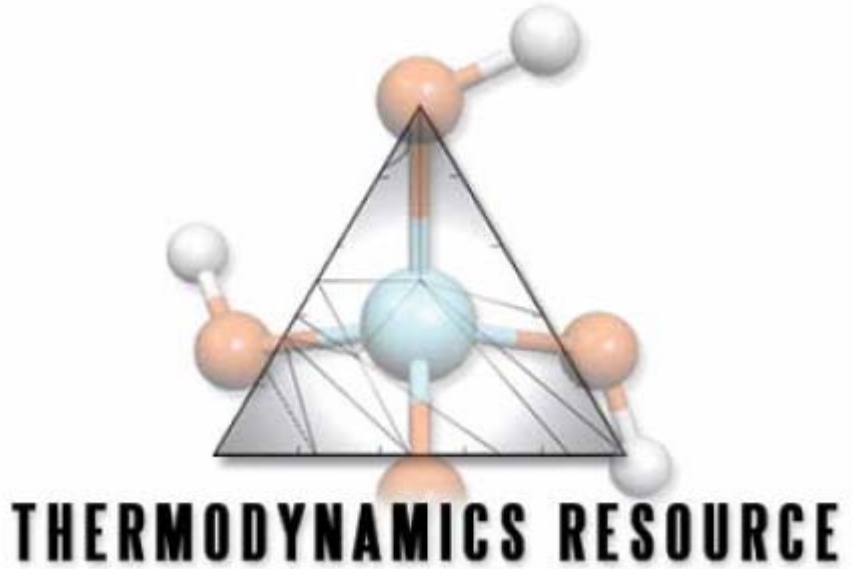
Thermochemical Models and Databases for High-Temperature Materials Processing and Corrosion

An internally consistent thermochemical database for refractory oxide materials will enable the prediction of the behavior of materials at high temperatures

Thermodynamic property data heats of formation, heat capacities, and entropies for both condensed- and gas-phase compounds) are the foundation of building accurate models for understanding all high-temperature processes. Such data has many uses, including: equilibrium calculations to predict corrosion of refractories and other materials heat-transfer modeling of furnaces and molten phases of glasses and metals modeling of high-temperature chemical reactions occurring in material synthesis prediction of process energy efficiency and pollutant formation for combustion and other high-temperature manufacturing processes and prediction of liquidus temperatures and the formation of crystalline inclusions in glass formulations. Without thermodynamic data, it is difficult or impossible to even begin to model many high-temperature processes. The technology roadmaps developed by various industry groups, including glass, aluminum, and chemicals, describe many high-priority technology barriers and research needs that in some way require detailed knowledge of materials thermochemistry. The computational methods used in this project provided an avenue for obtaining this critical data.



http://www.ca.sandia.gov/HiTempThermo/index.html

Benefits for Our Nation and Our Industry

- The availability of thermodynamic data for various glass systems lead to improved, higher-strength glass and thus lighter glass.
- Improved refractories that result from a better understanding of chemical behavior would lead to improved furnace designs, which were estimated to yield a 12.5% improvement over conventional furnaces.
- Estimated savings were in the vicinity of 12 trillion Btu/year for a 50% market introduction.

Applications in Our Nation's Industry

This project has applications throughout industry:

- Agriculture
- Metalcasting
- Aluminum
- Mining
- Chemicals
- Petroleum
- Forest Products
- Process Heating
- Glass
- Steel
- Heat Treating

Project Description

The goal of this project was to provide thermochemical data and models for an important set of materials -refractories and glasses. Such data are the basis for determining the potential for chemical interactions among materials and are essential for predicting stability and corrosion. All data were incorporated into a comprehensive web-based tool that provides the necessary input for commercial application.

Barriers

Major barriers addressed:

- Very limited data for refractories, glasses, and high temperature gas-phase species
- Absence of experimental data for model verification
- Lack of a consistent, documented, continuously updated, and fully open repository for data

Pathways

The objectives of this project were achieved through (1) the creation of models and the development of theory needed to predict thermochemistry from first principles; (2) teaming with NASA/Glenn to provide critical experimental data; and (3) creation of a user-friendly web site for distribution of project results.

Progress and Milestones

- Developed a refined, highly accurate base model for glass systems (Na-Ca-Al-B-Si-O) that agrees well with published phase diagrams
- Created a website that is open to the public with data available at no charge - site has over 850 compounds
- Developed methods to predict data for Zr, Y, Nb, Mo
- Expanded data relevant to combustion processes, especially NOx-related and halogenated hydrocarbons
- Completed software for CHEMKIN-FactSage format interconversion
- Provided user tutorials and examples for online equilibrium calculator
- Uploaded new condensed phase models to the website
- Explored educational possibilities via interactions with universities

Commercialization

A website is now live and available to the public at: http://www.ca.sandia.gov/HiTempThermo/index.html which contains the data available at no charge. The data is well documented with a clear pedigree, unlike most commercial (encrypted) databases. Since the site's launch on August 31, 2002, numerous upgrades have occurred, including: the addition of a recent news page; archived earlier versions of the data; an on-line equilibrium calculator; and an improved search engine. Users may now subscribe to the on-line user community.

Project Partners

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A Strong Energy Portfolio for a Strong America

Energy efficiency and clean, renewable energy will mean a stronger economy, a cleaner environment, and greater energy independence for America. Working with a wide array of state, community, industry, and university partners, the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy invests in a diverse portfolio of energy technologies.

U.S. Department of Energy
Energy Efficiency and Renewable Energy
Bringing you a prosperous future where energy is clean, abundant, reliable, and affordable

Ending FY2007
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