Thermoddem: an example of alive thermochemical database

LASSIN A.[1], BLANC P.[1], ANDRE L.[1], MARTY N.[1], PARMENTIER M.[1], MOYARD S.[2], AZAROUAL M.[1], PIANTONE P.[1], GAUCHER E.C.[1], KERVEVAN C.[1] AND TOURNASSAT C.[1]

[1]BRGM, 3 av. C. Guillemin, B.P. 36009, 45060 Orléans, France
[2]CASPEO, 3 av. C. Guillemin, 45060 Orléans, France

The basic goal of the Thermoddem thermochemical database [1] (http://thermoddem.brgm.fr/) is to gather standard thermodynamic data regarding chemical compounds encountered in most water-solid-gas systems, with a specific concern for environmental issues, cement phases and clay minerals. The construction of the database (since 2006) relies on a careful selection of published experimental data, constrained by a rigorous internal consistency. Data selection combines both solubility and calorimetric data in order to strengthen the coherence of the data set. A particular effort is paid to identifying the source of every data. Some examples will be presented for illustration.

A major objective of thermochemical databases (TDB) is to be integrated into coupled reactive transport modelling codes. Therefore, it is of key importance to provide database formats adapted to the most widely used calculation codes and to make them freely available on the Internet. In addition, Thermoddem includes mineralogical and geological information to help the modeller to define and to select the geochemical reactive system in agreement with the problematic to handle.

Geochemical and reactive transport modelling covers a wide range of temperature and pressure conditions, numerous reactive mechanisms (aqueous complexation, surface complexation and ionic exchanges, dissolution/precipitation or degassing reactions, kinetic processes, bacterial activity), and various contexts (dilute/saline waters, isobaric/anisobaric conditions). Models implemented in calculations codes for describing the different geochemical mechanisms evolve with time and new concepts are perpetually developed. Alive TDB have to adapt to these evolutions as for Thermoddem, which is this way developed. However one has to acknowledge that, despite the wide use of thermochemical databases, there is still a need for gathering a community that would actively contribute to help improving these tools. Furthermore a better scientific recognition could help supporting their development and maintenance.

[1] Blanc P., Lassin A., Piantone P., *et al.*. (2012) Appl. Geochem. 27(10), 2107-2116

How depleted is the upper mantle? Constraints from elemental-Os isotope correlations in abyssal peridotites and ocean island xenoliths

J.C. LASSITER*[1] AND B.L. BYERLY[1]

[1] Jackson School of Geosciences, University of Texas at Austin, Austin, TX, USA (* lassiter1@jsg.utexas.edu)

It is generally accepted that the convecting upper mantle is depleted in incompatible trace elements as a result of prior melt extraction. However, the amount of melt depletion that has occurred and the extent to which this has effected the major element composition of the mantle is less certain. *Workman & Hart* [1] estimated the composition of MORB-source mantle utilizing both MORB and abyssal peridotite (AP) compositional trends and inferred a relatively fertile bulk composition (e.g., Al_2O_3 > 4 wt.%) consistent with minor long-term melt depletion of ~3-4%, assuming a primitive mantle Al_2O_3 content of ~4.4 wt.% and that the melt extracted had a roughly MORB-like composition. *Walker et al.*. [2] also inferred limited long-term melt extraction (2-3%) based on Os-isotope systematics of ophiolite chromitites.

We have examined correlations between indices of peridotite fertility (Al_2O_3, spinel Cr#) and Os-isotopes in both APs and ocean island peridotite xenoliths (OIPs) to better constrain the average $^{187}Os/^{188}Os$ of the upper mantle, the average age of melt depletion, and the extent of melt depletion required to generate the observed major element-isotope correlations. APs and OIPs have statistically indistinguishable average $^{187}Os/^{188}Os$ (0.1244 versus 0.1245), and are considerably less radiogenic on average than chromitites derived from modern ophiolites (~0.1281; [2]). Both APs and OIPs display positive global correlations between fertility indices and $^{187}Os/^{188}Os$. The Al_2O_3-$^{187}Os/^{188}Os$ trends of both suites define aluminachron "ages" of ~1.5 Ga, similar to the average T_{Ma} ages of both populations. Combined, these trends suggest upper mantle peridotites have an average $^{187}Os/^{188}Os$ of ~0.1245 and the average age of melt depletion is ~1.5 Ga. If extraction of oceanic crust is the primary mechanism for depleting the upper mantle, then the degree of MORB melt extraction required to generate an average upper mantle Os-isotope value consistent with APs and OIPs is ~10-12%, significantly greater than previuos estimates of upper mantle depletion. During mantle upwelling, the degree of melt generated from a mantle packet is a function of initial fertility. MORB therefore oversample fertile components in the mantle, which likely accounts for the apparent conflict between our estimate of average mantle peridotite fertility and that of [1].

[1] Workman & Hart (2005), *EPSL* **231**, 53-72. [2] Walker *et al.*. (2002), *Geochim. Cosmochim. Acta* **66**, 329-345.

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