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Solubility data in physicochemical data collections and data banks

Adam Skrzecz

Thermodynamics Data Center, ul. Kasprzaka 44/52, 01-224 Warsaw, Poland

Abstract: Collections of experimental data on solubility, mutual solubility, and phase equilibria of liquid-liquid, gas-liquid, and solid-liquid systems are discussed. Bibliographies, handbooks on specific properties, books containing data collections, monographs and data banks in computerized form are reviewed. The data bank on solubility prepared by The Thermodynamics Data Center, Warsaw, Poland and The Thermodynamics Research Center, Texas, USA is discussed in detail.

Introduction

Accurate solubility and phase equilibrium data are needed for detailed calculations of separation processes. Often these data can only be found in monographs on particular substances, groups of substances or collected in specialized handbooks and computer data banks. Such collections of solubility data of non-electrolytes are discussed. Solubility data relate to the following phenomena:
- the dissolution of liquid in liquid and liquid-liquid equilibria;
- the dissolution of gas in liquid and gas-liquid equilibria (this is closely related to vapor-liquid equilibria);
- the dissolution of solid in liquid and solid-liquid equilibria.

Solubility data are very dispersed in the literature, thus making access to them difficult. Handbooks for general use often contain solubility data at one temperature only. In many cases it is only the solubility in water at 293 K which is given. It may be important to know the accuracy of experimental data and differences between experimental results obtained by various authors. In those cases critical evaluations of data are needed. A reliable evaluation ought to take into account the details of the method, the purity of the substances and the experimental experience of investigators. Data should be consistent with those for other similar systems and with other thermodynamic properties. The majority of data collections, both in hardcopy and electronic form, report only experimental data without critical evaluation. However there are some collections containing evaluations.

Bibliographies

Over the last twenty years, with the development of computer techniques, bibliographies of various properties have been prepared. These have been based on *Chemical Abstracts*. Bibliographies relating to various types of solubility have been published by Elsevier in the *Physical Science Data* series with subtitles *A literature source book* (see Table 1). In these bibliographies, the systems are ordered by molecular formula and contain codes of references. Each reference contains full details of the original publication and also the *Chemical Abstract* number. Unfortunately a significant number of these references do not contain quantitative solubility data.

TABLE 1. Bibliographies on Solubility Data

Wisniak, J.; Tamir, A. *Liquid-Liquid Equilibrium and Extraction (A literature source book)*
Parts A, B - Elsevier, Amsterdam, (1981); (7129 refs, period 1900 - 1981)
Supplement 1 - Elsevier, Amsterdam, (1985); (1556 refs, period 1982 - 1984)
Supplement 2 - Elsevier, Amsterdam, (1987); (1148 refs, period 1985 - 1986)
Wisniak, J.; Hreskowitz, M. *Solubility of gases and solids (A literature source book)*
Parts A, B - Elsevier, Amsterdam, (1984); (14530 refs, period 1900 - 1983)
Wisniak, J. *Phase Diagrams (A literature source book)*
Parts A, B - Elsevier, Amsterdam, (1981); (17400 refs, period 1900 - 1980)
Supplement 1 - Elsevier, Amsterdam, (1987); (4800 refs, period 1981 - 1986)

Handbooks, hardcopy data collections, monographs

The most important specialized handbooks containing solubility data are presented in Table 2.

