

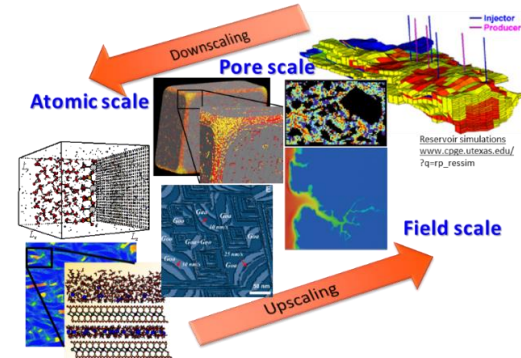
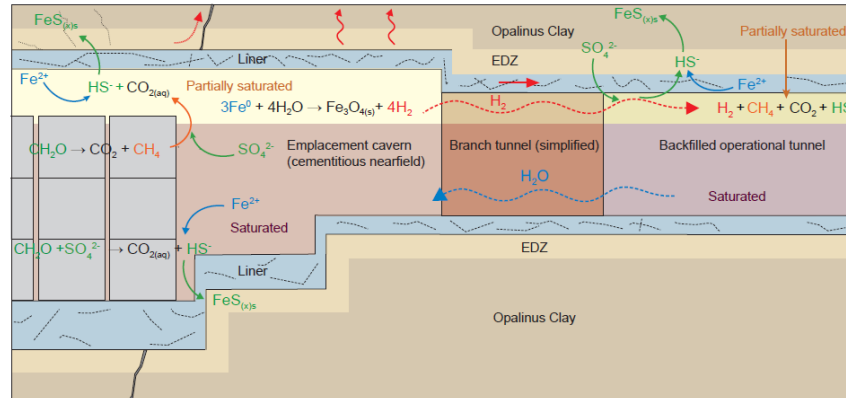
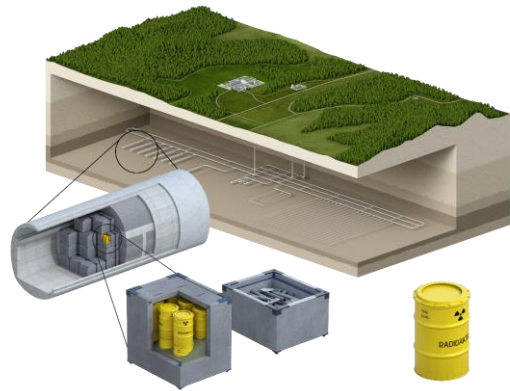


George Dan Miron :: Tenure Track :: Laboratory for waste management :: NES PSI
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THRACE: Traceable thermodynamic datasets for chemical modelling

Laboratory for waste management (part of NES)

- **Laboratory for waste management** - scientific basis for the safe geological disposal of radioactive waste
- Use of **geochemical modeling** for gaining fundamental understanding of chemical processes in natural and engineered geochemical systems.





Thermodynamic models

relations between thermodynamic properties,
calculation of measurable properties

+

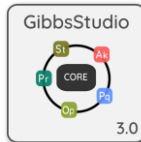
Thermodynamic datasets

actual values of thermodynamic properties
(compilation, derivation, consistency, errors,
bookkeeping)

<https://gems.web.psi.ch/>

Modeling tool package

chemical equilibrium speciation solver code





<https://gems.web.psi.ch/>

Open-Source GEMS codes

- Developed at LES PSI since early 2000s
- Open source (C++/Python) powerful research tool
- 900+ active users in geochemical community
- Do it all geochemical modeling tool (monolith)

The PSI/Nagra Chemical Thermodynamic database

- State of the art compilation of thermodynamic data
- Critical in-house reviews and data assessments (since 1990)
- Support in safety assessment for the planned repository
- Monumental work detailed in lengthy reports

