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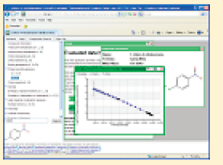
ThermoData Engine (TDE): Software Implementation of the Dynamic Data Evaluation Concept. 6. Dynamic Web-Based Data Dissemination through the *NIST Web Thermo Tables*

Kenneth Kroenlein,[†] Chris D. Muzny,[†] Vladimir Diky,[†] Andrei F. Kazakov,[†] Robert D. Chirico,[†] Joseph W. Magee,[†] Ilmutdin Abdulagatov,[†] and Michael Frenkel*[,†]

[†]Thermophysical Properties Division, National Institute of Standards and Technology, Boulder, Colorado 80305-3328, United States

ABSTRACT: *ThermoData Engine* (TDE) is the first full-scale software implementation of the dynamic data evaluation concept, as reported recently in this journal. In the present paper, we describe the development of a World Wide Web-based interface to TDE evaluations of pure compound properties, including critical properties, phase boundary equilibria (vapor pressures, sublimation pressures, and crystal−liquid boundary pressures), densities, energetic properties, and transport properties. This includes development of a system for caching evaluation results to maintain high availability and an advanced window-in-window interface that leverages modern Web-browser technologies. Challenges associated with bringing the principal advantages of the TDE technology to the Web are described, as are compromises to maintain general access and speed of interaction while remaining true to the tenets of dynamic data evaluation. Future extensions of the interface and associated Web-services are outlined.



1. INTRODUCTION

As discussed in the first five papers of this series,[1−5] the *NIST ThermoData Engine* (TDE) software represents the first full-scale implementation of the dynamic data evaluation concept[6,7] for thermophysical properties. This concept requires large electronic databases capable of storing essentially all relevant experimental data known to date with detailed descriptions of metadata and uncertainties. The combination of these electronic databases with expert-system software, designed to automatically generate recommended property values based on available experimental and predicted data, leads to the ability to produce critically evaluated data dynamically or 'to order'.

As TDE has evolved from a first release (version 1.0, released in 2004)[8] that was focused on thermophysical properties of pure compounds, the number of features and breadth of support has grown significantly. Additions have included on-demand generation of equations of state (EOS),[9] dynamic update of local data resources based on the *TRC-SOURCE*[10] data storage system, support for binary mixtures, including phase equilibrium,[11] and properties of chemical reactions.[12] The most recent version of TDE (5.0, released 2010)[5,13] included experiment planning support features and a product design tool for identification of compounds with specified properties.[5] Also included were advanced consistency tests for automated quality assessment for vapor−liquid equilibrium (VLE) data sets.[5]

TDE has proven to be a powerful software tool for thermophysical property data quality assurance,[14] validation of new experimental data,[15] and a variety of engineering applications including chemical process design.[16] It is also a critical component in implementation of the concept of *Global Information Systems in Science* with application to the field of thermodynamics.[17]

With the rise of the Internet, an inexpensive, effective, and rapid channel for the transfer of information has opened for scientific knowledge. Leveraging this opportunity, the Thermodynamics Research Center (TRC) migrated its statically evaluated tables of critically evaluated data covering physical and thermodynamic properties of pure compounds, TRC Tables-Hydrocarbons[18] and TRC Tables-Non-Hydrocarbons[19] (The *TRC Tables*), to a Web-based format: the Web Thermo Tables (WTT).[20] Over their 65-year history, the *TRC Tables* have been valued as a reputable source of evaluated thermophysical and thermochemical data. This migration facilitated more flexible, convenient, and up-to-date access to the data. The TRC tables were compiled by traditional static methods and, like all non-dynamic evaluations, suffered from the innate limitations of that approach, including inefficient use of expert personnel, high cost, and very slow incorporation of new research.[1] While this approach may be justified for a few key commodity chemicals,[21] it cannot be applied to the enormous and rapidly growing fields of modern specialty chemicals and new process design.

