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Window-Based Applications of TRC Databases: Structure and Internet Distribution[1]

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Thermophysical and thermochemical property data on organic compounds provide vital background information for scientific and engineering communities in both academic and industrial environments. The Thermodynamics Research Center (TRC) has collected an enormous amount of property data over the past 55 years. New advances in computer technology enable relatively large databases to have friendly "communications" based upon a PC Windows platform. Here we discuss the structure, upgrade procedures, and mechanisms for distribution over local PC networks and the Internet, with emphasis on three databases: TRC COMPOUNDS (Wincmp), SOURCE (WinSource), the archive of raw experimental data, and TRC TABLE (WinTable), the TRC collection of recommended data.

KEY WORDS: database evaluation; experimental data; recommended data; thermophysical property; Windows.

1. INTRODUCTION

The Thermodynamics Research Center (TRC) has performed physicochemical property collection, critical evaluation, and data management for more than 55 years. For the past 20 years, TRC has developed a number of electronic databases for thermophysical properties [1]. Among these databases, SOURCE and TABLE are the two major ones. SOURCE [2]

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has existed for 14 years and is an archive of original, experimentally measured values of thermophysical and thermochemical data covering over 100 properties of pure compounds, binary and ternary systems, and chemical reactions (Fig. 1). Recently, TRC has rebuilt the SOURCE database under the ORACLE client/server database system (ORACLE 8 Enterprise Edition) assuring robust maintenance and consistent data entry procedures [3].

The COMPOUNDS database is a subset of SOURCE representing a compound identification block. It contains Chemical Abstract Service Registry Numbers (CASRN), chemical formulas, and molar masses for more than 113,000 compounds with more than 218,000 alternative chemical names (Fig. 1).

The TABLE database is essentially an electronic version of TRC Tables–Hydrocarbons and TRC Tables-Non-Hydrocarbons [4, 5], published by TRC since 1942 and updated four times yearly. TABLE is supported by an ORACLE database system residing on a DEC-alpha workstation, and it contains 31 recommended thermophysical properties for 7446 compounds.

To provide users with easy access and multiple options to extract, display, and distribute data, TRC has developed new Window-based versions of TRC databases. TRC maintains three databases, with the ACCESS

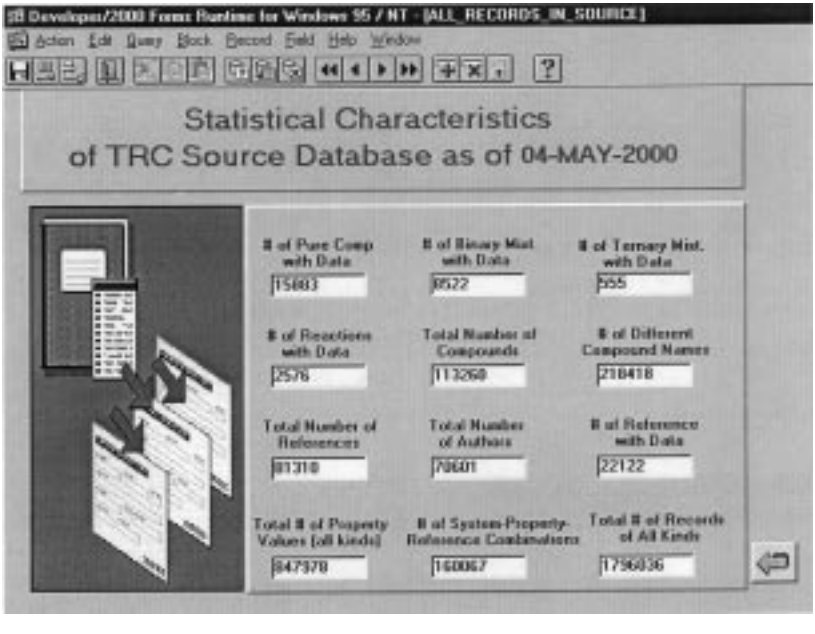

Fig. 1. Statistical characteristis of TRC SOURCE database.

database support system having retrieval functions written in Visual Basic. Efficient procedures exist to update these databases by converting data from ORACLE to ACCESS format, providing easy access through Windows GUI interfaces to display numerical data in tabular and graphic forms, to fit data with selected equations, and to distribute data through the internet.

