ELSEVIER

Fluid Phase Equilibria 158–160 (1999) 429–435

FLUID PHASE EQUILIBRIA

DETHERM®—a thermophysical property database

U. Westhaus *, T. Dröge, R. Sass

DECHEMA Deutsche Gesellschaft für Chemisches Apparatewesen, Chemische Technik und Biotechnologie e. V., Theodor-Heuss-Allee 25, D-60486 Frankfurt am Main, Germany

Received 14 April 1998; accepted 3 January 1999

Abstract

The DETHERM® database contains thermophysical properties of pure substances and mixtures and is one of the worlds largest data collection in this field. DETHERM® actually contains 2.85 million data sets for around 100,000 systems (16,000 pure components and 84,000 mixtures). Stored properties are: phase equilibria (vapour–liquid, liquid–liquid, gas–liquid, solid–liquid), azeotropic data, vapour pressures, critical data, caloric properties such as heat capacities, enthalpies and entropies, densities, compressibilities, transport properties such as viscosity, thermal conductivities and diffusion coefficients, surface tensions and electrolyte data such as solubility, electrical conductivities, activity coefficients, phase equilibrium data and transport properties. A bibliographic reference, descriptors and an abstract are always accessible with the numerical data. The article gives an overview about the contents of the DETHERM® database, access options and the features of the retrieval software package including numerical subroutines like parameter regression and interfaces to process simulator packages.

Keywords: Database; Data; Vapour–liquid equilibria; Liquid–liquid equilibria; Internet access

1. Introduction

Process synthesis, design and optimisation and also detail engineering for chemical apparatus depend heavily on availability and reliability of thermophysical property data for the pure substances and mixtures involved. If raw property data or parameter values for a suitable property model are not available, no process simulation or feasibility study is possible. If the data or parameters are not reliable, proper operation of apparatus cannot be guaranteed and costs figured out in advance may just be worthless numbers. Without access to a numerical database, containing either raw property data or parameter values for a reliable model, and if the available literature and notes do not contain a value, the only possibilities are to measure the data or to calculate them with a group contribution method or

* Corresponding author. Fax: +49-69-7564-201; e-mail: westhaus@dechema.de

0378-3812/99/$ - see front matter
PII: S0378-3812(99)00139-9

another estimation routine. The first alternative will be expensive and time consuming, the second one will produce data with unknown reliability in most cases. Therefore access to a thermophysical property database will be first choice. DETHERM® is such a numerical database package containing thermophysical properties of pure substances and mixtures. DETHERM® is an acronym for DECHEMA Thermophysical Property Database. It is one of the worlds largest databases in this field. Today 2.85 million data sets for around 16,000 pure components and 84,000 mixtures are stored in DETHERM®. The database is updated yearly. Parts of the data are also published in printed form as the 'DECHEMA Chemistry Data Series'.

2. Database contents

The DETHERM® database as a whole consists of several packages. The packages are property-oriented, for example, one package contains VLE-data at low pressures. Each package is produced and maintained by external experts. This guarantees checked and high quality data. Some of the packages are the foremost data collections in their area. Table 1 gives an overview of the main packages included in DETHERM®.

Each of the data records contains the numerical data itself, a bibliographic reference, an abstract and usually some index terms.

3. Access options

There are three possibilities to access the DETHERM® database: online via the STN International database hosts, inhouse with a locally installed system or with the DETHERM® Internet client via Internet connections.

Table 1
Packages of the DETHERM® database

Package name	No. of data tables	Contents
DDB, The Dortmund Database	245,000	Vapour–liquid equilibria of normal and low substances and electrolytes, liquid–liquid equilibria, activity coefficients at infinite dilution, gas solubilities, solid–liquid equilibria, azeotropic data, excess properties, pure component data
ELDAR, Electrolyte data collection	50,622	Densities, heats of solution, heat capacities, molar volumes, osmotic coefficients, solubilities, vapour pressures, electric conductivities, viscosities, dielectric properties, etc.
INFOTHERM, Thermophysical database	71,272	PVT-data, transport and surface properties, caloric properties, phase equilibria (VLE, GLE, LLE, SLE), basic data
COMDOR, Thermophysical parameters	20,131	Phase equilibria (VLE), excess enthalpies, transport and surface properties, caloric and acoustic data
C-DATA, Data collection Prague	7,043	20 physico-chemical properties for 593 components
BDBB, Base database Böhlen	18,041	Property/constant matrix with 24 fields for 1126 components
OTHERS, Several smaller packages	208,671	Chebyshev- and Antoine-constants, transport properties, caloric data, PVT-data, critical data

