



## 27-28 June 2019

Knowledge's frontiers in water unsaturated hydrogeosystems: interface dynamics, heterogeneities & couplings



ORLÉANS

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### LOCATION

Observatoire des Sciences de l'Univers en région Centre (OSUC) Campus Géosciences 1A Rue de la Férollerie 45100 Orléans - FR

### CONVENORS Dr Mohamed Azaroual & Prof. Lionel Mercury

Earth Sciences Institute of Orléans (ISTO) / University of Orléans, CNRS, French

Geological Survey (BRGM) - FR

ISTO 🔕 🔊 🌐 INRA



Dr Mohamed Azaroual & Prof. Lionel Mercury, Earth Sciences Institute of Orléans (ISTO) / University of Orléans, CNRS, French Geological Survey (BRGM) - FR

## LE STUDIUM WORKSHOP ORLÉANS | 2019 PROGRAMME & ABSTRACTS

Knowledge's frontiers in water unsaturated hydrogeosystems: interface dynamics, heterogeneities & couplings

LE STUDIUM WORKSHOP Knowledge's frontiers in water unsaturated hydrogeosystems: interface dynamics, heterogeneities & couplings | 27-28 June 2019

# EDITO

Created in 1996 on the CNRS campus in Orleans La Source, LE STUDIUM has evolved to become a multidisciplinary Loire Valley Institute for Advanced Studies (IAS), operating in the region Centre-Val de Loire of France. LE STUDIUM has its headquarters in the city centre of Orleans in a newly renovated 17th century building. The amazing facilities are shared with the University of Orleans. In 2014 new developments and programmes linked to the smart specialisation of the Centre-Val de Loire region came to strengthen existing IAS cooperative relationships with the local and the international community of researchers, developers and innovators.

LE STUDIUM IAS offers to internationally competitive senior research scientists the opportunity to discover and work in one of the IAS's affiliate laboratories from the University of Tours, the University of Orleans, National Institute of Applied Sciences (INSA) Centre Val de Loire and ESAD Orléans, as well as of nationally accredited research institutions located in the region Centre-Val de Loire (BRGM, CEA, CNRS, INSERM, INRA, IRSTEA). Our goal is to develop and nurture trans-disciplinary approaches as innovative tools for addressing some of the key scientific, socio-economic and cultural questions of the 21st century. We also encourage researchers' interactions with industry via the IAS's links with Poles of Competitiveness, Clusters, Technopoles, and Chambers of Commerce etc.

LE STUDIUM has attracted over one hundred and ninety LE STUDIUM RESEARCH FELLOWS and LE STUDIUM RESEARCH PROFESSORS for long term residencies. In addition to the contribution in their host laboratories, researchers are required to participate in the scientific life of the IAS through attendance at monthly interdisciplinary meetings called LE STUDIUM THURSDAYS and gathering members of the regional scientific community and industries.

For the period 2015-2021, LE STUDIUM operates with an additional award from the European Commission in the framework of the Marie Skłodowska-Curie Actions (MSCA) with the programme MSCA-COFUND for the mobility of experienced researchers. This co-funding instrument increases the number

of LE STUDIUM fellowships to be awarded each year. LE STUDIUM is also the official partner of the Ambition Research and Development 2020 (ARD 2020) initiated by the region Centre-Val de Loire, that supports the specialisation strategy around 5 main axes: biopharmaceuticals, renewable energies, cosmetics, environmental metrology and heritage intelligence.

Researchers are also invited and supported by the IAS to organise, during their residency and in collaboration with their host laboratory, a two-day LE STUDIUM CONFERENCE. It provides them with the opportunity to invite internationally renowned researchers to a cross-disciplinary conference, on a topical issue, to examine progress, discuss future studies and strategies to stimulate advances and practical applications in the chosen field. The invited participants are expected to attend for the duration of the conference and contribute to the intellectual exchange. Past experience has shown that these conditions facilitate the development or extension of existing collaborations and enable the creation of productive new research networks.

We thank you for your participation and wish you an interesting and intellectually stimulating conference. Also, we hope that during these days in our region some of you will see an opportunity to start a productive professional relationship with LE STUDIUM Loire Valley Institute for Advanced Studies and research laboratories in the region Centre-Val de Loire.

Yves-Michel GINOT

Chairman LE STUDIUM

Ung:wh

### CONTEXT

The understanding of the behavior of the Critical Zone (CZ) in response to the global changes requires the integration of geological, geochemical and biological cycles and their couplings at different and relevant time-space scales. The O-ZNS platform (Observatory of the Vadoze Zone (VZ) of the Beauce carbonate aquifer) is a part of the PIVOTS regional program (Innovation Platforms for the valorisation and optimization of environmental technologies: <u>https://plateformes-pivots.eu/</u>) with a main objective directed to the understanding of mass and heat transfer mechanisms and the fate of pollutants in the CZ compartments. The O-ZNS observatory consists of a well prospecting the entire thickness of the VZ up to the water table, with a finite diameter of ~ 4 m and a depth of ~ 20 m. The site is located in the Beauce region, in a heterogeneous carbonaceous formation, with a typical sequence (from top to bottom): ground/cryoturbated limestone / limestone marl / fractured micritic limestone. The well will be equipped with environmental monitoring, soil, and subsoil imaging tools in order to understand reactive transport phenomena and exchanges of mass and heat between phases (water - rock – gas) throughout the continuum «Soil - Unsaturated Zone - Capillary Fringe - Aquifer.

The field acquisitions of long-term environmental data target are crucial to identify the fingerprints of complex and coupled physical, physicochemical and microbiological processes as well as their role in fixation, degradation and / or transfer of pollutants in the VZ. This obviously requires multidisciplinary skills, complementary methods and result joint interpretations as well as renewed theoretical approaches. The development of O-ZNS platform aims to build a large and sustainable partnerships (academic, industrial, state agencies, etc.), at national and international scales, in a collaborative way that guarantees the continuity between the academic research, industrial needs and the academic training of young engineers and researchers.

Beyond the equipment itself, O-ZNS aims also at becoming a place to discuss the scientific issues related to unsaturated geological media. This

can be either naturally developed within the CZ compartments, or created by industrial purposes at various depths in the underground for  $CO_2$  and energy vectors storage and extraction of non-wetting energy substances where the active interfaces between phases play a key role in mass and energy exchanges inducing important petrophysical evolutions of targeted reservoirs and geological structures.

### AIMS

The workshop aims at gathering high-level scientists, to share their points of view, methodologies, certainties and open questions, within a pluridisciplinary and transversal approach to tackle complex problems. The exchanges are organized around the mechanistic understanding and the spatialized phenomenology of the multiphasic reactive transport within unsaturated hydrosystems impacted by global changes and man activities, as are the critical zone, the depleted aquifers, the deep underground targeted for nuclear wastes, energy and  $CO_2$  storages, and associated environmental issues.

Unsaturated hydrosystems express a multiplicity of coupled problems that can be tackled by a large range panel of scientists coming from diverse community and horizons: geologists, hydrogeophysists, soil and sedimentary scientists including thos turned to the structure of the reservoirs and petrophysics, carbonate rocks and karst sciences, field - experimental - theoretical geochemists, physical chemists of natural systems, fluid mechanics scientists, specialists into georeferenced mapping and information systems, geostatistics applied to environmental risk assessment and vulnerability maps, and associated geoscience domains.

Beyond the scientific themes, a key aspect of the workshop is the scale debate (from cap rocks and reservoirs of deep geosystems to the micromodels of the Lab-on-a-Chip emerging approach), with the familiar upscaling-downscaling issues to identify critical surfaces for mass/heat exchanges with associated electrokinetic and electrochemical processes.

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The workshop will gather scientists and engineers from academic laboratories, with specialists coming from the industry R&D groups, facing through different pathways, practices to the anthropogenic and global change pressure on the natural resources, and induced ecological issues.

### ORGANIZATION

The workshop is organized over two days as an open debate and free brainstorming among the participants, informal but intense and highly focused. To do this, the agenda of these two days (June 27 and 28) is structured as follows.

### DAY 1

The 1<sup>st</sup> day is focused on two main themes, with some dense lectures (10-15 mn) guiding the brainstorming of the group. Each lecturer has in charge the animation of a further dynamic stimulating very open and participative debate (20-30 mn) sharing and pushing deeply the thinking and questions emerging from the audience. At the end of each theme of discussions, a general synthesis and output will be lively elaborated to capitalize and mutualize new outcomes to progress in the shared steps of constructive discussions.

### DAY 2

The 2<sup>nd</sup> day, four round tables would have in charge of an extended and deepening exploitation of the challenges collected on the 1<sup>st</sup> day, re-expressed within the real context of O-ZNS and open perspectives. The workshop will come to the end with a final synthesis of the exchanges outcomes during the last half-day.

During these two scientific days of the workshop, each participant may propose a focused pitch of 3-5 minutes to contribute to the open debate and to stimulate the group brainstorming.

# Programme

### **THURSDAY 27<sup>TH</sup> JUNE 2019**

**08h30** Welcome & Introduction of the Workshop.

Anne BESNIER: Vice-President for Higher Education and Research, Center Region – Val de Loire Pierre TOULHOAT: Deputy CEO & Scientific Director of BRGM

Susan HUBBARD: Associate Laboratory Director, Berkeley Lab, Earth and Environmental Sciences

Ioan TODINCA: Vice-President of University, Research Services, University of Orléans

### **THEME 1: THE "FOUNDING STONES"**

09h00 Dr Mohamed Azaroual (ISTO, BRGM)

Renewing conceptualization combining laboratory and fields, measurements and modelling, nm- to km-scales: the DNA of 0-ZNS platform.

09h45 Dr Jennifer Druhan (University of Illinois)

Signatures of carbon respiration in deep Critical Zone structure and function.

**10h30** Dr Dani Or (*Dept. of Environmental Systems Science, ETH Zurich*) The challenges of monitoring the deep critical zone – going under the living skin of the Earth.

### 11h15 BREAK

### 11h30 Dr Pierre Toulhoat (BRGM)

Mechanistic-local vs. spatialized-distributed representations, geochemical vs. geophysical signatures, fields vs. labs: how to read deeply the nature ?

### 12h15 Dr Yuxin Wu (LBNL)

Mesoscale research: tools, workflows and lab - field co-design.

### GENERAL SYNTHESIS OF THE HIGHLIGHTS AND THE MAIN OUTCOMES

### 13h00 LUNCH

### THEME 2 : THE GEOSCIENCES CHALLENGES AND COUPLED/UNCOUPLED PROCESSES

### 14h00 Dr André Revil (CNRS, ISTerre, University of Grenoble)

Couplings coefficients in geophysics: a tool toward quantification and a mine of second order information for understanding key mechanisms. What are the interdisciplinary bridges ?

### 14h45 Dr Benoit Noetinger (IFP Energies Nouvelles)

A critical review of upscaling-downscaling procedures from geosciences perspective = mean-field petrophysic properties, heterogeneities. What are the relevant scales to capture meaningful signal ?

### 15h30 Dr Mohamed Azaroual (ISTO, BRGM)

Reactive transport and thermo-kinetic approaches – key mechanisms, recent advancements, some current limitations and perspectives.

### 16h15 BREAK

16h30 Dr Renaud Toussaint (CNRS, UNISTRA, University of Strasbourg)

Observing flow and deformation using different techniques - examples in fluid flow induced internal fractures and in landslide dynamics: comparing optical and seismic imaging.

17h15 Prof. Lionel Mercury (ISTO, University of Orléans)

Using micro-models to simulate critical zone's features: the analogy framework for hydro-chemo-poromechanical couplings.

### GENERAL SYNTHESIS OF THE HIGHLIGHTS AND THE MAIN OUTCOMES

FRIDAY 28<sup>TH</sup> JUNE 2019

**ROUND TABLE 1 - STATIC STRUCTURES - DYNAMIC PROPERTIES RELATIONSHIPS** 

**08h30** Moderated by Simon Andrieu (*BRGM*), Pascal Audigane (*BRGM*) & Gautier Laurent (*University of Orléans, ISTO*).

The following topics as well as related questions will be debated:

Karst developments, porous/fractured & dual media

Petrophysic properties of the carbonate rocks

Conceptualizing the mass flows and numerical models

Hosts vs. guests or Container vs. Content – key scientific challenges.

ROUND TABLE 2 - *IMAGERY, SPATIALIZATION AND DISCONTINUITIES IN GEOLOGICAL* **09h30** Moderated by Gilles Grandjean (*BRGM*), Renaud Toussaint (*CNRS*) & André Revil (*CNRS*). The following topics as well as related questions will be debated:

Physical chemical of interfaces and physical signatures

Data acquisition, localization, interpolation and joint interpretations

Visible and supposed/interpreting discontinuities

Scales and relevant supports to tackle the locks:

O-ZNS observatory – Mesoscale platforms as PRIME and EcoSENS – Lab scale: flow through columns and GLoCs.

Modelling challenges: hybrid mesh – deterministic/stochastic for predictivity – mechanistic calibration – micro-continuum approach and couplings.

### 10h30 BREAK

### ROUND TABLE 3 - HYDROSYSTEMS DYNAMICS AND COUPLINGS

11h00 Moderated by Mohamed Azaroual (ISTO, BRGM), Lionel Mercury (ISTO,

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### BRGM), Christophe Tournassat (ISTO)

### The following topics as well as related questions will be debated:

Interfaces = capturing discontinuities, concentrated driving forces, an aggregation area Buffered zones, quasi-steady states, reactive/moving fronts.

The inverse models, the role of the ghost zones and ephemeral phenomena.

From fields to the lab, from labs to model, and back to the fields: there any virtuous loop / workflow?

The virtuous linkage between research and training: from research to training, from training to the engineering & geotechnological needs and back to research.

### 12h00 LUNCH

**ROUND TABLE 4 - SMART SENSORS FOR ENVIRONMENT AND GEOSCIENCES** 

**13h30** Moderated by Raphaël Canals (*PRISME, University of Orleans*), Emeric Frejafon (*BRGM*), Yuxin Wu (*LBNL*)

The following topics as well as related questions will be debated:

Passive samplers and physical chemical monitoring tools.

How to install multi-parameter monitoring measurements for high resolution and massive data generation?

Smart architecture of multidisciplinary monitoring technics (T, µmovements, etc.).

### **ROUND TABLE 5 - ARTIFICIAL INTELLIGENCE FOR ENVIRONMENTAL ISSUES**

**14h30** Moderated by Charles Gumiaux *(ISTO, University of Orléans)*, Vincent Labbé *(BRGM)*, François Robida *(BRGM)* 

### The following topics as well as related questions will be debated:

Machine and deep learning for spatial environmental data.

How novel data science, data mining, and artificial intelligence techniques can innovate and inform environmental modeling practices.

Interoperability & Preparing and Architecturing for Machine Learning.

### 15h30 BREAK

GENERAL SYNTHESIS OF THE WORKSHOP

### 16h00 Academics, Industrials, The people in-between

What are the main outcomes?

What can we expect, who will do, when/where re-meeting to record advances and update the issues and objectives?

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## ARD 2020 PIVOTS PROGRAMME



The PIVOTS project is a coordinated set of seven experimental and analytical platforms focused on environmental quality monitoring and sustainable management of natural resources (soil, subsurface, surface water, groundwater, sediment and air) within a context of global change (increased anthropogenic pressure and climate change).