2. DESIGN AND PRODUCTION

Principal design and production schema for all three databases (Wincmp, WinSource, and WinTable) are similar as illustrated in Fig. 2. All three databases are essentially read-only versions of the TRC ORACLE in-house databases, SOURCE or TABLE. Converting the data from the ORACLE database into the ACCESS database through Open DataBase Connectivity (ODBC)—a common gateway for all kinds of databases—populates these databases. In turn, data entry into TRC ORACLE databases is possible either through the interactive Data Entry Form supported

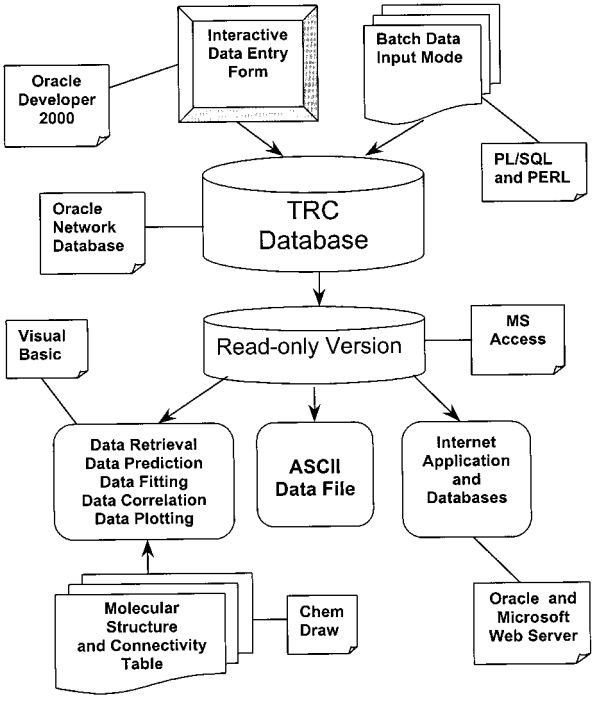

Fig. 2. Production lines for TRC Window-based databases.

by ORACLE Developer 2000 or using Batch Data Input Mode. The data stored in the MS ACCESS format can be retrieved, correlated, fitted to the selected equations, and represented in both tabular and graphical forms using the interfaces designed using Visual Basic. The tables of the MS ACCESS database can also be converted into an ASCII file for further use in other applications such as process simulation. Both ORACLE and MS ACCESS databases can be distributed *via* the Internet through the ORACLE or MS Web Server. Two files built with ChemDraw characterize each compound. One file is an image corresponding to the particular structural formula, while the other file contains the connectivity table.

3. WINCMP—TRC COMPOUND DATABASE FOR PC WINDOWS

We have produced and upgraded the ACCESS database for Wincmp from the compound identification block of the ORACLE SOURCE. Other TRC Windows databases use the retrieval functions and formats developed to represent output from Wincmp. Using Wincmp, it is possible to retrieve compound identification information by CASRN, chemical formula, formula fragment, chemical name, chemical name fragment, and any combination of these search criteria; the searches operate interactively as well as in batch mode. The formula fragment and name fragment functions permit a narrower search in case the net formula and full chemical name are unknown or doubtful. These options are also valuable if the search is related to the group of compounds characterized by the same formula fragment or name fragment. The search results obtained using the functions "formula fragment" or "name fragment" can be saved into a data subset for further search.

4. WINSOURCE—TRC SOURCE DATABASE FOR PC WINDOWS

We have produced and upgraded the ACCESS database for WinSource from the ORACLE version of SOURCE. Data entry for the ORACLE SOURCE is possible using both the Data Entry Form option (mostly in-house) and the Batch Entry Mode (to incorporate data files supplied by external contributors; Fig. 2). The available retrieval functions from WinSource fall into five groups: compound identification, pure compound properties, binary and ternary systems properties, chemical reaction properties, and references.

The compound identification block in WinSource is identical to Wincmp except it contains only those compounds which have numerical

data (over 15,800 compounds; Fig. 1). Pure compound property data records cover constants, properties at fixed conditions, and one- and two-variable properties, totaling 50 properties (Table I).

The retrieval functions developed for WinSource provide a variety of options for users to search all or any combination of property data available for a compound as well as particular property data for all or a selected group of compounds.

After having selected a particular compound and property for the search, the results appear in both textual and tabular forms and can be saved into a user-designated file. If the retrieved set contains more then two data points, the results of the search are available in graphical mode with options available for representation of uncertainties, selection of a particular range of the variables and properties, and particular user-designated data points. For constant and fixed-condition data, WinSource provides a display of the numerical data, deviation plots (as an option), average value, and average deviation. An example of the display from WinSource for a critical temperature search for methanol is shown in Fig. 3.