TABLE 2. Handbooks on Solubility Data

Seidel, A. vol. 1 *Solubilities of inorganic and metal organic compounds* (1600 p)
vol. 2 *Solubilities of organic compounds* (850 p) D. van Nostand Co., New York (1953).
Seidel, A.; Linke, W. F. *Solubilities of inorganic and organic compounds, Supplement to the Third Edition (1939-49)*, (1124 p), Am. Chem. Soc., New York (1952).
Timmermans, J. *The Physico-chemical Constants of Binary Systems in Concentrated Solutions*
vols 1 - 4, Interscience Pub., New York (1959-1960).
Kogan, V. B.; Friedman, V. M.; Kafarov, V. V. (editor in chief) *Spravochnik po Rostvorimosti (Handbook on Solubility)*, Izd. Akad. Nauk SSSR, Moskva (1961-1970).
vol. 1, *Binary systems*, (6540 tables, 2135 refs)
vol. 2, *Ternary and multicomponent systems*, (5199 tab, 1451 refs)
vol. 3, *Ternary and multicomponent inorganic systems*, (5587 tables, 2782 refs)
Stephen, H.; Stephen, T. (editors) *Solubilities of Inorganic and Organic Compounds*
vol. 1, part 1 and 2, Pergamon Press, Oxford (1963).
Domańska, U. Rolińska, J. *Solid-liquid Equilibrium Data Collection, vol. I, Monocarboxylic acids + Organic compounds*, PWN - Polish Scientific Publishers, Warszawa (1988).
Knapp, H.; Teller, M.; Langhorst, R. *Solid-liquid Equilibrium Data Collection,*
DECHEMA Chemistry Data Series, vol. VIII, Frankfurt/Main (1987)
Soerensen, J. M.; Arlt, W. *Liquid-liquid Equilibrium Data Collection,*
DECHEMA Chemistry Data Series, vol. V, Frankfurt/Main (1979-1980).
part 1, *Binary Systems,* (645 tables)
part 2, *Ternary Systems,* (625 tables)
part 3, *Ternary and Quaternary systems,* (391 tables)
part 4, *Supplement I,* (280 tables)
International Data Series, Selected Data on Mixtures
Kehiaian, H. V. (editor-in-chief 1973-1993); Marsh, K. N. (editor-in-chief 1993-)
Solubility Data Series
Kertes, A. S. (editor 1979-1989), vols 1 - 40; Lorimer, J. W. (editor 1989-1995), vols 41 - 60; Salomon, M. (editor 1996-)
Pergamon Press, Oxford (1979-1993); Oxford University Press, Oxford (1994-1996).

The first edition of the Seidel handbook was published in 1907. It contains only 353 pages of tables. The third edition, printed after the Second World War, covered data published before 1939 and, together with a supplement, contained 3600 pages of tables. The large monograph of Timmermans' *The Physico-chemical Constants of Binary Systems in Concentrated Solutions* is a useful collection of various thermophysical properties including solubility data. *Spravochnik po Rostvorimosti* (Handbook on Solubility) was published in 1961 - 1970. This huge Russian handbook was divided into 3 volumes, each volume in two parts of about 1000 pages. It covers experimental solubility data, in binary, ternary and multicomponent systems, of organic and inorganic compounds in 17,326 tables. Part of this work was published in English Pergamon Press in 1963, (editors - Stephen and Stephen).

The collection of data prepared by Domańska and Rolińska and published in the series *Thermodynamical Data for Technology* contains experimental data for binary and ternary systems of monocarboxylic acids (C_2 - C_{22}) with organic compounds. It contains 431 solubilities of solids in liquids for 24 acids, together with description of methods, materials and errors, and parameters of several correlation equations.

Another source of various experimental data is the DECHEMA Data Series. Volume VIII, entitled *Solid-liquid Equilibrium Data Collection* contains solid-liquid equilibrium data for 180 binary inorganic and organic systems. Calculated parameters for correlation equations are also included. Data for liquid-liquid systems have been published in volume V (3 parts) as *Liquid-Liquid Equilibrium Data Collection*. This collection contains only liquid-liquid equilibrium data (two phases in equilibrium) of binary, ternary and quaternary systems, and calculated parameters of NRTL and UNIQUAC equations.

International Data Series, Selected Data on Mixtures (IDS) is a continuous publication (4 issues per year available only on a subscription basis), of the Thermodynamics Research Center, Texas A&M University. It contains selected and well documented data of selected properties of binary mixtures. Uncertainties of each variable are stated together with purity of materials and methods of measurement. Material included since 1973 has included data for 188 liquid-liquid equilibria, 250 solid-liquid equilibria and 190 gas-liquid critical temperatures as functions of composition and pressure. These data are also available from the *IDS Data Bank*.

Another long term publication is *Solubility Data Series* - the project of IUPAC Commission on Solubility Data. The first volume was published in 1979 and 65 volumes will have been published by the end of 1996. Each of them is dedicated to a selected group of substances or systems and contains the compilations of experimental solubility data published in the original literature, together with an account of the method and apparatus, the substances used and likely errors. Experimental data are evaluated and appropriate data are recommended.

