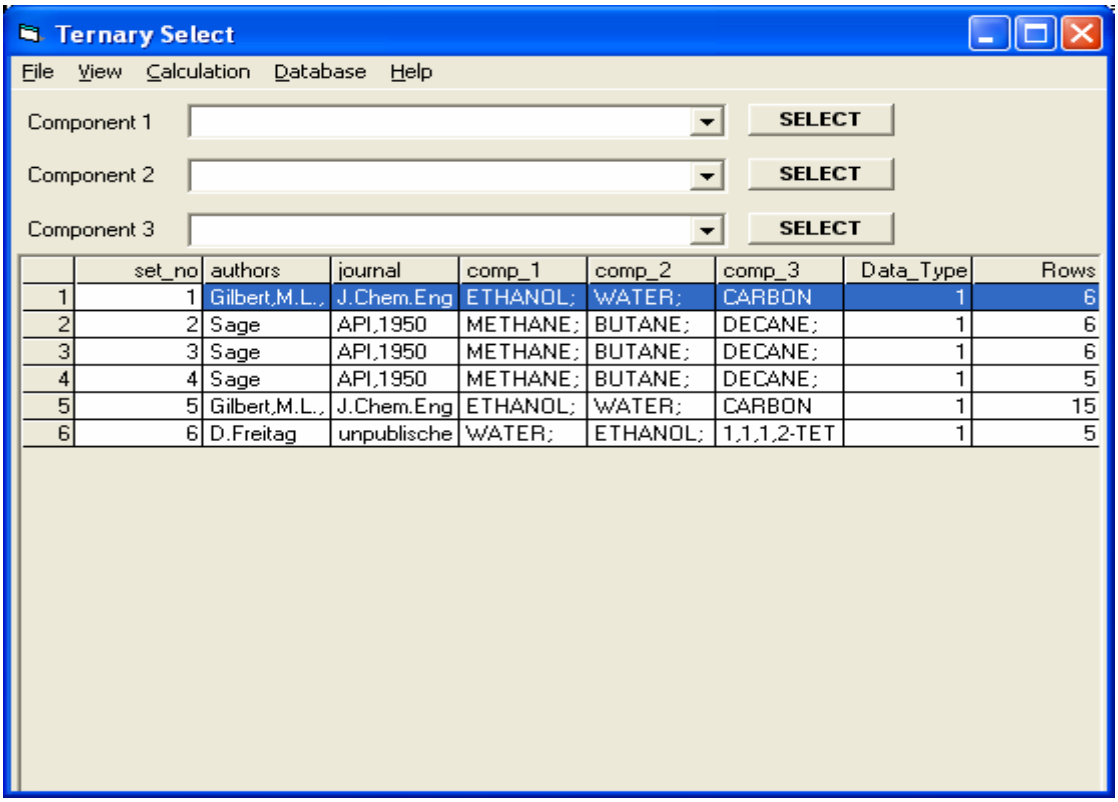
Fig. 3. Access database used by the PHEQ program

The database form for binary VLE data (called VLE2) is shown in Fig. 4. Using the sorted VLE data, it can be used to analyze and visualize the data and to offer the support for application of VLE models.