WinSource also provides a collection of more than 330,000 data points covering around 100 thermophysical properties for more than 8500 binary mixtures. It also includes all thermodynamic and transport property data collected by TRC during the development of the Design Institute for Physical Property Data (DIPPR) Project 882 [6]. To select a mixture for data retrieval, the user first selects one component of the binary mixture. WinSource then displays a list of all second components of the binaries, which, in combination with the first component, represent mixtures characterized by numerical data in the database. Upon selection of the second binary component from this list, WinSource displays the list of the available properties for the chosen mixture in the particular thermodynamic phase. Having defined the combination mixture/property, the search proceeds using retrieval functions similar to those developed for pure compound data retrievals. Figure 4 gives an example display of the results for a search of surface tension data for the binary mixture methanol–carbon tetrachloride.

WinSource contains about 10,000 data points covering 20 properties for 555 ternary mixtures. The ternaries can be selected directly from the complete list of ternary mixtures available or by a stepwise procedure similar to that for binaries. In addition to the options used to display the results of the data search for binary mixtures, ternary mixture data can be displayed in the triangle-type format when the variable properties are a function of mole (mass) fractions of the components.

WinSource contains thermodynamic data for more than 2500 chemical reactions. These data reside in two tables characterizing those obtained for

Table I. Properties of Pure Compounds Covered by the TRC Source Database

No.	Property	Code	Units
1	Adiabatic compressibility	VPA	kPa^{-1}
2	Boiling point temperature	TB	K
3	Coefficient of expansion	VTP	K^{-1}
4	Compressibility factor (PV/RT)	Z	
5	Critical density	VDC	$kg \cdot m^{-3}$
6	Critical molar volume	VC	$m^3 \cdot mol^{-1}$
7	Critical pressure	PC	kPa
8	Critical temperature	TC	K
9	Cryoscopic constant	YRC	K
10	Enthalpy	H	$kJ \cdot mol^{-1}$
11	Enthalpy of transition	HTR	$kJ \cdot mol^{-1}$
12	Enthalpy of vaporization at saturation	HVP	$kJ \cdot mol^{-1}$
13	Entropy	S	$J \cdot mol^{-1} \cdot K^{-1}$
14	Fugacity coefficient	FC	
15	Gibbs energy at 1 bar	G	$kJ \cdot mol^{-1}$
16	Heat capacity at constant pressure per unit volume	CPV	$J \cdot m^{-3} \cdot K^{-1}$
17	Heat capacity at constant pressure	CP	$J \cdot mol^{-1} \cdot K^{-1}$
18	Heat capacity at constant volume	CV	$J \cdot mol^{-1} \cdot K^{-1}$
19	Heat capacity at saturation	CS	$J \cdot mol^{-1} \cdot K^{-1}$
20	Heat capacity ratio (C_p/C_v)	CGM	
21	Internal energy	U	$kJ \cdot mol^{-1}$
22	Isothermal compressibility	VPT	kPa^{-1}
23	Joule–Thompson coefficient	TJT	$K \cdot kPa^{-1}$
24	Kinematic viscosity	NVK	$m^2 \cdot s^{-1}$
25	Molar density	VDM	$mol \cdot m^{-3}$
26	Molar volume	VM	$m^3 \cdot mol^{-1}$
27	Normal boiling point	TBN	K
28	Normal freezing point	TMN	K
29	Pressure at phase equilibrium	P	kPa
30	Pressure coefficient of enthalpy	HPT	$kJ \cdot mol^{-1} \cdot kPa^{-1}$
31	Reduced enthalpy, $(H-H_0)/T$	H/T	$J \cdot mol^{-1} \cdot K^{-1}$
32	Reduced Gibbs energy, $(G-H_0)/T$	G/T	$J \cdot mol^{-1} \cdot K^{-1}$
33	Refractive index for isotropic phase (Na D-line)	RID	
34	Refractive index of isotropic phase (other wavelength)	RIX	
35	Second acoustic virial coefficient	VVA	$m^3 \cdot mol^{-1}$
36	Second virial coefficient	VVB	$m^3 \cdot mol^{-1}$
37	Self-diffusion coefficient	NDC	$10^{-9} \cdot m^2 \cdot s^{-1}$
38	Specific density	VDN	$kg \cdot m^{-3}$
39	Specific volume	VS	$m^3 \cdot kg^{-1}$
40	Speed of sound	RSS	$m \cdot s^{-1}$
41	Surface tension	IST	$N \cdot m^{-1}$
42	Thermal conductivity	NTC	$W \cdot m^{-1} \cdot K^{-1}$
43	Thermal diffusivity	NTD	$m^2 \cdot s^{-1}$
44	Thermal pressure coefficient	PTV	$kPa \cdot K^{-1}$
45	Third acoustic virial coefficient	VVD	$m^6 \cdot mol^{-2}$
46	Third virial coefficient	VVC	$m^6 \cdot mol^{-2}$
48	Vapor pressure	PV	kPa
49	Viscosity	NVC	$Pa \cdot s$
50	Others		