Data banks

The most recent method of presenting thermophysical data is in the form of an electronic data bank. However access to some commercial data banks may be limited.

The electronic collections of National Institute of Standards and Technology, USA, contain evaluated and predicted properties of mixtures. Some of these data relate to solubility. The DECHEMA data bank also contains solubility data. It includes about 8,400 liquid-liquid equilibrium data sets and 6,800 gas-liquid equilibrium data sets. These are available through installation on a user's computer or by on-line access.

The data bank of the Thermodynamics Data Center in Warsaw is discussed in detail below. It contains over 66,000 experimental data sets of various thermophysical properties of pure substances and mixtures obtained from the open literature. The bank is the result of international collaboration and is operated in the Thermodynamics Data Center in Warsaw and in the Thermodynamics Research Center of Texas A&M University. It is managed by the Floppy Book Program adapted to IBM compatible computers operating under WINDOWS). This program is user friendly and allows the following:

- selection of a system by visual or pattern search,
- selection of a data set,
- display of the data in tabular and graphical forms,
- regression of the data,
- calculations when parameters of equations are available,
- saving of experimental and calculated data to external files.

The concept of *Floppy Books* was developed by A. Maczynski and J. Niedziela at the Polish Academy of Sciences. The program has been modified in conjunction with the IUPAC Commission on

Solubility Data, the CODATA Task Group on Phase Equilibrium Data and with the Thermodynamics Research Center at Texas A&M University.

The data bank is divided into thematic subcollections and contains:
- thermophysical properties of pure substances (33 properties e.g. triple point parameters, critical properties, density, saturated vapor pressure, refractive index, heat capacities, enthalpies of formation and transition, etc.); 13,474 data sets, 2,449 substances;
- boiling points; 13,533 data sets, 2,566 substances;
- freezing points; 7,573 data sets, 2,718 substances;
- flash points; 6,175 substances;
- viscosity; 1,060 data sets, 881 substances;
- virial and cross virial coefficients; 2,346 data sets, 907 systems, 350 substances;
- heats of mixing; 9,535 data sets, 4,744 systems, 864 substances;
- vapor-liquid equilibria (binary systems); 18,125 data sets, 4,824 systems, 1,081 substances;
- vapor-liquid equilibria (ternary systems); 1,271 data sets, 667 systems, 237 substances;
- solid-liquid equilibria; 1,175 data sets, 994 systems, 377 substances;
- solubility of gases in liquids; 485 data sets, 155 substances;
- liquid-liquid equilibria; 3,069 data sets, 927 systems, 659 substances.

All the above data collections are being updated.

Each of the subcollections is available as a separate database. The database entitled Liquid-Liquid Equilibria contains binary and ternary solubility and liquid-liquid equilibrium data. It now includes data for the systems: hydrocarbon - water, alcohol - water, alcohol - hydrocarbon, alcohol - hydrocarbon - water, ester - water, other organic compounds (containing oxygen) - water, and systems containing nitroalkanes.

The database entitled *Solubility of Gases in Liquids* contains experimental data and recommended equation parameters for dissolution of sulfur dioxide and of hydrogen sulfide but extension to include other gases is planned.

The mode of using the bank or its subcollections can be seen from illustrations of screens displayed when the *Liquid-Liquid Equilibria* database is accessed. The selected screens are:

fig.1, title page;
fig.2, selection of a component by pattern search;
fig.3, selection of a component by visual search;
fig.4, searching of the data set by author's name;
fig.5, display of the data set in graphical form;
fig.6, display of the data set in tabular form;
fig.7, display of the data together with the regression results in graphical form;
fig.8, calculations on the basis of model parameters obtained in regression.
Additional displays of the ternary liquid-liquid equilibrium data set are presented in fig. 9 and fig. 10: fig.9, display of the ternary data in graphical form; fig.10, display of the ternary data set in tabular form.

All subcollections in the data bank at the Thermodynamics Data Center may be presented in the same way.

Another data bank containing solubility data contains data presented in the *International Data Series, Selected Data on Mixtures.* It is the electronic form of the hardcopy data collection discussed above. Among nearly 6,000 data sets, 645 data sets contain solubility data. They are: solubilities of liquid in liquid, solid in liquid and gas in liquid. The bank is managed by the same Floppy Book software mentioned above.