The innovation through PIVOTS is founded on an integrated approach based on excellent research by academic and industrial experts together at all stages of the value chain, from fundamental research to validation of products and services.

The platforms are identified as:

DECAP: Development of Environmental Sensors and Pollutants Removal Processes

PRIME: Remediation and Innovation in the Service of Environmental Metrology

**O-ZNS:** Observatory of transport in the Unsaturated Zone

**PERMECA:** Testing and Research Platform in Collaborative and Applied Environmental Mechanics

**PESAT:** Soil - Atmosphere exchanges in peat bogs

**PESAA:** Soil - Atmosphere exchanges in Agricultural soils

**PRAT:** Atmospheric Reactivity

The teams involved originate from BRGM (French Geological Survey), University of Orléans, CNRS (National Center for Scientific Research), INRA (National Institute for Agricultural Research), Antea Group (consulting and engineering), DREAM (cluster of enterprises) and LE STUDIUM Loire Valley Institute for Advanced Studies.



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Prof. Lionel Mercury



### Dr Mohamed Azaroual

### CONVENOR

Earth Sciences Institute of Orléans (ISTO) / University of Orléans, CNRS, French Geological Survey (BRGM)

1A Rue de la Ferollerie 45100 Orléans - FR

Email: m.azaroual@brgm.fr Tel: 02 38 64 32 54

Mohamed Azaroual graduated in 1990 from the University of Paris 7 (DEA of IPGP). He obtained my PhD in Geochemistry (geothermal exchangers) at the Institute of Physics of the Globe of Paris - University of Paris 7, in 1993. He joined CNRS (Orleans) for two years to work on the aluminum dynamics in hydrothermal systems. He integrated the BRGM in 1996 as an engineer-researcher to work with BP and ELF on the scaling problems in oil reservoirs and the near well bore behavior. His scientific interest were focused on reactive transport between phases (water – gas – rock – "microorganisms") in complex hygrogeological systems throughout the continuum unsaturated and saturated zones for geo-resources and the environmental issues. He (co)published more than 50 peer review papers and developed R&D projects for ANR, Europe, international scientific collaborations (USA, China, Morocco, Japan,) including with industrials companies (i.e. TOTAL, ENGIE, etc.). Currently, he is deputy director of ISTO.

### Renewing conceptualization combining laboratory and fields, measurements and modelling, nm- to km-scales: the DNA of O-ZNS platform.

The PIVOTS (*Environmental Technology Innovation, Development and Optimization Platforms*) program is a regional (Centre Val de Loire) coordinated set of experimental and analytical platforms dedicated to the environmental quality monitoring and sustainable management of natural resources (soil, subsurface, surface water, groundwater, sediment and air) within a context of global change. The observatory (O-ZNS platform), a part of this platforms family, aimed to understand the water-rock-biosphere interactions and the mass (water and contaminants) and heat transfers throughout the continuum «atmosphere-vegetation-soil-vadoze zone-capillary fringe-saturated zone».

The O-ZNS, developed around an exceptional well dimensions (depth - 20 m & dimeter - 4m), offers a unique support for deciphering, at relevant scales (from nano- to metric scales), coupled phenomena in the environmental geosciences. The design of the well associated with laboratory experiments and numerical models allows the development/adaptation of innovative geophysical, physical and physico-chemical sensors for quantitative water transfers in the vadoze zone, and zooming around moving raid fronts, redox barriers, capillary fringe, in a porous/fissured limestone structure. The research field aimed identifying the level of coupling between the interfacial properties of multiphase hydrosystems, the electrical/electrokinetic/electrochemical properties.

This presentation aimed to discuss the project goals, the scientific challenges for renewing concepts of environmental monitoring technologies. The main objective is to identify the key processes promoted by the anthropogenic pressure (agricultural practices, etc.) along the soil-aquifer continuum, founding stone of a new generation of predictive modeling tools efficient for policy makers and industrials decisions.

#### Co-authors (with their institutions) :

Arnaud Isch *(ISTO)*, Clara Jodry *(ISTO)*, Gauthier Laurent *(ISTO University of Orleans)*, Thomas Jouen *(ISTO)* 

### **Dr Christophe Mouvet**

#### BRGM

3, Avenue C. Guillemin, BP 36009 45060 Orléans Cedex 2 - FR

Email: c.mouvet@brgm.fr Tel: 02 38 64 39 08

### PIVOTS - Environmental Technology Innovation, Development and Optimisation Platforms

The **PIVOTS** project is a coordinated set of seven experimental and analytical platforms focused on environmental quality monitoring and sustainable management of natural resources (soil, subsurface, surface water, groundwater, sediment and air), including remediation, and development of related ecotechnologies within a context of increased anthropogenic pressure and climate change. Environmental metrology for activities that consume a lot of natural resources is a priority theme chosen by the Centre - Val de Loire region, the main financial backer of PIVOTS, in the context of the European policy of intelligent specialization.

The innovation through PIVOTS originates from an integrated approach based on excellent research by academic and industrial experts together at all stages of the value chain, from fundamental research to validation of products and services. This will promote competitiveness among companies, particularly SMEs, and scientific excellence in the research teams involved.

The platforms are identified as:

- DECAP: Development of Environmental Sensors and Pollutants Removal Processes
- PRIME: Remediation and Innovation in the Service of Environmental Metrology
- O-ZNS: Observatory of transport in the Unsaturated Zone
- PERMECA: Testing and Research Platform in Collaborative and Applied Environmental Mechanics
- PESAt: Soil Atmosphere exchanges in peat bogs
- PESAaA: Soil Atmosphere exchanges in agricultural soils
- PRAT: Atmospheric Reactivity

The teams involved originate from Brgm (French Geological Survey), University of Orléans, CNRS (National Center for Scientific Research), INRA (National Institute for Agricultural Research), Antea Group (consulting and engineering), DREAM (cluster of enterprises) and Le Studium (Institute for Advanced Studies).

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### **Charles Nadim**

### ANTEA GROUP

803 Boulevard Duhamel du Monceau 45166 Olivet - FR

Email: charles-edouard.nadim@anteagroup.com Tel: 06 17 76 67 13

### Observation well geotechnical design

With regards to the project expectations, major adaptations had to be thought compared to a current classical geotechnical well design. For example:

- No concrete can be used for the works phase or for the definitive design, to avoid any chemical disturbance of the environment;
- No metallic elements can be used as well for the definitive well shielding not to disturb future geophysical measurements;
- The well must be waterproof, and must not create an artificial vertical drain;
- The digging phases must allow a direct and complete observation of the soil;
- Etc.

In order to fulfil all the expectations, a design inspired by ancient traditional stone wells was proposed. Actually, it is a fully limestone walled circular well that is proposed since it fits all the objectives: excellent geotechnical stability, no chemical influence, very low permeability, etc.

It will be surrounded by a specifically elaborated stuffing material on the outer side of the limestone structure which will ensure an extra protection to water intrusion and vertical circulation.

In addition, the stone structure is a guarantee of a high stability over the years which is also essential for this long-term project.

Co-authors (with their institutions) : Christophe Poinclou

### Dr Carlos Aldana, Dr Arnaud Isch

IST0

1A Rue de la Ferollerie 45100 Orléans - FR

Email: carlos.aldana@cnrs-orleans.fr Tel: 02 38 49 24 83

### O-ZNS Vadoze Zone hydrodynamics: fluid transfers and hydraulic properties of soils and limestone rocks of the observatory O-ZNS (Villamblain site)

The understanding of water flow and solute transport processes through the VZ is a cornerstone in the preservation of groundwater resources. An unconventional triaxial system is coupled to the multistep outflow (MSOF) method to measure the hydraulic properties of soils and rocks under both saturated and unsaturated conditions by means of a gas pressure-volume controller creating a three-phase unsaturated porous media. The purpose of this experiment is its versatility that allows the estimation of the hydraulic properties of all VZ samples using a unique assembly that runs the same specimen. This technique shows the benefits of using a triaxial cell, which allows reproducing overburden field conditions. The whole operating mode in saturated and unsaturated conditions may be successively carried out, thus avoiding sample being disturbed due to switching of the method or re-coring that could impact the reproducibility of measurements. Results show that the shape of the water retention curves and unsaturated hydraulic conductivity curves are in agreement with the information found in the literature according to the nature of the material. However, it seems that the effect of overburden decreases hydraulic properties when compared with other laboratory experiments. Fitting hydraulic parameters using the van Genuchten-Mualem model on the basis of multistep outflow experiments enables a first approach for validation hydraulic properties of each VZ material. These parameters will be used in a further study dedicated to the modelling of water flow and solute transport through the whole heterogeneous VZ.

> Co-authors (with their institutions): <u>Arnaud Isch</u> (ISTO), Yves Coquet (OSUC, Agro Paris Tech)

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#### Dr Jennifer Druhan

University of Illinois Urbana Champaign

1301 W Green St Urbana IL 61801 - US

Email: jdruhan@illinois.edu Tel: +15207306493

Jennifer is an Assistant Professor in the Department of Geology at the University of Illinois Urbana-Champaign. She joined the faculty in 2015 after completing an NSF postdoctoral fellowship at Stanford University. She holds a Ph.D. from the University of California Berkeley Department of Earth and Planetary Sciences and an M.S. from the University of Arizona Department of Hydrology and Water Resources. Her research centers on the relationship between the physical heterogeneity and chemical reactivity of aquifers, and ways in which stable isotope ratios are sensitive to this relationship.

### Signatures of carbon respiration in deep Critical Zone structure and function

In many terrestrial environments, rooting depths extend into the weathered regolith and bedrock beneath soils. However, the effect of deep rooting on the associated storage and respiration of organic carbon (OC) via rhizodeposition and root penetration is poorly constrained, due to the difficuly of sampling water and gas in unsaturated, weathered rock. Here we present two years of data collected at the Eel River Critical Zone Observatory (ERCZO) in a novel vadose zone monitoring system (VMS) that samples water and gas over an 18 m thick, variably saturated argillite weathering profile. We observe significant CO, production which peaks meters beneath thin soils, leading to low pH, increased dissolved inorganic carbon (DIC), and a net efflux of CO, from the vadose zone to the base of the soil which persists throughout the year. The source of this OC is critical to accurate model development for both respiration and weathering. Reasonable descriptions may involve (1) the delivery of surface-derived labile carbon through rapid transport pathways; (2) the deposition of root exudates by mature trees reaching many meters into the weathered regolith; and (3) the oxidation of lithogenic OC derived from the shale bedrock. To discern these pathways, fraction modern (FM) radiocarbon of solid phase OC recovered from drill cuttings were contrasted with gas phase CO, collected both at the height of the dry and wet seasons. These result indicate that respired OC is of a modern origin, delivered from the surface to the vadose zone, and that the concentrations of this labile source is highest between 5 - 8 m below the soil surface, thus strongly suggesting rhizodeposition.

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#### Dr Fatima Laggoun

ISTO - Orléans

1A Rue de la Ferollerie 45100 Orléans - FR

Email: fatima.Laggoun@univ-orleans.fr Tel: 02 38 49 46 63

### Platform for gases Exchange at the 'Soil - Atmosphere' interface in peatlands (PESAt)

PESAt (**P**latform for gases **E**xchange at the '**S**oil - **A**tmosphere' interface in **t**urf forming system: peatlands) is one of the platforms of the PIVOTS project whose main objective is to develop an innovative metrology to estimate the carbon (C) budget of peatlands and to characterize the spatial and temporal variability of greenhouse gases (GHGs,  $CO_2$  and  $CH_4$ ) emitted by these ecosystems. Peatlands soils can strongly influence the climate as they contain a 1/3 of the C stock of the world. The metrology deployed in PESAt allows the acquisition of time series that can reduce uncertainties on the estimates of GHG emissions by peatlands and thus contribute to the improvement of global models of climate prediction in which the large stock of C of peatlands is not taken into account yet. PESAt includes 5 actions:

- 1. Eddy covariance station for high time frequency measurements of GHG emissions.
- 2. Development of automatic chambers to estimate spatial variability of GHG emissions.
- 3. Acquisition of automatic and mobile chambers.
- 4. Adaptation of sensors for the measurement of soil CO<sub>2</sub> production at different depths.
- 5. Study of C microbial metabolism (exoenzyme activities) in peat soil to link small scale processes in the peat soil to ecosystem carbon emissions.

PESAt is deployed mostly in the La Guette peatland site (Neuvy-sur-Barangeon, Cher, Sologne) and in the laboratory at ISTO-OSUC conducting field, mesocosms, and microcosms experiments.

Co-authors (with their institutions): Sébastien Gogo+23, Christophe Guimbaud+56, Laurent Perdereau+23, Adrien Jacotot+23, El Houssain Ait Mansour+23, Fabien Leroy+23, Juanita Mora-Gomez+23, Frédéric Savoie+23, Stéphane Chevrier+56 Gilles Chalumeau+23 'Université d'Orléans, ISTO, UMR 7327, 45071 Orléans, France 2 CNRS, ISTO, UMR 7327, 45071 Orléans, France 3 BRGM, ISTO, UMR 7327, BP 36009, 45060 Orléans, France 4 Université d'Orléans, LPC2E, UMR 7328, 45071 Orléans, France 5 CNRS, LPC2E, UMR 7328, 85071 Orléans, France 4 CNES, LPC2E, UMR 7328, BP 36009, 45060 Orléans, France

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### **Dr Romain Millot**

**BRGM - French Geological Survey** 

45060 Orléans - FR

Email: r.millot@brgm.fr Tel: 02 38 64 48 32

### Chemical weathering of a granitic watershed: coupling Lithium isotopes and reactive transport modeling, preliminary results

In the present study, we report lithium concentrations and Li isotopic compositions for different samples within a granitic watershed (Margeride, France). We investigate unweathered bedrock and samples displaying different stages of weathering in order to characterize Li isotopic fractionation. This was achieved by coupling lithium isotope geochemistry and reactive transport modeling during granite weathering at the scale of this watershed.

The first stages of this work were intended to building a robust alteration model considering the initial minerals within the bedrock (wt.% and Li concentration). This weathering model was developed using the PHREEQ-C code and simulates a weathering sequence in agreement with the products observed within the soils, saprolites and sediments for Li concentrations. This first stage was important in order to conserve the mass balance for lithium. The next step, we are working on now, is to implement Lithium isotope fractionation during weathering reactions. This model for coupled chemical and isotopic equilibration explicitly considers isotopic equilibration in the absence of bulk chemical disequilibrium by making use of a solid-solution model for the precipitating mineral phase (no isotopic fractionation is likely to occur during mineral dissolution).

