International Journal of Thermophysics (2026) 47:142
https://doi.org/10.1007/s10765-026-03814-7

Challenges and Research Opportunities in Chemical Thermodynamics, Thermophysics, and Materials Property Science

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Received: 19 June 2026 / Accepted: 10 July 2026 / Published online: 31 July 2026

Abstract

There is robust industrial demand for thermodynamic and thermophysical property data for chemical substances and materials. Unresolved inconsistencies and unexplained anomalies in the data are frequently revealed by data users. Inconsistency appears when either multiple measurements significantly deviate from each other beyond reasonable uncertainties or different reported properties do not obey thermodynamic relations between them. Anomaly here means a reported value or behavior significantly deviating from expectation based on theory or correlation. To address such issues, we have launched the new Thermodynamics Research Center (TRC) Research Challenge Search website. The goals of this service are to encourage researchers to address these problems, identify the need for additional theoretical and experimental development, support the justification of related research proposals, and ultimately provide users with reliable data. This publication provides an overview of the service, presents the current collection of cases, and describes the procedures for user feedback and contribution.

Keywords Research challenges · Thermodynamic properties · Thermophysical properties · Web service · Inconsistencies · Anomalies

1 Introduction

There is a constant demand for thermodynamic/thermophysical properties of chemical substances and materials from various industries [1]. When the need for specific thermodynamic/thermophysical data appears, the first question is: "*Have they*

Extended author information available on the last page of the article *already been measured and is the existing information reliable?*" If the answer to either of these is negative, the next obvious question can be: "*Is a relatively cheap and sufficiently accurate computational method available to reliably predict them?*" Progress in theoretical methods constantly opens new avenues that may help fill experimental gaps in many domains (*e.g.*, quantum chemical calculations for enthalpies of formation [2] or dilute gas properties for small molecules [3]). Machine-learning methods [4, 5] are emerging and can be used for resolution of challenges after a robust assessment of their accuracy, especially for extrapolation beyond training sets. If, after all attempts to obtain the needed data or to identify reliable information in cases of inconsistencies, the problem still exists, additional research may be required. Despite the huge industrial importance of thermodynamic/thermophysical information, the corresponding research in this field is frequently considered routine and not deserving much attention. This leads to insufficient funding for reliable thermodynamic measurements (that are often expensive and labor intensive) or development of theoretical methods with new predictive capabilities. Related research sometimes happens as a byproduct of other objectives. As a result, thermodynamic data needs are not always addressed. Exact industrial needs are typically not made public because of their confidential nature. Remarkable exceptions include some crowdsourcing projects inviting researchers to develop and test theoretical and prediction methods, such as the Industrial Fluid Properties Simulation Challenge [6] or the Solubility Challenge [7, 8]. These industrial challenges [6–8] sparked attention and led to productive competition, which increased the visibility of the field.

If a researcher who identified a data issue does not have resources or connections to initiate additional research, finding a solution may be challenging. Publishing such an issue may encourage others to find a solution. A prominent example developed as follows: a previously published enthalpy of sublimation of cubane was questioned in Ref. [9], and the authors of Ref. [10] experimentally confirmed that suspicion and provided a more accurate value. Although proven to raise awareness, publishing separate articles on each identified experimental thermodynamic/thermophysical challenge may be too time-consuming and would lead to unconsolidated information. Instead, the authors of this work believe that a separate dedicated web-resource is the most optimal platform for sharing such knowledge because it can provide single-point access to various reported challenges, their fast dissemination and communication, on-demand searching, and collaboration to resolve them. Due to these advantages, we have developed a new web service [11] for sharing unresolved inconsistencies and unexplained anomalies in thermodynamic/thermophysical data.

The goals of this project are in line with those of the above-mentioned challenges [6–8] and are somewhat broader: to attract researchers to solving the problems, reveal the need for additional theoretical and experimental developments, support justification of related research proposals, and serve final users with reliable data. Moreover, additional research can refine our knowledge of the abilities of experimental and theoretical methods, as well as the reliability of reported values in the absence of alternative ways to get the property of interest. We hope that our proposed service will facilitate coordination and collaboration in the field of thermodynamics/thermophysics. While the previous industrial challenges [6–8] can be compared to batch operation in chemical engineering, the proposed project should provide continuous, or "flow," operation by providing an online service allowing users to search cases by chemical substances and/or properties, see their updated status, and contribute by giving comments and sharing their cases.