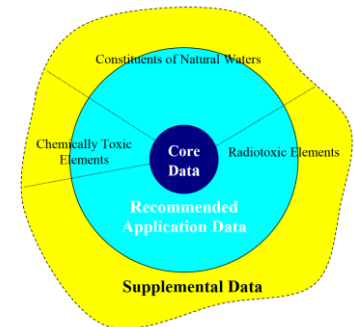
I am a member in the development teams and responsible for future development of GEMS and TDB)



The PSI/Nagra Chemical
Thermodynamic Database 12/07

Nuclear Energy and Safety Research Department
Laboratory for Waste Management (LES)

Thes Thoenes, Wolfgang Hummel, Urs Berner, Enzo Curti
Paul Scherrer Institut, Villigen PSI, Switzerland



1300 p.

PSI Bericht No. 14-04
December 2014
ISBN 10219-0643

Problems/questions of a modeler

- Appropriate **code and database package** for my application?
- What thermodynamic data** should I use?
- What sources do data come from**, how was it compiled/derived?
- What is the **quality** of the data, errors?
- How can I use it** in a modeling code?
- How to compare **alternative models and datasets**?
- How can I **manage** (Create, Read, Uppdate, Delate, Search) **the thermodynamic database**? How can I **import/export** the data?
- Is there a way to **check formal consistency** between properties?
- How can I **retrieve new sets of internally consistent parameters**?