It is likely that data collected and evaluated by the IUPAC Commission on Solubility will eventually be published in electronic form.

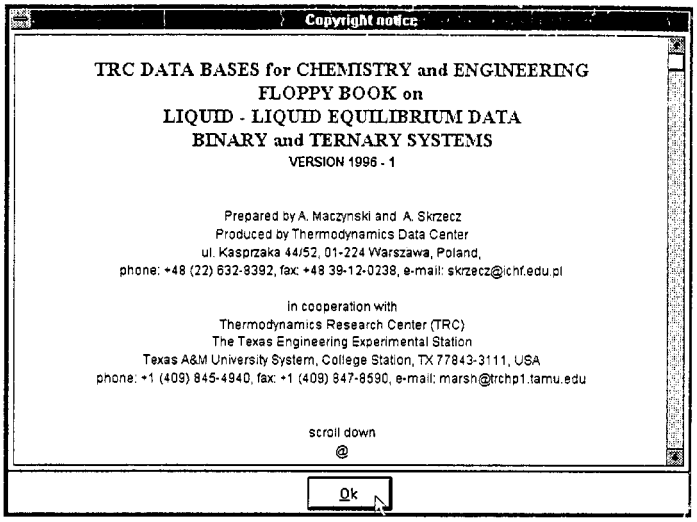

Fig. 1. Title page.

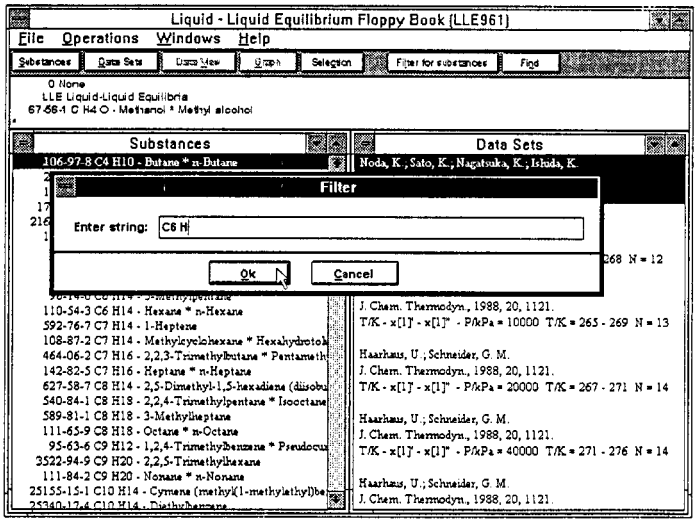

Fig. 2. Selection of a component by pattern search.

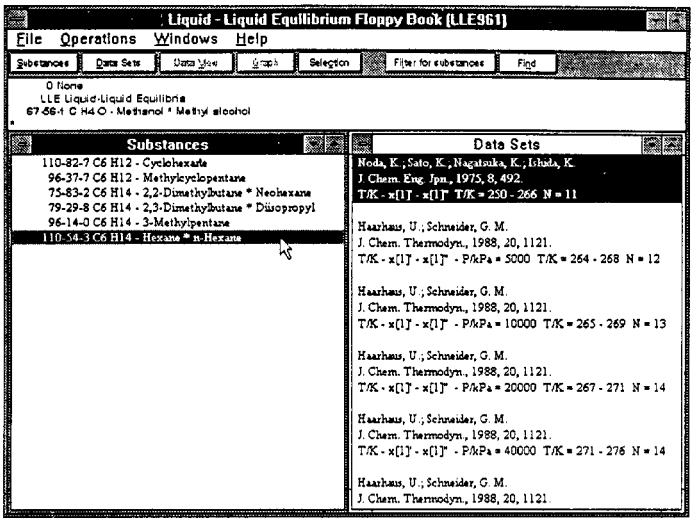

Fig. 3. Selection of a component by visual search.