The next logical stage in the evolution of this data resource was to update the data recommendations of WTT by utilizing the dynamic data evaluation concept and algorithms embodied in TDE.[1] To accomplish this, the core software libraries of TDE were automated and coupled with Web service technologies and a novel, dynamic Web interface. "Core libraries" refer to those portions of the TDE codebase responsible for data evaluation and computation but not those associated with the user interface. This coupling allowed access not only to recommended values and fit parameters for critically evaluated property regressions but also to

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on-demand calculations of property values at specified state points. A key feature of TDE is full traceability to original data sources. This is maintained in the Web implementation, where users are provided easy access to comparisons of the critically evaluated data with the underlying experimental data. Another key feature of the TDE technology is automatic application of appropriate prediction methods for limited data sets. Full traceability for these predicted values is also maintained in the present application.

2. SCOPE OF CHEMICAL SYSTEMS CONSIDERED

While key industrially important inorganic compounds (e.g., ammonia, water, sulfur dioxide, etc.) are within the scope of TDE, the focus is molecular organic compounds composed of the elements C, H, N, O, F, Cl, Br, I, S, and P. This is unchanged from previous versions. As the underlying archive of this system is based on data pre-evaluated with TDE (as compared to that generated on demand), it becomes necessary to generate a list of target compounds. Compounds are selected if they possess either thermophysical data in the *TRC-SOURCE*[10] data archive or a manually reviewed molecular structure. The list of compounds is re-evaluated on a quarterly basis following the growth of the underlying data resource and is culled automatically as necessary during the evaluation process.

For well studied compounds such as water, it is unlikely that an automated treatment will generate recommendations that are of higher quality than recent recommendations from expert manual review. Further, there is a risk of generating a recommendation of poorer quality for various reasons, including inadequacies in the processing technology and insufficient data coverage in the underlying database. (For example, the internationally accepted equation of state for water[22] has more than 50 parameters, which far exceeds the present modeling capabilities of TDE.) As a preventive measure and to help guarantee the highest quality information, this interface utilizes the NIST Reference Fluid Thermodynamic and Transport Properties Database, REFPROP,[21] as an underlying mathematical model for 68 common compounds. As the REFPROP recommendations are limited to fluid properties, they are augmented by TDE where possible and appropriate.

As this interface replaces the historical TRC Thermodynamic Tables,[20] a small amount of evaluated data from that source was replicated. For systems of specialized interest, such as radical species and fullerenes, that lie outside the scope of TDE, these data are presented to the user without constraint or validation from the TDE core libraries.

3. GENERAL ARCHITECTURE

To provide a high-quality data resource over a network, we require a series of high-availability data services on a host computer, a well-defined data-transfer protocol, and an easily navigable interface on the client computer. Conventionally, data access over the World Wide Web has involved a heavy processing load on the host computer, where information is retrieved from a database, processed into a final form, and padded with styling and formatting metadata in the form of HTML tags and attributes. This relatively bulky format would then be serialized according to the standard Internet Protocol Suite and transferred to the client, where a Web browser would render the final product according to the embedded HTML metadata. Today, JavaScript technologies have become standard in Web browsers, allowing the computational burden to be shifted more to the client machine