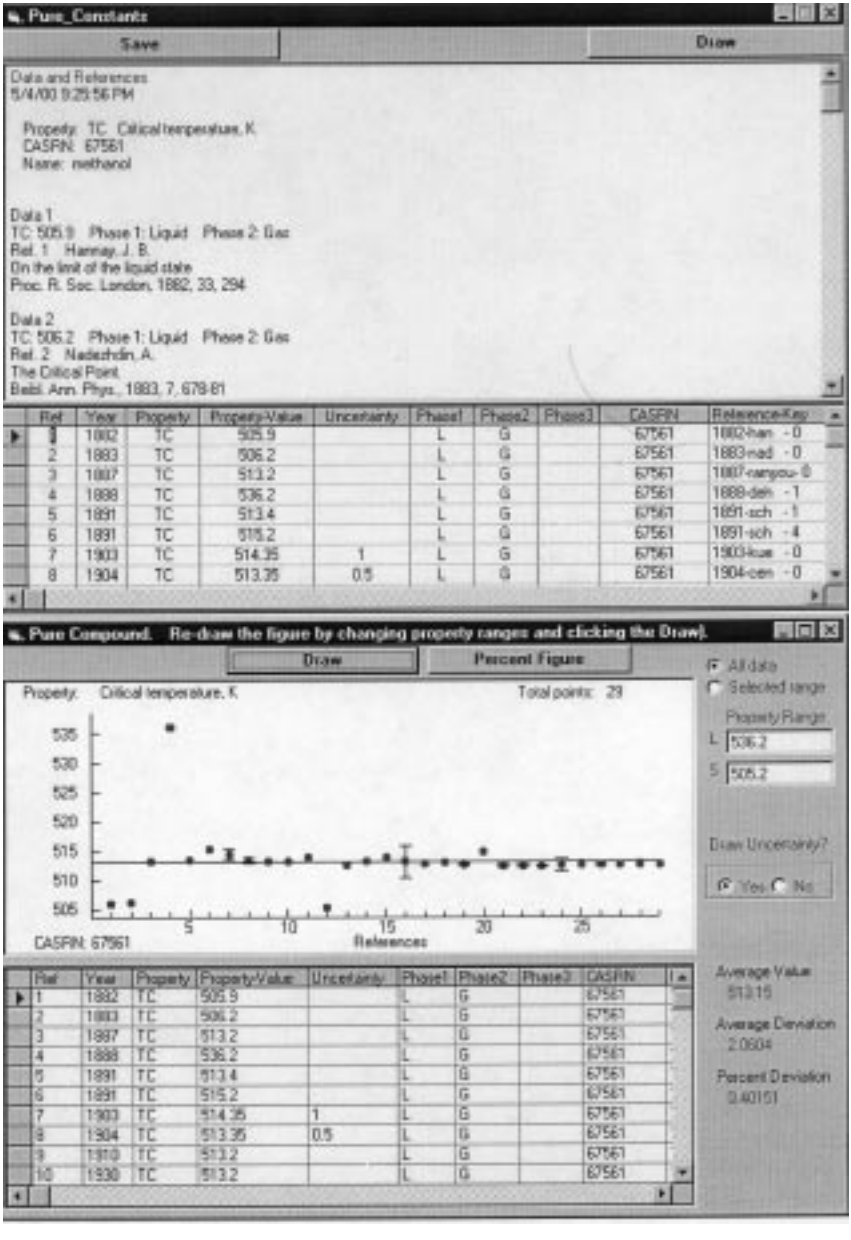

Fig. 3. Example display of the critical temperature data search for methanol from WinSource.