	set_no	authors	journal	comp_1	comp_2	ca_comp_1	ca_comp_2	Data_T
1	10707	GASEM,K.A	FLUID	ETHYLENE	NITROGEN	74-85-1	7727-37-9	
2	10708	GASEM,K.A	FLUID	ETHYLENE	NITROGEN	74-85-1	7727-37-9	
3	10730	LHOTAK,V.,	FLUID	ETHANE;	BUTANE;	74-84-0	106-97-8	
4	10731	LHOTAK,V.,	FLUID	ETHANE;	BUTANE;	74-84-0	106-97-8	
5	10751	JAIN,D.V.S.	J.CHEM.TH	1,4-DIOXAN	METHYLCY	123-91-1	108-87-2	
6	10754	JAIN,D.V.S.	J.CHEM.TH	TETRAHYD	METHYLCY	109-99-9	108-87-2	
7	10763	CRESPO	J.CHEM.TH	2-PROPANC	CYCLOHEX	67-64-1	110-82-7	
8	10764	CRESPO	J.CHEM.TH	2-BUTANOI	CYCLOHEX	78-93-3	110-82-7	
9	10765	SIPOWSKA	J.CHEM.TH	CYCLOHEX	HEPTANE;	108-93-0	142-82-5	
10	10766	SIPOWSKA	J.CHEM.TH	CYCLOHEX	HEPTANE;	108-93-0	142-82-5	
11	10782	ISHIDA,K.,N	ASAHI	PROPANE;	HEXADECA	74-98-6	544-76-3	
12	10787	ISHIDA,K.,N	ASAHI	PROPANE;	HEXANE;	74-98-6	110-54-3	
13	10796	HAKUTA,T.	MEM.FAC.T	1-PROPENE	2-BUTANOI	115-07-1	78-93-3	
14	10799	HAKUTA,T.	MEM.FAC.T	1-PROPENE	1-PROPANC	115-07-1	71-23-8	
15	10800	HAKUTA,T.	MEM.FAC.T	1-PROPENE	1-BUTANOL	115-07-1	71-36-3	
16	10801	HAKUTA,T.	MEM.FAC.T	1-PROPENE	2-PROPANC	115-07-1	67-64-1	
17	10866	HSU,FU-JU/	AICHE	BUTANAL;	METHYLBE	123-72-8	108-88-3	
18	10867	HSU,FU-JU/	AICHE	BUTANAL;	METHYLBE	123-72-8	108-88-3	
19	10905	ZURITA,J.L	J.SOLUTIOI	DICHLOROI	2-PROPANC	75-09-2	67-63-0	
20	10918	ZUDKEVITC	AICHE	1-METHYL-:	1,2-DICHLO	872-50-4	95-50-1	

Fig.4. Screen image for the binary VLE database and applications (VLE2)



	set_no	authors	journal	comp_1	comp_2	comp_3	Data_Type	Rows
1	1	Gilbert,M.L.,	J.Chem.Eng	ETHANOL;	WATER;	CARBON	1	6
2	2	Sage	API,1950	METHANE;	BUTANE;	DECANE;	1	6
3	3	Sage	API,1950	METHANE;	BUTANE;	DECANE;	1	6
4	4	Sage	API,1950	METHANE;	BUTANE;	DECANE;	1	5
5	5	Gilbert,M.L.,	J.Chem.Eng	ETHANOL;	WATER;	CARBON	1	15
6	6	D.Freitag	unpublische	WATER;	ETHANOL;	1,1,1,2-TET	1	5

Fig.5. Database form for ternary VLE data and calculations (VLE3)

