

Thermal analysis and computational thermodynamics: From experiment and theory to application

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Thermodynamics plays a central role in processing of materials and the prediction of system behavior. While the theory is well established, the first and second laws are empirically derived with fundamental yet simplified equations that describe only highly ideal cases. Many of the most sophisticated models rely on constructs and/or mathematical expressions with adjustable parameters to correctly describe the behavior of real systems. Experimental data, like those from thermal analysis, provide fundamental information used to determine thermodynamic values and tune adjustable parameters. The semi-empirical models derived from theory and optimized from measurements can then be applied to develop materials and processes for advanced technologies. The usefulness of computational thermodynamics with a particular emphasis on nuclear fuel technology will be discussed.

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