TCIII- 2019- 07E

ThermoChimie

Technical report

ThermoChimie guideline 4: Data traceability

E. Colàs, O. Riba, D. Pérez, I. Campos and L. Duro (Amphos 21)

A.J. Fuller (Galson Sciences Ltd)

25 October 2019

The ThermoChimie database was first developed in 1995 by Andra, the French national radioactive waste management agency. They have since been joined by Radioactive Waste Management (RWM) from the UK, and ONDRAF/NIRAS from Belgium.

ThermoChimie provides an accurate and consistent set of data specifically chosen for use in modelling the behaviour of radionuclides in waste packages, engineered barriers, and both the near surface and deep geosphere. The database can be used to model the speciation and solubility of a wide range of stable and radioactive elements, organics, and solid phases including cements, clay minerals and degradation products (such as zeolites). The database is suitable for use within the range of conditions expected in both near-surface and geological disposal facilities: pH 6-14, ionic strength up to SIT, Eh within the stability fields of water, and temperatures from 15 to 80°C.

ThermoChimie is intended for use across the radioactive waste management community, to support repository performance assessment, research and development activities and decision making. To maximise their utility the data are therefore provided in formats suitable for use with common geochemical modelling codes. The database can be viewed and downloaded from the project website: https://www.thermochimie-tdb.com/, where additional information and supporting documents are also available.

This fourth guideline for ThermoChimie, details the processes followed and the documents produced to guarantee the traceability to ThermoChimie, which is one of the main requirements of the database.

TCIII-2019-07E

ThermoChimie guideline 4: Data traceability

VERSION 2, OCTOBER 2019

Written by: Amphos 21 (Colàs, E., Riba, O., Pérez, D., Campos, I., Duro, L.)

Revised by: Galson Sciences Ltd (Fuller, A.J.)

Approved by: ThermoChimie steering committee: Andra (Madé, B.); RWM (Hibberd, R.); ONDRAF/NIRAS (Brassinnes, S.).

TCIII-2019-07E

DOCUMENT VERSIONS

Version	***Date***	***Comment***
2	*Oct. 2019*	*Full revision to support the release of v10a*
1	*Jul. 2015*	*First version uploaded in ThermoChimie website*

Index

1. Introduction

Traceability is one of the main requirements of the ThermoChimie (TC) database. A database can be defined as traceable if it provides a history of the included data and keeps track of the successive changes.

The selected data must be traceable to the original source, associating each thermodynamic parameter with the corresponding original bibliographic reference. Calculations used to obtain the data must also be traceable (see Guideline 2: Data integration and consistency and Guideline 5: Bibliographic references recording process). Likewise, every single change, update and/or correction made to ThermoChimie during its development must be recorded.

This guideline describes how changes between different versions of ThermoChimie are recorded and provides details on the two traceability reports, which track the changes and modifications made in the database: Track-Changes and Track-Error documents.

2. ThermoChimie versions

ThermoChimie versions are identified using a number and a letter (e.g. version 9.b, 10.a, etc.).[1] If significant modifications are made to the database (for example, if a new element is included, or if a large number of values are modified) the identification number is changed. If modifications affect only to a small number of parameters, then only the letter is changed.

Modifications carried out between different ThermoChimie versions are automatically recorded by the XCheck© tool. This tool is a VB.net based programme specifically developed to automate various processes related to ThermoChimie development, avoiding “man-made” typos or wrong assumptions, and ensuring consistency with auxiliary data and also among the fundamental laws of thermodynamics (see Guideline 2: Data integration and consistency). The XCheck© tool is able to keep an automatic record of any changes and modifications made between different database versions, including changes in the values of thermodynamic parameters, deleted or added species, or most changes in the bibliographic references.

3. Traceability documents

The Track-Changes document describes the evolution of the database and the Track-Error document describes the corrections performed in the new releases to address errors in previous versions of ThermoChimie. If it is considered appropriate, both documents can be integrated in a single report. Those documents will be elaborated by ThermoChimie database

[1] Some ThermoChimie versions older than version 10.a included also a third level number (e.g. version 9.b.0). The third-level number indicated minor variations among versions.

administrators, taking into account the information provided by the different project contributors.

3.1 Track-Changes document

All the changes made in a new version of ThermoChimie with respect to the previous version are summarised in the ***Track-Changes document***. This document allows the ThermoChimie end users to understand the differences between versions and thus, the reasons for different simulation results when different versions of ThermoChimie are used in geochemical calculations. The document is made available to users through the ThermoChimie website.

The Track-Changes document must clearly and accurately define the versions that are being compared, and the date of the modifications. Information related to the following issues must be summarised in a ***brief and practical way*** in the document (when applicable):

- **New systems:** New systems (e.g., a new element, a new organic ligand) added in the database must be documented.
- **Updated values:** Updates made to thermodynamic data already included in the database must be documented. Changes, such as elimination of species, inclusion of new species, changes in the name of an existing compound, inclusion of SIT coefficients, inclusion of entropy values, etc. must also be reported.
- **Changes in extracted files**[2]**:** The information contained in the ThermoChimie database is extracted into the different required formats for use with various geochemical codes (e.g. PhreeqC, ToughReact, Geochemist Workbench, etc.)[3] and the Track-Changes document must also report the changes in those extracted files. For example, the parameter “molar volume” for solid phases is included in the PhreeqC file of ThermoChimie version 10a. As this parameter was not extracted in previous versions, it has been appropriately reported in the corresponding Track-Changes document.

3.2 Track-Errors document

ThermoChimie is continuously revised by the database developers to address potential errors and mistakes. Furthermore, feedback and comments from final users are received through the ThermoChimie website and these are a good source of information for the identification of errors and potential improvements.

[2] Those specific changes are not registered by the XCheck tool
[3] See Guideline 2: Data integration and consistency.

Examples of typical mistakes can be:

- Incorrect values or typos in thermodynamic data (e.g. S_m^0 ($J \cdot K^{-1} \cdot mol^{-1}$)=122.000 instead of S_m^0 ($J \cdot K^{-1} \cdot mol^{-1}$)=121.960).
- Incorrect notation of aqueous and solid species (e.g. NpO_2)OH) instead of NpO_2(OH).
- Typos in bibliographic references (e.g. 14/GIF/GRI instead of 14GIF/GRI).

When mistakes are noticed, an alert is set up on the website in order to notify users of the problem.

The identified errors and their solutions are summarised in a ***brief and practical way*** in a **Track-Error document**. When a new version of the database is released, the full document is made available to all users through the ThermoChimie website.

4. Summary

This guideline provides detailed information on how changes between different versions of ThermoChimie are registered and reported, and summarises the information needed to prepare the Track-Changes and Track-Errors documents. These documents allow ThermoChimie users to understand the differences between versions of the database and thus, to understand the reasons for differences in simulation results when different versions of ThermoChimie are used in geochemical calculations.