

**SOFTWARE DESIGN FOR THERMODYNAMIC MODELING
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In the contemporary landscape of computational materials science, the complexity of multicomponent systems necessitates a rigorous architectural distinction between thermodynamic models and the numerical algorithms employed to solve them. Inspired by the C++ Standard Template Library (STL), where the separation of algorithms and data structures serves as a cornerstone of efficiency and flexibility, this report proposes a similar approach for thermodynamic databases and corresponding software.

The crucial part of this methodology is usage of the TDB (Thermodynamic Database) text format. While the TDB format is traditionally used as a static repository for Gibbs free energy parameter, we also demonstrate that the TDB format can serve as a universal, high-level abstraction layer. For example, it has object-oriented features, which are inherently useful for definition of parameters of phases utilizing diverse thermodynamic models in a structured, hierarchical manner.

TDB format provides means for seamlessly merging of multiple sub-databases while maintaining strict human-readability. Being just plain text files, it enables seamless integration with version control systems, essential for tracking of the evolution and highlighting differences of thermodynamic assessments.

This report introduces specific software features of our developed suit, focusing on the parsing and internal representation of TDB files as dynamic data structures. We discuss how these technical choices directly translate into a superior User Experience (UX). Treating the TDB file not just as a flat data source but as a modular codebase enables advanced search capabilities, support for language extensions for setting additional settings of computational environment, and a streamlined workflow for the assessment and refinement of thermodynamic data.

The authors gratefully acknowledge the financial support of the Program “Chemical Thermodynamics and Theoretical Material Science” (№ 121031300039-1), Lomonosov MSU