Progresses on Thermodynamic Databases

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Abstract. Chemical production is accompanied by heat generation and the generation of new substances. The use of these calories and products, for sustainable development and environmental protection is of great significance. Thermodynamics is the understanding and mastery of the nature of heat and the law of energy conversion. It is a macroscopic theory based on experiment and has a high degree of universality and reliability. Thermodynamic data is an essential basic data for chemical design, simulation, and production. Therefore, thermodynamic data is of great significance to the sustainability of chemical production and environmental protection. Several relatively complete thermodynamic database around the world such as FactSage, THERMO-CALC, HSC Chemistry, inorganic thermochemical database, metallurgical thermodynamic database and so on were summarized and discussed.

1. Introduction
So far, although several relevant monographs, monographs, manuals around the world on thermodynamic databases were compiled and published, the query and calculation of thermodynamic data in accordance with traditional methods need to spend a lot of time and effort. The combination of database technology and thermodynamics greatly reduces the time it takes for this process.

2. Development Status of Thermodynamic Database

2.1. Factsage Thermodynamic Database.
In 2001, the FACT software developed by the University of Montreal fusion with ChemSage software developed by GTT Germany, becoming one of the world’s largest integrated systems for fully integrated databases in the field of chemical thermodynamics named Factsage. The FactSage not only has a built-in CRCT database of the oxide database that has been accumulated over the past 30 years, but also links to other well-known international databases [1]. With FactSage you can calculate the conditions for multiphase, multi-component equilibria, with a wide variety of tabular and graphical output modes, under a large range of constraints. For example, general N-component phase diagram sections can be easily generated with a wide choice of axis variables; matte/metal/slag/gas/solid equilibria can be accurately calculated, tabulated and plotted for industrial systems; multicomponent predominance and EpH diagrams can be readily produced; the course of equilibrium or non-equilibrium solidification can be followed; complex heat balances can be computed; and so on [2,3].
The FactSage 7.1 Update/Installation (2017) package was released in January 2017. The software interface is shown in Figure 1. It contains three modules:

1. Database modules: This module scans the databases and enables you to display the standard state thermodynamic properties of the compound species and to list the solution phases. And you can build a user's private compound (pure substance) database.

2. Calculate modules: This module is used to calculate changes in extensive thermodynamic properties (H, G, V, S, Cp, A) for a single species, a mixture of species or for a chemical reaction, calculate and plot isothermal predominance area diagrams and Eh vs. pH (Pourbaix) diagrams for one-, two or three-metal systems. There are other calculations and graphics functions. Specific functions are shown in Table 1.

3. Manipulate modules: This module is used for data input, results in output and calculation results chart generation.

2.2 THERMO-CALC Software.
Thermo-Calc Software was founded in 1997, but it all really started much earlier, even traced back to the mid 1970’s. The place was the department for physical metallurgy at the Royal Institute of Technology in Stockholm, Sweden.

Thermo-Calc Software offers a wide spectrum of high-quality thermodynamic and mobility databases for use with Thermo-Calc, the add-on Diffusion module (DICTRA) and/or Precipitation module (TC-PRISMA), as well as SDKs for various applications. The databases supplied by Thermo-Calc Software have all been produced by critical assessments and evaluations based on experimental data. Used in 70+ countries by industry, Government, and academia. More than 2500 licenses sold worldwide [4,5].

Thermo-Calc Software can be divided into Thermo-Calc and Thermodynamic database:

Thermo-Calc has over the past 30 years gained a worldwide reputation as the best and most powerful software package for thermodynamic calculations. It is widely used for a variety of calculations including calculating: Stable and meta-stable heterogeneous phase equilibria; Amounts of phases and their compositions; Thermochemical data such as enthalpies, heat capacity and activities; Transformation temperatures, such as liquidus and solidus; Driving force for phase transformations; Phase diagrams (binary, ternary and multi-component); Solidification applying the Scheil-Gulliver model; Thermodynamic properties of chemical reactions; And much, much more.

The thermodynamic database offers an extensive selection of high-quality thermodynamic databases for use with Thermo-Calc, as well as other software products. All databases have been produced after a critical assessment of all relevant experimental and theoretical information, followed by optimization and validation. Include TCS Steels/Fe-alloys Database; TCS Ni-based alloys Database; TCS Aluminum-based Alloys Database; TCS Magnesium-based Alloys Database; TCS Cu-based Alloys Database; and so on [6].
Figure 1 The window of FactSage software

| Module      | Functions                                                                 |
|-------------|---------------------------------------------------------------------------|
| Reaction    | Calculate changes in extensive thermodynamic properties (H, G, V, S, Cp, A) |
| Predom      | Calculate and plot isothermal predominance area diagrams for one-, two or three-metal systems |
| EpH         | The Eh-pH diagram of metal system in ideal state is calculated and plotted |
| Equilib     | Calculates the concentrations of chemical species when chemical equilibrium. |
| Phase Diagram | Calculate, plot and edit unary, binary, ternary and multicomponent phase diagram |
| OptiSage    | Optimize the thermodynamic parameters and set up a personal database       |

