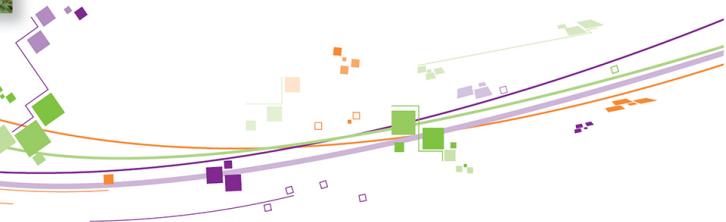




Science@ifpen

Issue 46 - November 2021



Written on 14 December 2021



15 minutes of reading



News

Fundamental Research



As confirmed by the recent IPCC report, the energy and ecological transition is more essential than ever to tackle global warming and move towards sustainable development, shifting from a carbon-based economy to carbon neutrality by 2050.

IFPEN's Earth Sciences and Environmental Technologies division is a key player in this ambition. Building on its experience in the oil and gas sector, it is evolving and channeling its expertise to support the development of innovations that will provide solutions to societal and industrial challenges related to energy and climate. To this end, the division relies on a knowledge basis that enables it to characterize, understand and model the soil, the subsurface and the fluids that flow through it. It also relies on many laboratory facilities specializing in a broad range of fields, including geochemistry and gas analysis, complex fluid transfer in porous media, thermodynamics and materials characterization.

The division thus successfully combines multi-scale characterization (from laboratory to field) with the development of models and simulations capable of numerically reproducing the behavior of the media studied. This characterization-modeling combination is now complemented by data science approaches. With its experimental capabilities, the division conducts a variety of research projects ranging from the understanding of systems and mechanisms to the development of technological objects.

In this issue of *Science@ifpen*, you will find an overview of the subjects tackled by the division's researchers, illustrating significant advances in research themes in recent years and the invaluable contributions of a multidisciplinary approach, whether within IFPEN itself or via collaborative projects with academic teams and industrial partners.

I hope you enjoy reading it.

Benjamin Herzhaft

Director of the Earth Sciences and Environmental Technologies Division

LES BRÈVES

One way to decrease the amount of atmospheric CO₂ is to reduce greenhouse gas emissions of fossil origin, but it is also possible to increase the quantities of carbon stored in the soil. This option brings into play soil organic matter (SOM), categorized into three functional groups depending on the speed with which CO₂ decomposes: fast (from a few days to a year), intermediate (from a few years to a few decades) or slow (from several decades to more than a century). In connection with the chemical composition of organic matter, the time the latter remains in the soil depends on its interactions with the minerals present and its mineralization induced by the action of microorganisms.

In the current context of climate change, understanding the evolution of carbon in the ground is critically important. It is for this reason that IFPEN wanted to study the potential offered by Rock-Eval®, a flagship of oil research, as a tool that can be used to provide reliable and fast characterization data. This characterization is based on simpler thermal analyses than the fractionation and incubation protocols currently proposed in soil and environmental sciences. The efficiency of the method, which consists in subjecting samples to heating programs (pyrolysis and combustion), has been widely demonstrated in the oil and gas context to characterize organic matter, both qualitatively and quantitatively^[1]. By differentiating carbon fractions of varying thermal stabilities (labile^a, resistant and refractory), the method also makes it possible to identify the different functional categories of SOM and demonstrate the capacity of samples to mineralize.

Thus an original method using Rock-Eval® was recently developed at IFPEN to better quantify soil organic carbon (SOC) and soil inorganic carbon (SIC) (patents pending), at the same time providing a better understanding of COS stability. In this respect, two new functional criteria based on the analysis of the pyrolysis thermogram were identified to represent and monitor the mineralization and stabilization dynamics of carbon on a diagram^[2].