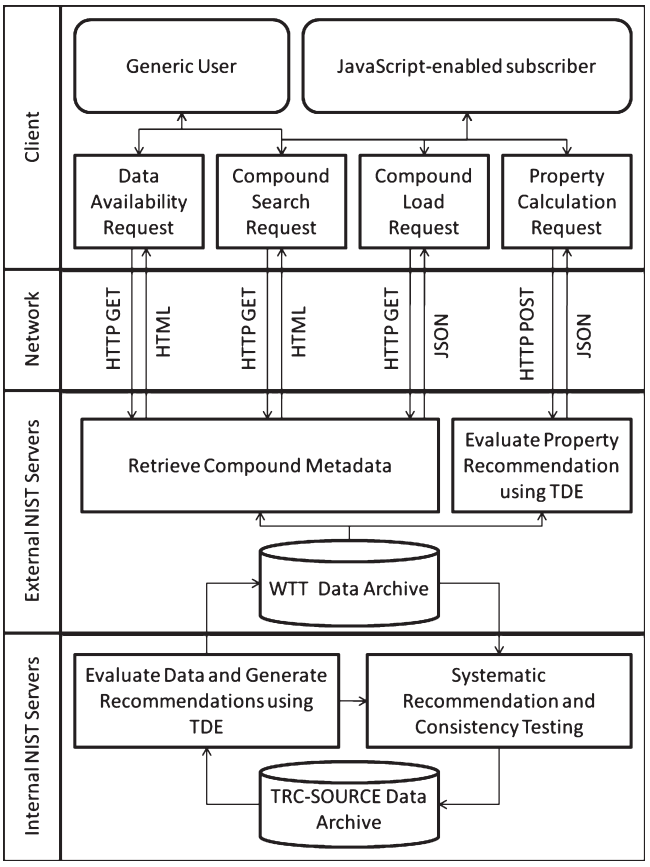

Figure 1. Schematic of data flow through the application stack.

as compared with static HTML pages. This results in reduced server loads and faster network transactions due to decreased payload size and more flexible and intuitive interface design. This stack of technologies is often termed Asynchronous JavaScript and XML or AJAX.[23] [While the name of the technology stack includes both the terms 'asynchronous' and 'XML' (Extensible Markup Language), implementations termed AJAX do not necessarily operate asynchronously nor do they necessarily leverage XML technology. To a significant extent, the terminology remains only for historical reasons. In this Web application, data requests are performed asynchronously, but XML is not used for data transmission.]

The new data dissemination scheme described here required that an AJAX application stack be developed with JavaScript Object Notation (JSON)[24] as a compact, easily parsed transaction protocol. In addition, the Google Web Toolkit[25] suite of tools was used to build a dynamic user interface that provides a consistent user experience across a broad range of operating systems and Web browsers. [Products or companies are named solely for descriptive clarity and neither constitute nor imply endorsement by NIST or by the U.S. government.] This new, complete stack consists of preliminary evaluation and serialization of data with a feedback for quality control, dissemination of data and metadata over a series of Web services, and a dynamic JavaScript-based user interface (Figure 1).

4. THE WTT DATA ARCHIVE

On a typical modern computer, the TDE software requires a few seconds to several minutes to complete data evaluation for a

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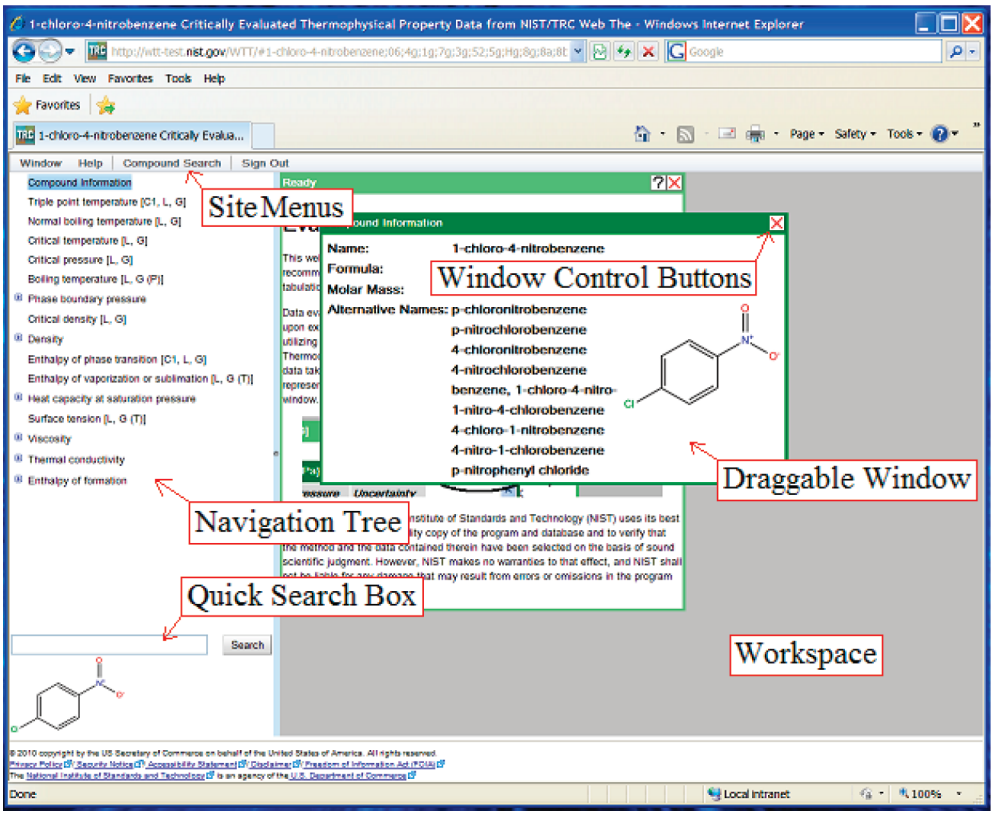