Co-authors (with their institutions) : Joachim Tremosa, Philippe Négrel



### Prof. Dani Or

ETH Zurich

Universitätstrasse 16 8092 Zürich - CH

Email: dani.or@env.ethz.ch Tel: +41 44 633 60 75

**Dani Or** is a professor of *Soil and Terrestrial Environmental Physics* at the Swiss Federal Institute of Technology [ETH] Zurich. His research focuses on mass and energy transport in porous media; mechanics of shallow landslides and debris flows; evaporation from porous surfaces, and on linking physical processes with biological activity in soil. Dr. Or has authored and coauthored over 280 ISI publications, co-authored a book, and over 400 proceeding papers and abstracts. Dr. Or is the former Editor in Chief of the Vadose Zone Journal, recipient of the Kirkham Soil Physics Award (2001), 2004 Fellow of the Soil Science Society of America, chair of the 2008 Gordon Research Conference on Flow and Transport, and 2010 Fellow of the American Geophysical Union. He was the 2013 Birdsall-Dreiss distinguished lecturer, recipient of Helmholtz Inter. Fellow Award (2013); elected 2014 Fellow of Geological Soc. Am.; the 2017 recipient of the European Geosciences Union Dalton Medal and 2018 AGU Langbein lecturer.

http://www.step.ethz.ch/people/scientific-staff/prof-dani-or.html

### The challenges of monitoring the deep critical zone – going under the living skin of the Earth surface

A widely accepted definition of the Earth's critical zone: a near-surface zone where complex interactions among rock, soil, water, air, and living organisms modify weathering rates and form soil thus regulating fluxes through this highly dynamic compartment that is essential for terrestrial life. This living skin of the Earth provides numerous ecosystem services (from food to wood, water filtration, nutrient cycling) and regulatory functions (terrestrial carbon and water cycles) and is the domain with which humans interact most. The inherent feedbacks between hydrology, geology, geochemistry, biology and climatology make the study of this zone a frontier of interdisciplinary Earth sciences. A key step for advancing understanding and harnessing knowledge from different disciplines is to better monitor and understand key processes and transformations occurring in this domain. Present observational capabilities are limited in space and time and remain too fragmented (different disciplinary foci) to effectively address complexities of observing the deep critical zone. The scientific community needs a strategy to better link the highly dynamic shallow part of the critical zone with the stable deep zone including key processes and transformations. The presentation will highlight feedbacks among biology and hydrology that mediate and transform subsurface fluxes; the challenges of subsurface parameterization and observation methods, and discuss promising new observational methods for improved understanding of deep critical zone process.

### Prof. Mikael Motelica-Heino

### ISTO UMR 7327 Cnrs-Université d'Orléans-BRGM

1A rue de la Férollerie 45071 Orléans Cedex 2 - FR

Email: mikael.motelica@univ-orleans.fr

### Can we track trace elements "hotspots" in reactive zones of the critical zone ?

Surface environments are made of a tridimensional mosaic of micro-habitats with various oxygenation gradients and redox conditions that alter the diagenetic processes. Trace elements in the critical zone are involved in dynamic geochemical transformations that are often driven by biologically controlled processes. While changes in redox state offer general mechanisms for supply and removal of metal(loid)s from solution, there may be specific linkages of particular elements of precise mechanistic linkages between the geochemistry and biota will be best achieved if measurements are made at a scale that relates directly to the individual organism or its species-specific grouping. Correspondence between fine structure observed for the different trace metals and fine structure in sulfide, iron, manganese and nutrients distribution has provided insight into the linkages of the supply/removal processes of metals at a small scale, particularly the role of Fe, Mn and S(-II) phases and microorganisms.

Future research is concerned with what happens next: what is the fundamental mechanism of release of metals and S on a small scale. For example, what processes would result from a small (microns) parcel of fresh organic material introduced at depth? This work investigates the reactive transport principles that could be employed to address these microniche sources and their impact on natural systems in terms of fluxes across diverse spatial and temporal scales in tandem with the possible application of advances in quantitative imaging, reactive interface characterization techniques and in-situ chemical sensors and probes.

### **Dr Nicolas Deaveau**

### BRGM

3, Avenue C. Guillemin, BP 36009 45060 Orléans Cedex 2 - FR

Email: n.devau@brgm.fr Tel: 02 38 64 35 51

### Modeling fate of emerging contaminants in soil aquifer treatment experiment: insight into new modelling tools

The use of treated wastewater in indirect non-potable reuse (InPR) practices are frequently happening in worldwide. However, unknowns still raise concerning transfer to surface waters and groundwater of the emerging contaminants and pathogens that adversely affect aquatic life as well as human health. The 3-years project FRAME funded by the Water JPI program has been done to investigate the InPR practices. Among the different tasks targeted by the project, one is to simulate the fate and transport of emerging contaminants in soil aquifer treatment (SAT) experiments. The modelling approach is based on the use of the flow and reactive transport code MARTHE-PHREEQC. Several organic emerging contaminants as well as their transformation products have been tested. Flow rates was simulated according to the Richards' equation. Mass transfer in aqueous phase was considered to occur through advection-dispersion equation while gas diffusion is simulated by Fick's law. To describe the geochemistry, microbial driven degradation reactions of emerging contaminants, aerobic respiration, nitrification, solid organic matter solubilisation as well as adsorption reactions (both hydrophobic and electrochemical reactions) were taken into account. The transition of redox states during the SAT experiment has been accurately simulated. Models is able to give new insights on the complex degradation pathways of emerging contaminants and how they are impacted by sorption reactions.

> Co-authors (with their institutions) : Pettenati M.<sup>1</sup>, Picot-Colbeaux G.<sup>1</sup>, Blanc P.<sup>1</sup>, Thiéry D.<sup>1</sup>, Drewes J.E.<sup>2</sup>, Hübner U.<sup>2</sup>, Ternes T.<sup>3</sup> <sup>1</sup>BRGM, UMR 7327, Orléans France. <sup>2</sup>Technical University of Munich, Chair of Urban Water Systems Engineering, 85748 Garching, Germany. <sup>3</sup>Bundesanstalt für Gewässerkunde, 56068 Koblenz, Germany.



### Dr Pierre Toulhoat

### BRGM

3, Avenue C. Guillemin, BP 36009 45060 Orléans Cedex 2 - FR

Email: p.toulhoat@brgm.fr Tel : 02 38 64 38 70

Pierre Toulhoat graduated in 1980 from the École Normale Supérieure in Paris, where he completed a PhD thesis in geochemistry. He then joined the CEA to work on the hydrogeochemistry of uranium and, later, on underground confinement of radionuclides and nuclear waste disposal. In parallel, he developed analytical chemistry for environment in a joint research unit he established with the University of Evry. In 2002, he joined CNRS and the University of Lyon, to set up the Institute of Analytical Sciences, which he directed until 2012. In 2005, he became the scientific director of Ineris, French national institute for industrial environments and risks. Fellow of the French Academy of Technologies since 2010, Pierre Toulhoat joined the BRGM in 2016 as deputy CEO and scientific director.

### Mechanistic-local vs. spatialized-distributed representations, geochemical vs. geophysical signatures, fields vs. labs: how to read deeply the nature?

The critical zone exhibits a large variety of scientific challenges: highly variable boundary conditions, highly variable fluxes of nutrients, contaminants, highly variable features and properties (mineralogy, porosity, transport properties, texture...), steep chemical gradients, biogeochemical activity. It is probably one of the best example of a complex system, with entangled evolving structure and moving reactive fronts in time and space.

A fully coupled deterministic approach aiming at a predictive approach is certainly out of reach, at least in the future decades. But if specific answers can be prioritized, operational approaches can be developed...

For example: if the contamination of an underlying aquifer is at stake, the transfer function of contaminants through the CZ or VZ has to be determined. Experimental design approaches can be used, with a limited number of key variables. It requires a sound determination of the key parameters, and the use of tracers. This kind of "black box" approaches are currently used in chemical engineering.

However, this type of approach can be invalidated in the case of strongly coupled processes, or slow dynamic processes. It the reason why such approaches need to be controlled by multi-scale investigations of the system behaviour: contaminant displacement, redox front displacement, changes in the distribution of microorganisms, time and space variation of transport properties.

In the frame of the PIVOTS project, Brgm has developed PRIME; a pluri-metric experimental facility, in which a reconstructed 3D unsaturated and/or saturated porous system. It can be studied in operando thanks to a large variety of sensors and modelled as "digital twin".

In OZNS, a natural system can be investigated in situ, either with a direct access through physical and chemical sensors, but also remotely imaged and scanned, using innovative geophysical methods. Data mining, machine learning, data assimilation, new approaches in geostatistics and modelling, such as the use of SPDE, will be tested.

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### Dr Xu Tang

### UNIVERSITY OF NOTTINGHAM

Room B44a, School of Chemistry, University Park, Nottingham, NG7 2RD - GB

Email: xutang2050@outlook.com Tel : 44 7512469842

### Nanoscale chemical-mechanical heterogeneity characterization of shale

Understanding mechanical and chemical properties of rock is essential for evaluating the long term performance of subsurface rock engineering projects, such as geological carbon storage, radioactive waste storage and disposal and hydrocarbon production. Fine-grained shales are usually caprocks, source rocks and host rocks for these projects. Investigation of the stability and reactivity of shale for subsurface rock engineering projects requires a thorough understanding of material properties of shale such as mechanical properties and surface chemistry at nanoscale. **This work reports a simultaneous nanoscale chemical-mechanical mapping of a shale sample using a novel peak force infrared microscopy (PFIR)**. The results show that thesilicon-oxygen band, aliphatic band, aromatic ring stretching band and carbonyl/carboxyl band are dispersively distributed at a resolution of 10 nm. A spatial correlation between aliphatic/aromatic band and mechanical properties such as reduced modulus, deformation and dissipation are obtained by using the Pearson's correlation. This work demonstrates that the PFIR has the capacity to reveal the nanoscale chemical-mechanical heterogeneity of shales. This high spatial resolution technique thus opens the door for researchers to probe the coupled chemical-mechanical processes pertinent to subsurface rock engineering projects at the nanoscale.

Co-authors (with their institutions) : Devon S. Jakob, Xiaoji G. Xu (Lehigh University) Robert Mokaya (University of Nottingham) Nino Ripepi (Virginia Tech)

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### **Dr Arnault Lassin**

### BRGM

3, Avenue C. Guillemin, BP 36009 45060 Orléans Cedex 2 - FR

Email: a.lassin@brgm.fr Tel: 02 38 64 30 25

### Dynamics of a two-step mechanism of calcium carbonate formation: an integrated study involving microfluidic experiments and reactive transport modelling.

The description of coupled processes that control mass transfers in porous media is a scientific issue for which research activity remains very dynamic. As a contribution to this activity, a new kinetic model was developed based on a transition-state-theory (TST) / surface-complexation-model (SCM) coupling. It aims to describe the successive precipitation of amorphous calcium carbonate (ACC) and calcite, taking account of their mutual influence: ACC precipitates according to the standard TST and creates surface complexation sites from which calcite can form and create new surface complexation sites. When the kinetics of calcite precipitation are fast enough, the consumption of dissolved matter leads to the re-dissolution of ACC. This model is first compared to batch experiments and, then, applied with a reactive transport calculation code to a dynamic experiment carried out on a microfluidic device composed of a single straight channel. The results show a good match between experiments and reactive transport modelling: the combination of simple experimental microfluidic devices and reactive transport modeling could be a promising integrated methodology to study the dynamics of geochemical reactivity at the pore scale, before application to more complex and larger systems.

The study also reveals issues to address regarding the description of the transport of reactive (i.e. growing/shrinking) particles in porous media and the related hydrodynamic and physico-chemical mechanisms.

Co-authors (with their institutions) : Laurent André (BRGM, UMR ISTO), Nicolas Devau (BRGM), Adeline Lach (BRGM), Thomas Beuvier (Univ. du Maine), Alain Gibaud (Univ. du Maine), Stéphane Gaboreau (BRGM), Mohamed Azaroual (BRGM, UMR ISTO).

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### Dr Yuxin Wu

STAFF SCIENTIST

Lawrence Berkeley National Laboratory 1 Cyclotron Rd, Berkeley CA, 94720 - US

Email: ywu3@lbl.gov Tel : 5104864793

Dr Yuxin Wu is a staff scientist at the Earth & Environmental Sciences Area at Lawrence Berkeley National Lab. He is trained in near surface and environmental geophysics, and has expertise in hydro-/bio- geophysics, and joint applications of geophysical, hydrological and biogeochemical methods for multi-disciplinary research. His research interests include geophysical monitoring of subsurface hydro-biogeochemical processes; characterization and monitoring of fracture flow related to energy production and waste storage; enhanced geophysical imaging approaches; and the development of novel imaging approaches for ecosystem interactions. Dr Wu is a member of AGU and SEG, and has published 40 + peer-reviewed papers.

### Mesoscale research: tools, workflows and lab - field co-design

In soil and hydrological sciences, mesoscale is typically referred to at the scale of multiple meters. Research at mesoscale provides critical link between key mechanisms at smaller scales with observations of coupled processes at field scales that are often multi-physics with multiscale heterogeneities. The complexity and heterogeneities of the physical, chemical and biological interactions observable at mesoscales are relevant to the field scales, yet this intermediate scale is small enough to allow intense control, observations and manipulation, which allows the decoupling of the multi-scale and complex problems.

This presentation will focus on two key components that are critical to mesoscale research, and include the following aspects (1) sensing, monitoring and data capabilities needed to tackle the multi-physics problems across scales, (2) Cross-scale linkages between different data types, and (3) Laboratory and field interactions and co-design. Examples and mesoscale research efforts at LBL will be discussed, which includes reactive processes in the soil and hydrological/rhizosphere dynamics at both lab and field scales. We will also focus on how geophysical methods can be used jointly with other measurement techniques at mesoscales to better understand the hydrobiogeochemical dynamics of the complex soil system.

#### Co-authors (with their institutions) :

Chunwei Chou (LBL), Luca Peruzzo (LBL), Eoin Brodie (LBL), Ken Williams (LBL), Kate Scow (UC Davis), Elison Blancaflor (Noble Research Institute), Susan Hubbard (LBL)

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#### **Dr Christophe Mouvet**

BRGM

3, Avenue C. Guillemin, BP 36009 45060 Orléans Cedex 2 - FR

Email: c.mouvet@brgm.fr Tel : 02 38 64 39 08

The PRIME platforms (Platforms for Remediation and Innovation in Environmental Metrology)

The objective of the set of PRIME platforms is to develop services in environmental metrology and remediation based on the understanding and quantification of reactive transport processes of pollutants in soils, sub-soils, sediments and aquifers.

PRIME provides experimental means on a variety of scales, ranging from ml-reactors up to a 100 m3 pilot. These facilities make it possible to validate tools (sensors, samplers...), methods and techniques (physical, chemical and biological) dedicated to the remediation or the monitoring of degraded environments. All the means afforded by PRIME are applicable in the framework of research projects that can be subsidized, collaborative or of service provision. Classified ICPE, the hall that houses PRIME provides partners with all the guarantees associated with this status, notably for industrial processes.

### Means

- Centimetric or decimetric-sized reactors of the "batch-type" (closed containers)
- Decimetric to metric-sized columns and tanks (H = 0.2 to 5 m, interior diameter = 0.05 to 1 m)
- Plurimetric Pilot (PPM 10 x 4 x 4 m which can be broken down into 4 independent modules)
- Laboratories and equipment for monitoring physical, chemical and microbiological parameters. Sampling (water, gas, solids) appropriate to all the spatio-temporal scales under study
- Scientific expertise and technical know-how that can be mobilized starting with the conception of the studies down to the interpretation and valorization of the results

### Application examples

- Simulation of ground water circulation in order to test sensors and passive samplers
- Migration and fate of contaminants through either fragmented solid matrixes (soils, sediments) or consolidated ones (rock) under non-saturated, saturated conditions, or a continuum of both, in aerobic or anaerobic environments
- Implementation and validation (comparison with standardized methods, mass balance, costbenefit analysis) of remediation tools and processes (physical, chemical, biological) on various scales up to that of the industrial pilot.