2.3 HSC Chemistry.

HSC Chemistry is the world's most widely used integrated thermodynamic database software developed by the Outokumpu research center in Finland. Its latest version 7.0 has a database of detailed thermodynamic properties of more than 20000 inorganic substances and 24 calculation modules designed for different applications (The main sub-databases are shown in Table 2). The simulation chart can be edited and the data can be exported in various forms to facilitate third-party software to analyze and plot [7].

HSC Chemistry is designed for various kinds of chemical reactions and equilibria calculations, The main modules and functions are shown in Table 3[8].

The name of the program is based on the feature that all fourteen calculation options automatically utilize the same extensive thermochemical database which contains enthalpy (H), entropy (S) and heat capacity (C) data for more than 17000 chemical compounds. This database is equivalent to more than seventeen thick data books.

The objective of HSC is to make conventional thermodynamic calculations fast and easy to carry out using personal computers. Therefore HSC has a wide range of application possibilities in scientific education, industry, and research. Thermochemical calculations are useful, for example, when developing new chemical processes and improving old ones. HSC Chemistry is also a useful tool for universities and schools in chemical practices and studies.
Traditionally, thermodynamic calculations based on experimental or assessed data have utilized stability functions in various thermodynamic data books and papers in scientific journals. The difficult searching stage and complicated calculations, as well as inconsistencies arising from different selections of standard and reference states, have made this calculation procedure quite time-consuming.

HSC Chemistry offers powerful calculation methods for studying the effects of different variables on the chemical system at equilibrium. For example, if the user gives the raw materials, amounts and other conditions of almost any chemical process, the program will give the amounts of the product as a result. HSC also makes heat and material balance calculations of different processes much more easily than any manual method. The Eh-pH-diagrams option of HSC also offers a very fast way of studying the dissolution and corrosion behavior of different materials.

Of course, HSC does not solve all chemical problems, because it does not take into account the kinetics (rates) of the chemical reactions and non-ideality of solutions. However, in many cases, it is a very inexpensive and useful tool which helps to find the optimum reaction conditions and yields for experimental investigations without expensive trial-and-error chemistry [9,10].

| Table 2 The Main Databases of The HSC |
|--------------------------------------|
| Database                             | Contents                                                                 |
| HSC Thermochemical Database          | The thermochemical database contains 20000 kinds of pure substances and water soluble substance |
| Heat Conduction Database             | Heat transfer database containing more than 700 materials                  |
| Heat Convection Database             | The heat transfer database containing 111 substances and 4 equations       |
| Surface Radiation Database           | The surface diffusion database containing more than 60 materials           |
| Minerals Database                    | Including a mineral database of 3581 minerals, users can add new minerals into the database |

| Sim                                  | Simulation and modeling of chemical processes                                |
| LCA Evaluation                       | Complete recycling chains can be simulated and their environmental impact evaluated |
| Mass Balance                         | Common data reconciliation                                                   |
| Reaction Equations                   | The equilibrium constant and the heat of reaction are calculated by the reaction equation |
| Heat and Material Balances           | Calculate, plot and edit unary, binary, ternary and multicomponent phase diagram |
| Heat Loss Calculations               | Optimize the thermodynamic parameters and set up a personal database        |
| Equilibrium Compositions             | Calculate the equilibrium composition and amounts of prevailing phases in any reactor |
| Energy Balance                       | Calculate the energy, mass and heat balance for a system                    |
| Eh-pH Diagrams - Pourbaix H, S, Cp and Ellingham Diagrams | Draw diagrams with only an element or several elements                  |
| Tpp Diagrams - Stability Diagrams    | Drawing an Eh-pH diagram for a single element or multiple elements          |
| Lpp Diagrams - Stability Diagrams    | Calculates the diagrams on the basis of minimum Gibbs energy (area graphs) |
| Water - Steam Tables, etc            | Calculates the phase stability boundaries as lines based on the reaction equations |
| $H, S, Cp$ Estimates                 | $P - T$ diagram                                                             |
| Benson Estimation                    | Estimates $H, S$ and $C_p$ values for chemical compounds.                    |
|                                      | Estimation tool for organic species                                         |
Species Converter: Convert an elemental analysis to a species analysis and vice versa.
Periodic Chart Elements: Periodic table of elements
Measure Units: Easy tool for fast unit conversions in thermochemistry as well as in other fields of engineering.
HSC Add-In Functions: Thermochemical and mineralogical calculations in Excel
Geo-Mineralogical calculations: Mineralogical calculation and analysis
Map-GPS material stock: Reserves of raw materials control chart
Fit-Numerical Data fit: Multivariate regression, curve fitting and statistical properties
Data-Statistical analysis: Statistical analysis of data

2.4 Part of the free foreign thermodynamic database.
The rapid development of network technology, so that it is combined with the various disciplines faster and faster. Many domestic and foreign scholars tend to use the network to get a lot of information they need, can save a lot of time and research funding, and real-time information updates.