Figure 2. Dynamic window-in-window interface developed for this product with annotations specifying viewport components. The example shows the initial view displayed for 1-chloro-4-nitrobenzene.

single compound. Evaluation includes checks for data validity and consistency as well as an automated selection of optimal functional forms and fitting constants. Large data sets, such as those for many common compounds, necessarily involve longer processing time. While this is acceptable for desktop applications, a delay of several minutes between request and response is unacceptable in a Web context. These time issues would be further exacerbated under a Web services model, where each invocation of the service would require reloading and reevaluating all data. Thus, a usage pattern involving generation of multiple tables and graphs would be unacceptably slow.

In order to address this issue and avoid possible complications associated with synchronization of data, all data sets are evaluated offline with TDE, and the results are encoded and stored to disk in the *WTT Data Archive*. This approach guarantees high data availability at the cost of requiring a predefined list of target compounds and introducing a delay between population of data into the *TRC-SOURCE Data Archive* and presentation to subscribers. Members of the list of target compounds are removed during the evaluation by TDE if reliable recommendations cannot be generated based upon available data and implemented predictive methods. The files of the *WTT Data Archive* contain identifying metadata (e.g., compound names, Hill-order chemical formula), equation parameters and covariance matrices for property recommendations, and experimental data sets with associated metadata. For compound properties with extensive experimental data, only a subset is selected (currently 50 numerical values) to prevent performance problems from arising in downstream technologies. The experimental values for display are selected based upon their evaluated quality and relative

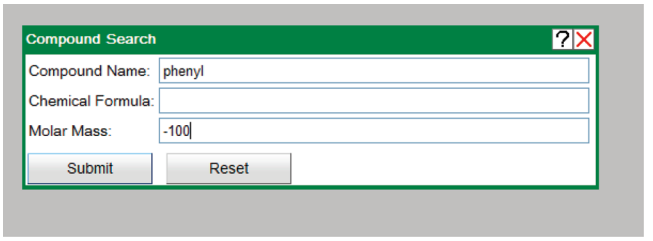


Figure 3. Compound Search window; the interfacial component used for detailed compound searches. Parameters entered as shown will generate a query for all compounds with "phenyl" in the name that have a molar mass less than or equal to 100 g/mol.

constraint upon the property evaluations by TDE. The *WTT Data Archive* files can be parsed explicitly, for example to populate a database for compound search support, or can serve as a basis for calculation of property values (with uncertainties) for user-specified state conditions (e.g., temperature and pressure). This is equivalent to access of results from TDE in a postevaluation state for a particular compound. For those compounds that possess validated molecular structures, images of the two-dimensional structure are retrieved and populated into the archive as well.

Uncertainties are estimated for all properties evaluated with TDE and are propagated into the WTT framework. These uncertainties are based on the covariance approach, which was described fully in the first two papers of this series.[1,2] Both experimental uncertainties and curve deviations are taken into account when calculating statistical weights for the covariance

matrix evaluation. For those 68 compounds for which results were obtained from the REFPROP database, a covariance matrix evaluation was infeasible, and uncertainties were based upon the coarse uncertainty recommendations documented for each compound in REFPROP.