Co-authors (with their institutions): S. Dupraz (BRGM)

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### **Dr Dominique Thiéry**

### BRGM

3, Avenue C. Guillemin, BP 36009 45060 Orléans Cedex 2 - FR

Email: d.thiery@brgm.fr Tel : 02 38 64 34 37

An efficient approach to model flow and heat transfer through unsaturated Chalk from the ground surface to the aquifer

A vertical numerical flow model based on Richards' equation has been developed to simulate infiltrating rainwater flow through the vadose zone from the ground surface to the saturated Chalk aquifer. The MARTHE computer code, which models the unsaturated-saturated continuum, was adapted to handle the double permeability effects that are observed high saturation periods. Composite constitutive functions (hydraulic conductivity-saturation and pressure-saturation) that integrate the increase in hydraulic conductivity near saturation and extra available porosity resulting from fractures were introduced into the code. Using these composite constitutive functions, the model is able to reproduce the data monitored during 2.5 years at an experimental site located in the Hallue basin (France) from the ground surface down to the water table. 26.5 m below ground level. The water content and pressure monitored at all depths over the entire monitored period, including infiltration tests is accurately simulated. The soil temperature is also well simulated over a depth of 8 m, except during the infiltrations tests, which contributes to the model validation. The model enables to calculate the aquifer recharge over long periods including droughts and floods. The calculated recharge is realistic as it makes it possible to simulate the corresponding monitored groundwater level, which increases confidence in the modelling approach.

This modelling approach contributes to improve the understanding of groundwater flooding in Chalk catchments basins overlaid by an unsaturated fractured chalk formation.

Co-authors (with their institutions): N. Amraoui (BRGM)

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### **Dr Anfré Revil**

CNRS

Université Savoie Mont-Blanc ISTERRE CNRS, Rue du Lac d'Annec, Campus scientifique Savoie Technolac, Bâtiment Belledonne, Bureau 252 73376 Le Bourget-du-Lac - FR

Email: andre.revil@univ-smb.fr Tel : 06 75 58 00 75

André Revil is currently Directeur de Recherché 1st class with the CNRS at ISTERRE [Institut des Sciences de la Terre, Chambéry, France] and Université Savoie Mont-Blanc [Chambéry]. He is interested in the developments of electrical and electromagnetic methods with a vast range of applications including volcanic activity, permafrost and hydrogeophysics. He has a special interest in pushing forward geoelectric methods such as the electrical conductivity, the self-potential and seismoelectric methods, and induced polarization. He has published over 300 peer-reviewed papers. In 2015, he was awarded the 1st Nishida Prize for Promotion of Geoscience from the Japan Geoscience Union (JpGU) with the entry «Theoretical studies on coupled hydromechanical and electromagnetic phenomena in porous media and their applications to the geosciences. He was elected AGU Fellow by the American Geophysical Union in 2016.

Couplings coefficients in geophysics: a tool toward quantification and a mine of second order information for understanding key mechanisms. What are the interdisciplinary bridges?

In porous and fractures materials, there is a set of cross-coupling phenomena in the key constitutive equations describing transport phenomena. These cross-couplings effects allow extending the constitutive equations beyond the classical Ohm's, Darcy's, Fourier's and Fick's laws. These cross-coupling phenomena are also essential bricks to formulate the underlying physics behind some geophysical methods such as the induced polarization method, the self-potential method, and the seismoelectric and electro-seismic methods. In this talk, I will describe the key physics of these processes, and how they can be applied to these geophysical methods, and what is the resulting gain of information in hydrogeophysics. Especially important in the near-future will be to directly connect these methods to key multi-phase reactive transport modelling softwares to bring 4D information directly in the numerical modelling of important transport processes in environmental geosciences. Several practical applications will be demonstrated.

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### **Dr Philippe Leroy**

#### BRGM

3, Avenue C. Guillemin, BP 36009 45060 Orléans Cedex 2 - FR

Email: p.leroy@brgm.fr Tel : 02 38 64 39 73

"Investigating the electrochemical properties of the air/water interface from the atomic to the micrometric scale" (in link with the presentation of Prof. Lionel Mercury)

The unsaturated zone in the subsurface is a multiphasic porous medium where the capillary water plays a significant role. At the interface between air and the capillary water, there is a very thin water layer governed by an electrostatic potential due to the specific orientation of the water molecules and ion distribution. This very thin layer may contribute to controlling the rock's wettability, hence the distribution of water in the pores, and can adsorb some pollutants such as titanium dioxide nanoparticles. There is no consensus on the exact nature of the difference forces existing at the air/water interface. The goal of our work is to use atomic simulations to better describe these forces and the resulting ion distributions at the mesoscopic scale for the case of brines (salinity above 0.1 mol L-1) where surface tension strongly varies with salinity. However, atomic simulations can give different results depending on the model assumptions and only microscopic measurements such as NAPXPS (Near-Ambient Pressure X-ray Photoelectron Spectroscopy) can reveal the specific behaviour of the air/water interface. Geophysical measurements such as selfpotential and induced polarization can also indirectly reveal it. However, downscaling information from the macroscopic (centimetric to plurimetric) to the microscopic (nanometric) scale is very challenging and will need reactive transport modelling at the pore and laboratory scales as well as atomic simulations to constrain them.

#### Co-authors (with their institutions):

Arnault Lassin (BRGM), Vivien Ramothe (BRGM, UMR PHENIX, Paris, IRSN, Paris), Virginie Marry (UMR PHENIX, Paris), Magdalena Dymitrowska (IRSN, Paris), Olivier Bernard (UMR PHENIX, Paris).

### Dr Géraldine Picot-Colbeau

### BRGM

3, Avenue C. Guillemin, BP 36009 45060 Orléans Cedex 2 - FR

Email: g.picot@brgm.fr Tel : 02 38 64 31 37

Land use effect on nitrate storage and transport through the unsaturated zone of chalk aquifer: a pluridisciplinary and transversal approach

Chalk aquifer is the main water resource for domestic water supply in many parts in northern France. In this region, groundwater is frequently affected by quality problems concerning nitrates. Often close to or above the drinking water standards, nitrate content in groundwater is mainly due to historical agriculture practices, combined with aguifer recharge through the vadose zone. The complexity of processes occurring into such an environment leads to combine a lot of knowledge in agronomy, geochemistry and hydrogeology in order to understand, model and predict the spatiotemporal evolution of nitrate content and provide a decision support tool for the water producers and stakeholders. To succeed in this challenge, conceptual and numerical models representing accurately the aguifer are developed, including a multidisciplinary approach to simulate storage and transport from the soil surface to the underlying groundwater. This involves a new agronomic module "MONICA" (MOdelling NItrates transfert taking into account Crops and Agricultural practices), a soil-crop model calculating the nitrogen mass balance in arable soil, integrated in the 3D transient groundwater numerical code "MARTHE". The numerical development is applied on a 1D and 2D vertical cross-section in the vadose zone representing experimental nitrate vertical measurements in soil profiles (0-22 m depth) in the Somme region (France). The experiment results highlight the land use management effect on nitrate evolution into the vadose zone (forest and crops). Simulations constrained by climate forcing, land use and nitrogen inputs over several decades reproduce the nitrate spatial and temporal distribution. This numerical tool will help the decision-making in all activities in relation with water uses.

> Co-authors (with their institutions): Thiéry Dominique, Devau Nicolas, Surdyk Nicolas, Pettenati Marie, Parmentier Marc, André Laurent (*BRGM*).

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### Dr Benoît Noetinger

**IFPEN** 

1 avenue de Bois Préau 92852 Rueil Malmaison - FR

Email: benoit.noetinger@ifpen.fr Tel : 01 47 52 61 01

Dr B Noetinger, graduated from Ecole Polytechnique in 1985 holds a Master in Liquid State Physics from UPMC in Paris. He completed his PhD in ESPCI Paris in 1989 about Modelling of rheology and Sedimentation of suspensions. He was hired at IFPEN in 1989, where he occupied many positions in research. He was habilitated to manager research In October 2000.

His research interest are up scaling flow in heterogeneous and fractured media, using techniques arising from statistical physics. He is interested by the macroscopic effect of the small scale disorder on the global behaviour of subsurface reservoirs.

# A critical review of upscaling-downscaling procedures from geosciences perspective = mean-field petrophysic properties, heterogeneities. What are the relevant scales to capture meaningful signal?

Up-scaling remains an unavoidable task in applied geoscience studies when dealing with full field applications. As pore-scale modelling is impracticable at field scale, a cascade of up-scaling sequences allowing to pass from a pore scale description to a Darcy scale one and then to a "pseudo" large scale model (such as the dual porosity description" of flow in fractured media) has been the subject of numerous studies since mid XIX century.

In addition, the incomplete data sets that are available (few measurements on samples of small support sizes) render unavoidable any complete deterministic description of the system. Quantifying uncertainties and identifying critical parameters controlling the overall behaviour of the case under investigation is part of the problem. This process is very time consuming, and thus expansive.

Up-scaling procedures involve techniques such as homogenization or volume averaging to deduce the form of effective equations at the relevant scales. These large scale equations contain parameters that may be determined by solving an appropriate closure or "cell problem" to be solved at the smaller scales. Analogous considerations can be followed in the stochastic context when model uncertainties are accounted for.

Developing more realistic process-based and/or geostatistical models allowing to develop shared Digital twins models is also a constant concern of research. Practical use of these models will always imply exploring parameter space of very large dimensions, implying using adapted Big Data and IA techniques to get efficient workflows for the geo-engineer.

The talk will focus on some recent results and practices, from simple to more complex cases involving strong non-linearity, case in which the form of large scale equations may be different that their small scale local counterparts.

### **Dr Cyprien Soulaine**

### BRGM

3, Avenue C. Guillemin, BP 36009 45060 Orléans Cedex 2 - FR

Email: c.soulaine@brgm.fr

### Quantifying the reactive surface area from pore-scale simulations

It exists sometimes several orders of magnitude difference between the reaction rate measured in the lab and the reaction rate obtained from field measurements. The difference comes from the fact that not all the surfaces of the minerals react because of a complex interplay between chemical reaction, minerals distribution, and fluid flow. In this talk, we discuss the use of porescale simulations to assess the effective reactive surface area.

### **Dr Laurent Gauthier**

ISTO 1A Rue de la Ferollerie 45100 Orléans - FR

Email: gautier.laurent@univ-orleans.fr

### Linking static structures and alterations of continental carbonates to hydrodynamic properties

Understanding the hydrodynamic context of the critical zone calls for tackling three main scientific challenges: (1) the characterisation of the parameters that are controlling the hydrodynamic properties and their interactions with structures, (2) the upscalling of these properties and geometries, and (3) their integrations into simulations of transport processes.

In this framework, the prediction of the spatial repartition of reservoir properties is particularly complex for carbonates, and in particular continental carbonates. The main factors in play are the conditions of deposition, the evolution post-deposition including diagenesis, and later alterations of the rock that can lead to karstification. These alterations often depend on existing structuration of the rocks that rely on lithological structures or fractures. These alteration episodes can also be related to remobilisation of elements and precipitation of peculiar minerals that may affect the hydrodynamic properties and play a critical role in the hydrodynamic and chemical processes that take place in the unsaturated zone.

To be addressed the challenges call for a better understanding of the 3D spatialisation of the properties and processes of formation and alteration of carbonate rocks, and their integration into a hydrodynamic modelling workflow.

Co-authors (with their institutions): Simon Andrieu (BRGM), Eglantine Husson (BRGM)

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### **Dr Mohamed Azaroual**

Earth Sciences Institute of Orléans (ISTO) / University of Orléans, CNRS, French Geological Survey (BRGM) 1A Rue de la Ferollerie 45100 Orléans - FR

Email: m.azaroual@brgm.fr Tel: 02 38 64 32 54

Mohamed Azaroual graduated in 1990 from the University of Paris 7 (DEA of IPGP). He obtained my PhD in Geochemistry (geothermal exchangers) at the Institute of Physics of the Globe of Paris - University of Paris 7, in 1993. He joined CNRS (Orleans) for two years to work on the aluminum dynamics in hydrothermal systems. He integrated the BRGM in 1996 as an engineer-researcher to work with BP and ELF on the scaling problems in oil reservoirs and the near well bore behavior. His scientific interest were focused on reactive transport between phases (water – gas – rock – "microorganisms") in complex hygrogeological systems throughout the continuum unsaturated and saturated zones for geo-resources and the environmental issues. He (co)published more than 50 peer review papers and developed R&D projects for ANR, Europe, international scientific collaborations (USA, China, Morocco, Japan,) including with industrials companies (i.e. TOTAL, ENGIE, etc.). Currently, he is deputy director of ISTO.

### Reactive transport and thermo-kinetic approaches – key mechanisms, recent advancements, some current limitations and perspectives

The understanding of reactive transport phenomena in the unsaturated zone at different time and space scales requires couplings of physical, physicochemical, microbiological and thermo-kinetic mechanisms acting essentially at the phase interfaces (minerals - water - gas - «micro-organisms»). Currently, numerical models cannot satisfactorily integrate these coupled mechanisms even their effects have been highlighted in both laboratory experimentations, industrial processes and field observations systems. In this context, it is necessary to seek developing modeling concepts to circumvent certain numerical difficulties, computation time or lack of data at relevant scales.

The accumulation of knowledge on the evolution of some natural geosystems allowed significant advances in particular by identifying buffered systems «ie, mineral assemblages and characteristic reactive facies, Eh - pH buffer zones, pCO2 of carbonate hydrosystems». When it is applicable, the quasi-stationary approach could made it possible to reproduce efficiently the evolution of complex hydrological systems. The fine observations of natural phenomena at relevant scales (i.e., O-ZNS observatory) with derived experimentations at mesoscales (i.e., PRIME, EcoSENS, LBBIO, etc.) will help to identify the critical parameters and the key variables. The geophysical imagery could bring independent constraints. The development of a workflow based on these different scales and steps could improve the quality of the predictive modeling.

We are currently unable to develop inverse geochemical models because of many ephemeral phenomena and the past ghost zones shaping the present evolution state. Integrating massive field data at relevant scales with simplified modeling approaches allow the development of more efficient direct models.

Some current limitations and challenges of reactive transport modeling for environmental and energy applications will be discussed.

Co-authors (with their institutions) :

Laurent André (BRGM, ISTO), Arnault Lassin (BRGM)

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#### **Dr Christophe Tournassat**

BRGM - 1A Rue de la Ferollerie, 45100 Orléans - FR UMR 7327 - Institut des Sciences de la Terre d'Orléans, 45071 Orléans - FR LAWRENCE BERKELEY NATIONAL LABORATORY - 1 Cyclotron Road, Berkeley, CA 94720 - US

Email: c.tournassat@brgm.fr

## Modeling of coupled processes in nanoporous media. From molecular dynamics information to reactive transport modeling

Nanoporous media exhibit a remarkable array of macro-scale properties with marked departures from those observed in conventional porous media such as permeable aquifers, for the study of which reactive transport models and codes have been historically developed. These properties arise from the interactions of charged nanopore surfaces with water and solutes. The presence of an electrostatic potential field at the surface–water interface and of the so–called diffuse layer leads to coupling between flux terms. Reactive transport models have been developed recently to take into consideration the presence of this diffuse layer. In this presentation, we will show how some of the parameters that describe the properties of the diffuse layer porosity can be rooted in small scale information gained from molecular scale modeling methods.

