Web Database of ThermoChemical Properties Now Available to Industry

The web-based ***Thermodynamics Resource*** is now available to help industries engaged in high-temperature processing address critical technology challenges. Scientists at Sandia National Laboratories and Oak Ridge National Laboratory created this user-friendly database to aid in modeling and exploring processing solutions involving high-temperature materials and corrosion. This free resource on thermochemistry for gas-phase and condensed species currently includes pages specifically for the *glass* manufacturing and *petrochemica*l industries; similar pages focused on the *chemical*, *forest products*, *steel*, and *aluminum* industries will be added soon. See Figure 1 and the Thermodynamics Resource web site (www.ca.sandia.gov/HiTempThermo/index.html) for further description and contact information.

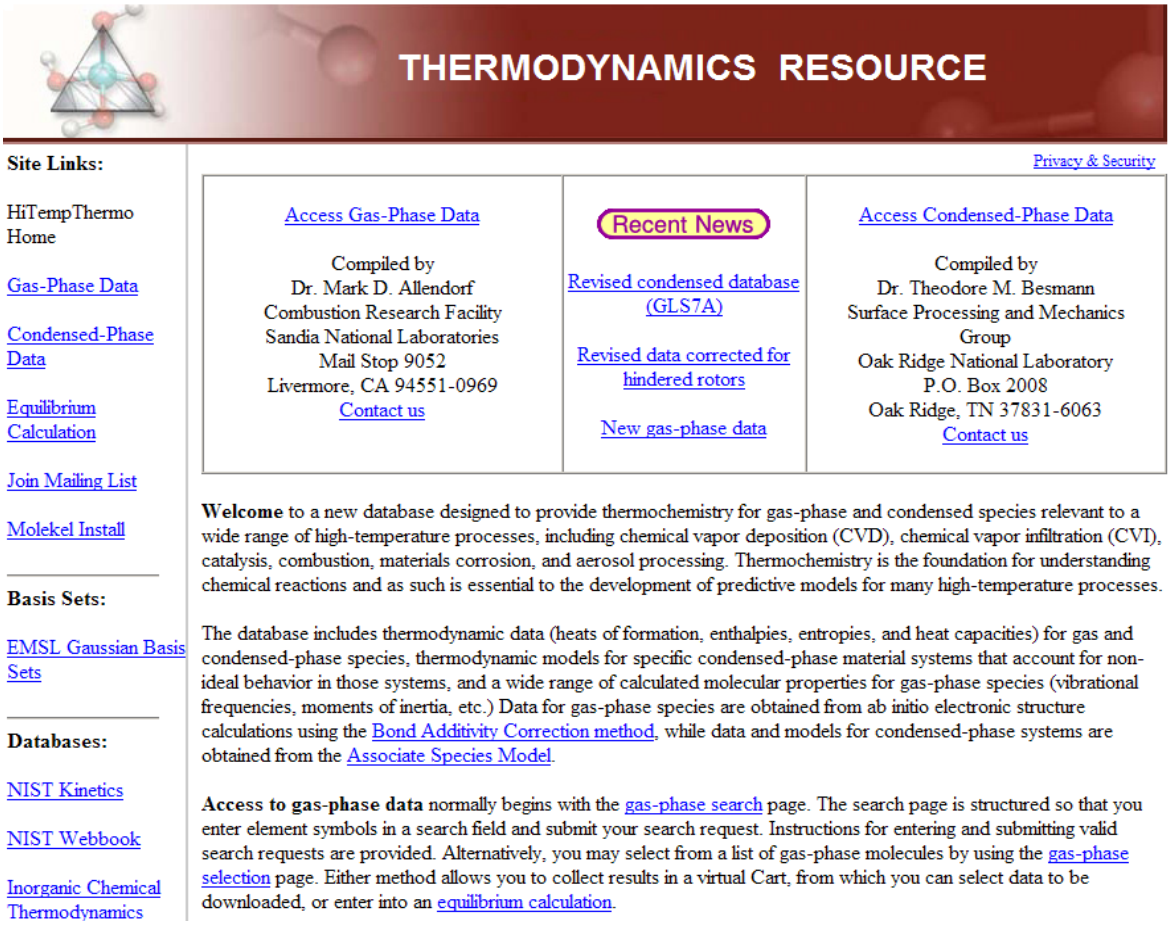


Figure 1: Thermodynamics Resource Home Page

The ***Thermodynamics Resource*** database includes thermodynamic data (heats of formation, enthalpies, entropies, and heat capacities) for gas and condensed-phase species; thermodynamic models for specific condensed-phase material systems (that account for non-ideal behavior in those systems); and a wide range of calculated molecular properties for gas-phase species (vibrational frequencies, moments of inertia,

etc.). Data for gas-phase species were obtained from *ab initio* electronic structure calculations, primarily using Bond Additivity Correction methods, while data and models for condensed-phase systems were obtained from the Associate Species Model.

