

ThermoChimie

Technical report

ThermoChimie guideline 5: Bibliographic references recording process

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

A.J. Fuller (Galson Sciences Ltd)



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 document is the fifth guideline for the ThermoChimie database. It defines how the database containing the bibliographic references for ThermoChimie is built. It also includes indications on how the different types of publications should be referenced in the ThermoChimie development reports.



ThermoChimie guideline 5: Bibliographic references recording process

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-2019-08E

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.....	1
2. BIBLIOGRAPHIC CITATIONS.....	1
2.1 REFERENCE LIST.....	1
2.2 IN-TEXT CITATIONS	2
2.3 REFERENCES WITHIN THERMOCHIMIE DATABASE.....	3
3. BIBLIOGRAPHIC DATABASE	3
4. SUMMARY.....	5

1. Introduction

The development of the ThermoChimie database requires the consultation of peer reviewed scientific publications and technical reports. In order to provide traceability to this process, it is necessary to systematically organise this bibliographic information.

The present document provides instructions on how the different types of publications (books, articles published in journals, proceedings, technical reports, etc.) should be referenced and it also explains how these references are included in the bibliographic database.

2. Bibliographic citations

The bibliographic references used to update and develop ThermoChimie and those included in the different project reports must contain sufficient information to identify and trace the original data sources. It is advisable that this information is presented in a consistent and standardised manner throughout the project reports, as described below.

2.1 Reference list

The references included in any ThermoChimie report have to be systematically compiled at the end of the document to form of a reference list or bibliography. The references should be arranged in alphabetical order by the first authors' last name. If possible, **Harvard citation style** should be followed. Other citation styles can be used if enough information to identify and trace the original source is provided. Examples of the different reference formats for different types of publications are presented below.

Articles in journals and magazines

The complete reference of an article from a journal/magazine should include the following information: author(s), date of publication, article title, journal title, volume number, issue number (if applicable), and page numbers. Example:

Giffaut, E., Grivé, M., Blanc, P., Viellard, P., Colàs, E., Gailhanou, H., Gaboreau, S., Marty, N., Madé, B. & Duro, L. 2014. Andra Thermodynamic database for performance assessment: ThermoChimie. *Applied Geochemistry*, 49, 225-236.

Books and book chapters

Reference to an entire book or to a book chapter must include the following information: author(s) and/or editor(s), date of publication, title, and the name of the publisher. Example:

Grenthe, I., Puigdomenech, I. & Allard, B. 1997. *Modelling In Aquatic Chemistry*, Nuclear Energy Agency

TCIII-2019-08E

(NEA).

Blanc, P., Vieillard, P., Gailhanou, H., Gaboreau, S. 2013. Chapter 6 - Thermodynamics of Clay Minerals, in: *Developments in Clay Science*. Bergaya, F. and Lagaly, G. (Ed.), Elsevier, pp. 173-210.

Technical reports

Reference to a report should include the following information: author(s), date of publication, title and name of publisher. If the issuing organization assigns a number (e.g., report number, contract number, or monograph number) to the report, it should also be specified. Example:

Campos, I., Colàs, E. 2019. Bibliography. ThermoChimie technical report TCIII-2019-02E.

PhD thesis

The information needed to reference a thesis includes the following information: author of the thesis, date of publication, title, type of thesis (eg PhD, MSc) and the university or institution in which the thesis was completed. Example:

Colàs, E. 2014. Complexation of Th(IV) and U(VI) by polyhydroxy and polyamino carboxylic acids. PhD Thesis, Universitat Politècnica de Catalunya, Barcelona.

Entire website

When citing a Web site, no reference list entry is required if the address for the site is cited in the text of the document. When possible, the date of the consultation should be included.

<https://www.thermochimie-tdb.com/> (02 September 2019)

2.2 In-Text Citations

Citations are placed in the body of the document to identify the sources and to guide the reader to the source of the cited information in the reference list. The citations are referred with the name(s) of the author(s) and the year of publication (e.g. Giffaut et al., 2014). Citations using numbers (example [1], [1-3], etc...) are not recommended.