Co-authors (with their institutions): Carl I. Steefel (Lawrence Berkeley National Laboratory)

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#### Dr Laurent André

**ISTO** 

1A Rue de la Ferollerie 45100 Orléans - FR

Email: l.andre@brgm.fr Tel :02 38 64 31 68

#### Kinetic modelling of bacterial processes in aqueous systems: application to denitrification mediated by micro-organisms

In many environments, the chemical reactions like the redox reactions are intimately linked to micro-organisms who are often catalysts. During such reaction, bacteria use a part of the produced energy to drive the cells metabolism. Intracellular mechanisms include numerous reactions like synthesis of adenosine triphosphate (ATP) from adenosine diphosphate (ADP) and orthophosphate ion  $(PO_4^{-3})$ . Because of the number and the complexity of the involved elementary reactions, the numerical modelling simulating these processes requires the implementation of powerful and relevant theoretical approaches. The geochemical codes initially devoted to simulate the reactive transport processes must be adapted to integrate microbiological phenomena including the bacterial growth.

The difficulty is to choose an adequate biological model to implement in the geochemical code. Many theoretical and empirical approaches coupling kinetic, thermodynamic and bacterial growth were developed since the first model of Michaelis-Menten. If they are very useful for batch systems, these modelling comprise however inherent limitations. More recent comprehensive approaches consider both the chemical characteristics of the reactive system and the thermodynamic driving force of metabolism reaction. If the energy of the corresponding redox reaction is not sufficiently high to provide ATP synthesis, the redox reaction stops.

This global and semi-empirical approach is implemented in the geochemical code PHREEQC and applied to denitrification process, both in batch and column systems. The agreement between experimental measurements and simulation results is relatively good demonstrating that the chosen numerical approach is suitable to simulate biogeochemical processes.

Co-authors (with their institutions): H. Pauwels (*BRGM*), M.-C. Dictor (*BRGM*), M. Parmentier (*BRGM*), M. Azaroual (*BRGM*, ISTO).

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#### Prof. Reneaud Toussaint

IPGS, CNRS/University of Strasbourg, PoreLab, University of Oslo

IPGS - EOST, 5 rue Descartes 67000 Strasbourg - FR

Email: renaud.toussaint@unistra.fr Tel: 06 73 14 29 94

Research Prof. [Directeur de Recherche au CNRS] at Earth Physics Institute of Strasbourg (IPGS) and Adjunct Professor (Professor II) at the Center of Excellence "Porous Media Laboratory", University of Oslo. Renaud Toussaint is heading the group "Experimental Geophysics". His research focuses on subjects at the boundary between physics, geophysics and hydrology: Physics and Mechanics of Geomaterials, Complex Systems in Earth Science, Fluid and granular mechanics, deformable porous media, Earthquake sources and landslide dynamics. He studied Theoretical Physics (Magistère, DEA) and Mathematics (Agrégation) at ENS Lyon, and Geophysics (DEA) at IPG Paris, completed a PhD on Fracture and statistical physics at the University of Rennes I and a Habilitation at the University of Strasbourg. He authored/co-authored over 120 peer reviewed scientific publications, and was granted some academic recognition prizes, incl. a "Hope of the University of Strasbourg" in 2013.

# Observing flow and deformation using different techniques - examples in fluid flow induced internal fractures and in landslide dynamics: comparing optical and seismic imaging

In geophysics, subsurface imaging focuses on highly heterogeneous propagation media for the physical fields used, and the objects imaged often present complex geometries, as fractal ones, or highly branched ones. We focus different types of systems, and compare their imaging using direct optical imaging together with numerical simulations and image treatment, possible in laboratory experiments, and more classical geophysical imaging, using acoustic emissions, microseismics or saturation / pore pressure measurements.

Three classes of systems are examined:

1. When fractures are induced by sufficiently pressurized fluid flow in porous media, branched fractal structures can arise. A comparison of their structure and dynamics will be presented, with the dynamics of the solid path, of the pore pressure, a direct optical imaging of the fracturing process using fast cameras, and localization techniques using the seismic wavefield monitored by transducers.

2. The force chains transmitting stress between grains during landslides and their dynamics are responsible for a complex seismic signal generated. Direct optical imaging during experiments will be compared to the seismic imaging of the same laboratory landslides ("slidequakes").

3. During biphasic flow in porous media, fractal structures of displacing fluid arise, with fractal dimensions depending on the Bond and Capillary number, and on the global configurations (more or less dense fluid arriving from the top, least or most viscous fluid displacing the other). We will see how these structures gain fractal dimensions, depending on the scaling range and the dynamics, and how this impacts the fields imaged in hydrology, as pressure, saturation and their relationships. We will show how a distribution of saturation can give information on the flow speed that displaced water/air interface.

Co-authors (with their institutions) :

Antoine Turquet (*IPGS*, Fredrik Eriksen (*IPGS*), Shahar Ben Zeev (*IPGS*), Cécile Clément (*IPGS*), Vincent Bachelet (*IPG Paris*), Maxime Farin (*IPG Paris*), KJ Maloy (*Univ. of Oslo*), Eirik G Flekkoy (*Univ. of Oslo*), Einat Aharonov (*Univ. Ben Gurion*), Stanislav Parez (*Acad. Of Scinces*), Anne Mangeney (*IPG Paris*), Julien de Rosny (*Inst. Paul Langevin, Paris*).

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#### **Dr Damien Jougnot**

SORBONNE UNIVERSITÉ UMR 7619 METIS, Campus Pierre et Marie Curie, 4 place Jussieu 75005 Paris - FR Email: damien.jougnot@upmc.fr

## Streaming potential monitoring of water flow in the vadose zone, benefits and challenges from the effective excess charge density approach

The self-potential (SP) method is a passive geophysical method that relies on the measurement of naturally occurring electrical field. One of the contributions to the SP signal is the streaming potential, which is of particular interest in hydrogeophysics as it is directly related to both the water flow and porous medium properties. The streaming current is generated by the relative displacement of an excess of electrical charges located in the electrical double layer surrounding the minerals of the porous media. We developed a physically based analytical model to estimate the effective excess charge density dragged by the water flow under partially saturated conditions. The proposed model is based on the assumption that the porous media can be represented by a bundle of tortuous capillary tubes. The excess charge that is effectively dragged by the water flow is estimated using a flux averaging approach. Under these hypotheses, this new model describes the effective excess charge density as an analytical closed-form, function of saturation and relative permeability while also depending on the chemical and interface properties, and on petrophysical parameters of the media. The performance of the proposed model is succesfully tested against previous models and different sets of laboratory and field data from the literature. This new model proposes a simple and efficient way to model the streaming current generation for partially saturated porous media that can be applied to the monitoring of water flow in the vadose zone.

Co-authors (with their institutions): Mariangeles Soldi, Luis Guarrracino (Facultad de Ciencias Astronomicas y Geofisicas, La Plata, Argentina), Flore Rembert, Alexis Maineult (UMR 7619 METIS, Paris - France), Philippe Leroy (BRGM, Orléans - France)

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#### **Dr Florian Osselin**

IST0

1A Rue de la Ferollerie 45100 Orléans - FR

Email: florian.osselin@cnrs-orléans.fr Tel :06 32 58 04 43

## Modeling crystallization pressure in the context of $CO_2$ storage in deep saline aquifers

 $CO_2$  storage in deep saline aquifers appears as a solid mid-term solution for coping with global warming, taking advantage of the huge storage capacities of these geological formations. However, the injection of supercritical carbon dioxide deeply disturbs the geochemical equilibrium of the aquifer in a very coupled way, especially in the critical zone next to the well. In particular, the evaporation of the formation brine (drying-out) and the subsequent precipitation of salts in the vicinity of the well can be potentially problematic as it clogs the percolation paths and decreases injectivity. However, salt precipitation in confined media is also known to create strong stresses on the porous matrix, often high enough to fracture the rock. This phenomenon, known as crystallization pressure, could counterbalance the clogging by salt precipitation through the opening of a new percolating network of fractures. Here, we present coupled poromechanical modelling allowing the estimation of the crystallization pressure in the context of CCS in deep saline aquifers. We show that in most cases, the generated stresses are moderate, but could in some cases overcome the mechanical resistance of the aquifer host rock.

Co-authors (with their institutions): Teddy Fen-Chong (IFSTTAR), Antonin Fabbri (ENTPE), Jean-Michel Pereira (ENPC), Patrick Dangla (IFSTTAR), Mohamed Azaroual (BRGM, ISTO).

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#### Prof. Lionel Mercury

Earth Sciences Institute of Orléans (ISTO) / University of Orléans, CNRS, French Geological Survey (BRGM) 1A Rue de la Ferollerie 45100 Orléans - FR

CONVENOR

Email: lionel-mercury@univ-orleans.fr Tel: 02 38 49 49 75

I got my PhD in 1997 on the role of capillary geochemistry in arid zones, through thermodynamic a priori calculations. Assistant professor at Orsay (France) in 1998, I pursued my studies on the capillary physics together with the adsorptive and confinement properties of liquid water in porous surficial systems. These physical states can (conceptually) drive peculiar water-rock interactions. After obtaining a habilitation degree (2006), I moved to Orléans in 2007, where I became full professor in 2011. The reactivity of interphases related to their curvatures and/or short-scale complex effect (disjoining pressure) became the core of my researches, with a predominance of experimental (spectroscopic) measurements to establish the generic features of pore-scale processes. My present researches are to observe these processes within reactive transport schemes to make them scalable up to the critical zone reasoning.

## Using micro-models to simulate critical zone's features: the analogy framework for hydro-chemo-poromechanical couplings

Unsaturated hydrosystems are complex systems with large compositional diversities and specific pore structure arrangements that concurrently drive the continuum properties. In this complex 'reservoir', the basic processes are indeed determined at the very local scale, based on the interactions between the pore network local 'infrastructure' and the short-scale composition of the resident materials. Typically, any porosity change due to a given mass transfer fails to result in a correct estimate of the permeability change, because of the localization of the crystalline deposits which drive a specific transformation of the local microstructure.

To predict how the rock microstructure may evolve under reactive transport, experiments have started to explore how interphases properties were able to control the phase transitions, to which extent, and under which dependence. We also plan to observe and quantify how the reactive schemes across interphases assembles with the transport processes to build the reactive transport mass balances, also considering explicitly the associated stress fields in the solid host.

Processes can be observed and quantified by using synthetic porous materials: silica capillaries, fluid inclusions, labs on a chip. The chemical systems and the associated phase transitions are drastically simplified, to mechanistically connect the established cause(s) to the observed effect(s) through properties scalable throughout the diversity of one given hydrosystem. The notion of scalability and the relevance of the simplifications (the 'analogy problem') will be debated, and some intriguing and stimulating observations will be presented as well as renewed thermodynamic schemes of interpretation.



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#### Dr Sophie Roman

#### UNIVERSITY OF ORLEANS

#### 1A Rue de la Ferollerie 45100 Orléans - FR

Email: sophie.roman@univ-orleans.fr

Tel : 02 38 25 50 26

#### Interface breakup and viscous coupling in porous media at the pore-scale

Multiphase flow in porous media is important in a number of environmental and industrial applications including flows through unsaturated hydro systems. Capillary, viscous and gravitational forces determine the dynamics of two-phase immiscible flow and the competition between these forces can lead to highly unstable flow. Using micromodels experiments we explore pore scale mechanisms and their consequences on the upscaling of rock and fluid properties.

Micromodel systems are transparent pore networks that allow direct and in situ visualizations of pore scale interface dynamics. We use micro-Particle Image Velocimetry (PIV) in microfluidics models to visualize the velocity distributions during two-phase flow.

With this setup, we investigated the snap-off mechanism of a gas bubble in constricted capillaries. During the displacement of water by air, snap-off is responsible for disconnecting and thus trapping of the gas phase. On a larger scale this phenomenon has implications for the residual trapping of a gas phase and on our modelling of fluid-fluid displacement processes.

We use micro-PIV measurements in micromodels to visualize the velocity distributions inside immobile globules of water while an immiscible phase in injected. In some cases, we observed a recirculating motion within the water phase that is due to the shear stress at the fluid-fluid interface. These observations and further characterization are particularly important for our modelling of immiscible two-phase flows at the continuum scale and for our understanding of transport properties.

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#### **Dr Yves Méheust**

GÉOSCIENCES RENNES (UNIV. RENNES 1) Bât. 14B, Campus de Beaulieu, Université de Rennes 1 35042 Rennes - FR

Email: yves.meheust@univ-rennes1.fr Tel : 02 23 23 62 51

#### Mixing and reactions in unsaturated porous media: analog experiments

The mixing and reactive transport of chemical elements is a primary controlling process for biogeochemical cycles and contaminant transport in the vadose zone. Reaction kinetics measured in well-mixed laboratory reactors are much faster than those measured on the field, and Darcyscale models based on Fickian transport/mixing often cannot explain measurements in the unsaturated zone. This is due to the interplay between advection by the strongly heterogeneous pore scale velocities, molecular diffusion, and chemical reactions. We use a millifluidic setup based on 2D porous media to investigate that interplay. The setup provides pore scale measurement of the velocity field and concentration field. The presence of the air phase results in an anomalous temporal scaling of the scalar dissipation rate, and, hence, of product masses in chemical reactions occurring between miscible liquids (e. g., an injected solution and a the resident water). The impact of the medium's saturation on reactive mixing is not controlled by geometry of the medium, but depends on the type of injection (continuous or finite volume). If the solute species are charged (i.e., ions), the effective electrical conductivity is strongly sensitive to their spatial distribution, but electrical resistivity tomography (ERT) performed on the field often results in a large discrepancy (of up to 80%) between the measured and injected masses of solute. Our experiment provides hints on why this is to be expected.

#### Co-authors (with their institutions):

Joaquin Jimenez-Martinez<sup>1\*</sup>, Pietro de Anna<sup>1\*</sup>, Régis Turuban<sup>1\*\*\*</sup>, Hervé Tabuteau<sup>2</sup>, Damien Jougnot<sup>34</sup>, Tanguy Le Borgne<sup>1</sup>, Niklas Linde<sup>3</sup>

> <sup>(2)</sup> Géosciences Rennes, Université de Rennes 1, Rennes, France <sup>(2)</sup> Département Milieux Divisés, Institut de Physique de Rennes, Rennes, France <sup>(3)</sup> Faculté des Géosciences et de l'Environnement, UNIL, Lausanne, Suisse <sup>(4)</sup> METIS, Université Pierre et Marie Curie, Paris, France

> > <sup>(\*)</sup> Now at ETH Zürich, Zürich, Switzerland <sup>(\*\*)</sup> Now at (3) <sup>(\*\*\*)</sup> Now at IUSTI, Univ. Marseille, France

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### **ROUND TABLE 1 (8:30 - 9:30)**

STATIC STRUCTURES - DYNAMIC PROPERTIES RELATIONSHIPS

MODERATED BY SIMON ANDRIEU (*BRGM*), PASCAL AUDIGANE (*BRGM*) & GAUTIER LAURENT (*UNIVERSITY OF ORLÉANS, ISTO*). THE FOLLOWING TOPICS AS WELL AS RELATED QUESTIONS WILL BE DEBATED:

Karst developments, porous/fractured & dual media Petrophysic properties of the carbonate rocks Conceptualizing the mass flows and numerical models Hosts vs. guests or Container vs. Content – key scientific challenges.