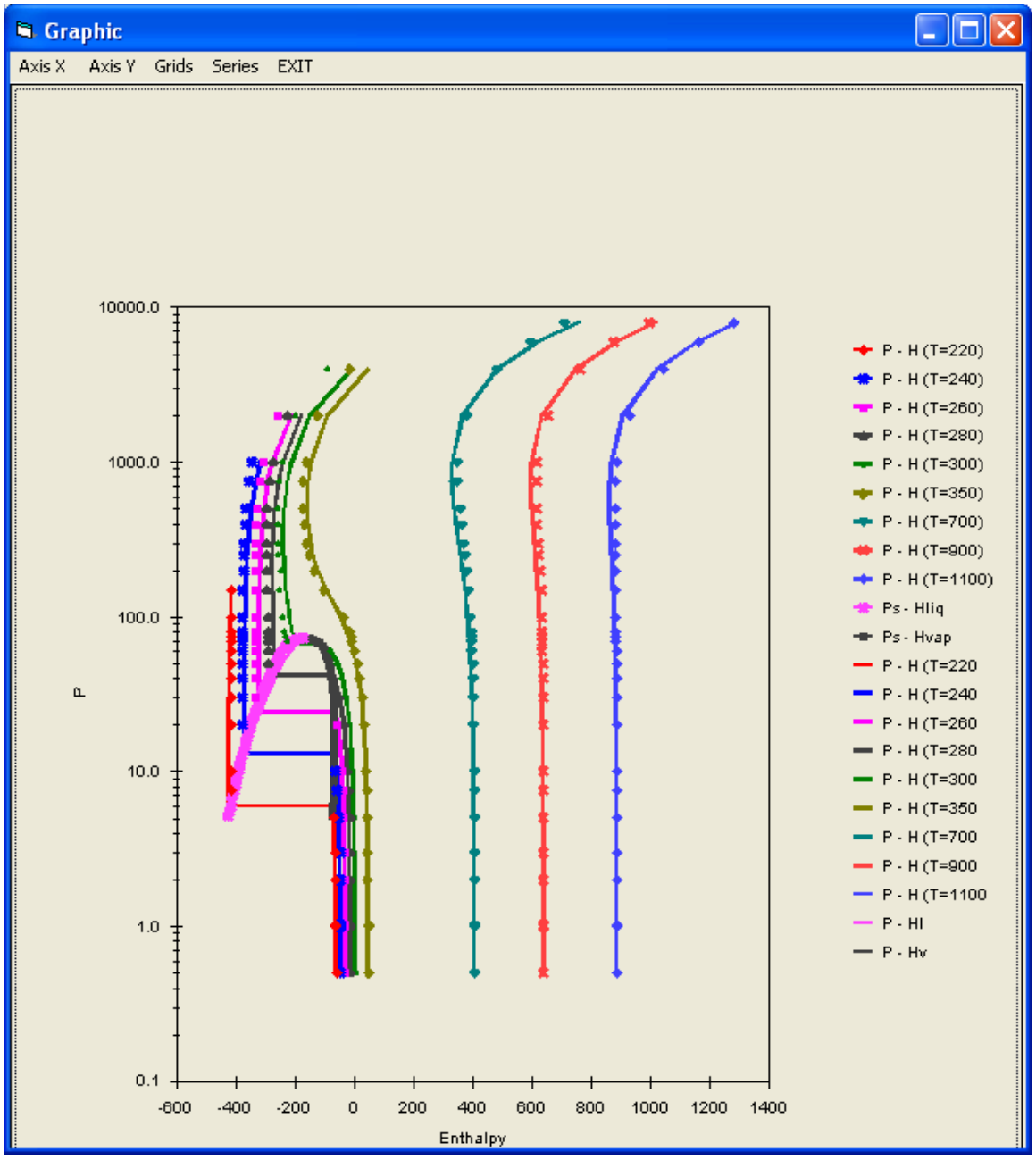
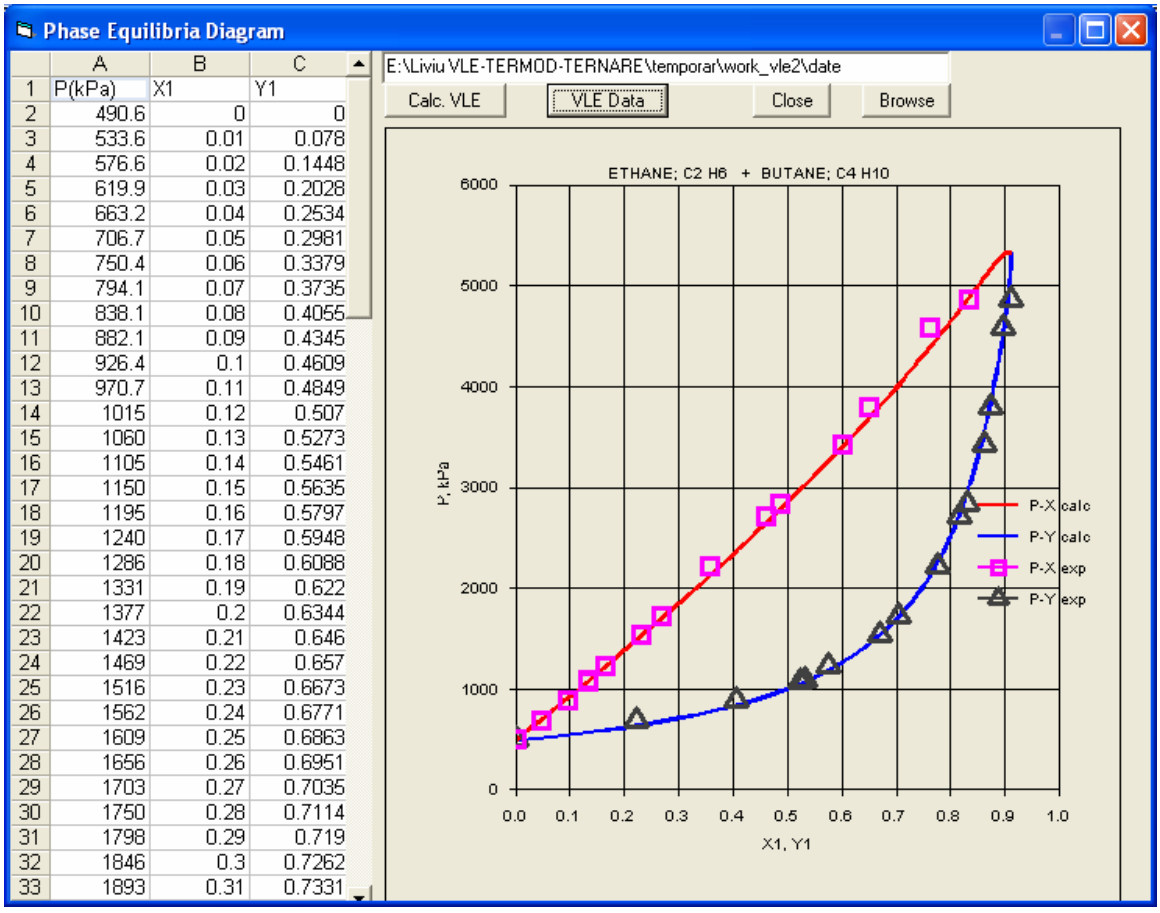


