

IUPAC Project Progress Report

Date : December 2005 ; Period: July 2005 – February 2006

Project number: 2002-031-1-500

Project Title: Solubility data of compounds relevant to mobility of metals in the environment. Alkaline earth metal carbonates

Task Group Leader: Alex De Visscher

Starting date:

Report:

1. *Projected completion date (documents ready for external review):*
December 2006

2. *Have the project objectives been modified during the last 6 months?*
The scope of the modelling part of the project was clarified during the SSED annual meeting in Portoroz. No major changes.

3. *Please list the task group members involved in the work during the last 6 months.*
Alex De Visscher, Jan Vanderdeelen

4. *Difficulties encountered (or concerns):*
I have been informed by J. Lorimer that the compilation is incomplete as he is still preparing some compilations. This could potentially lead to substantial delays as it might require me to redo the evaluation and modelling parts.

5. *Please list the to-date results (outputs) of the project:*
Compilation: (nearly ? see above) complete
Evaluation: Data arranged in tables, except for aragonite and vaterite. An evaluation had been done, but this is being thoroughly reworked by introducing more appropriate empirical equations. A Pitzer model was developed for the metal carbonate – H₂O – CO₂ data and tentative thermodynamic constants were derived. These still need to be checked against independent thermodynamic data, eg. on the calcite-aragonite transition.

6. *Please list the dissemination events (viz. articles, CD, conference presentations; etc.)*
(i) already accomplished:

De Visscher A. & Vanderdeelen J. Estimation of the solubility constant of calcite, aragonite and vaterite at 25°C based on primary data using the Pitzer ion interaction approach. *Monatsh. Chem.* **134**, 769–775 (2003).

De Visscher A. & Vanderdeelen J. Consistency issues of aqueous solubility data and solution thermodynamics of electrolytes. *Pure Appl. Chem.* **77**, 619–629 (2005).

Aveiro, Portugal, 26–29 July 2004, 11th International Symposium on Solubility Phenomena, Oral presentation: De Visscher A. & Vanderdeelen J., Consistency issues of solubility data and solution thermodynamics of electrolytes.

(ii) planned: A volume of the IUPAC-NIST Solubility Data Series is in preparation for publication in *J. Phys. Chem. Ref. Data*.

7. If your project is within 6 months of completion, how do you plan to utilise any remaining budget for this project?

Not applicable

8. Work on this project may have identified new problems, issues, challenges, emerging topics, opportunities for related projects, etc.

Future work should emphasize high-pressure work, because there is an increased interest in the carbon dioxide storage capacity of deep underground aquifers, often in the presence of carbonate minerals. This includes evaluation of CO₂ volumetric properties near its critical point, and high-pressure CO₂ solubility data.