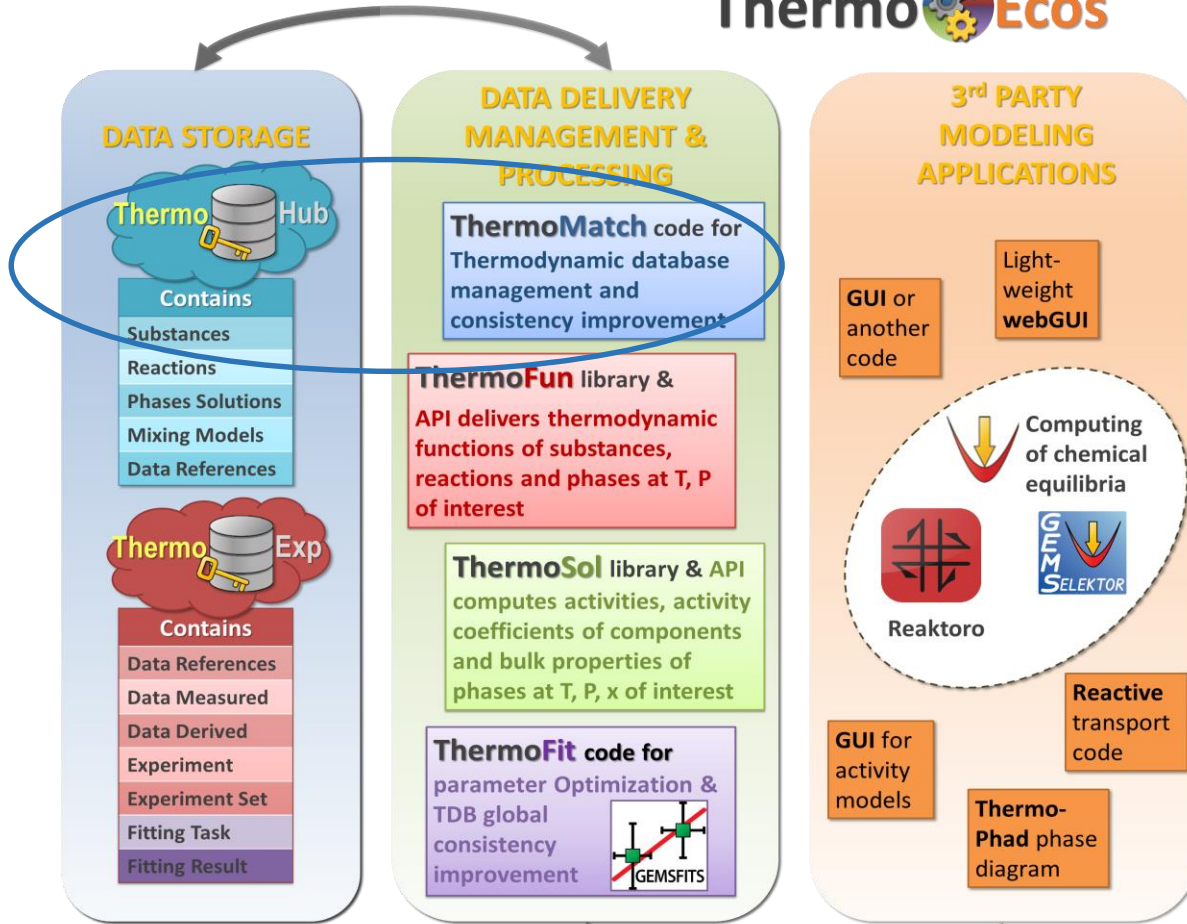
Developer issues

- Lack of funding**, staff support (**IT engineer technicians** like lab technicians)
- Usually **in-kind development**, 3rd party secondary support through main scientific projects

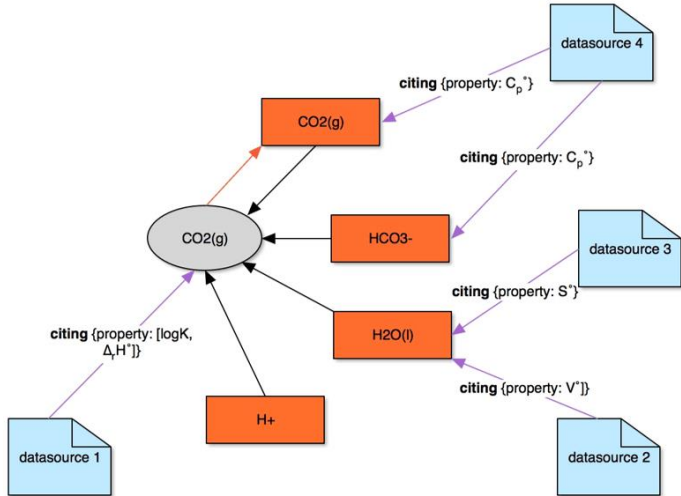
Not yet



ORD project focus



- Is an **online property graph database** that stores thermodynamic datasets
 - Stores various type of **structured data**
 - **Flexible structured format** (JSON) storage of diverse data types (schemas)
 - **Data consistency** and **traceability** through property graph links
 - **Easy-access** local or remote (cloud) storage



- **psinagra-12-07** | ¹ – waste disposal
- **slop98-inorganic and slop98-organic** | ² – aqueous geothermal (revised SUPCRT92)
- **cemdata18** | ³ – suitable for cement systems
- **heracles** | ⁴ – modeling of U and fission products
- **mines16** | ⁵ – modeling magmatic-hydrothermal ore forming processes
- **aq17** | ⁶ – modeling fluid rock interaction at hydrothermal conditions
- **slop16** | ⁷ – aqueous geothermal (organic and inorganic)
- ...

- Main data management operations: **Querying – Editing – Importing – Exporting**
- Queries and import/export scripts as user-defined JSON documents that can also be saved into the ThermoHub database
 - Define a **format file that matches the data fields** of the imported file to those in our own data format
 - **Import from foreign formats**: structured data, text stream, key-value, or CSV
 - Define a **reverse match to export data** from the database format into other formats



Aim of the contribute project

- **Bring ThermoHub to its full potential** and demonstrate its ORD/FAIR
- Ensure the **consistency traceability** of thermodynamic datasets
- A unified thermodynamic database in a general JSON format, with datasets **ready to use for geochemical modelling applications**
- Some mainstream databases used in chemical modeling, to be curated and imported to ThermoHub during the work proposed in the project
- Writing and **adapting the import export scripts**
- Adapting the **JSON schemas of data and metadata**
- Setting up an **automatic suite of tests** for the import/export procedure
- Semiautomatic **workflow for contributing to the ThermoHub** database after the end of the project

