Thermochemical software tools for research and practice: FactSage, ChemApp and SimuSage

Stephan Petersen, Moritz to Baben, Klaus Hack
GTT-Technologies, Herzogenrath, Germany

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GTT-Technologies‘ activities, since 1983

Thermochemical Data

Application Software

Consulting
Modelling and simulation tools

- **FactSage™**
  - The Integrated Thermochemical Databank System
  - → ... to perform interactive and phase diagram calculations

- **ChemApp™**
  - The Thermochemical Library (Gibbs Energy Minimizer) for your Software
  - → ... to add thermochemical equilibrium calculations to your or third-party software

- **SimuSage™**
  - The Component Library for Rapid Process Modelling
  - → ... to create ChemApp-based complex process simulations with Delphi/Lazarus

- **ChemSheet™**
  - The Thermochemistry Add-In for Microsoft Excel ®
  - → ... To add equilibrium calculations to your spreadsheets
Why care about Gibbs energy?

The laws of thermodynamics are among the most fundamental laws describing ALL processes in the universe.

→ Only those processes are possible that lead to a decrease in Gibbs energy

→ Without kinetic constraints, Gibbs energy minimizes

→ For that reason, a Gibbs Energy Minimizer (GEM) is the core of all of our calculation software

→ Our customers use our software tools and Gibbs energy databases to predict and understand processes and materials
What is CalPhaD?

Phase diagram database

- System A-B
- System A-C
- System B-C

PhaseLiquid

Phase β

Phase α

G = f(X_A, X_B, X_C, T, p)
Some General Application Examples

- Sintering
- Roasting
- Waste Treatment
- Heat Treatment Cycles
- Al-alloys
- Precipitate Investigations
- Hard Metal Phases
- Coal Combustion and Gasification
- Slags
- Steels
- Non-Oxide Refractories
- Cement Production
- Dioxins
- Glasses

- Aluminium Electrolysis
- Casting Processes
- Waste Incineration
- Electro Steel Making
- Ore Reduction
- Corrosion
- Nuclear Materials
- Electronic Materials
- High-$T_C$ Superconductors
- Ceramics and Refractories
- Nitrate in Water
- Salt Melts
- Recycling Processes
- Geochemistry/Planetology
- …
Available Databases for FactSage

FACT
• FactPS - FACT pure substances database
• FToxid - oxide database for slags, glasses, ceramics, refractories
• FTsalt - salt database
• FThall - Hall aluminum database
• FThelg - aqueous (Helgeson) database
• FTmisc - miscellaneous database for sulfides, alloys, etc.
• FTpulp - pulp and paper database (also for corrosion and combustion)
• FTfrtz - fertilizer database (also for explosives)
• FTOxCN - oxycarbonitride high temperature database
• FTlite - light metal database

GTT
• GTOX - GTT oxide database
Available Databases for FactSage

Cooperative development (CRCT – Spencer Group – GTT)
• FScopp - copper alloy database
• FSlead - lead alloy database
• FSstel - steel database
• FSupsi - ultrapure silicon database

SGTE (Scientific Group Thermodata Europe)
• SGnobl - noble metal database
• SGnucl - nuclear database
• SGTE - alloy database
• Gold - solders database

Spencer Group
• SpMCBN - Non-Oxide Refractories Database

Other suppliers
• TDNucl - Thermodata nuclear database
FactSage – The Integrated Thermodynamic Databank System (ITDS)
Example: Adiabatic Combustion of CH4 with air

\[
\begin{align*}
&<1-A> \text{ CH}_4 + <2A> \text{ O}_2 + <8A> \text{ N}_2 \\
&\text{Adiabatic flame temperature}
\end{align*}
\]

![Graph showing adiabatic flame temperature vs Alpha](image)
Example: Adiabatic Combustion of CH4 with air

\[ \text{CH}_4 + \text{O}_2 + \text{N}_2 \]

Species at \( T_{\text{adiab}} \)

\[ \text{CH}_4(g) \]
\[ \text{H}_2(g) \]
\[ \text{CO}_2(g) \]
\[ \text{H}_2\text{O}(g) \]
\[ \text{O}_2(g) \]
Example: Slagging und Fouling of Hard Coals

[Graph showing temperature (T) vs. wt% liquid with curves for SKR, SKU, SKC, and SKK]
Example: Slagging und Fouling of Hard Coals

![Graph showing the slagging and fouling of SKC Hard Coal](image-url)
CaCl₂-NaF-CaF₂-NaCl ternary reciprocal salt polythermal liquidus projection

Na - Ca - Cl - F
(Na⁺ + 2Ca²⁺) = (Cl⁻ + F⁻), 1 atm

Equivalent fraction Ca

Equivalent fraction F

(NaF)₂

(996°C)

(NaCl)₂

(801°C)

CaCl₂

(772°C)

CaF₂

(1418°C)

T(min) = 486.03 °C
T(max) = 1418.02 °C
T(inc) = 50
The reality: Processes are not simple equilibrium states

- Processes take place in time and space
- $T$ is not constant throughout reaction space
- Composition is not constant
- Heat is released or added

➢ The solution is to consider multiple, local equilibria instead of one global equilibrium
ChemApp - The Thermochemical Library (Gibbs Energy Minimizer) for your Software