This new approach was applied to a series of soil samples taken from different depths in a managed beech forest in Normandy (France), records for which date back 200 years^[3]. This study highlighted a relationship between the particle size of the soil fractions and the thermal stability of the SOM, probably indicating its biogeochemical stability. These field results were corroborated by incubation experiments on a model soil (figure 1), which established the link between microbial diversity, the molecular complexity and the thermal stability of the SOM^[4]. Similarly, the impact of adding a mixture of biochar^b and organic fertilizer on fertility and long-term carbon sequestration in the ground^[5] was studied.

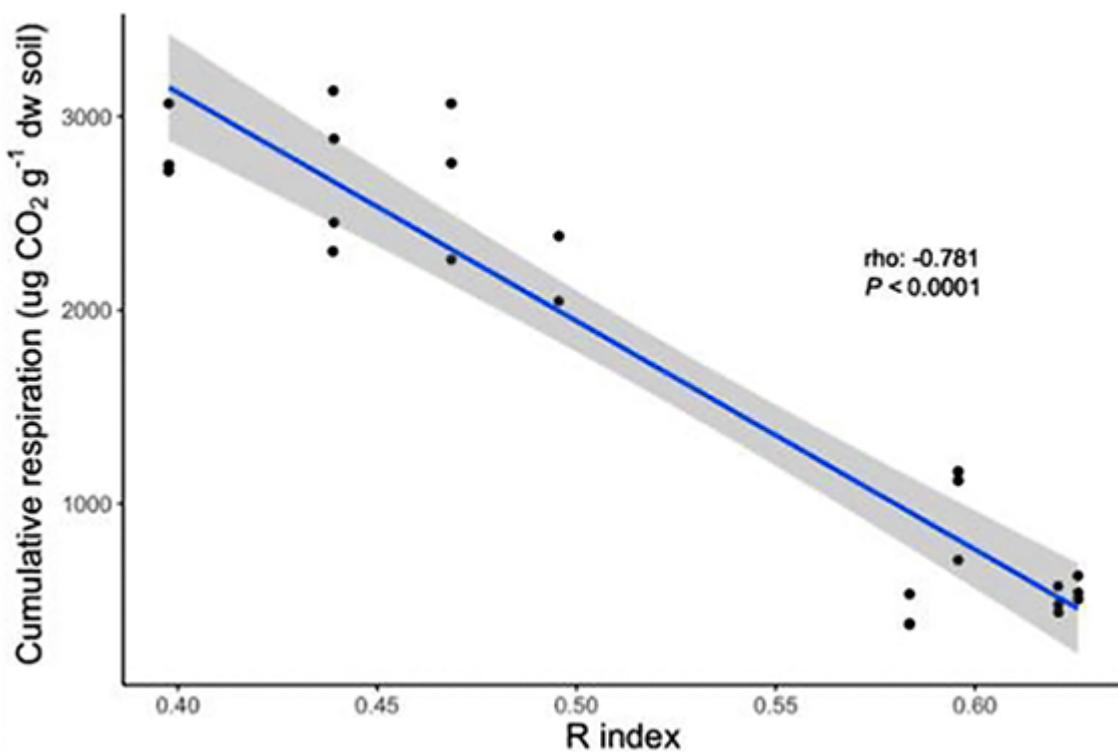


Figure 1: Determination of the CO₂ generated by SOM mineralization
(R-Index: descriptor of SOC stability obtained from the Rock-Eval® analysis) [4]

This recently acquired expertise by IFPEN is already being used in collaborative projects:

- an ANR (French National Research Agency) project aimed at gaining a better understanding of the impact of plastics on soil ecosystems^[6];
- a [Belmont Forum](#) project focusing on the impact of recent climate changes and the use of arctic and equatorial soils on carbon storage^[7].

Original and promising for carbon characterization in soils in numerous pedologic^c and agronomic contexts (figure 2), these activities illustrate IFPEN's capacity to transfer expertise in order to address the challenges of the environmental transition.