2 Overview of the Collection

Within the framework of this project, unresolved inconsistencies and unexplained anomalies are collected and communicated to the scientific community. Inconsistencies are identified when measurement results reported by different researchers disagree by more than the claimed uncertainties and/or the typical uncertainties associated with the experimental methods employed. Within TRC, such inconsistencies are typically detected through automated data screening performed by the ThermoData Engine (TDE) program [12], with uncertainty assessments based on the methodologies described in Ref. [13]. In other instances, decisions to add specific inconsistency cases can be based on observations and expertise of the project participants. Anomalies are typically revealed in a similar way, with the difference that the comparison is made between experimental data and models or predictions rather than between different experimental studies. In general, the extent of the deviation triggering an addition to the collection should exceed three times the joint uncertainty of the sources being compared. However, it is impossible to strictly define the threshold; therefore, expert assessments, such as the expected impact and feasibility of conducting additional research, are also taken into account. Revealed cases are added to the project collection if they cannot be resolved by discarding obviously erroneous reports, and/or by means of additional literature search or corroboration through reliable theoretical predictions or correlations.

The present collection of problem cases [11] is based on the ambiguities and anomalies accumulated during recent years of maintaining the NIST SOURCE database [14], as well as contributions from the project participants. It contains 619 cases, of which 180 belong to pure chemical substances and their reactions, 402 to binary mixtures, and 37 to ternary mixtures. Each case is a combination of the system (compound, mixture, or reaction) and property (such as density or vapor–liquid equilibrium pressure). Some typical examples are discussed below.

The most abundant property is solid solubility, 256 cases (a typical example is illustrated in Fig. 1). Issues related to condensed-phase transitions in pure compounds give 72 cases, and vaporization and sublimation give 41 cases. There are 51 liquid–liquid equilibrium (LLE) cases (a typical example is illustrated in Fig. 2) and 36 vapor–liquid equilibrium (VLE) cases registered. Other significant properties are shear viscosity (39 cases), density (29 cases), and activity coefficients (28 cases).

There are many experimental difficulties, mistakes, and oversights that can lead to inconsistent property data. A few illustrative examples are listed below:

- One of the most common problems is insufficient data reporting. Data reporting may be incomplete and/or ambiguous, leaving readers to guess the meaning of the reported data. Following the Good Reporting Practice [15] and undergoing

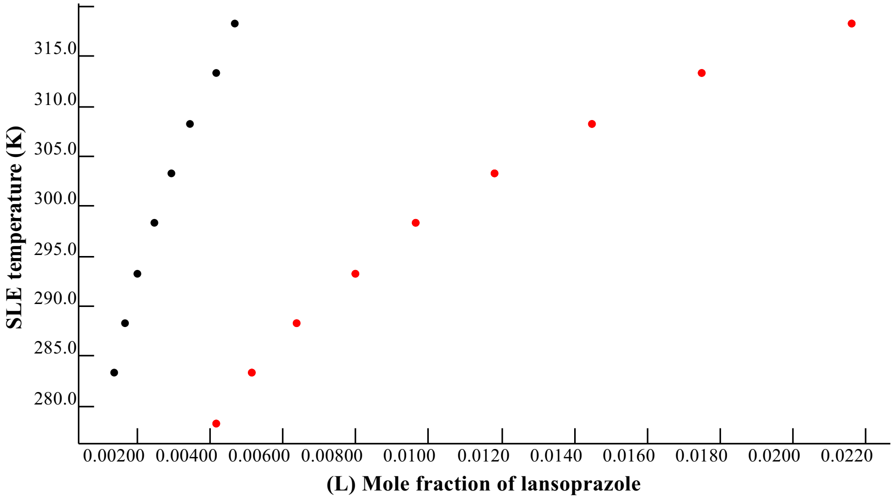

Fig. 1 An illustrative example of two (black and red dots) inconsistent solid–liquid equilibrium (SLE) reports for lansoprazole + ethyl acetate (Case 24 in the database web service [11] Color figure online)