... is partially contained in other GTT products

(FactSage)

... is a module for 3rd party programs

CFX®, OpenFOAM®, Fluent®, AspenPlus®, PRO/II®, BALAS®, Comsol®, gPROMS®

... is used in custom programs

Dedicated simulation programs by GTT, Customers’ own programs

... is contained in other GTT products

ChemSheet SimuSage KilnSimu (VTT)
Coal Combustion and Mineral Matter Transformation

- \( H_2O \) Evaporation
- \( C_xH_y \) Devolatilization
- CO Char burnout
- Na, K, S, Cl evaporation and transformation of mineral matter, calculation of liquid (slag) phase fraction and composition

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Particle Tracks and Temperature Profiles

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Preprocessing (ChemApp)

- Change in Mineral Compounds during Combustion
- Particle History has to be considered
- Look-up Table
SimuSage – The Component Library for Rapid Process Modelling

SimuSage is a ChemApp-based set of Delphi/Lazarus components for process simulation/flowsheeting tasks (sequential modular approach)

ChemApp + Delphi™ Lazarus =

- Stream
- Stream
- Stream
- Stream
- Stream
- Stream
- Stream
- Stream
- Stream
Full Model
SimuSage model (Dohrn – IEK-2)

Input data:
- \( \text{Mg}_{\text{a-\%}} \)
- \( \text{H}_{2}\text{O} \)
- \( \text{C} \)
- \( \text{H}_{\text{a-\%}} \)
- \( \text{N} \)
- \( \text{Cl} \)
- \( \text{Ash content} \)
- \( \text{Al}_{2}\text{O}_3 \) to \( \text{TiO}_2 = 100\% \)
- \( \text{Fe}_2\text{O}_3 \)
- \( \text{MgO} \)
- \( \text{Na}_2\text{O} \)
- \( \text{P}_2\text{O}_5 \)
- \( \text{SO}_2 \)
- \( \text{SO}_3 \)
- \( \text{TiO}_2 \)
- \( \text{Lambda} \)

Lambda-Calculation
1. Calculate amount of \( \text{O}_2 \) necessary for: \( \text{C} \to \text{CO}_2, \text{H} \to \text{H}_2\text{O}, \text{S} \to \text{SO}_2 
2. 100-\( \text{H}_{2}\text{O} \cdot \text{C} \cdot \text{H}_{\text{a-\%}} \cdot \text{S} \cdot \text{Ash-Cl} = \text{O}_2
3. Subtrast Calculation 1 - 2
4. Multiply by Lambda
5. Multiply by 3.773 (for value of Nitrogen) and add both values
6. Separate this amount to Air 1, Air 2 and Air 3

Output data M1
- \( \text{Mg}_{\text{a-\%}} \)
- \( \text{H}_{2}\text{O} \)
- \( \text{C} \)
- \( \text{H}_2 \)
- \( \text{N} \)
- \( \text{Cl} \)
- \( \text{AshAl}_2\text{O}_3 \)
- \( \text{Ash(HCaO}_3 \)
- \( \text{Ash(Fe}_2\text{O}_3 \)
- \( \text{Ash(K}_2\text{O}_3 \)
- \( \text{Ash(MgO} \)
- \( \text{Ash(Na}_2\text{O}_3 \)
- \( \text{Ash(P}_2\text{O}_5 \)
- \( \text{Ash(S}_2\text{O}_3 \)
- \( \text{Ash(TiO}_2 \)
- \( \text{O}_2 \)
- \( \text{O}_2 \) (+100-all)

Air \( \text{Mg}_{\text{a-\%}} = 23.4\% \text{O}_2, 76.6\% \text{N}_2 \)
The present state of the GTOX database

The GTOX database contains the assessment of the \( \text{Al}_2\text{O}_3-\text{Al}_2\text{S}_3-\text{CaF}_2-\text{CaO-}\text{CaS-}\text{CaSO}_4-\text{CrO-Cr}_2\text{O}_3-\text{CrS-FeO-Fe}_2\text{O}_3-\text{FeS-K}_2\text{O-K}_2\text{S-K}_2\text{SO}_4-\text{Na}_2\text{O-Na}_2\text{S-Na}_2\text{SO}_4-\text{MgO-MgS-MgSO}_4-\text{MnO-Mn}_2\text{O}_3-\text{MnS-P}_2\text{O}_5-\text{SiO}_2-\text{TiO}_2-\text{ZnO} \) system

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New viscosity module based on ChemApp and GTOX

- Modeling the viscosity of an 8-component system
  - Lubricant effect
  - Charge compensation
  - Weak lubricant effect
  - Effect of p(O₂)

- Future developments:
  - Addition of further components, e.g. P₂O₅ and TiO₂
  - Extension of the model to the solid-liquid area: effect of solid particles
Summary

- GTT-Technologies provides state-of-the-art thermochemical software and data for coal combustion and gasification
- Unique, high-quality thermochemical data for slags
- Software for interactive and phase diagram calculations (FactSage)
- Software module (DLL, library) for 3rd party programs and customers’ own software (ChemApp)
- Redistributable software tools for the development of specialized in-house and commercial software (ChemApp, SimuSage)
- Current development: unique viscosity module for slags based on our thermochemical database (GTOX) and Gibbs energy minimization code (ChemApp)