The *WTT Data Archive* also facilitates automated testing of property recommendations. In addition to the data consistency verification that is performed in the TDE core libraries during recommendation generation, a battery of fundamental consistency checks were developed to ensure functional recommendations, and associated uncertainties display physically realistic behaviors. These checks include tests for mathematical properties, such as positive definiteness, monotonicity, and comparative scaling, as appropriate for a particular thermophysical property. This test suite is executed against every compound state file in the archive prior to deployment, thereby providing a breadth and thoroughness not possible via manual review.

5. WEB SERVICES

The *WTT Data Archive* functions as the underlying data source for four data services: compound search, data availability, compound metadata, and property calculation. Search capabilities exist for compound name, chemical formula, and molar mass. Compound name searches are performed as case-insensitive substring searches against all names in the data archive. Chemical formula search terms are reordered into Hill format that is, in turn, used for an exact-match search against chemical formulas in the database. This guarantees results are independent of the order in which elements are specified (e.g., CH3COOH will yield identical results to C2H4O2). Finally, the molar mass queries perform a ranged search against molar masses. If a single number is entered, a range of 1.0 g/mol about the specified value is searched. A range can be specified using (-). Open ended searches can be performed by appending (-) to the limit, e.g., '-100' (molar mass <100) or '32-' (molar mass >32). Returned results conform to all provided criteria. Results are returned in an HTML table with links to load each compound that matches all provided criteria. Matches are ordered by (1) molar mass and (2) compound name, with the exception of an exact name match, which is listed first. At most, 200 search results are displayed at any time. Compound search requests are performed via HTTP GET with a key/value pair for each search term. [The Hypertext Transfer Protocol (HTTP) is the underlying communication technology of the World Wide Web. GET and POST are two of the request methods specified in the protocol. For purposes here, the most significant difference is that a POST request can contain significantly more data (i.e., more state points) than a GET request. In Web services, these protocols act as interfaces to computations done on a remote server in a manner similar to a subroutine call to a library in common programming languages.]

The data-availability service provides a compound-based summary of all available property recommendations, including ranges of applicability and a count of underlying experimental values. To aid users in verifying compound identity, the resultant page also includes identifying compound metadata and a two-dimensional molecular structure, if available. The service is implemented via HTTP GET requests keyed off of a site-specific unique molecular identifier and returns results in an HTML-formatted response. This service functions primarily as a convenience for nonsubscribers interested in determining data availability for compounds of interest. It also functions as a fallback for browsers without JavaScript enabled and for automated search engine Web crawlers.

When a validated subscriber loads a new compound into the interface, a request is submitted to the compound-metadata service. Again implemented via HTTP GET requests keyed off of a site-specific unique molecular identifier, this service returns a JSON structure that contains nearly all information contained in the TDE state file for the desired compound. This includes names, chemical formula, molar mass, model parameters, ranges of applicability, and covariance matrix entries.

A property-calculation service is also available for determining numerical values associated with given thermophysical states. The service, implemented via HTTP POST, requires as arguments information identifying the compound and the property of interest and can utilize either range and increment information or can compute property values and associated uncertainties at prescribed state points. Again, this service is available only to validated subscribers, and requests to this service are generally made via the AJAX interface. Responses are returned as simple

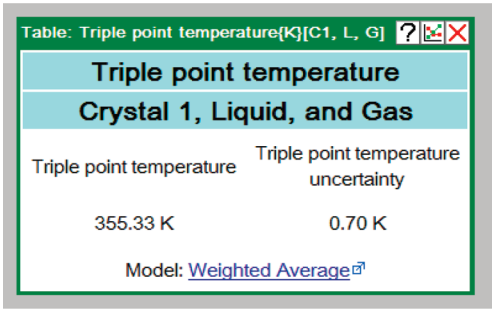


Figure 4. Example of a single-valued property recommendation. The example is for the crystal−liquid−gas triple point temperature of 1-chloro-4-nitrobenzene.

