

Subsurface Environmental Simulation Benchmarking Workshop V



www.turismocoruna.com

A Coruña (Spain)
October 13th -15th, 2016

J. Samper, L. Montenegro & A. Naves Eds.



UNIVERSIDADE DA CORUÑA



CICA
ADVANCED SCIENTIFIC
RESEARCH CENTER

Background

The complexity and detail of subsurface processes, properties and conditions to be addressed in subsurface science and engineering has significantly increased in order to provide accurate assessments of risk and engineering. In order to guarantee confidence and reliability of simulation tools, benchmark problems are indispensable to qualifying appropriate modelling approaches and codes.

The Subsurface Environmental Simulation Benchmarking workshops are an initiative for benchmarking subsurface environmental simulation methods with a current focus on reactive transport processes.

Each benchmark exercise consists on several cases with gradually increasing complexity. The aim is to provide a basis for resolving the discrepancies between code bases, but should also increase the number of problems that can be attempted by interested modelers.

The first workshop, organized by Carl Steefel and Steve Yabusaki, took place in Berkeley in 2011. After, the workshop series continued in Taiwan, Leipzig (Germany) and Cadarache (France):

- SS Bench I, organized by LBNL, in Berkeley (USA) in November of 2011
- SS Bench II, organized by the Graduate Institute of Applied Geology of National Central University and the National Science Foundation of Taiwan, in Taiwan between October and November of 2012
- SS Bench III, organized by Helmholtz Centre for Environmental Research – UFZ, in Leipzig (Germany) in November of 2013
- SeS Bench IV, co-organized by CEA, Andra, BRGM and Mines Paristech, in Cadarache (France) in August of 2014.

The University of A Coruña hosts and organizes the SeS Bench V which will take place in A Coruña from the 13th to the 15th of October of 2016.

Scientific Committee

- Olivier Bildstein. CEA. Cadarache (France).
- Francis Claret. BRGM. Orleans (France).
- Laurent De Windt. EMP. Paris (France).
- Olaf Kolditz. UFZ. Leipzig (Germany)
- Uli Mayer. UBC. Canada
- Javier Samper. UDC. La Coruña (Spain).
- Carl Steefel. LBNL. California (USA)
- Tianfu Xu. Changchun (China)
- Steve Yabusaki. PNNL. Handford (USA)
- George Yeh. NCU. Taiwan.
- Georg Kosakowski. PSI. Switzerland

Organizing Committee

- F. Javier Samper Calvete
- Luis Montenegro Pérez
- Antonio Paz González
- Acacia Naves García-Rendueles
- Bruno Pisani Veiga
- Alba Mon López
- Jesús Fernández Águila

From: Water and Soil Research Group
Centro de Investigacións Científicas Avanzadas (CICA)
Universidade da Coruña

Workshop program

Thursday 13th

Welcome to SeS bench V

14:30	Welcome	Javier Samper
	Program and organization	Organizing committee
	SeS Bench overview	Scientific committee

Session 1 – Geological Storage of Radioactive Waste *Chairman: F. Claret*

15:00	Modelling of Radionuclides Migration in the Low Ph Cement/Clay Interface	Vanessa Montoya
15:30	Benchmarking of Caesium Migration through Opalinus Clay Calculated by a Single-Species Model Using a Measured Non-Linear Sorption Isotherm and a Multi-Species Transport Model	Jesús Fernández
16:00	Modelling Approach to the Evolution of Physicochemical Conditions in Deep Geological Repository Conditions: Alteration of Engineered Materials And Redox Control	Olivier Bildstein

16:30  *Coffee break*

Session 2 – Redox processes and reactive transport at interfaces and dynamic update of parameters *Chairman: S.Yabusaki*