#### PITCH 1: Dr Marwan Fahs

Laboratoire d'Hydrologie et Géochimie de Strasbourg (LHYGES)

École Nationale de Génie de l'eau et de l'environnement de Strasbourg (ENGEES)

1 rue Blessig 67084 Strasbourg - FR

Email: fahs@unistra.fr

#### Efficient discrete fracture model for unsaturated flow in fractured porous media

Flow in fractured porous media is encountered in a spectrum of applications such as carbon dioxide sequestration, management of karstic aquifers and geothermal systems. The literature in modeling of flow in fractured media is abundant. Most of the existing studies deal with saturated porous media. Unsaturated flow in fractured porous media is marginally investigated and the related processes are still not fully-understood.

The flow in the vadose zone is often modeled using Richards' equation (RE). Accurate numerical solution of the RE remains a challenge. Fractures compounds these challenges as they typically involve complex geometry that requires dense grids. The discrete fracture network (DFN) approach, in which the fractures are embedded as 1D elements in 2D-dimensional domain, is commonly used to deal with such a difficulty.

To the best of our knowledge, the DFN approach has not been used for flow in unsaturated porous media which is often modeled using the traditional equivalent porous media approach. In this work, we develop an efficient model for unsaturated flow in fractured porous media, based on the DFN approach. In this model, we use Richard's equation for both matrix and fractures. We use advanced numerical techniques for both space discretization and time integration in order to avoid numerical artifacts. Further work is oriented towards a real field application in an epikarst site. An upscaling technique to capture two-phase flow in fractures is investigated.

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#### **PITCH 2: Dr Fabienne Battaglia**

UNIVERSITÉ D'ORLÉANS, CNRS, BRGM, ISTO, UMR 7327 45071 Orléans - FR Email: f.battaglia@brgm.fr

# Diversity and abundance of microbial communities along the non-saturated zone profile of the O-ZNS platform

The O-ZNS platform of the PIVOTS project will be a large experimental well that will allow investigations of the non-saturated zone functioning through a range of complementary approaches (geophysics, geochemistry, probes, microbiology). Microorganisms play a key role in transformation and transfer of chemical species in soil and sub-soil. In particular, microbes present in the non-saturated zone, acting as a filter bioreactor, can transform the compounds transferred from the surface to groundwater, in particular dissolved organic matter and other chemical species potentially used by living organisms as electron donors or acceptors (ammonium, nitrate, sulfur species, dissolved iron of manganese...). However, up to now, the microflora of the non-saturated zone was less studied than the micro-organisms of the surface soil or groundwater.

In the O-ZNS site, samples of cores will be taken at 50 cm intervals, and in all different facies, in particular in the heterogeneous zones. These samples will be crushed and stored at -20°C until DNA extraction. Then, the ribosomal 16S gene will be amplified and analyzed using a molecular fingerprint method (t-RFLP) in order to perform a first screening of spatial distribution of bacterial diversity and to elaborate a map of the bacterial communitie structure along the O-ZNS platform profile. A selection of extracted DNA will further be submitted to high-throughput sequencing in order to acquire qualitative and quantitative data about the taxonomic biodiversity of bacteria and archaebacteria along the profile. In parallel, DNA samples will be stored at -80°C for further studies targeting specific functional genes that will be interesting for future projects.

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## **ROUND TABLE 2 (9:30 - 10:30)**

IMAGERY, SPATIALIZATION AND DISCONTINUITIES IN GEOLOGICAL BODIES

MODERATED BY GILLES GRANDJEAN *(BRGM)*, RENAUD TOUSSAINT *(CNRS)* & ANDRÉ REVIL *(CNRS)*. THE FOLLOWING TOPICS AS WELL AS RELATED QUESTIONS WILL BE DEBATED:

Physical chemical of interfaces and physical signatures Data acquisition, localization, interpolation and joint interpretations Visible and supposed/interpreting discontinuities Scales and relevant supports to tackle the locks:

O-ZNS observatory – Mesoscale platforms as PRIME and EcoSENS – Lab scale: flow through columns and GLoCs. Modelling challenges: hybrid mesh – deterministic/ stochastic for predictivity – mechanistic calibration – micro-continuum approach and couplings.

#### PITCH 1: Dr Clara Jodry

IST0

1A Rue de la Ferollerie 45000 Orléans - FR

Email: clara.jodry@cnrs-orleans.fr

#### The DNA of O-ZNS platform, the geophysical objectives

The observatory (0-ZNS platform), a part of the family of PIVOTS (Environmental Technology Innovation, Development and Optimization Platforms) program, aimed to understand the water-rock-biosphere interactions and the mass (water and contaminants) and heat transfers in the vadose zone (VZ). The 0-ZNS, developed around an exceptional well dimensions (depth - 20 m & dimeter - 4m), offers a unique support for deciphering, at relevant scales (from nano- to metric scales), coupled phenomena in the environmental geosciences.

Contribution of geophysical imagery technique is key to spatialize relevant information within the vadose zone. To this purpose, the platform allows the development and adaptation of innovative geophysical in situ monitoring technique. Use of multi geophysical measurements from the surface and boreholes in addition to the well itself will allow highlighting different scales and resolutions. Whether it is definition of lithologies, descriptions of seasonal hydric behaviour of the vadose zone, or even observations of the solution/precipitation phenomenon in fractures.

Laboratory complementary measurements will help understanding origins of the geophysical measurements evolution throughout time and space as well as link those responses to bio-physico-chemical properties by means of empirical petrophysical relationship.

Geophysical data interpretation are combined with geological and hydrogeological informations by way of joint inversion, which takes into account sensitivity and resolution of the different

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methods. The observatory aimed to establish in fine predictive transfer models based on these multiple observations and petrophysical relationships.

This project represents a great opportunity to compare and contrast measurements made in a controlled environment such as laboratory testing to field conditions and thus deconvolute the multiphase reactions in the vadose zone.

#### PITCH 2: Dr Céline Mallet

#### LABORATOIRE LAMÉ, UNIVERSITÉ D'ORLÉANS

8 rue Léonard de Vinci 45100 Orléans - FR

Email: celine.mallet@univ-orleans.fr

#### Seismic characterization of transport properties of cracked rocks

Cracks control the transport properties of reservoir porous rocks in whatever saturated or unsaturated conditions. Due to their field uses, seismic tools have to be considered in laboratory studies to investigate the characterization of fractured rocks. Especially, the attenuation of seismic waves in fractured porous media is governed by the fracture interconnectivity. It offers the perspective of linking seismic observations to the transport properties of fractured rocks.

I worked with a numerical model based on porous mechanics in order to interpret mechanical data in terms of wave velocity dispersion. It has been used to validate the signature of a low cracked material. Then, this process has been applied to a large branch of data in order to determine the effect of crack density, rock permeability, thermal and hydraulic conditions on the wave dispersion. It appears that the wave velocity dispersion is much more pronounced when (i) crack density increases and (ii) between unsaturated and saturated cases. However, temperature seems to decrease this dispersion. This study is a first step to understand the link between transport properties and wave velocity dispersion. It has to be tested on more various materials with more or less complex crack networks.

Yet, scale issues have to be discussed especially in terms of frequency variation. This is an important issue to deal with when trying to link laboratory interpretations and field applications.

#### BREAK (10:30 -11:00)

#### **ROUND TABLE 3 (11:00 - 12:00)**

HYDROSYSTEMS DYNAMICS AND COUPLINGS BETWEEN PROCESSES

#### MODERATED BY MOHAMED AZAROUAL *(ISTO, BRGM)*, LIONEL MERCURY *(UNIVER-SITY OF ORLÉANS, ISTO)* & CHRISTOPHE TOURNASSAT *(ISTO, BRGM)*. THE FOL-LOWING TOPICS AS WELL AS RELATED QUESTIONS WILL BE DEBATED:

Interfaces = capturing discontinuities, concentrated driving forces, an aggregation area Buffered zones, quasi-steady states, reactive/moving fronts

The inverse models, the role of the ghost zones and ephemeral phenomena From fields to the lab, from labs to model, and back to the fields: there any virtuous loop/workflow?

The virtuous linkage between research and training: from research to training, from training to the engineering  $\vartheta$  geotechnological needs and back to research.

#### PITCH 1: PhD Student Alexandra Mattei

MINES ParisTech PSL University / GEOTOP UQAM

35 rue Saint-Honoré 77300 Fontainebleau - FR

Email: alexandra.mattei@mines-paristech.fr

#### Are pore water stable isotopes a powerful tool for soil model calibration ?

Accurate estimates of soil hydraulic parameters and dispersivities are crucial to simulate water flow and solute transport in the vadose zone. However, parameters determined from laboratory experiments have low accuracy to describe field-scale processes. The inverse modeling approach is an established method that results in effective parameters, which lump the system's subscale heterogeneity and describe its behavior at the targeted field scale. A key question to the inverse modeling approach is whether the measurements contain sufficient information to estimate the effective hydraulic parameters with the required accuracy.

The type of data used for model calibration is investigated here. We compared 4 strategies for model calibration, with the use of (i) one single depth profile of water content at a given sampling time, (ii) one depth profile of both water content and pore water isotope composition at a given time and monthly monitoring of water content/pore water isotope composition at 15cm depth, (iv) one depth profile of both water content and pore water isotope composition at a given time and daily monitoring of water content at 4 different depths. A realistic calibration is possible without temporal continuous monitoring data using only water content/pore water isotopic composition profiles at a given and single sampling time. However, even if not continuous, temporal data, and especially pore water isotope data, prove to be useful for model calibration.

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#### **PITCH 2: Dr Florian Osselin**

IST0

1A Rue de la Ferollerie 45000 Orléans - FR

Email: florian.osselin@cnrs-orléans.fr

#### Karst-on-chip, dissolution patterns of gypsum dissolution in an analogue fracture

Dissolution of rocks is a fundamental process in the shaping and weathering of natural landscapes. Additionally, the study of dissolution processes is also of highest importance in engineering applications such as EOR or CCS.

If batch dissolution processes are well known and explored, the coupling of dissolution and flow rate during reactive percolation is much more challenging. For example, the coupling of flow and reaction is evidenced through the reactive infiltration instability where heterogeneities in permeability cause differential dissolution leading to a positive feedback at the origin of wormholes and fingering.

In order to study this phenomena and coupling, we have designed a very simple and efficient microfluidic device consisting of a chip of pure gypsum inserted between two polycarbonate plates and subjected to a constant flow rate of pure water. Thanks to this device, we are able to control all parameters such as flow rate, fracture aperture, roughness of the walls... but also to observe in situ the progression of the dissolution thanks to the transparency of the polycarbonate. We have been using this experimental set-up to explore and investigate all aspects of the dissolution in a fracture, such as initial instability patterns formation, and to compare it with theory and simulations.

#### LUNCH (12:00 -13:30)

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## **ROUND TABLE 4 (13:30 - 14:30)**

SMART SENSORS FOR ENVIRONMENT AND GEOSCIENCES

#### MODERATED BY RAPHAËL CANALS (UNIVERSITY OF ORLEANS, PRISME), EMERIC FREJAFON (BRGM) & YUXIN WU (LBNL), THE FOLLOWING TOPICS AS WELL AS RE-LATED QUESTIONS WILL BE DEBATED:

Passive samplers and physical chemical monitoring tools How to install multi-parameter monitoring measurements for high resolution and massive data generation?

Smart architecture of multidisciplinary monitoring technics (T, µmovements, etc.)

#### PITCH 1: Dr Isabelle Cousin

INRA

UR0272 Sols, 2163 avenue de la Pomme de Pin, CS40005 Ardon F-45075 Orléans Cedex 2 - FR

Email: Isabelle.Cousin@inra.fr

#### The soil-atmosphere interface: a front and exit door to the unsaturated zone

At the top of the unsaturated zone, the soil, at the interface with the atmosphere, is the location of interactions of this unsaturated zone with climate and human activities, especially agricultural practices. In contrast to the major part of the unsaturated zone, whose structure can be considered as stable at the year or decade scale, the soil structure evolves at a short timescale - from the second to the season - under the combined influences of i) the living organisms activities (rhizosphere, mesofauna and macrofauna), ii) the action of the climate (succession of rainfall events bringing water for infiltration, and sunny periods favorable to evaporation), and iii) human activities (cropping, tillage). The dynamics of fluids exchange in soil is therefore complex, because the structure of the porous network is not stable, and because the gas and water flow direction, ascending or descending, changes at high frequency. A better understanding of the determinism of these hydric and gas exchanges requires addressing the following research questions: i) characterising and modelling the plant root dynamics in interaction and in feedback with the water and gaseous functioning of the soil, ii) as a consequence of the previous point, quantifying the contribution of the deep soil layers (or even of part of the unsaturated zone) to the water supply of the plants, iii) improving our understanding of the determinism of gas emissions from the soil towards the atmosphere, in relationships with the soil structure dynamics and the soil hydric functioning. Our presentation will present some innovative tools to address these issues.

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#### **PITCH 2: Dr Frédérick Gal**

BRGM

1A Rue de la Ferollerie 45100 Orléans - FR

Email: f.gal@brgm.fr

#### Investigations techniques for near surface monitoring

Understanding the unsaturated zone relies on investigating compartments strongly influenced by atmospheric processes or, until water-saturated horizons are reached, influenced by deeper processes. Consequently, the use of a wide spectrum of monitoring techniques is required to investigate appropriately each of these compartments. Here, some of these techniques used at BRGM will be presented. It consist in the coupling of soil gas concentration and soil gas flux monitoring techniques, including the monitoring of isotope of C-rich gas species. Such approaches have been applied successfully in Environmental Baseline Assessment in CO, storage applications or hydrocarbon applications. Below ground level, it may still be the characterization of gas footprint in the soil and subsoil but also the determination of the chemical characteristics of pore water, especially under the frame of better understanding infiltration and percolation processes in a complex bio-geological matrix. Once in the capillary fringe being described, again an interesting compartment to focus on, the challenge of well describing the processes of e.g. gas emissions from an aquifer to the unsaturated zone is still pregnant. Last, in the saturated zone, the corpus of monitoring techniques ranges from common purging techniques to less frequently used passive sampling techniques, for which devices aiming to standardize trapping of dissolved elements are developed and implemented. In the case of layered aguifers, whose vertical heterogeneities are assessed through chemical logging, investigations techniques may also rely on the use of deep sampling techniques or point sampling techniques to stress precisely the subtle chemical variations that may exist along a water column.

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## **ROUND TABLE 5 (14:30 - 15:30)**

ARTIFICIAL INTELLIGENCE FOR ENVIRONMENTAL ISSUES

MODERATED BY CHARLES GUMIAUX (*ISTO, UNIVERSITY OF ORLÉANS*), VINCENT LABBÉ (BRGM) & FRANÇOIS ROBIDA (*BRGM*). THE FOLLOWING TOPICS AS WELL AS RELATED QUESTIONS WILL BE DEBATED:

Machine and deep learning for spatial environmental data How novel data science, data mining, and artificial intelligence techniques can innovate and inform environmental modeling practices, Interoperability & Preparing and Architecturing for Machine Learning.