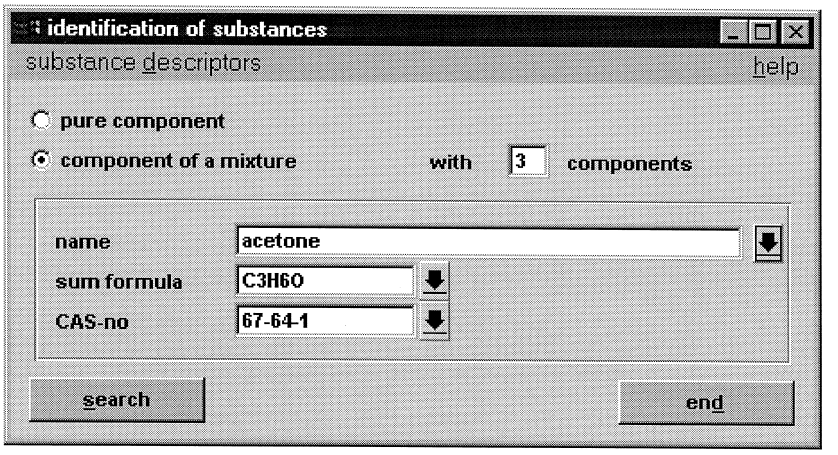

Fig. 1. Identification of substances.

3.1. Online access

If data are needed only sporadically, online access is the right choice. Access to DETHERM® is possible via STN-International and actually DETHERM is loaded on the hosts in Columbus, OH,

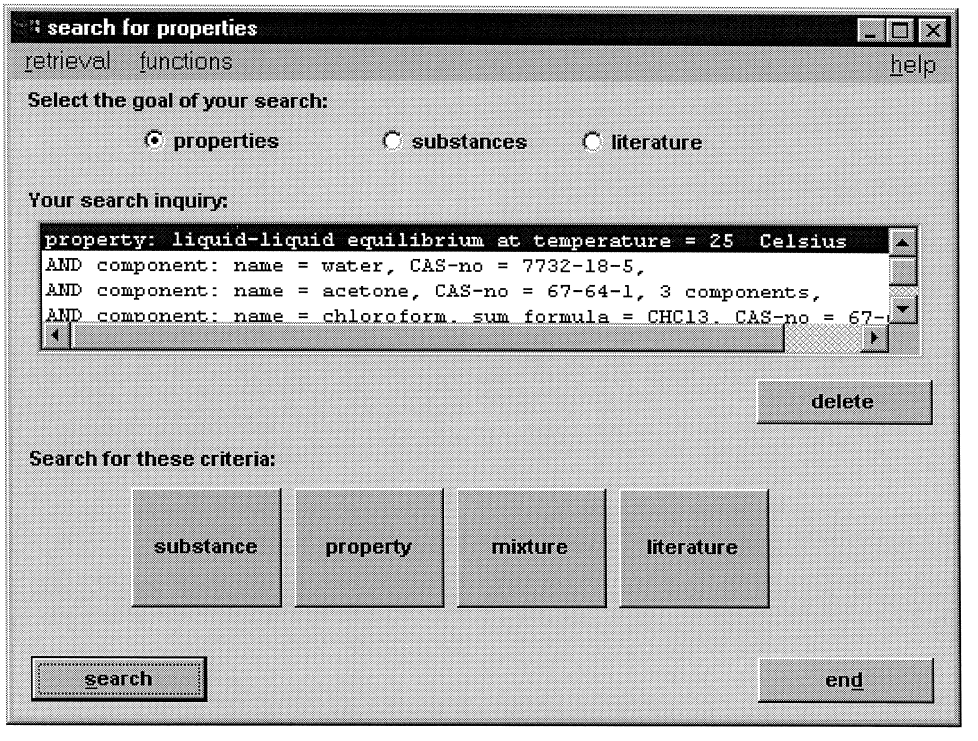

Fig. 2. Combined search request.