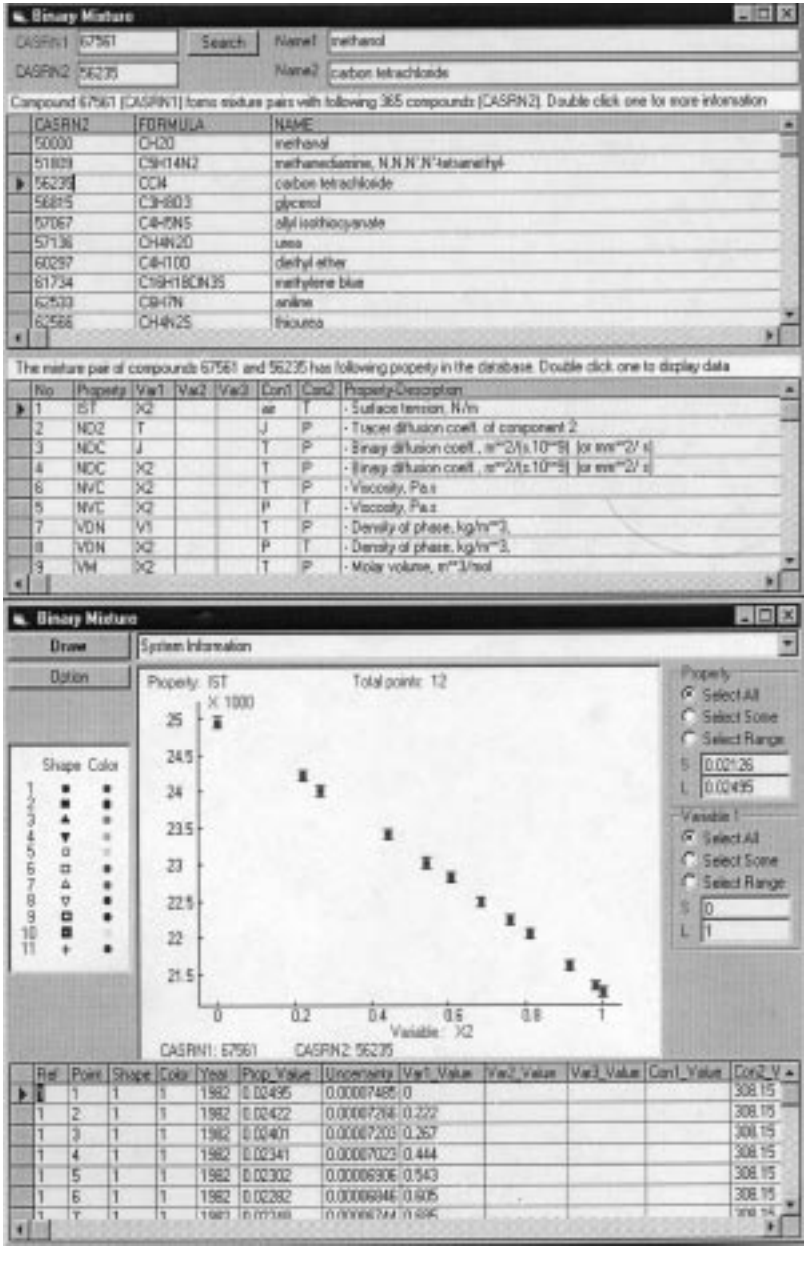

Fig. 4. Example display of the surface tension data search for the binary mixture methanol–carbon tetrachloride from WinSource.

Table II. Properties of Chemical Reactions Covered by the TRC Source Database

No.	Property	Code	Units
1	Apparent equlibrium constant in terms of molalities	KM	
2	Apparent equilibrium constant in terms of molarities	KJ	
3	Apparent equilibrium constant in terms of mole fraction	KX	
4	Apparent equilibrium constant in terms of partial pressures in gas phase	KP	
5	Enthalpy change	H	$kJ \cdot mol^{-1}$
6	Heat capacity at constant pressure	Cp	$J \cdot mol^{-1} \cdot K^{-1}$
7	Heat of combustion at constant volume	UV	$J \cdot g^{-1}$
8	Internal energy change	U	$kJ \cdot mol^{-1}$
9	Thermodynamic equilibrium constant for the specified standard state	KT	

reactions with initial thermodynamic state change (usually irreversible chemical reactions studied by bomb and reaction calorimetry) and those characterizing chemical reactions at equilibrium. Most of the first type of data encompass properties such as change of internal energy and heat and enthalpy of reaction. Various types of equilibrium constant properties (usually as a function of temperature at constant pressure) characterize the second type of data. The collection of equilibrium data in WinSource essentially covers all the experimental data of this type available including those previously selected by Frenkel *et al.* [7]. Nine properties are available from the reaction block in WinSource (Table II).

All the reactions are subdivided into 18 types: addition of unsaturated compounds to other compounds, combustion with oxygen, combustion with other compounds or elements (Cl_2, F_2, etc.), homonuclear dimerization, esterfication, exchange of alkyl groups, exchange of hydrogen with other groups, formation from elements, halogenation (addition or replacement), addition of water to liquid or solid compounds to produce a hydrate, other reactions with water, hydrogenation (addition of hydrogen to unsaturated compounds), hydrohalogenation, structural isomerization, stereo isomerization, neutralization (acid plus base), oxidation with oxygen (not complete combustion), and other reactions (not in any other class).