Thermodynamic property data are essential for building a broad range of predictive models for high-temperature processes (see inset). Valuable applications include the following:

- Development of equilibrium calculations to predict corrosion of refractories and other materials
- Modeling of heat transfer in furnaces and in molten phases of glasses and metals
- Modeling of high-temperature chemical reactions occurring in material synthesis
- Prediction of energy efficiency and pollutant formation during combustion and other high-temperature manufacturing processes
- Prediction of liquidus temperatures and the formation of crystalline inclusions in glass formulations

Examples of Data Available via the *Thermodynamics Resource*

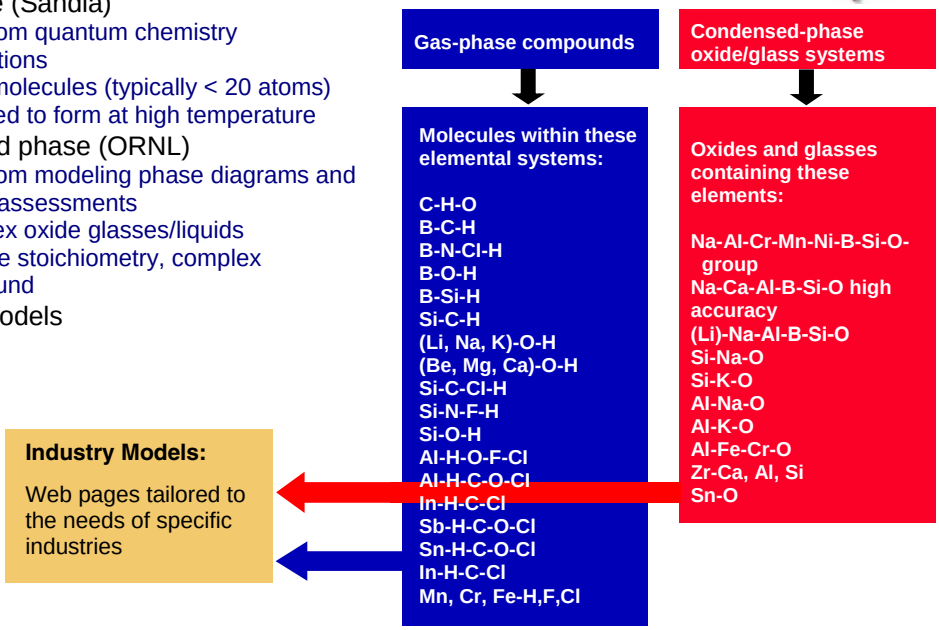
- Data on carbon and hydrocarbon species for coal gasifier applications, enabling equilibrium modeling to simulate
  - Refractory corrosion
  - Interactions that could cause solids deposition (coking)
  - Influence of refractory on gas composition
- Information about high-temperature chromia refractories used in combustion to support evaluation of their reaction with contaminants—particularly alkali and calcia, which are common in bio-fuels. Data can be used in the following applications:
  - Aluminum production, impurity removal
  - Alkali corrosion of refractories in glass furnaces
  - Corrosion of Cr-containing refractories in gasifiers
  - Production of coated float glass
- Thermochemical data for transition metal compounds that have applications as metal interconnects in solid-oxide fuel cells and refractories for such applications as
  - Black liquor gasifiers
  - Coal gasifiers
  - Air/fuel glass melting furnaces
  - Aluminum smelting
  - Steel making

The database incorporates input from an advisory committee representing the glass, chemicals, aluminum, petrochemical, forest products, refractory, and software industries. The theoretical approaches used to determine thermochemical data for transition metal compounds were validated via experiments conducted at the NASA/Glenn Research Center. The web site includes FactSage, an on-line equilibrium calculator used for predicting phase equilibria in high-temperature systems. A CHEMKIN data conversion tool allows thermodynamic data in NASA polynomial format to be used by ChemSage and FactSage. Contents of the ***Thermodynamic Resource*** web site are summarized in Figure 2 (below) and available to the public free of charge. See the project factsheet (http://www.eere.energy.gov/industry/imf/pdfs/1788_thermochemicalmodels.pdf) or visit the ***Thermodynamic Resource*** web site (www.ca.sandia.gov/HiTempThermo/index.html) for points of contact and further information.

Thermodynamics Resource

a user-friendly source of industrially relevant thermochemical data

- Gas phase (Sandia)
  - Data from quantum chemistry calculations
  - Small molecules (typically < 20 atoms) expected to form at high temperature
- Condensed phase (ORNL)
  - Data from modeling phase diagrams and critical assessments
  - Complex oxide glasses/liquids
  - Variable stoichiometry, complex compound
- Industry models



Site is open to the public and all data are available at no charge

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

Figure 2: Summary of data available through the Thermodynamics Resource