Click on the picture to enlarge

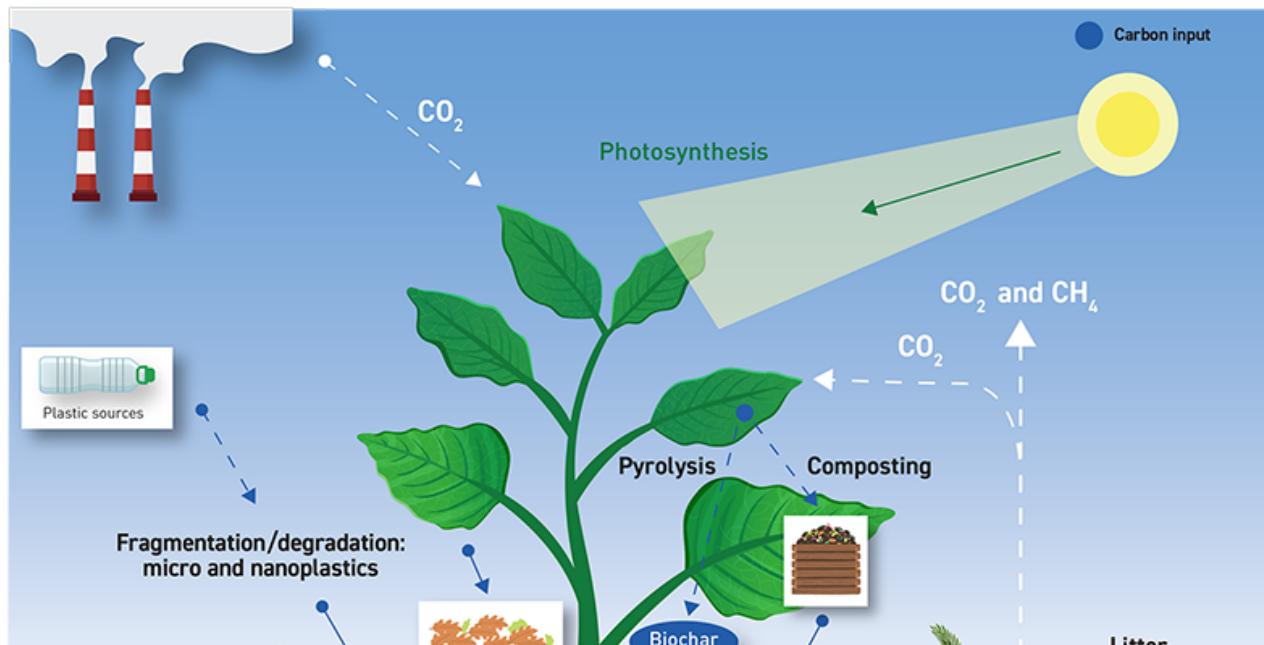


Figure 2: Illustration of research conducted at IFPEN

- a- Unstable.
- b- Solid carbon-rich residue obtained via the pyrolysis of organic matter of diverse origins (agricultural residues, manure, forestry residues, etc.).
- c- Relating to the study of soils.

Publications:

- [1] <https://www.ifpenergiesnouvelles.com/brief/rock-evalr-thermal-analysis-rocks-and-soils>
- [2] Sebag D., Verrecchia E.P., Cécillon L., Adatte T., Albrecht R., Aubert M., Bureau F., Cailleau G., Copard Y., Decaens T., Disnar J.-R., Hetényi M., Nyilas T., Trombino L., 2016. *Geoderma* 284, 185-203. <https://doi.org/10.1016/j.geoderma.2016.08.025>.
- [3] Sebag D., Verrecchia E.P., Adatte T., Aubert M., Cailleau G., Decaens T., Kowalewski I., Trap J., Bureau F., Hedde M., 2021. *Pedosphere*, 2021, *in press*.
- [4] Domeignoz-Horta L. A., Shinfuku M., Junier P., Poirier S., Verrecchia E., Sebag D., De Angelis M., ISME COMMUN., accepted (preprint <https://doi.org/10.1101/2021.04.23.441131>).
- [5] Aubertin M.L., Sebag D., Jouquet P., Girardin C., Houot S., Kowalewski I., Lamoureux-Var V., Pillot D., Rumpel C., 2021. *Eurosoil 2021 (virtual congress)*, 23-27 août 2021, *oral paper*.
- [6] ANR e-Dip project: “*Dynamique environnementale et impacts des cocktails de contaminants provenant des plastiques dans les écosystèmes terrestres*” (*Environmental dynamics and impacts of cocktails of contaminants from plastics in land ecosystems*). Project coordinator: Marie-France Dignac, INRAE, iEES Paris.
- [7] *Projet VULCAR-FATE* : “*Global change impact on vulnerable carbon reservoirs: carbon sequestration and emissions in soils and waters From the Arctic To the Equator*”, financed by the Belmont Forum. Project coordinator: Jean-Jacques Braun, IRD, Géosciences Environnement Toulouse.