#### PITCH 1: Dr Emilio M. Sanfilippo

#### LE STUDIUM, LOIRE VALLEY INSTITUTE FOR ADVANCED STUDIES, ORLÉANS & TOURS

Université de Tours, 59 rue Néricault-Destouches 37020 Tours - FR

Email: emiliosanfilippo@gmail.com

# Ontology engineering by stressing the use of ontologies for geological knowledge representation and data modeling

I will give in the talk a flash overview of ontology engineering by stressing the use of ontologies for geological knowledge representation and data modeling.

Ontology engineering is an interdisciplinary area of research at the intersection between computer science, artificial intelligence, logics, linguistics, cognitive science, and philosophy (e.g., mereological theories to model part-of relations). Its purpose is the development of formal models, called ontologies, to represent human knowledge in a way that is transparent and accessible to both human and artificial agents. Ontology-based information systems and applications are nowadays exploited in various domains (e.g., medicine, manufacturing, robotics, agriculture, architecture and civil engineering, archaeology, etc.) for different purposes, e.g., to support data sharing, model the inter-relations between data, annotate visual models with experts' knowledge or automatically reason over knowledge and data, just to mention few cases. In particular, the core advantage of ontology-based architectures is to make explicit the intended semantic (meaning) of data, which is necessary to allow multiple agents and systems to interoperate without the loss of relevant information.

In the context of geology, ontologies are used at both the research and industrial levels (e.g., ISO 15926 for the gas and oil industry) to formally describe domain entities of geological interest (e.g., what is a void?), disambiguate and align heterogeneous experts' terminologies to facilitate communication and systems interoperability.

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#### **PITCH 2: Dr Vincent Labbe**

BRGM

3 Avenue Claude Guillemin 45100 Orléans - FR

Email: v.labbe@brgm.fr

## Modeling by machine learning in addition to the classic models of the subsoil: yes but ... need explanations.

To predict natural phenomena related to the subsoil (presence of mineral resources, groundwater dynamics, seismic risks ...) presents important issues: from anticipation of crisis to the sustainable management of natural resources. The amount of available data on these phenomena grow rapidly but the societal need to anticipate them grows as well.

Historically, different kinds of models have been used to predict these phenomena: especially empirical, physical and statistical models. Each type of modelling comes with their pros and cons. Independently, the scientific community in the domain of Artificial Intelligence – from machine learning field in particular - has developed algorithms leading to efficient, general, industrialized and agnostic predictive models. These models prove each day a little more their superiorities in certain tasks (image recognition, text classification, speech recognition ...) in terms of efficiency and should complement the existing panel of the subsoil models in a very relevant way.

However, they often present themselves like «black boxes»: we do not know why, in fine, the predictions are made. The resolution of this particularity constitutes an emerging scientific trend, which aims to improve both the confidence we have in these models (ensure that a good prediction is made for good reasons), and the understanding of the underlying phenomena.

#### **PITCH 3: Dr Léo Fourrier**

**BRGM / LIFAT / UNIVERSITY OF TOURS** 

BRGM - 3 Avenue Claude Guillemin 45100 Orléans - FR

Email: l.fourrier@brgm.fr

#### Prediction of groundwater level with Machine Learning methods

In this talk, we will present a way to predict groundwater level using machine learning.

Predicting groundwater level is an important task in the efficient management of groundwater resources. In our society, these resources are widely used by many actors, most notably industry, farming and domestic usage. Being able to accurately predict groundwater level allows to alleviate various risks like droughts and floods.

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To ease the deployment on a larger scale of models such as already existing semi-empirical models currently in use, we use a LSTM, a type of recurrent neural network dedicated to timeseries. We feed it with signals of a specific watershed: groundwater level captured by piezometers, evapotranspiration, pluviometry, debit, pumping. We compare our model, that does not require tuning by experts, to an existing humanly parametrized semi-empirical model, t o ensure that performances are at least comparable. Our first results show that both models indeed play in the same ballpark leaving room for future work on the confidence of black-box prediction model.

### BREAK (15:30 -16:00)

#### **GENERAL SYNTHESIS OF THE WORKSHOP** (16:00 - 17:00)

What are the main outcomes? What can we expect, who will do, when/where re-meeting to record advances and update the issues and objectives?

AUDIENCE : Academics, Industrials, The people in-between.

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24/06/2019 11:13:37

# POSTERS

## • Use of Harmonic pumping tomography for identification of groundwater flow paths in a karstic and fractured aquifer

A.Jardani<sup>1</sup>, P. Fischer<sup>1</sup>, H.Jourde<sup>2</sup>

<sup>(1)</sup> Normandie Univ, UNIROUEN, UNICAEN, CNRS, M2C, 76000 Rouen - FR

<sup>(2)</sup> Laboratoire Hydrosciences, Université de Montpellier, CNRS, 34000 Montpellier - FR

The exploitation of karst water resources relies on the identification and characterization of the preferential flow paths developed around fracture and karst networks. In this poster, we discuss the relevance and effectiveness of harmonic pumping tomography in the localization of fracture networks. The method involves applying an oscillatory pumping with multiple frequencies and interpreting the hydraulic responses recorded at different wells in terms of transmissivity and storativity fields, through an inversion algorithm in which the groundwater flow equation solved in frequency mode. This approach has been tested on an experimental site (Terrieu) with 13 wells set up on a karstic area (2500 m2).

#### Fiber optic sensors for environmental monitoring

#### Bouamama Abbar<sup>1</sup>

<sup>(1)</sup> Waves and Complex Media Laboratory (LOMC), UMR 6294 CNRS, University Le Havre - FR

Email: bouamama.abbar@univ-lehavre.fr

Fiber optic sensors represent a new and innovative measurement technology in different fields, such as security, energy, civil engineering, and environmental monitoring (geotechnical zones, rivers and sea monitoring ...). Their interest lies mainly in the intrinsic properties of optical fibers: electromagnetic neutrality, large multiplexing capability and access to long measurement distances. These advantages allowed them to measure a large number of factors and phenomena such as position, vibration, temperature and pressure (Bremer et al., 2017), CO2 and humidity (Stolberg-Rohr et al., 2011, Starecki, et al., 2015) and groundwater flow monitoring (Drusová et al., 2019). The advantages of fiber optic sensors are thus strongly differentiating, with the possibility of use in hazardous environments, and excellent metrological performance in terms of sensitivity, or response time. In addition, this type of sensor offers new measurement functionalities: integrated, distributed or in grating. The implementation of optical fiber grating sensor thus considerably reduces the cost of a measuring point, allowing the pooling of the information processing system for many sensors. In this poster, the principle, the advantages of optical fiber sensors and some applications in civil engineering and environmental monitoring are presented.

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## • Experimental and numerical assessment of transient stream-aquifer exchange during disconnection

A.Rivière<sup>1</sup>, J.Gonçalves<sup>2</sup>, A.Jost<sup>3</sup>

<sup>(1)</sup> MINES PARISTECH - FR

<sup>(2)</sup> CEREGE - FR

<sup>(3)</sup> METIS - FR

Email: agnes.riviere@mines-paristech.fr

Understanding the state of connection processes of stream-aquifer systems is of great interest for water resources management, particularly in semi-arid regions and where groundwater is extracted in the vicinity of a river bank. Here we present a combined experimental-numerical study to explain physical processes involved in disconnected stream-aquifer systems. A streamaquifer sand box was built to measure the infiltration rate through the stream bed during aquifer drainage. The pressures in the saturated zone of the aquifer and the infiltration rate were measured in order to quantify the fluid flow in this system. The transient transitional stage between connected and disconnected flow regimes, which was obtained experimentally, is characterised by a maximum infiltration rate across the stream bed before a decrease towards a constant value. This behaviour is analysed by means of transient numerical simulations using relevant hydrodynamic parameters. The importance of the drainage kinematics and unsaturated zone parameters for the temporal variation of the infiltration rate is demonstrated. The possible occurrence of a maximum infiltration rate value during the transitional stage is characterised into a general view of the stream-aquifer disconnection with direct implications for pumping near a stream.

#### Numerical modeling of water flows in unsaturated media using time-lapse MRS measurements

<u>A. Legchenko<sup>1</sup></u>, Jean-Michel Baltassat<sup>2</sup>, Céline Duwig<sup>1</sup>, Marie Boucher<sup>1</sup>, Jean-François Girard<sup>3</sup>, Alvaro Soruco<sup>4</sup>, Alain Beauce<sup>2</sup>, Francis Mathieu<sup>2</sup>, Cedric Legout<sup>5</sup>, Marc Descloitres<sup>1</sup>, Gabriela Patricia Flores Avilés<sup>4</sup>

IGE - IRD - FR
BRGM - FR
IPGS/EOST - FR

<sup>(4)</sup> INSTITUTO DE INVESTIGACIONES GEOLÓGICAS
Y DEL MEDIO AMBIENTE - BO
<sup>(5)</sup> UNIV. GRENOBLE ALPS, IGE - FR

Email: anatoli.legtchenko@ird.fr

We have developed and tested on real data a new hydrogeophysical approach to investigate the water processes taking place in the unsaturated zone composed of non-magnetic materials (chalk, limestone, ...). The method consists of combining Magnetic Resonance Sounding (MRS) time-lapse measurements with numerical modeling of water flows in partially saturated media. We use the NUMIS MRS instrument for measurements and an existing software HYDRUS-1D for water modeling. The data assimilation program developed specifically for this study, facilitates the exchange of information between the geophysical and hydrogeological interpretation procedures. Obtained hydrodynamic properties of the subsurface correspond to an average throughout the investigated volume defined by the loop size (75 x 75 m<sup>2</sup>). Obtained results are consistent with the known hydrogeological conditions and the limitations of the approach are summarized to help geophysicists and hydrogeologists to apply this approach.

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# • PESAa - Platform for studying Soil–Atmosphere Exchanges on agricultural soils. An agro-environmental equipment for experimentation and acquisition of agro-environmental references

I.Cousin<sup>1</sup>, A. Ayzac<sup>1</sup>, L. Cottenot<sup>1</sup>, H. Gaillard<sup>1</sup>, G. Giot<sup>1</sup>, A. Grossel<sup>1</sup>, M. Lacoste<sup>1</sup>, C. Le Lay<sup>1</sup>, C. Pasquier<sup>1</sup>, M. Seger<sup>1</sup>

<sup>[1]</sup> INRA - FR

#### Email: Isabelle.Cousin@inra.fr

The PESAa platform - Platform on « Soil – Atmosphere » Exchanges of agricultural soils – is an agro-environmental equipment, consisting in a support for experimentation and acquisition of agro-environnemental references on soil functions and services, especially on gas and hydric exchanges between the soils, the water and the atmosphere. The PESAa platform is dedicated to the characterization of the physical (water retention, structural stability, soil structure, ...) and biological properties of soils (nitrification, denitrification,...), of their hydrological functioning and of their greenhouse gas production. It may likewise engage experimentations in relation to their waterflow and biogeochemical operations, in laboratory controlled conditions (rainfall simulation); or in situ, on two Inra sites.

The facilities available on the platform are: i) a rainfall simulator, ii) laboratory facilities for the characterisation of the physical properties of soils, iii) analyzers of gas samples, iv) measurement chambers for  $N_20$  emissions from soils, v) numerical soil-analysis tools for the analysis of the spatial soil functioning (GIS, geostatistics). In the near future, the platform will be equipped with vi) a high-precision irrigation facility on the experimental plot of Nouzilly, vii) automated chambers for the continuous measurements of  $N_20$  emissions, viii) micro-meteorological measurement devices for  $N_00$  emissions on the  $0S^2$  experimental plot.

· Gas transfer in soils: application to the case of peatlands

L.André<sup>1</sup>, S. Gogo<sup>1</sup>, F. Leroy<sup>1</sup>, A. Jacotot<sup>1</sup>, F. Laggoun<sup>1</sup>

<sup>(1)</sup> BRGM - FR

Email: l.andre@brgm.fr

Northern hemisphere peatland soils contain ~33% of global soil carbon, while accounting for only 3-5% of total land area. Many of these peatlands are degraded and emit rather than store carbon. Global annual GHG emissions from drained organic soils are ~1,600 MT  $CO_2$  eq., twice that from aviation. In NWE this is ~150 MT/year, more than Belgium's emissions. Yet emission estimates from degraded peatlands are inadequate and we lack effective strategies and methods to combat degradation and promote recovery.

It is then necessary to develop integrated approaches able to estimate the gas transfers from field measurements but also to predict them through modelling approaches according to impacting parameters such as climate changes. This methodology is applied in the INTERREG Care-Peat project, where five knowledge institutes from three European countries work together to develop and test new techniques and methods necessary to understand the best ways of restoration to reduce carbon emissions and increase the C-sequestration function in peatlands. These pilots are also necessary to develop better methods and decision-making tools (i.e., modelling approaches) and to identify sustainable best practices and strategies for widespread incorporation.

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#### Ecodynamics of trace metals in reactive zones of the critical zone: evidence for redox "microniches"

M.Motelica-Heino<sup>1</sup>

<sup>[1]</sup> ISTO - FR

Email: mikael.motelica@univ-orleans.fr

Measurements of trace metals in sediments, soils and water columns of lakes and rivers soils have

shown that they are involved in dynamic geochemical transformations that are often driven by biologically controlled processes. While changes in redox state offer general mechanisms for supply and removal of metals from solution, there may be specific linkages of particular elements. Almost all of the redox transformations are microbially mediated. Identification of precise mechanistic linkages between the geochemistry and biota will be best achieved if measurements are made at a scale that relates directly to the individual organism or its species-specific grouping. The key is to identify the reactional mechanisms related to biogeochemical processes that control their bioavailability and global cycling at the relevant spatial scale. We present in-situ investigations of the microdynamics of trace metals in natural environmental systems with in-situ sensors such as DGT (diffusive gradients in thin-films).

Our work is contributing to the emergence of a new paradigm for the behaviour of trace elements. In sediments small-scale remobilisation within a 3-dimensional framework ("microniches" as localized hot-spots of reduced organic matter) appears to be superimposed on the relatively macro-features of systematic vertical changes associated with redox zones. Correspondence between fine structure observed for the different trace metals and fine structure in sulfide, iron, manganese and nutrients, has provided insight into the linkages of the supply/removal processes of metals at a small scale, particularly the role of Fe, Mn and S(-II) phases and microorganisms.

# • Effects of temperature and saturation changes on dielectric permittivity and complex electrical resistivity of porous media saturated with DNAPLs: a laboratory study

M.Iravani<sup>1</sup>, J.Deparis<sup>1</sup>, H.Davarzani<sup>1</sup>, S.Colombano<sup>1</sup>, R.Guerin<sup>2</sup>, A.Maineult<sup>1</sup>,

<sup>(1)</sup> BRGM - FR <sup>(2)</sup> SORBONNE UNIVERSITÉ - FR

Email: a.iravani@brgm.fr

Few studies have discussed effects of temperature and saturation changes on electric properties of multiphase porous media polluted by Dense Non-Aqueous Phase Liquids (DNAPLs). This study attempts to characterize variations of relative permittivity and electrical complex resistivity in these porous media. All measurements were carried out using a column and a 2D tank. Spectral Induced Polarization (SIP) and Time Domain Reflectometry (TDR) were used to measure complex electrical resistivity and relative permittivity, respectively. Results for two DNAPLs with water and canola oil with ethanol on different temperatures (20 °C to 50 °C) and saturations were investigated. Concerning to temperature change, results demonstrated that real parts of relative permittivity and electrical resistivity are functions of temperature. The temperature increase leads to decrease in amplitude and phase shift of complex electrical resistivity of DNAPLs.