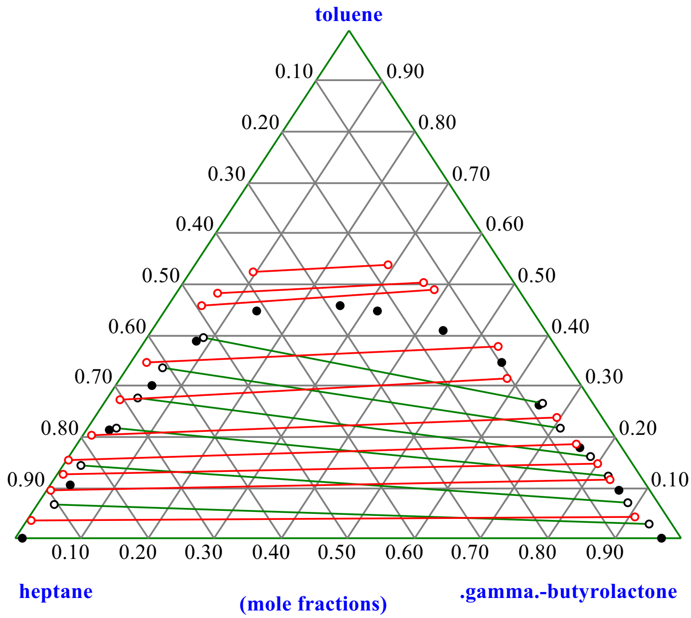

Fig. 2 An illustrative example of two (black and red dots) inconsistent LLE reports involving tie-line and binodal data for toluene + heptane + γ-butyrolactone (Case 3 in the database web service [11] Color figure online)

thorough reviewing [16] should reduce the number of such issues during publication.

- Identity and purity of the studied compounds are sometimes questionable, especially if compounds, which are synthesized by authors, are unstable, hygroscopic, able to hydrolyze, or change their composition (such as protic ionic liquids or deep eutectic solvents).
- Low solubilities and infinite dilution properties (such as activity coefficients and Henry's law constant) are difficult to measure because they require high measurement precision with numerous precautions and careful calibrations. Moreover, many experimental methods are not applicable to measuring low solubilities (*e.g.*, titration).
- Low solubilities are susceptible to such factors as impurities in solvents and surface phenomena. For example, non-aqueous condensed-phase equilibria may be sensitive to unaccounted moisture. In addition, kinetics of equilibration and formation of metastable states add ambiguity to results of solid–liquid and liquid–liquid equilibrium studies.
- Low electrical conductivities can be dramatically altered by trace amounts of water or electrolytes.
- High shear viscosities are difficult to measure, compounds may exhibit non-Newtonian or thixotropic behaviors, and any measured viscosity data may be wrong if measurement techniques were used outside of their applicability ranges. Any properties of highly viscous substances are also difficult to measure; that may explain the scatter of various property data reported for systems involving glycerol and deep eutectic solvents.
- Interpretation of the measured values may be unfounded, or data processing errors can occur (*e.g.*, not accounting for water from hydrates or misidentification of compounds).

For the data challenges currently posted in the web service [11], additional information may exist but be unavailable to the project participants, so additional input from readers may contribute to their resolution. Consistency analysis and correlations may sometimes indicate which measurement of a set of conflicting results is the most probable, but the accuracy of those derivations may be insufficient. Additional analyses may reveal flaws in either or even all conflicting reports. It would be useful to corroborate the correct results and improve the methods for corroboration. The solutions must be convincing, considering all factors affecting the considered data and the full uncertainty budget. It is anticipated that new methods contributing to solving the challenges will be developed and published, and the existence of unresolved issues will justify and support such developments.

3 Web Implementation

The developed web service [11] (Fig. 3) is based on the above-described database of identified data issues. Each issue is composed of one to three chemical compounds, type of property (such as SLE solubility or enthalpy of formation), and its status. A