In general, for citations in the body of the document the following rules should be applied:

- If the cited study has two authors, both authors should be cited in the signal phrase or in brackets, followed by the year of publication. The word "*and*" should be used to separate the authors:

Parkhurst and Appelo (2013) or (Parkhurst and Appelo, 2013)

- If the cited study has more than two authors, only the first author's last name followed by "et al." and the year of publication, should be used in the signal phrase or in brackets:

Giffaut et al. (2014) explained.... or (Giffaut et al., 2014).

- If two or more cited studies have the same author and year, they must be differentiated by adding letters.

Giffaut et al. (2014a) and (Giffaut et al. 2014b).

- If the author is an organisation or a government agency, the citation should mention the organisation in the signal phrase or in brackets:

According to the Nuclear Energy Agency (2013)..... or (Nuclear Energy Agency, 2013)

- If the report is authored by ThermoChimie consortium, the citation should mention ThermoChimie in the signal phrase or in brackets:

According to ThermoChimie (2019)..... or (ThermoChimie, 2019)

2.3 References in ThermoChimie database

In the ThermoChimie database, references are stored using the format [YYAAA/BBB], where "YY" represents the last digits for the year of publication, "AAA" represents the three first letters of the first author's last name, and "BBB" the three first letters of the second author's last name. Examples are provided below:

[90CIA] Ciavatta, L. 1990. The specific interaction theory in equilibrium analysis. Some empirical rules for estimating interaction coefficients of metal ion complexes. *Annali di Chimica*, 80, 255-263.

[14GIF/GRI] Giffaut, E., Grivé, M., Blanc, P., Viellard, P., Colàs, E., Gailhanou, H., Gaboreau, S., Marty, N., Madé, B. & Duro, L. 2014. Andra Thermodynamic database for performance assessment: ThermoChimie. *Applied Geochemistry*, 49, 225-236.

3. Bibliographic database

Each contractor participating in the ThermoChimie project has to provide the database administrators with a list of all the literature references cited in their work. These files will be managed by the database administrators to create a bibliographic database that will fulfil the traceability requirements of ThermoChimie.

The bibliographic database needs to include:

- References available in the open literature: peer-reviewed articles, technical reports from agencies or institutions, etc.
- References not available in the open literature, for example documents reporting the results from the data acquisition program supporting ThermoChimie. These documents will be quoted as technical reports not available in open literature. It is worth mentioning that the general policy of ThermoChimie is to publish in peer-reviewed journals all the information generated in the development of the database. Nevertheless, due to time constraints and delays in publication, this is not always possible.

Usually, reference managers such as Endnote or Zotero are used during the development of the database. The main function of these reference managers is to store, manage and allow searching of references in a personal library. In addition, reference managers allow the reference library to be exported in different file formats. It is accepted, however, that contractors will deliver their bibliographic files to the database administrators in different formats according to their own preference. Examples of common bibliography formats are provided below:

- a) **EndNote:** the EndNote software (<http://endnote.com/>) is currently being used as a reference manager system for the ThermoChimie project. Thus, if EndNote is used by the contractor, a full EndNote library (.enl file) should be provided to the database administrators.
- b) **Other reference management system:** many other reference managers such as Zotero, Citavi, JabRef or Mendeley can generate reference lists in formats compatible with EndNote. When those reference managers are used, the contractor should provide to the database administrators an exported file in a format (.ris, .xml...) compatible with Endnote. A .txt document containing the references in Harvard citation style must also be delivered.
- c) **No reference manager system:** If the contractor does not use any reference manager compatible with EndNote, a full list of bibliographic references in Harvard citation style should be provided in a Word document.

The bibliographic reference list will be integrated in ThermoChimie database using the XCheck tool©. This tool is a VB.net based programme specifically developed to automate various processes related to ThermoChimie development (see Guideline 2: Data integration and consistency). The XCheck© tool is able to automatically link the full bibliographic references in the bibliographic database with the corresponding [YYAAA/BBB] internal citation.

4. Summary

This guideline summarises the way that the different types of publications (books, articles in journals, proceedings, technical reports, etc.) are referenced in ThermoChimie, and how the bibliographic database supporting ThermoChimie is developed.