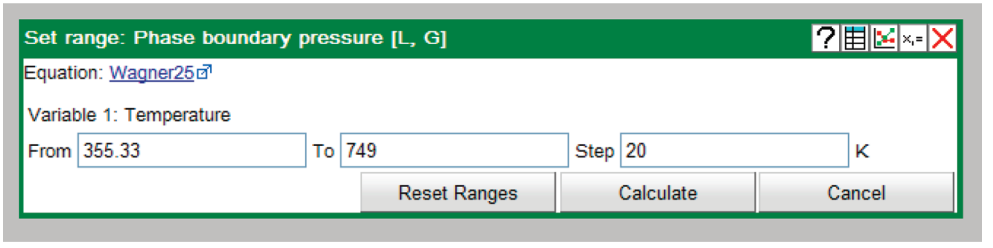


Figure 5. Range Specification window; the interfacial component used for specifying the ranges for a model calculation. The example is for a liquid−gas phase boundary pressure (vapor pressure) calculation between temperatures of 355.33 and 749 K with a calculation step of 20 K. The underlying model for the example is Wagner25. Full details of the Wagner25 model are accessed through the indicated link.

two-dimensional arrays of decimals, formatted as necessary to conform to the JSON standard. This service provides the underlying information for all dynamically generated tables and graphs in the interface.

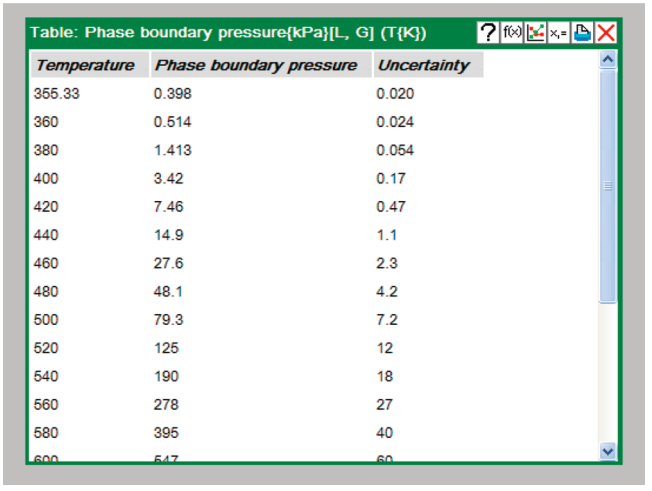
The set of Web services is made complete by including auxiliary services for user validation and session management as well as providing images of two-dimensional molecular structures.

6. USER INTERFACE

With the reduction in computational load associated with migration to host-based data services, there follows a correspondingly significant increase in data-handling requirements and display-logic complexity for the client machine in order to parse and present data in an easily interpretable format. Here, a dynamic window-in-window interface (Figure 2) was developed to allow alternative views of the property information. Users can drag and resize windows as with standard desktop environments. A capability exists to dynamically generate tabulated results and present graphs for comparison of the critically evaluated results with the underlying experimental and predicted data values.

The Web application provides a dynamic, window-based interface to a collection of critically evaluated thermodynamic property data. Windows can be reorganized and resized within the workspace by a standard drag-and-drop interface. This interface also includes support for using the browser's back button to undo actions, support for bookmarking a particular state of the workspace, and provides Universal Resource Locators (URLs) that can be copied, pasted, and distributed to other authorized users to share a particular workspace state. If a user has either provided valid credentials or if the client's IP address corresponds to a registered range, the user is granted access to the full data archive; otherwise, users are provided with complementary information regarding compound, property, and data availability via the search services described above.

Primary search functionality is accessible via the Compound Search window (Figure 3), which provides compound name, chemical formula and molar mass-based searches. Returned results satisfy all specified constraints. For simple searches based upon only one criterion, a Quick Search field is available in the left-hand panel of the interface. Search terms submitted through this interface are automatically interpreted based upon format into one of the above-listed search criteria. For example, if a provided string contains a series of capital letters separated by digits, the service will assume that a chemical formula search is intended and then process the request accordingly.