WinSource provides thermodynamic data for chemical reactions by performing searches based upon reaction type, property, and one component in the reaction mixture. The reaction block in WinSource contains more than 3000 components. Structure files created using ChemDraw (Fig. 2) characterize all components and permit display of chemical reactions in a structural form. The equilibrium data as a function of temperature can be represented graphically using normal or logarithmic

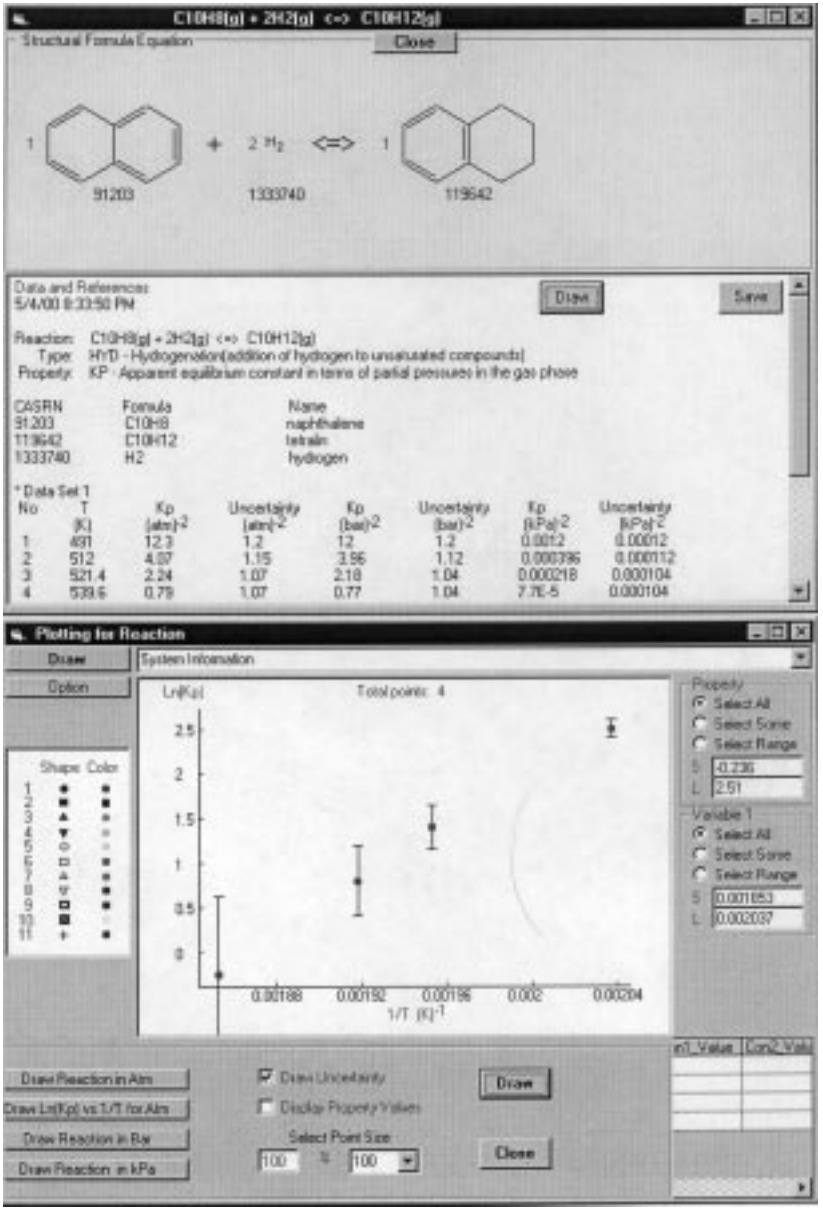

Fig. 5. Example displaying results of the equilibrium constant data search for the hydrogenation of naphthalene from WinSource.

coordinates. Figure 5 presents an example display of the results for an equilibrium data search for the hydrogenation of naphthalene.

WinSource provides additional retrieval functions for information related to the original sources of experimental data totaling more than 81,000 references. References can be searched by (1) reference code consisting of the year of the publication, three or six characters corresponding to the first three letters of the author's last name or of the first and the second author's last names (when the reference is authored by more than one author) and additional sequence number in case the combination year/author(s) is not unique; (2) author name or name fragment; (3) given period of time, with the option to use the author name or name fragment as additional search criteria; and (4) given period of time and type of the property data reported.