USA, Karlsruhe, Germany and Tokyo, Japan. Access to STN is possible via every international packet switched network (e.g., DATEX-P) or via the Internet. Users can either initiate a terminal session or use a graphical interface under Windows. In both cases, searching is only possible utilizing the MESSENGER command language.

3.2. Inhouse version

For more frequent use and even for inexperienced users, the inhouse system is the first choice. In contrast to the online version it offers the following advantages:

- designed as client–server–application using an ORACLE database
- easy-to-use graphical interface to carry out the formulation of retrieval questions
- graphical representation of the data possible
- export and import filters to various data formats
- some data regression routines already included
- possibility of data input and maintenance

The inhouse version is designed as client–server–application. The client can be any networked computer with Windows or Motif. The client runs the retrieval software and the graphical user interface. The server needs an ORACLE database and stores the data. The amount of disk space

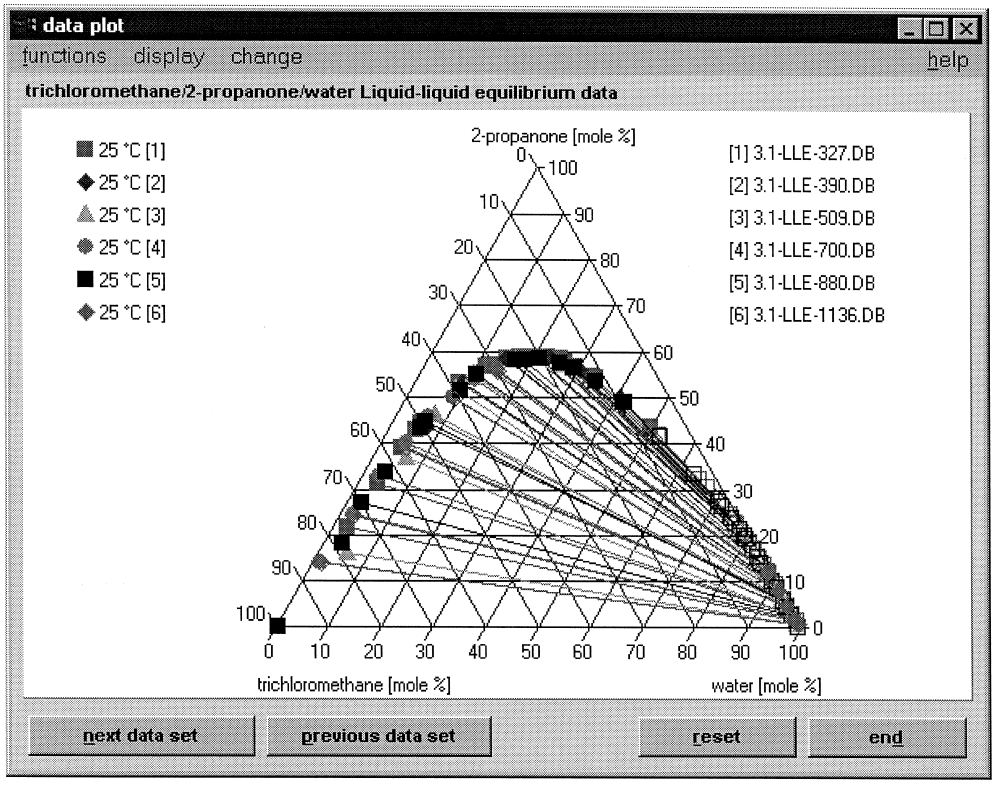

Fig. 3. Graphical representation of liquid–liquid equilibrium data.

needed on the server can be large, for example, 2 Gigabytes for the whole database. A workstation or nowadays a high end PC is needed to ensure adequate response times. UNIX workstations are normally used to run the database server. The communication between client and server is handled via SQL∗NET. This software is part of any ORACLE server database installation and allows communication independent of the network protocol used (e.g., TCP/IP, SPX/IPX, DECNET).