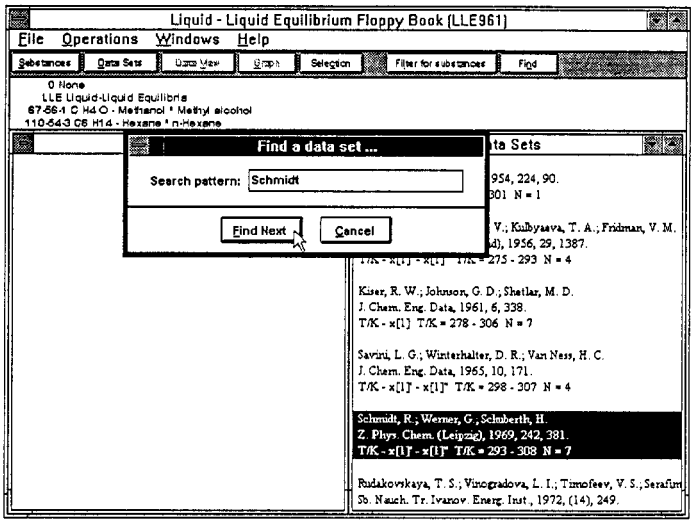

Fig. 4. Searching of the data set by author's name.

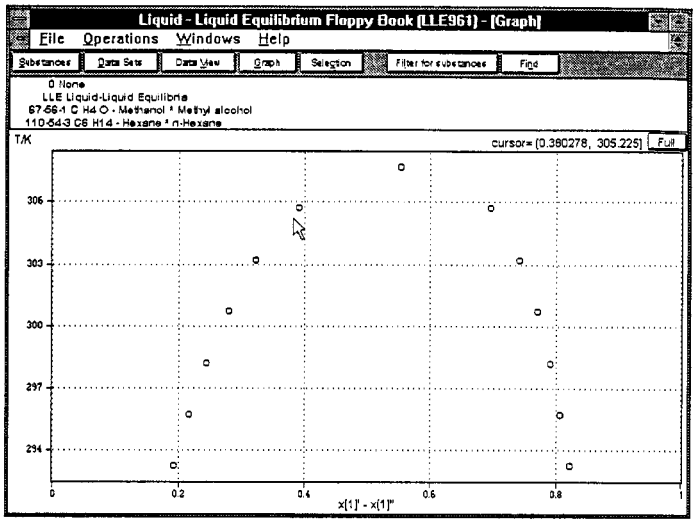

Fig. 5. Display of the data set in graphical form.

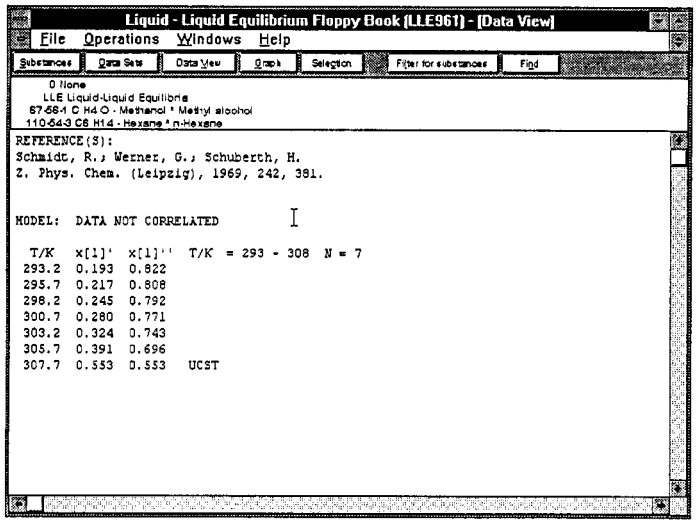

Fig. 6. Display of the data set in tabular form.

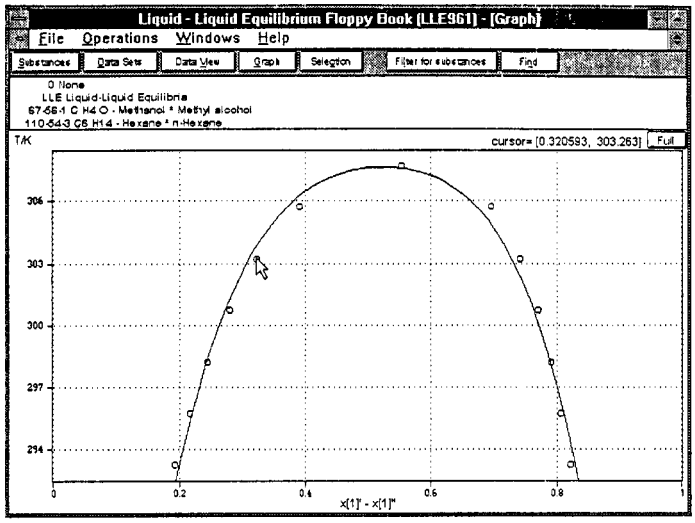

Fig. 7. Display of the data together with the regression results in graphical form.