5. WinTable—TRC TABLE DATABASE FOR WINDOWS

The ACCESS database for WinTable comes from the ORACLE version of the TABLE database. This database stores recommended data for a selected list of thermodynamic properties of pure organic compounds. It is populated with data using specially developed procedures which take data directly from input files used to update the on going loose-leaf serial publications, TRC Thermodynamic Tables–Hydrocarbons [4] and TRC Thermodynamic Tables–Non-Hydrocarbons [5]. The properties currently covered in WinTable are listed in Table III.

The retrieval functions for WinTable are similar to those available for the pure compound block in WinSource. In addition, WinTable has particular tables designed to store the coefficients of fitting equations used for interpolation and extrapolation (when possible).

6. FUTURE DEVELOPMENT

The availability of critically evaluated and recommended thermodynamic and thermophysical property data is crucial for a great variety of scientific and engineering applications. Therefore, in the near future, TRC intends to expand significantly the amount of recommended data available in electronic form beyond the coverage of TRC Thermodynamic Tables (Fig. 6). The combination of recommended data currently available from WinTable with data previously evaluated by TRC for a variety of properties (density [8–14], vapor pressure [15, 16], ideal gas properties [17]) provides data in the form of equation coefficients along with data generated directly from SOURCE using the principle of dynamic compilation [18]. Predicted values generated using group contribution methods

Table III. Thermophysical Properties Covered by the TRC Table Databes

No.	Property	Code	Units
1	Adiabatic compressibility	Z	
2	Compressibility factor (PV/PT)	Z	
3	Critical compressibility factor (PV/PT)	ZC	
4	Critical density	VDC	$kg \cdot m^{-3}$
5	Critical molar volume	VC	$m^3 \cdot mol^{-1}$
6	Critical pressure	PC	kPa
7	Critical temperature	TC	K
8	Enthalpy of combustion of gas	HCG	$kJ \cdot mol^{-1}$
9	Enthalpy of combustion of liquid	HCL	$kJ \cdot mol^{-1}$
10	Enthalpy of formation	HF	$kJ \cdot mol^{-1}$
11	Enthalpy of phase transition	HTR	$kJ \cdot mol^{-1}$
12	Enthalpy of vaporization at equilibrium	HVP	$kJ \cdot mol^{-1}$
13	Enthalpy, H(equil., T) − H(crystal, 0), of liquid or crystal	HVP	$kJ \cdot mol^{-1}$
14	Entropy of ideal gas and condensed state	S	$J \cdot mol^{-1} \cdot K^{-1}$
15	Entropy of phase transition	STR	$J \cdot mol^{-1} \cdot K^{-1}$
16	Entropy of vaporization at saturation	SVP	$J \cdot mol^{-1} \cdot K^{-1}$
17	Gibbs energy of formation	GF	$kJ \cdot mol^{-1}$
18	$-(G(T) - H(0))/T$ of ideal gas and condensed state	G/T	$J \cdot mol^{-1} \cdot K^{-1}$
19	$(H(T) - H(0))/T$ of ideal gas	H/T	$J \cdot mol^{-1} \cdot K^{-1}$
20	Heat capacity at constant pressure	CP	$J \cdot mol^{-1} \cdot K^{-1}$
21	Heat capacity at equilibrium temperature and pressure	CS	$J \cdot mol^{-1} \cdot K^{-1}$
22	Kinematic viscosity at atmospheric pressure	NVK	$m^2 \cdot s^{-1}$
23	Normal boiling point	NBP	K
24	Normal freezing point	TMN	K
25	Refractive index	RIX	
26	Second virial coefficient	VVB	$m^3 \cdot mol^{-1}$
27	Specific density of gas and liquid	VDN	$kg \cdot m^{-3}$
28	Surface tension at atmospheric pressure	IST	$N \cdot m^{-1}$
29	Thermal conductivity	NTC	$W \cdot m^{-1} \cdot K^{-1}$
30	Triple-point temperature	T	K
31	Vapor pressure	PV	kPa
32	Speed of sound	RSS	$m \cdot s^{-1}$
33	Viscosity of gas and liquid	NVC	$Pa \cdot s$

based upon the connectivity table files created with chemical structure image files (Fig. 2) can fill existing "gaps" in available experimental data. Currently, the structural information for more than 4000 compounds exists in a database. The molecular adjacency matrix, distance matrix, topological index, and group types for group contribution methods and some molecular descriptors result from this information. This comprehensive collection of the recommended data with thermodynamic consistency creates the foundation for a new database, SELECT, whose direct output applies to numerous applications.