The graphical user interface of DETHERM® inhouse allows even unskilled users to query the database. A typical retrieval case is to search for the properties of a specific substance or mixture. Substances can be identified either by name, synonym, sum formula or CAS-number. Combination of entries and use of wildcards is also allowed (see Fig. 1).

For more complex requests, it is possible to combine different search items. This allows, for example searching for liquid–liquid equilibrium data of the three component mixture chloroform/acetone/water at 25 °C (see Fig. 2).

A result window lists all available data sets matching this query. Viewing, printing and plotting of the data (see Fig. 3) is possible.

Furthermore, it is possible to search for substances or mixtures with given properties. Queries of this type are called inventor questions. The questions ''Which liquid substance has a thermal conductivity greater than X (cP) in a given temperature range and a melting point greater than Y (°C)?'' or ''Which substance builds up a mixture gap with the miscible mixture A/B and has an

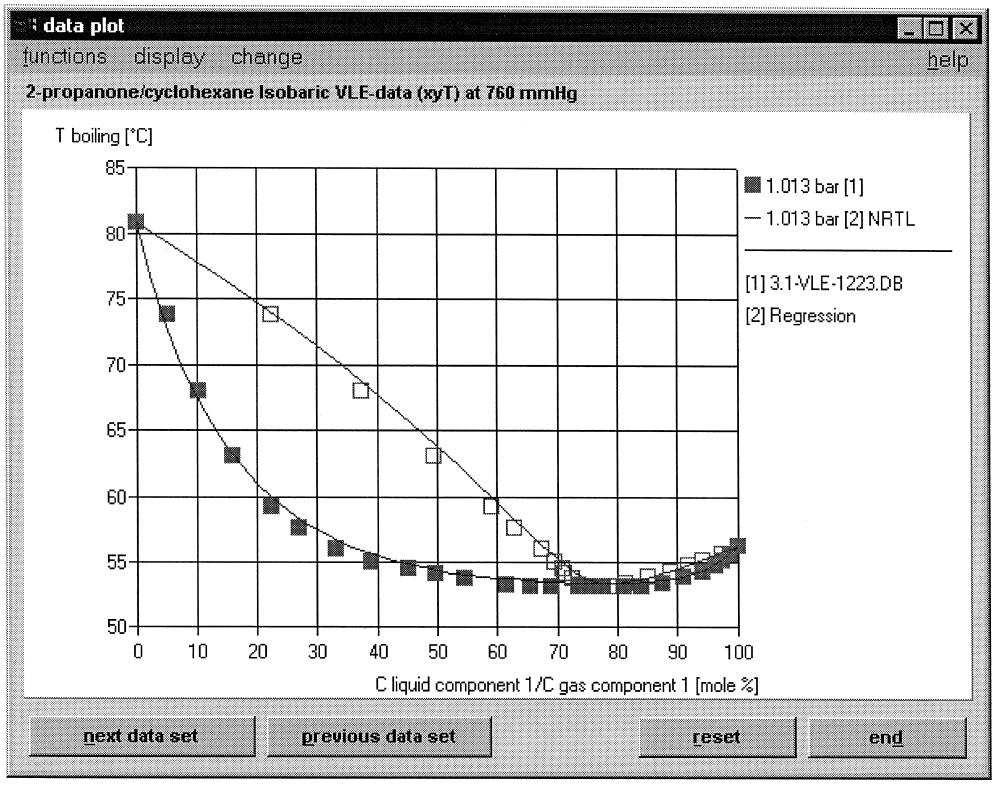

Fig. 4. Result of an automated NRTL parameter regression.

azeotrope with component A?'' are examples for this type. Running inventor questions through large databases can offer significantly reduced response times in comparison to guessing by human experts.

The retrieved data can be exported for further manipulation or use in other programs. Export in EXCEL, IK-CAPE and ASPEN-DRS formats is feasible. The IK-CAPE format originated in the German chemical industry is strongly related to the European CAPE OPEN activities. It will be replaced by the CAPE-OPEN results for raw data exchange in future. The ASPEN-DRS format allows direct inclusion of the data in the ASPEN Data Regression module for parameter regression within the ASPEN PLUS simulation software package.