Fig. 6. Enthalpy-pressure diagram of CO_2 in PHEQ program. Points are literature data, and lines are calculations with GEOS3C EOS.

Fig. 5 shows database form for ternary VLE data (called VLE3). An example of the results analysis is shown in Fig. 6, for the calculation of enthalpy-pressure diagram of CO_2. Fig. 7 shows another example of the output of PHEQ program, for a binary P-X-Y phase diagram of the high-pressure ethane-butane system. The Fig. 8 presents a graphic output of a ternary VLE diagram of the high-pressure methane-butane-decane system at 344.15 K and 27.58 bar.



	A	B	C
1	P(kPa)	X1	Y1
2	490.6	0	0
3	533.6	0.01	0.078
4	576.6	0.02	0.1448
5	619.9	0.03	0.2028
6	663.2	0.04	0.2534
7	706.7	0.05	0.2981
8	750.4	0.06	0.3379
9	794.1	0.07	0.3735
10	838.1	0.08	0.4055
11	882.1	0.09	0.4345
12	926.4	0.1	0.4609
13	970.7	0.11	0.4849
14	1015	0.12	0.507
15	1060	0.13	0.5273
16	1105	0.14	0.5461
17	1150	0.15	0.5635
18	1195	0.16	0.5797
19	1240	0.17	0.5948
20	1286	0.18	0.6088
21	1331	0.19	0.622
22	1377	0.2	0.6344
23	1423	0.21	0.646
24	1469	0.22	0.657
25	1516	0.23	0.6673
26	1562	0.24	0.6771
27	1609	0.25	0.6863
28	1656	0.26	0.6951
29	1703	0.27	0.7035
30	1750	0.28	0.7114
31	1798	0.29	0.719
32	1846	0.3	0.7262
33	1893	0.31	0.7331

Fig. 7. Binary P-X-Y phase diagram of the ethane-butane system at 323.15 K. Symbols are experimental data and lines are calculations by GEOS3C equation of state

The calculation of different problems of phase equilibria is the main task in applications of the PHEQ package. Several equations of state have been evaluated to determine their accuracy in predicting and correlation of phase equilibria. 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[7].