17:00	Benchmarking of Reactive Transport Codes for a 2D Setup with Mineral Dissolution/Precipitation Reactions and Feedback on Transport Parameters	Jenna Poonoosamy
17:30	A Benchmark for Microbially Mediated Chromium Reduction under Denitrifying Conditions in a Biostimulation Column Experiment	Andreas Rupp
18:00	Modeling Laboratory Scale Experiment (TRACE and SPECY) of Fe-Cr Redox Reaction along with Precipitation and Porosity Change	Jérôme Carrayrou

 *Let's have some "tapas"!*

Friday 14th

Session 3 – Coupled THMC problems *Chairman: G. Kosakowski*

9:00	Benchmarking of an Explicitly Coupled THMC Model with a Tailing Site	George Yeh
9:30	Calibration of Water-Granite Interaction with Pressure Solution in a Flow-Through Fracture Under Confining Pressure	Renchao Lu

Session 4 – Isotopic Fractioning**Chairman: B. Cochepin**

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| 10:00 | A Reactive Transport Benchmark for Kinetic Isotope Fractionation Associated with Mineral Precipitation | Carl I. Steefel |
| 10:30 | Stable and Radioactive Carbon Isotope Partitioning in Soils and Saturated Systems: A Reactive Transport Modeling Benchmark Study | Jennifer Druhan |
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11:00  *Coffee break*

Session 5 – Integrated Surface-Subsurface Models**Chairman: C. I. Steefel**

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| 11:30 | A Benchmark Problem for Biogeochemical Cycling Induced by Seasonal Water Table Dynamics in A Heterogeneous, Variably-Saturated Floodplain | Steve Yabusaki |
| 12:00 | Modeling Integrated Surface Subsurface Water Flow and Biogeochemical Cycling in the Hyporheic Zone | Dwivedi Dipankar |
| 12:30 | Benchmarking Integrated Surface-Subsurface Models along a Hillslope Transect | Bhavna Arora |
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13:00  *Lunch at MUNCYT*

Session 6 – Unsaturated/multiphase processes**Chairman: G. Yeh**

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| 14:00 | A Benchmark for Multiphase Multicomponent Flow with Geochemical Reactions | Peter Knabner |
| 14:30 | Numerical Modeling of Coupled Two-Phase Multicomponent Flow with Reactive Geochemical Transport in Porous Media | Etienne Ahusborde |
| 15:00 | A Numerical Investigation on the Influence of the Water Availability on the Temporal Evolution of the Waste Package | Yonghui Huang |
| 15:30 | Compressible Multicomponent Two-Phase Flow in HYTEC: Some Applications to Gas Injection and Impact of Impurities | Vincent Lagneau |
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16:00  *Coffee break*

Session 7 – New Topics, New Challenges**Chairman: O. Bildstein**

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| 16:30 | A Benchmark for Mineral Dissolution at the Pore Scale | Sergi Molins |
| 17:00 | Grain-Scale Modelling of Cesium Transport in Fracture – Rock Matrix Systems: A Benchmark Case for Upscaling Mineralogical Heterogeneity at Sub-Millimetre Scale | Paolo Trinchero |
| 17:30 | Diffusion in The Diffuse Layer at Clay Mineral Surfaces. Solving Boundary Conditions and Discontinuity Problems | Christophe Tournassat |

18:30 *Panoramic tour through A Coruña shore*



20:45



Dinner

Restaurante Coral

Avenida de la Marina 9

<http://www.restaurantecoralacoruna.com/es/>


Saturday 15th

Session 8 – Less developed benchmarks

Chairman: J. Samper

9:00	Non-isothermal benchmark of interactions of concrete, bentonite and clay	Alba Mon
9:30	A Benchmark Problem for Tc in Cementitious Waste Forms	Steve Yabusaki
10:00	A Benchmark Problem for Root Structure and Function in Soil	Steve Yabusaki

Summary and conclusions

10:30	Summary of outcome	All
11:00	 <i>Coffee break</i>	
11:30	Summary of outcome (continued) Integration, synthesis and development of milestones	All
13:00	<i>End of the workshop</i>	