Another feature of DETHERM® inhouse is the possibility of parameter regression just inside the program. Fig. 4 shows the result of a NRTL parameter regression using vapour–liquid equilibrium data of an acetone/cyclohexane mixture. The values calculated with the resulting NRTL parameters are displayed together with the raw data. The parameters themselves can be viewed, printed or exported on demand.

Another advantage of the DETHERM® inhouse system is the possibility of data maintenance. This allows users to append their own data to the database and enables companies to merge their own data pool with the one delivered. This data can be retrieved together with the rest of the database, as mentioned before. The maintenance of literature and components or mixtures is also feasible.

3.3. Internet access

A third alternative to access DETHERM® is the usage of the DETHERM® Internet client. This software allows database searching and data downloads via Internet connections to an online

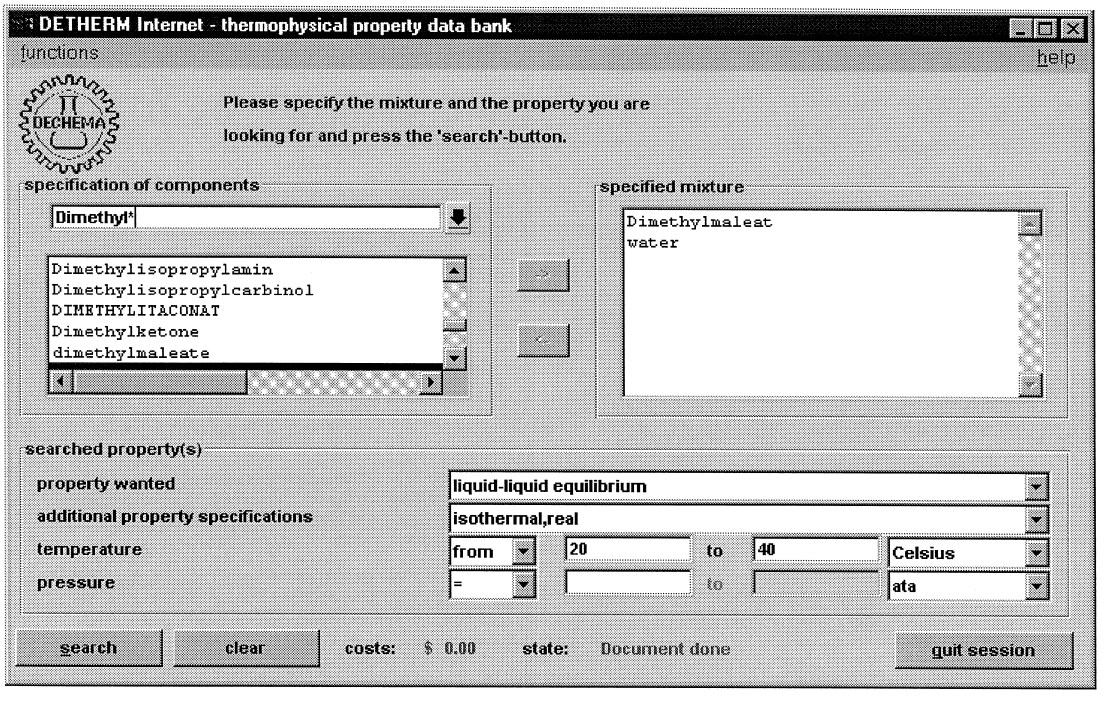

Fig. 5. DETHERM® Internet client.

DETHERM® database server (see Fig. 5). At present, this option is already available for customers of the ASPEN PLUS simulation software package. The DETHERM® Internet client provides a seamless interface between the new ASPEN PLUS Version 10 and the DETHERM® database. Starting from the ASPEN PLUS user interface, engineers are able to access, search and display data either online or inhouse. Desired datasets can be downloaded and are imported into ASPEN PLUS automatically. A public version of this software for free searching and scanning of the DETHERM® database can be downloaded from the DECHEMA Internet homepage located at 'http://www.dechema.de'.

4. Conclusion

The DETHERM® database package offers access to wide variety of thermophysical property data. One of the main focuses of DETHERM® is phase equilibrium data. The various access options are tailored to meet the needs of a wide range of different users. Interfaces to data regression tools and process simulation packages offer especially chemical engineers an integrated environment for data retrieval, maintenance and preparation.