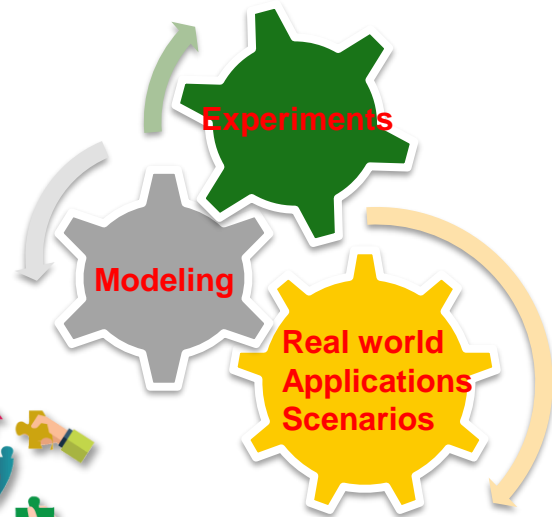
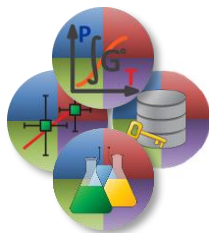


Contains
Substances
Reactions
Phases Solutions
Mixing Models
Data References

Thermo  Match

Future vision

High-quality traceable thermodynamic data and tools for accurate (geo)chemical modeling of real-world scenarios.



- **Open Research Data:** Databases, code tools and web services for chemistry and thermodynamic modelling.
- **Databases** for experiments and thermodynamic data
- **Tools** for optimization and prediction, chemical modeling
- **Microservices** and web applications, tuned for specific application.
Running locally or in the cloud.

Acknowledgments:

ORD PSI and ETHZ

LES/NES

Dmitrii Kulik

Barbara Lothenbach

Sergey Churakov

Thank you!

Questions?

ThermoMatch

data consistency
improvement

ThermoFun

thermodynamic
functions

ThermoSol

phase-solution
models

ThermoFit

model
optimization

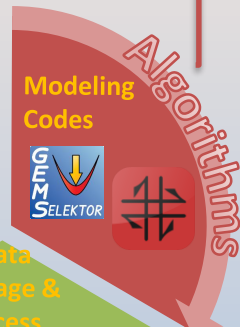
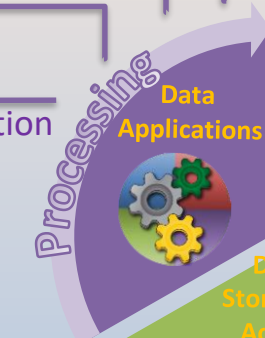
ThermoEcos



online database

PSI-Nagra TDB
Cemdata TDB

Radiotoxic										Chemotoxic										Groundwater										...	Ha																																																									
PSI Chemical Thermodynamic Data Base 2020																																																																																								
H	Li	Be																																	B	C	N	O	F	Ne	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	Fr	Ra	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og



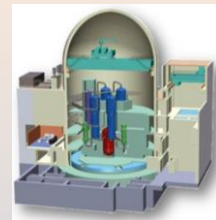
experimental data:
solubility, spectroscopy,
...



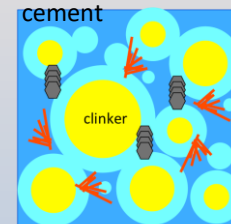
web services
CemGEMS



reactor chemistry



cement
chemistry



● C-S-H ● Portlandite ▲ Ettringite

reactive
transport



<http://gems.web.psi.ch/>
<https://thermohub.org/>
<https://cemgems.app/>
<https://geoml.eu/>