Temperature	Phase boundary pressure	Uncertainty
355.33	0.398	0.020
360	0.514	0.024
380	1.413	0.054
400	3.42	0.17
420	7.46	0.47
440	14.9	1.1
460	27.6	2.3
480	48.1	4.2
500	79.3	7.2
520	125	12
540	190	18
560	278	27
580	395	40

Figure 6. Data Table window; the interfacial component used for display of tabulated results. The example shows a liquid−gas phase boundary pressure (vapor pressure) calculation for 1-chloro-4-nitrobenzene.

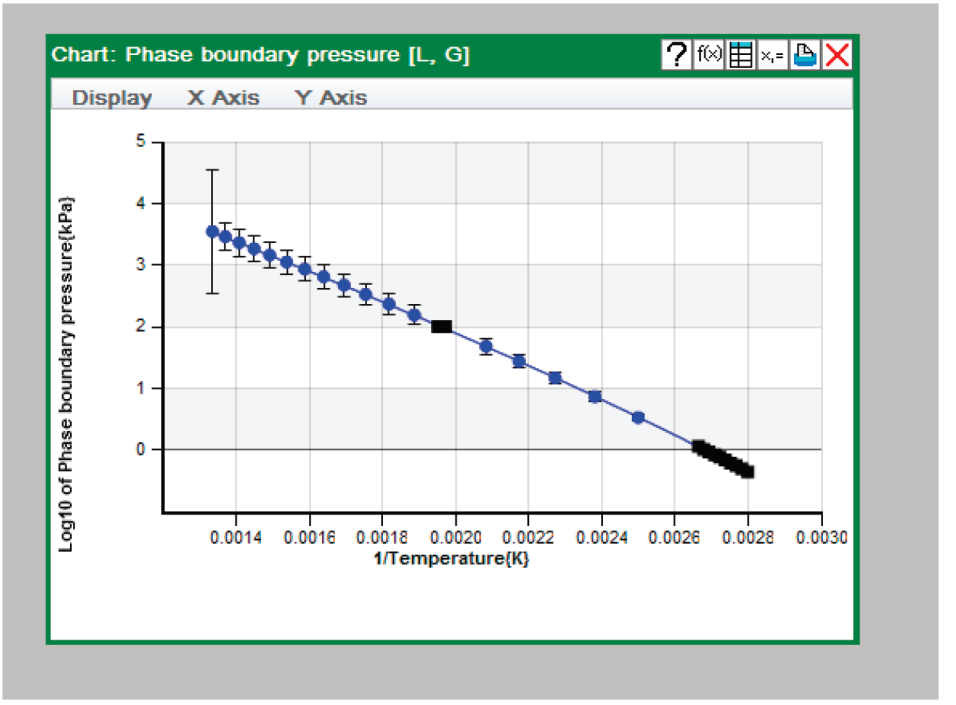


Figure 7. Graphical Plot window; the interfacial component used for display of model contours and comparisons with independent property predictions and underlying experimental data. The example shows a liquid−gas phase boundary pressure (vapor pressure) calculation for 1-chloro-4-nitrobenzene.

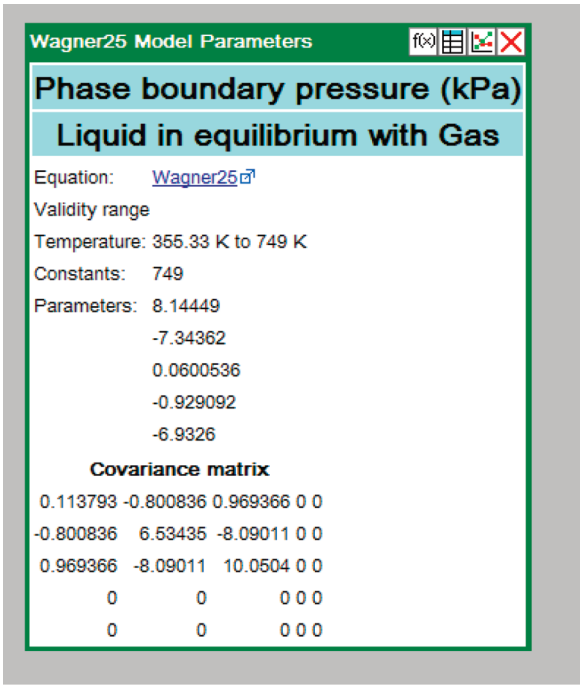


Figure 8. Model Summary window; the interfacial component used for display of model parameters and covariance matrix. The example shows the parameters for the liquid−gas phase boundary pressure (vapor pressure) model for 1-chloro-4-nitrobenzene.