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Two sets of experiments examined impacts of saturation changes on these two geophysical parameters. Our findings show that due to high resistivity of oil and coal tar, increase in water saturations leads to decrease in resistivity and phase. Resistivity and relative permittivity evolutions with saturation were compatible with Generalized Archie's law and CRIM mixing models, respectively. Moreover, effects of temperature and saturation on complex resistivity on frequency domain and Cole-Cole parameters in Pelton model were evaluated in this work. Results for a 2D tank DNAPL pumping test under non-isothermal conditions will be also presented.

## • Measurement of hydraulic properties of soils and rocks using an unconventional triaxial system coupled to the multistep outflow method

C.Aldana<sup>1</sup>, A.Isch<sup>1</sup>, A. Bruand<sup>1</sup>, Y.Coquet<sup>2</sup>

ISTO - FR
OSUC - FR

#### Email: carlos.aldana@cnrs-orleans.fr

The understanding of water flow and solute transport processes through the vadose zone is a cornerstone in the preservation of groundwater resources. For many years, various laboratory techniques and equipments have been designed to estimate soil hydraulic properties. We present an unconventional triaxial system adapted to 70 mm-diameter samples that is coupled to the multistep outflow method (MSOF) to measure the hydraulic properties of soils and rocks under both saturated and unsaturated conditions by means of a gas pressure-volume controller creating a three-phase unsaturated porous media. The purpose of this experiment is its versatility that allows the estimation of the hydraulic properties of all vadose zone samples using a unique assembly that runs the same specimen. This technique shows the benefits of using a triaxial cell, which allows reproducing overburden field conditions. The whole operating mode in saturated and unsaturated conditions may be successively carried out, thus avoiding sample being disturbed due to switching of the method or re-coring that could impact the reproducibility of measurements. Among the advantages of the device is the high accuracy of the outflow measurement since the pressure-volume controller has a 1 mm3 resolution. Void ratio is also measured throughout the experiment in order to evaluate the volume change of the samples as a consequence of each pressure step. As a testing material a large range of samples with different textures and hardness were used such as repacked silty loam, undisturbed silty clay loam soil with plastic behavior, loamy sand sediment, as well as highly cemented limestone. After several tests, the effectiveness of the system has been evaluated according to the nature of the samples. Results show that the shape of the water retention curve and unsaturated hydraulic conductivity curves are in agreement with the information found in the literature according to the nature of the material. However, it seems that the effect of overburden decreases hydraulic properties when compared with other laboratory experiments. Void ratio measurements showed that porosity values decreased slightly in the order of 3-5% at the end of the whole experiment.



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• Possible positive feedback in geochemical and hydrogeological processes in a clay till, hill slope

R.Jakobsen<sup>1</sup>

[1] GEUS - DK

Email: raj@geus.dk

A 2D transect along the flow was sampled 3 times over a year. Data show variations in NO, and  $NH_{\star}^{\star}$  distributions as well as the position of the undulating redox interface (seen as an increase in  $SO_{2}$  appearing to coincide with stable water isotope signals and variations in the saturation for SiO<sub>2</sub> (SI<sub>singl</sub>. Nitrification appears to be slower in a zone where stable isotopes and SISiO2 indicate that infiltration is higher, related to a flat part in the 2D transect. Perhaps the depth to the reducing zone where nitrate disappears relates to small-scale variations in the topography affecting precipitation. A first attempt, looking into possible effects of variations in infiltration was made using the reactive saturated transport code PHAST, but only slight undulations could be created even with large variations in infiltration along the surface, indicating that effects of infiltration variations on the water saturation need to be included. Perhaps small variations in local topography, leading to small variations in precipitation and infiltration, affects the O2 flux to reduced compounds in the deposited till, via the water content and thereby diffusivity. Lower precipitation implies more oxidation of e.g. pyrite and higher acid production, increasing the dissolution rate of carbonate dispersed in the glacial till sediment, increasing porosity, reducing saturation, increasing diffusivity, further increasing oxidation, acid production and carbonate dissolution. This positive feedback loop could lead to an undulating redox interface formed since infiltration and oxidation started after the last glaciation. However, to model it requires that the changes in diffusivity over time, as a result of mineral weathering are included in the model

## Semi-analytical solutions and numerical approach for reactive transfer in a saturated pore network model

T.Kamtchuenq<sup>1</sup>, J-L.Rouet<sup>134</sup>, M.Azaroual<sup>134</sup>, O.Rozenbaum<sup>234</sup>, E.Le Trongl<sup>134</sup>, S.Adil<sup>4</sup>

ISTO - FR
CEMHTI - FR
CNRS - FR
BRGM - FR

Protection and remediation of ground water resources are a major societal challenge. It implies to understand the transport mechanisms of organic and inorganic pollutants in the saturated and unsaturated zones. For that purpose numerous studies have been conducted to model the multiphase reactive transport in a porous media. The Pore Network Models (PNM) simplify drastically its geometry and consider pores linked by straight throats of constant section. With such geometry the solution of the Stokes'equation is directly integrated so the computational effort is dramatically reduced.

As chemical reactions are very sensitive to the reactant concentration it is important to be

able to follow precisely their values throughout the pore network. Using Laplace transform, the reaction-transport equation is integrated in throats, based on the main assumption that pores act as perfect reactors. Furthermore, we exhibit a semi-analytical solution of the time evolution of the concentrations in both throats and pores. The solutes transport consists in a Volterra equation system. Its convolution kernels are expressed as a summation of exponentially decreasing time functions (except the first term which is constant). The time constant is driven by the diffusion time (td). As td goes to zero, keeping the Peclet number fixed, each term of the summation reduces to a Dirac. The response of the system is then instantaneous. When the volume of the pore is large enough it is possible to neglect all the terms of the kernel except the constant one. In the limit where the Peclet number goes to zero, usual models are recovered. Numerically, the exponential decay time of the kernel allows optimizing the computational time according to a given precision.

#### Permeation Research Activities of The P2CF Team

S.Abdelhakim<sup>1</sup>, K.Chetehouna<sup>1</sup>, N.Gascoin<sup>1</sup>

<sup>[1]</sup> INSA - FR

Email: abdelhakim.settar@insa-cvl.fr

P2CF (Permeation, Pyrolysis, Combustion and Fire) is a research team affiliated to the CE (Combustion-Explosion) axe of the PRISME laboratory, Orleans university. The team is composed from 9 members with 3 full professors. The research activities cover a multitude of themes related to pyrolysis, fire behaviour of heterogonous materials, fire safety and flow/porous materials interaction, including particles deposition.

In the present workshop, focus on the permeation research activities of P2CF team will be presented. Scientific problems in this field are related to the interaction between fluid flows and porous media, using experimental and numerical approaches. Many application sectors are concerned, among them, the use of porous media as thermal protection of combustion chamber walls, i.e. those of scramjets, attracts considerable attention within P2CF team. Especially with regard to the transpiration cooling process. In fact, porous media improve the heat extraction involved by the high thermal load endured by scramjets. However, the transpiration process can be subject to coke formation caused by the pyrolyzed fuel. To address this issue, experimental and numerical studies are conducted to enhance the process. Conducting experimental study in conjunction with numerical one allows to explore the transpiration cooling efficiency.

#### Labbio pilots

M.Crampon<sup>1</sup>, S.Stephant<sup>1</sup>, H.Thouin<sup>1</sup>, S.Dupraz<sup>1</sup> <sup>(1)</sup> BRGM - FR

Email: m.crampon@brgm.fr

The Platforms for Remediation and Innovation in service of Environmental Metrology (PRIME) is

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one of the seven platforms of the PIVOTS program. The PRIME platforms, managed by the BRGM, aim to (1) identify and quantify soil, sub-soil and groundwater pollution, (2) predict their potential impact on the environment in the short and medium term, (3) offer solution to remedy and study affected areas. PRIME is composed of centi- to pluri-metric experimental pilots. These facilities make it possible to validate tools, methods and techniques dedicated to the remediation or monitoring of degraded environments.

The LABBIO pilots are three metric devices (mesocosms), which aim at studying contaminant transfers in soil, both in the root zone and at the interface of the unsaturated/saturated zones. The mesocosms are composed of a sealed stainless steel columns of about 1 cubic meter. These are instrumented to control and manage the experimental conditions (temperature, humidity, lighting, water sprinkle, water table level). The columns are instrumented with an automated sampling system to monitor the physical, chemical and microbiological changes occurring in the system.

Like other PRIME platforms, LABBIO pilots are usable in the framework of research projects that can be subsidized, collaborative, or considered as service delivery. The scientific expertise, technical knowledge and analyses can all be mobilized in BRGM, from the studies conception to interpretation and valorisation of the results.

#### Time monitoring of electrical resistivity in the vadose zone

M.Serger<sup>1</sup>, G. Guillaume<sup>1</sup>, I.Cousin<sup>1</sup>

<sup>[1]</sup> INRA URSOLS - FR

#### Email: maud.seger@inra.fr

Climate change modifies the precipitations and temperatures, changing the distribution of water supply in soil during the growing seasons of cultivated plants. To help farmers to optimize their irrigation, the description of water processes in agricultural soils is essential. In this context, we have evaluated a new geophysical device to characterise water exchanges in the vadose zone, both in the soil (area prospected by the roots), and at the soil / subsoil interface. We were especially interested in identifying ascending fluxes linked to capillary rise. About 50 meters from the O'ZNS area, the studied soil has been equipped with a drilling device measuring the electrical resistivity on 21 levels up to 3.1 m several times a day: the "Subsurface Monitoring Device" (SMD). After a 2 years measurements period, we are optimistic about the whole quality of the measured data recorded by the SMD since April 2017, despite the low level quality of some surface measurements due to soil / electrode contact problems. Comparisons of SMD data with independent resistivity measurements demonstrated the good coherence of data. The device allows us to acquire data at a resolution in depth that would not be accessible by a surface geophysical device. The temporal analysis suggested that water transfers exist between the different soil and subsoil levels in depth. This hypothesis still needs to be validated by a comparison with complementary data over a longer observation period as well as by confronting the data that will be collected on the long-term observatory of the O'ZNS platform being installed on the study site.

## • TriNappe, a mesoscale platform to study the water level effect in the critical zone

S.Stephant<sup>1</sup>, M.Crampon<sup>1</sup>, H.Thouin<sup>1</sup>, S.Dupraz<sup>1</sup>, C.Mouvet<sup>1</sup> <sup>(1)</sup> BRGM - FR

Email: s.stephant@brgm.fr

PRIME is one of the seven PIVOTS' platforms dedicated to the Remediation and the Innovation in service of Environmental Metrology. PRIME consists in several pilots, which allow carrying out experiments at different scales. One of them is called TriNappe and is dedicated to study vertical water transfers on several meters. The originality of this set up comes from the possibility to simulate groundwater rises, which could strongly impact the biogeochemistry of the system (especially RedOx conditions) and thus the fate of contaminants.

The set-up is made of 3 interconnected columns (H: 1m; *Dia*: 1m). The top of the first column can control lighting, temperature, humidity and water intakes in order to reproduce environmental conditions of the surface. The bottom of each column is connected through pipes to the top of the next column in order to mix lixiviates and thus nullify the effect of flow preferential pathways between each stage. Several ceramic suction lysimeters are implemented in each column so as to perform water sampling at any times. These water samples can be analysed on-line (pH, Eh, conductivity, and  $O_2$  concentration) or stored for further studies. The water circulation and the sampling sessions are fully automated.

The pilot may be used to develop new tools for environmental metrology, to study the efficiency of new remediation methods, or to understand the processes involved in the mobility and/or degradation of contaminants. TriNappe is especially suitable for studying systems with high groundwater level variation and/or systems composed of several layers of soils that could interact.



## NOTES

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### 2019

Dr Carmen Díaz Orozco & Dr Brigitte Natanson

Forging glances. Images and visual cultures in XIXth century Latin America

28-29 May 2019

Dr Marcelo Lorenzo & Prof. Claudio Lazzari New avenues for the behavioral manipulation of disease vectors 21-23 May 2019

Dr Agnieszka Synowiec & Dr Christophe

Hano Biological Activities of Essential Oils

13-15 May 2019

Prof. Yiming Chen & Prof. Driss Boutat 2019 International Conference on Fractional Calculus Theory and Applications (ICFCTA 2019) 25-26 April 2019

25-26 April 2019

Prof. Temenuga Trifonova & Prof. Raphaële Bertho On the Ruins and Margins of European Identity in Cinema: European Identity in the Era of Mass Migration

2-3 April 2019

Dr Patrizia Carmassi & Prof. Jean-Patrice Boudet Time and Science in the Liber Floridus of Lambert of Saint-Omer 27-28 March 2019

Dr Vincent Courdavault & Prof. Nathalie Guivarc'h

Refactoring Monoterpenoid Indole Alkaloid Biosynthesis in Microbial Cell Factories (MIAMi)

5-6 February 2019

Dr Denis Reis de Assis & Prof. Hélène Blasco Induced Pluripotent Stem Cells (iPSCs): From Disease Models to Mini-Organs 28-30 January 2019

### 2018

Pr Igor Lima Maldonado & Prof. Christophe Destrieux

Frontiers in Connectivity: Exploring and Dissecting the Cerebral White Matter 5-6 December 2018

December 2010

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detection to removal

Prof. Guoxian Chen & Prof. Magali Ribot Balance laws in fluid mechanics, geophysics, biology (theory, computation, and application) 19-21 November 2018

Dr Volodymyr Sukach & Prof. Isabelle Gillaizeau Progress in Organofluorine Chemistry 15-17 October 2018

Jens Christian Moesgaard, Prof. Marc Bompaire,

Bruno Foucray & Dr Guillaume Sarah Coins and currency in the 10th and 11th centuries: issuing authorities, political powers, economic influences 11-12 October 2018

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Dr Renaud Adam & Prof. Chiara Lastraioli Lost in Renaissance 20-21 September 2018

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Prof. Abdelwahid Mellouki & Dr Véronique Daële The 6th Sino-French Joint Workshop on Atmospheric Environment

10-12 September 2018

Prof. Emre Erdem & Dr Guylaine Poulin-Vittrant Frontiers in Nanomaterials for Energy Harvesting and Storage 27-29 August 2018

27-27 August 2018

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## 2014

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Dr Eric Reiter **3rd International Congress on Gonadotropins & Receptors - ICGRIII** 7-10 September 2014

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Prof. Chandani Lokuge & Prof. Trevor Harris Postcolonialism now 4-5 February 2013

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8-9 April 2013

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# CONTACT

# Dr Aurélien Montagu

Scientific Relations Manager +33 2 38 21 14 86 aurelien.montagu@lestudium-ias.fr

# LE STUDIUM

Loire Valley Institute for Advanced Studies

# www.lestudium-ias.com

1, rue Dupanloup • 45000 Orléans • FR