Table 4 lists some of the foreign free thermodynamic databases.

| Database            | Function                                                                 |
|---------------------|--------------------------------------------------------------------------|
| NPL                 | Basic constant, energy conversion factor                                  |
|                     | Including Chemistry Web-book thermodynamics data, 5000 compounds at 298K|
| NIST                | 298K conditions $\Delta H$, $\Delta S$, and $C_p$, 3000 chemical reaction |
|                     | heat and 14000 ion energy                                                 |
| NEA DataBank        | High radiation waste U, TC, Np, Pu, Am in the 298K conditions of $\Delta H$|
| CS ChemFinder       | The properties of more than 40,000 compounds                             |

3. Development Status of Domestic Thermodynamic Database

3.1 Metallurgical thermodynamic database.
METHEDAS is modeled on the database of the Institute of theoretical metallurgy, Rheinisch Westfaelische Technische Hochschule Aachen University, Germany [7]. It consists of three parts:

a. Two databases: One is a database of the thermochemical properties of 2,200 inorganic compounds. The second is the thermodynamic database of 400 binary alloys.

b. Application library. This is the most important part of the database. Rely on these procedures can be data to deepen the processing, through the formula to get the user needs a variety of thermodynamic data, these programs include: (1) Retrieve, (2) Calculate the thermochemical properties of inorganic matter at each temperature, (3) Equilibrium chemical reaction equation, (4) Calculated chemical reaction equilibrium constant, (5) Calculate the maximum temperature of reaction products, (6) Calculation of multivariate multiphase chemical reaction equilibrium composition, (7) Generation of Predominance Area Phase Diagram.

c. Control system. Coordinate calls to data and programs [11,12].

The metallurgical thermodynamic database system has reached the international and domestic advanced level and has been serving the production, teaching and scientific research of metallurgy, material, chemical and other fields in our country [7].

3.2 Inorganic thermochemical database.
ITDB by the Chinese Academy of Sciences Institute of Chemical Metallurgy in 1979 the completion
of the preliminary construction work, in 1982 began to promote, provide online service started in the middle of 1990s[7].

ITDB database currently includes 35000 thermochemical data of 2020 inorganic compounds. In addition to the data retrieval and thermodynamic calculation, it can also calculate the interaction between the compounds, four coefficients regression of the calculation formula of heat capacity, diagram calculation and mapping of thermodynamic functions and temperature, predominance area phase diagram of $\log P_i - \log P_j$ and $\log P_i - 1/T$. ITDB can provide the best experimental conditions, the choice of the best process conditions, and the accurate calculation of energy consumption and so on. It will help to improve the efficiency of scientific research and increase the economic benefits [13,14].

4. The Database of Salt-water Systems.

The solubility data are among the most important basic physicochemical parameters widely used in chemical processing. The dissolution of salt minerals, the evaporative crystallization of production materials, choose and confirm the suitable process and conditions in technological design and new technologies, processes and products are developed according to the temperature variation effect all need the fundamental theoretical guidance by the solubility data of salt-water systems.

With the development of science and technology, finding and using the increasing solubility data poses the main difficulty for scientists and engineers. Moreover, due to the different experimental apparatus and methods, the solubility data for the same systems will be biased at the same temperatures and hence cannot satisfy the users’ needs. It is imperative and innovative to query and assess the solubility data of salt-water systems effectively in the inorganic salt chemical industry.

Our team collected the solubility data for more than 9,000 systems, which had been published since 1910, and classified them as binary, ternary, quaternary and multiple systems, creating a Salt-water System Database that can be used to query data based on system composition and temperature. The operation interface is shown in Figure 2 [15].

![Figure 2 The webpage window of the Database of Salt-water Systems](image)

5. Conclusions

Thermodynamic databases established based on the web have brought great convenience for thermodynamic research and improved the efficiency of research and production, provide large data support for the sustainable development and environmental protection of chemical productions. However, the data needs to be further authoritative and standardized, which is the basis for the further implementation of the implementation of the migration of various systems.

Acknowledgements

Financial supports from the National Natural Science Foundation of China (Grants U1607123, U1407113 and 21773170), the Postdoctoral Science Foundation (2016M592872) and the Innovative Research Team of the Chinese University (IRT17R81) are acknowledged.
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