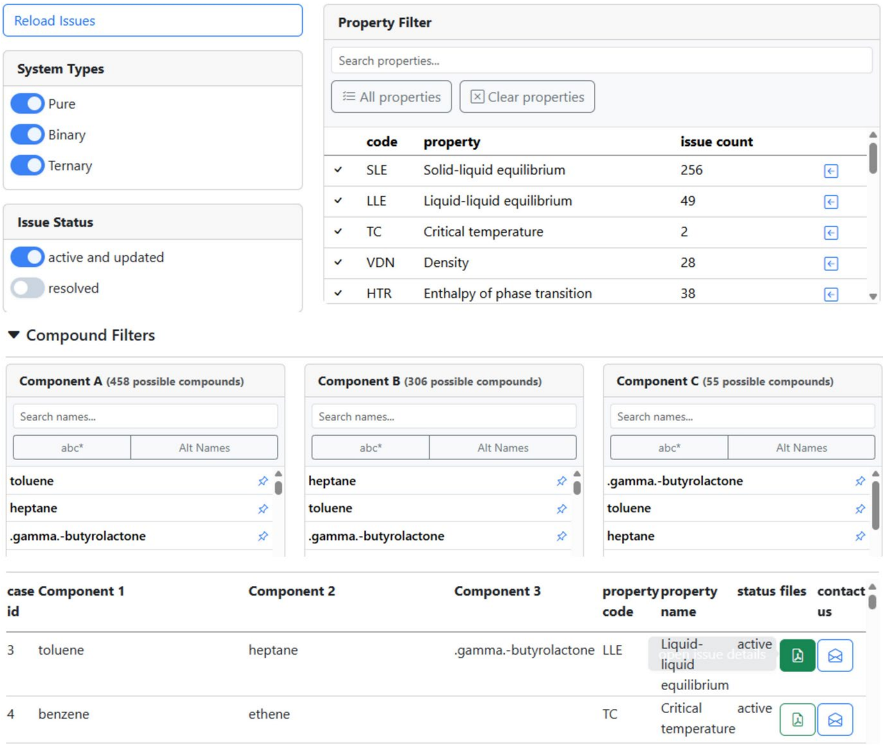

Fig. 3 Interface of the developed research challenge web service [11]

PDF file is supplied for each case describing and illustrating the problem and giving references.

The search site is a Vue3 wrapper for this database and allows users to browse by property, system type, or compound. Filtering by property can help experimentalists identify data needs in their areas of expertise. The compound filters allow searching by compound. Additionally, selecting one compound restricts the other compound filters based on identified binary or ternary system issues. Together, these features help experimentalists identify what needs they can investigate with their existing sample inventory or a couple of additional samples.

Beyond browsing, users are encouraged to provide comments or suggest new problem cases, which will be reviewed by the project participants and can be added to the collection, if unresolved. This reporting functionality is supported by the corresponding buttons, which initiate emails to the service point of contact with the corresponding subject titles. Upon receiving additional information, the database of identified issues will be periodically updated, and the status of all cases resolved to date will be changed from "active" to "resolved."

To foster transparent scientific discourse and ensure the scalability of community feedback, the Research Challenge Search application also utilizes a public issue-tracking ledger powered by GitHub. Rather than routing discrepancy inquiries through private communication channels, each identified data conflict in the

TRC database is programmatically linked to a dedicated, public GitHub Issue. This architecture will allow researchers worldwide to openly discuss data anomalies, share new experimental measurements, and collaboratively peer-review resolutions, thereby creating a permanent, searchable record of the community's efforts to refine thermophysical data.

New cases and updates are reviewed by the project participants on a voluntary basis. As the web service is hosted on the TRC platform, the TRC staff is ultimately responsible for its content and makes final decisions regarding its maintenance and updates. The project aims to update information on active cases and process user-submitted data promptly upon receipt of feedback. Cases identified through activities of TRC will be added to the database periodically (once or twice a year). In future, as more efficient algorithms are developed, the frequency of updates may be increased. In principle, the criterion for resolving a case is the elimination of the underlying issue(s) that prompted its inclusion in the collection (as described in the previous section). While individual assessments may involve some degree of subjectivity, considering the opinions of multiple project participants and contributors should help minimize ambiguity.

4 Conclusion

In line with our previous projects, we hope this initiative will promote collaboration and coordination, which should increase the efficiency and reliability of research in materials science.

Author Contributions VD contributed to initiation, initial database content, and writing of the initial draft. DR and PD contributed to development of web services. All co-authors involved in discussion of the concept, reviewing the service, database content, and the manuscript, and making suggestions and additions.

Funding No funding was received for this work.

Data Availability No datasets were generated or analyzed during the current study.

Declarations

Competing interest The authors declare no competing interests.

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