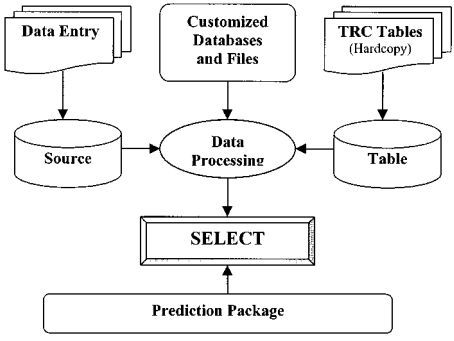

Fig. 6. Schema of the potential expansion of the WinTable.

7. DISTRIBUTION VIA THE INTERNET

The benefits of developing and deploying applications over the World Wide web become apparent when combining databases and Web technology. Internet applications that count on fast and reliable database systems are deployed and maintained on centralized application servers, from which they are downloaded to the end-user's web browser at runtime. This distribution method reduces the time, cost, and complexity of deploying applications to a large or geographically dispersed end-user base, all without installing application software on individual desktop machines.

WEBTRC is an ongoing project at TRC concerned with building a dynamic web site for thermophysical property data distribution. The site uses a three-tier architecture. The first tier is the web browser. The middle tier consists of Oracle Developer Server and Microsoft Internet Information Server running on a Microsoft Windows NT server. The third tier is the database tier that includes Oracle 8I running on a DEC-alpha workstation. The goal of the project is to enable end users to retrieve data interactively or order data products through the browser and internet access. Another key role of this site is to provide data centers and individual experts around the world with the ability to input experimental data directly into a mirror database of SOURCE, Source Feeds, through a standard data entry form.

Completion of the first phase in this project includes the following.

(1) A distributed data collection system consisting of Source Feeds and the Data Entry Form. Incoming data from the Source Feeds through the Data Entry Form are analyzed by the database rules established at TRC as SQL triggers that generate an error report

on the incoming data. TRC staff tests and checks for erroneous data in the mirror database before loading data into SOURCE.

(2) A web retrieval system consisting of the Compound database, the Table database, and the Source database. The anticipated goal is to provide end-users with identical feature-rich functions such as the standard desktop versions described in this paper.

Web-based architecture represents a shift back to a server-centric deployment model. This model enables an effective and efficient distribution mechanism without relying upon individual client configurations. A web database application process flow designed for the WEBTRC site appears in Fig. 7. To start and run any database from WEBTRC, end-users can deploy their selected web browser to access a URL. The URL corresponds to a web page on the web server. An HTML page and Form client scripts (for an Oracle process) or other client-site scripts such as Active Server Page scripts (for a Microsoft process) are generated accordingly and then downloaded to the user's browser. These functions contact the Form runtime engine or ASP server scripts to initiate a new database process or to join an existing process. The web server engine is then in charge of communicating with databases on the database server. The engine sends the

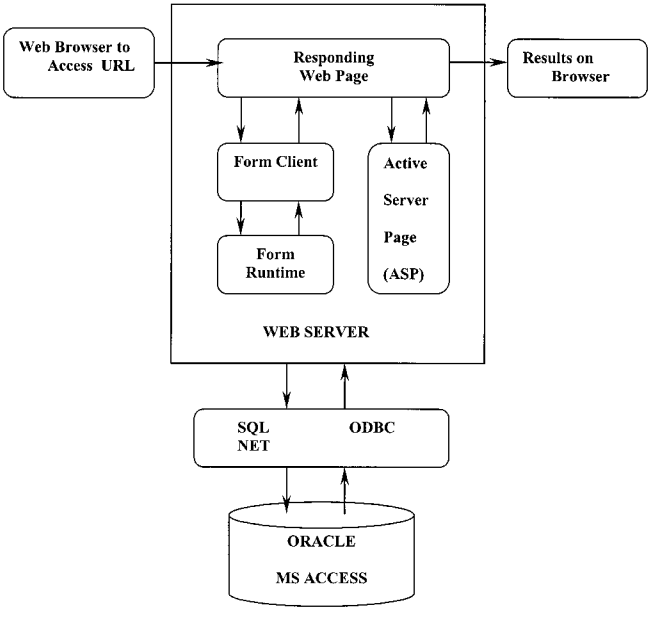

Fig. 7. Web database process flow.

retrieved results back to the client's browser. This Internet distribution schema allows connection of a large number of users worldwide to the database collection available at TRC for customized or standard applications.

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