Once the property data are loaded, a navigation tree is dynamically populated for exploration of the available properties. As windows are requested, they dynamically appear in the workspace and are added to a window menu. This menu enables quick navigation if the workspace becomes crowded. The navigation tree is controlled by mouse input or though the keyboard.

If only one data type (i.e., a phase combination) is available for a given property, it is displayed as an ordinary tree node with phases and variables indicated in brackets (e.g., '[L, G(T)]' for liquid in equilibrium with gas as a function of temperature). If data are available for more than one combination of phases, these sets are populated into a collapsed node. Expanding the node reveals the combinations available. For properties of saturated liquids and gases, the phase of the property is indicated first.

For single-valued properties, a simple table is presented that gives a recommended value and its associated uncertainty (Figure 4). For properties that are functions of state variables, a form is displayed for specification of the range(s) of interest (Figure 5). At the top left of the window, the underlying mathematical model is specified with a link to a detailed description. Below that, the maximum, minimum, and steps for each variable are specified. By default, the fields are populated with the model limits. The default step size is set to yield about 20 property values in each dimension. The defaults can be recovered at any time with the Reset Ranges button. The Calculate button initiates calculation of the requested values, which are returned and displayed in a data table (Figure 6). The Cancel button can be used to cancel the request. The returned data table can be sorted.

Simple plotting is supported for all properties that have a functional form and for single-valued properties with directly comparable experimental data (Figure 7). In order to view plots, the browser must have Adobe Flash technology installed. The plotting technology supports normal, inverse, and logarithmic scaling as well as absolute and relative deviation plots. In addition, plots include the experimental and predicted data values used by TDE in generation of the evaluated results. Provenance of each datum is provided to users via tooltips, made visible when the user hovers the cursor over the point of interest. In this way, the core tenet of full traceability, which is central to the NIST implementation of dynamic data evaluation in TDE, is maintained in this new implementation of WTT.

Access to underlying model parameters is available (Figure 8). The property, units, and phases are specified at the top of the window. The model name is provided as active text, linking directly to the model documentation with details of the functional form therein. The window also provides ranges of applicability, parameters and constants of the model, and the associated covariance matrix.

7. CONCLUSIONS AND FUTURE DEVELOPMENT

The core libraries of the NIST ThermoData Engine (TDE) were utilized in building a Web-based infrastructure for the calculation, exploration, and dissemination of critically evaluated thermophysical property data for pure compounds. A Web-based system for the dissemination of property results based on dynamic data evaluation was described. This system was shown to retain the principal advantages of the dynamic evaluation approach, while exploiting the convenience of the Web.

The data system described here was deployed to a NIST public server at the end of 2010. Access is available via the NIST Standard Reference Data Program. Public release of WTT is available in two editions: Professional (http://wtt-pro.nist.gov) and Lite (http://wtt-lite.nist.gov). The Professional edition contains records for more than 23,000 compounds and more than 500,000 critically evaluated experimental data values. The Lite edition restricts the data to those for 150 common (primarily organic) compounds and contains more than 86,000 experimental values. These systems include 32 thermophysical and thermochemical properties. At present, the underlying chemical systems are re-evaluated against the continuously growing *TRC-SOURCE* data archive on a quarterly schedule. Information about the availability of specific data (properties for a given compound, parameter ranges, number of experimental values) can be accessed at each respective URL.

Plans for future development include leveraging the developed software stack to extend the experimental planning capabilities of TDE,[5] including those for binary chemical systems, to the broader research community.

AUTHOR INFORMATION

Corresponding Author

*E-mail: frenkel@boulder.nist.gov.

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