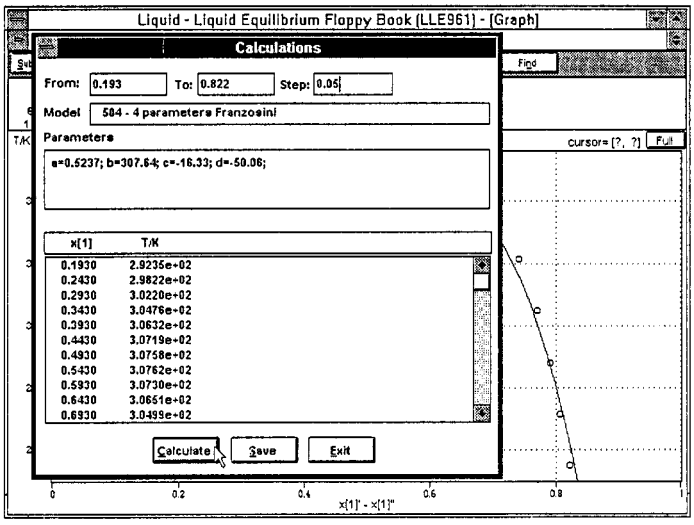

Fig. 8. Calculations on the basis of model parameters obtained in regression.

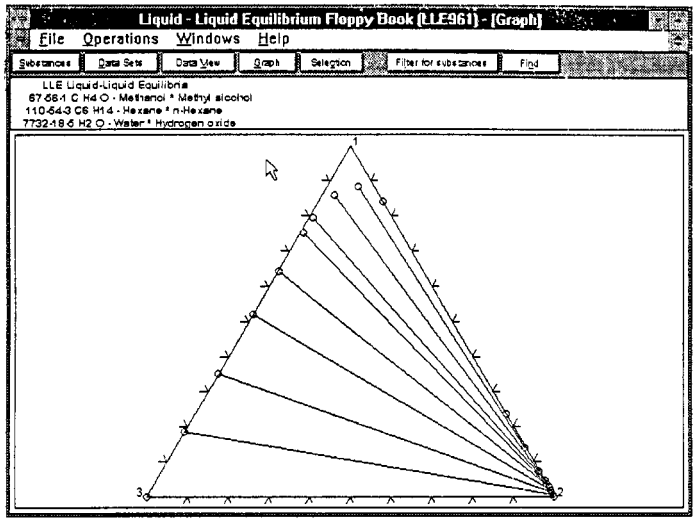

Fig. 9. Display of the ternary data in graphical form.

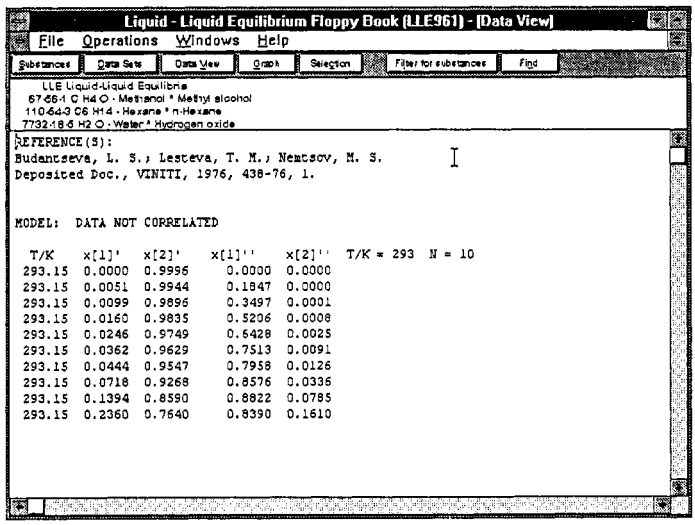

Fig. 10. Display of the ternary data set in tabular form.