

IUPAC Project Progress Report

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

Project number:2005-016-1-100

Project Title: Developments and Applications in solubility

Task Group Leader: Trevor Letcher

Starting date: June 2005

Report:

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

The book is nearing completion and so far I have received and edited most of 15 of the total of 26 chapters. If any authors fail to meet the deadline they will be axed. The next step is to complete the remaining editing and get the final copy to the Royal Society for Publication. I expect this to happen in April or May and the book should be published in December 2006. On the advice of my Task Group, the title has changed to reflect the proper message of the book

2. Have the project objectives been modified during the last 6 months? No

3. Please list the task group members involved in the work during the last 6 months.

Professor Rubin Battino (Wright State University), Dr Justin Salminen (Berkeley, California) and Glen Hefter (Perth)

4. Difficulties encountered (or concerns):

nil. It has been a trouble free project and I must thank my colleagues for their input.

5. Please list the to-date results (outputs) of the project

DEVELOPMENTS AND APPLICATIONS IN SOLUBILITY – 26 CHAPTERS

Theory, Techniques and Results

1. Thermodynamics of Nonelectrolyte Solubility by Professor Emmerich Wilhelm (Vienna), Emmerich.Wilhelm@univie.ac.at

2. Thermodynamics of Electrolyte Solubility by Professor Earle Waghorne (Dublin) earle.waghorne@ucd.ie

3. Solubility of Solids in Bayer Liquors by Professor Glen Hefter (Murdoch), Professor Eric Koenigsberger and Professor Peter May. g.hefter@murdoch.edu.au

4. Solubility of Solids in Radioactive Waste Repositories by Dr Wolfgang Hummel (Paul Scherrer Institute, Switzerland). wolfgang.hummel@psi.ch

5. Solubility of Gases, Ionic Liquids, Solvents and Aqueous Solutions by Professor G Maurer (Kaiserslautern). gmaurer@rhrk.uni-kl.de
6. Solubility Phenomena in “green” Quaternary Mixtures (ionic liquid + water + alcohol + CO₂) by Professor Luis P N Rebelo and Professor M Nunes da Ponte (New University, Lisbon). luis.rebelo@itqb.unl.pt .
7. Solubility in Water and Seawater by Professor Rubin Battino (Wright State) and Professor Larry Clever. rubin.battino@wright.edu and hlclever@worldnet.att.net
8. Isotopic Effects in Solubility by Professor Alexander van Hook (Tennessee, Knoxville) and Professor Luis P N Rebelo (New University, Lisbon). avanhook@utk.edu
9. Solubility of Organic Solids for Industry by Professor U Domanska (Warsaw). ula@ch.pw.edu.pl
10. Solubility of Gases in Molten Salts by Professor Reg Tomkins (New Jersey.) tomkinsr@adm.njit.edu
11. Solubility of Impurities in Cryogenic Liquids by Professor Dominique Richon (Ecole Des Mines, Paris), richon@paris.ensmp.fr and Dr V de Stefani (Imperial College, London).
12. Solubility of BTEX and Acid Gases in Alcanolamine Solutions in relation to the Environment by Professor Dominique Richon (Ecole des Mines, Paris) and Dr C Coquelet. richon@paris.ensmp.fr

Modeling and Simulation

13. Solubility and Molecular Modeling by Professor M Costa Gomes (Clermont Ferrand). margarida.c.gomes@univ-bpclermont.fr .
14. Molecular Simulation Approaches to Solubility by Professor J Ilja Siepmann and Professor Kelly E Anderson (Minnesota). siepmann@chem.umn.edu
15. "Predicting Solubility with COSMO-RS" by Dr Frank Eckert (COSMOGermany) Eckert@cosmologic.de

Industrial Applications

16. Solubility of Gases in Polymers by Professor Jean-Pierre Grolier and Dr S Boyer (Clermont Ferrand). j-Pierre.grolier@univ-bpclermont.fr
17. Solubility in the Metallurgical and Hydrometallurgical Processes by Dr J Salminen and Professor T Khashiala (Helsinki). justin.salminen@hut.fi

18. Solubility related to Reaction and Process Design by Professor Ralf Dohrn (Bayer, Germany), Dr Ricarda Leiberich (Bayer, Germany) and Dr Ljudmila Fele (NIC, Slovenia) ralf.dohrn@bayertechnology.co
 19. Solubility in the Pharmaceutical Industry by Professor Jacques Fages (Ecole des Mines, d'Albi). jfages@enstimac.fr
 20. Solubility in Food, Pharmaceutical and Cosmetic Industries by Professor Maria Eugenia Macedo (Porto) and Professor Simão Pedro de Almeida Pinho (TI Bragança) eamacedo@fe.up.pt
 21. Solubility Data and Predictions in Industry by Professor Jürgen Gmehling (Oldenburg) and Dr W Cordes (DDBST). gmehling@tech.chem.uni-oldenburg.de
 22. Solubility of Gases in Industry by Professor Joan Brennecke (Notre Dame). jfb@nd.edu or joan.brennecke.1@nd.edu
 23. Solubility of CO₂ in Industrial Applications by Professor John Prausnitz and Dr J Salminen (Berkeley). justin.salminen@hut.fi
 24. Solubility of the Oil Industry by Dr Tony Goodwin (Schlumberger Products) and Professor K Marsh(Canterbury) agoodwin@slb.com
 25. Solubility in Super Critical Fluids by Professor Cor Pieters (Delft). cor.pieters@tnw.tudelft.nl
 26. Solubility of Inorganic solids and their importance in Industry by Professor Wolfgang Voigt (Freiberg) wolfgang.voigt@chemie.tu-freiberg.de
6. Please list the dissemination events (viz. articles, CD, conference presentations; etc.)
- (i) already accomplished; 15 of the above are almost complete and edited and the remainder will be done by April – May.
 - (ii) planned All going to plan.
7. If your project is within 6 months of completion, how do you plan to utilise any remaining budget for this project?
- Visiting Cambridge to sort out editing issues with the publisher, payment for faxes, computing etc . (I no longer have free University computing as I have retired to ther UK for the duration of writing and editing books), and visiting London to discuss issues of two chapter that need some advice.
8. Work on this project may have identified new problems, issues, challenges, emerging topics, opportunities for related projects, etc. Please indicate these here so that the Division can follow up on them.
- There are no new problems but many new and exciting issues that are coming from the chapters.