Concluding remarks

The PHEQ software is an intelligent Windows-based package for the management of large amounts of phase equilibrium data, involving three types of systems (pure components, binary mixtures and ternary/multicomponent mixtures) and calculation programs for the correlation and/or prediction of phase behavior of the above systems. The project enables to develop the

program at three software levels: the intelligent user friendly interface, calculation programs for phase equilibria problems, implementing the new models (our and from the literature), and the data base with the considered types of systems.

Phase equilibrium data and applications can be easily added for subsequent operation of PHEQ program. PHEQ program enables the prompt extraction of data and facilities for analysis of calculation results.

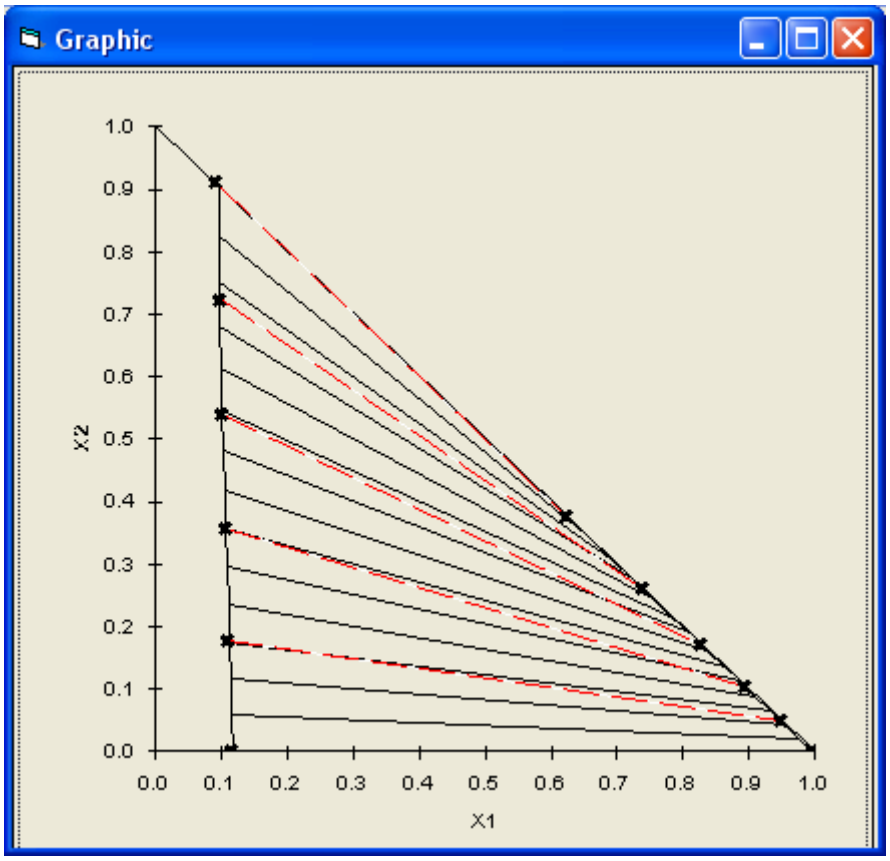


Fig.8. Graphic output of a ternary VLE diagram of the high-pressure methane-butane-decane system at 344.15 K and 27.58 bar

Furthermore, development of the software in Visual Basic.Net is intended, as well as new calculation programs to integrate the last models and algorithms appeared in literature. Several similar packages are available. A program, called PE (Phase Equilibria) was developed at Technical University Hamburg-Harburg, since 1985, in the group of the professor Gerd Brunner.[8] The last free versions, after 1998, run on PC under Windows 98, NT, Me, XP. Another program[9], called MULTIFLASH is commercially available, by the firm INFOCHEM, Computer Services Ltd, UK. A third package[10], called COSMOTHERM, is

commercially available, by the firm COSMOlogic GMBH, De. More or less elaborated programs for phase equilibria calculations can be found on many sites in Internet.

References

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