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Modelling clay diagenesis using a combined crystalchemistry and thermochemistry approach: a case study on smectite illitization

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Abstract

A general procedure that integrates laboratory mineral analysis and numerical tools is proposed to investigate the main diagenetic processes occurring in clayey and arenaceous sediments. The methodology relies on the use of experimental data from natural samples as input, on the use of numerical algorithms to estimate the thermodynamic parameters of site-specific dehydrated phyllosilicates, and produce an internally consistent thermodynamic database in a ready-to-use format for the Geochemist's Workbench, PHREEQC, and TOUGHREACT simulators. A set of non-isothermal 0D and 1D numerical models is set-up to explore the efficiency of smectite-illite transformation under variable geochemical conditions.

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Keywords: Clay diagenesis; stoichiometry; illite; smectite; geochemical modelling, thermochemistry

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1. Introduction

Nomenclature

EDX	Energy Dispersive X-Ray
BRGM	Bureau de Recherches Géologiques et Minières
TDB	Thermodynamic Data Base
FESEM	Field Emission Scanning Electron Microscopy
GWB	Geochemist's WorkBench
I/S	Mixed layer illite/smectite
LogK	Logarithm of the thermodynamic constant of mineral formation
PEPITA	Parameter Estimation and Parameter Interpolation for Thermodynamic Analysis
PSM	Petroleum System Model
RTM	Reactive Transport Model
SSP	SUPCRT92 software package
XLS	MS Excel tool to estimate standard thermochemical parameters of phyllosilicate formation
XRD	X-Ray Diffraction
WDX	Wavelength Dispersive X-Ray

Diagenetic transformations occurring in layered sand and shale successions are complex processes depending on many parameters and coupled phenomena that should be taken into account when trying to formalize the web of reactions occurring in the sediments [1]. The main diagenetic process taking place in the clays is the smectite illitization that is considered to proceed more efficiently with the increase of depth (increase of pressure and temperature) and availability of potassium. This reaction greatly influences the chemical and physical evolution of the sediments, both clays and sandstones, and proceeds through the formation of I/S that are characterized by a progressive reduction of Si (as others cations as Fe, Ca), increase of Al and K and ordering in the structure [2, 3].

Numerical models may represent valid tests to check and verify the conceptual picture of such a diagenetic scheme although they may suffer the high crystalchemistry variability of the clay mineral phases and the lacking of the thermodynamic and kinetics parameters to describe their reactive behaviour. The kinetics parameters are usually not available and sensitivity is the generally accepted approach used to overcome these limitations. On the contrary, the thermochemical parameters can be estimated from the stoichiometry and the structure of the pure mineral phase through different methods [4].

The aim of the present activities is the compilation of a consistent thermodynamic database to describe and model the smectite illitization reaction in burial diagenesis environments. This reaction has a pivotal role in influencing the physico-chemical and mechanical properties of the sediments, mainly due to:

- mobilization and redistribution of the chemical elements (as K,Al,Si, Fe, Ca, Mg and H_2O);
- changes in sediment porosity (silica precipitation);
- overpressure (water release).

2. Methodology

A procedure that combines (i) laboratory analysis of the clays, (ii) estimation of specific thermochemical parameters and (iii) geochemical numerical models is proposed to investigate the illitization of smectite in different geochemical contexts.

The numerical procedure (PEPITA) consists of the following steps (Fig. 1):

- smectite, illite and I/S from natural samples are firstly investigated in the laboratories for their structural characteristics and analyzed for their chemical composition;