Scientific contact: **Isabelle Kowalewski**

>> ISSUE 46 OF SCIENCE@IFPEN

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Innovation and Industry



News

November 2020

SI Celestite (SrSO_4)

ze for Rock-Eval® 7S



Fundamental Research



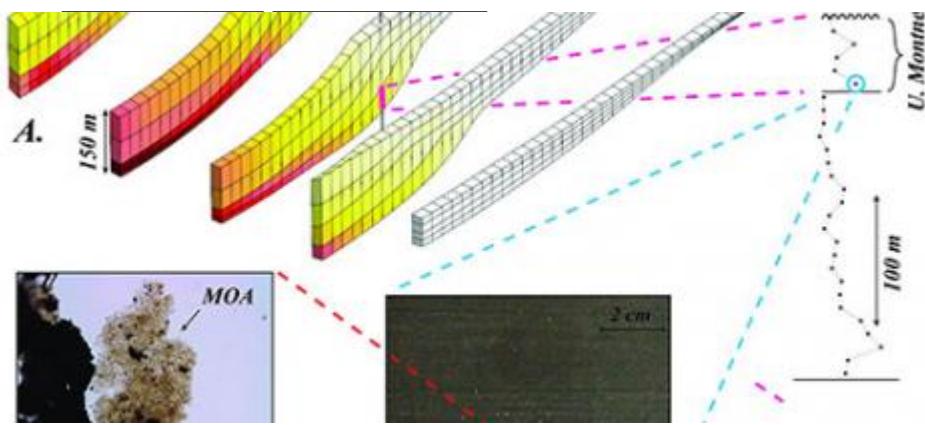
News

March 2020

The energy transition and geothermal energy: Knowledge that is difficult to uncover

Renewable energies

Geothermal energy



Rock-Eval® : to find out more

Méthodes analytiques (détails), interprétation pour l'exploration pétrolière, littérature

Responsible oil and gas

Basins and reservoirs modeling and simulation

Carnot IFPEN Ressources Energétiques

Today, the impact of climate change and human activities on the evolution of landscapes and water resources is a major challenge. Predicting it requires dedicated tools capable of evaluating, 100 years ahead, the consequences of different scenarios on watersheds and groundwater.

To this end, IFPEN is developing modeling approaches targeting erosion-transport-deposition phenomena combined with surface and subsurface flows. To do so, it is drawing on its longstanding expertise in the field of Earth sciences, particularly stratigraphic modeling^[1] and multiphase transport in complex porous media. The models under development are designed to predict the evolution of soil erodibility, sediment flows in rivers, potential flood zones, quantitative and qualitative aquifer recharge, etc. The objective is to define risk maps that can be used by local players to adapt risks prevention plans and regional planning projects.

Of course, the “critical zone”, which extends from the canopy to the bedrock, lies at the heart of these problems. It is exposed to soil erosion, that can induce catastrophic mud slides during extreme rainfall events. Moreover, erosion leads to the loss of organic matter, causing disruption to ecosystems. Hence its characterization is essential. Modeling these phenomena involves understanding the influence of vegetation cover and human occupation, via a scientific approach hinged around the study of recent past systems (from -10,000 years to the present day)^[2].

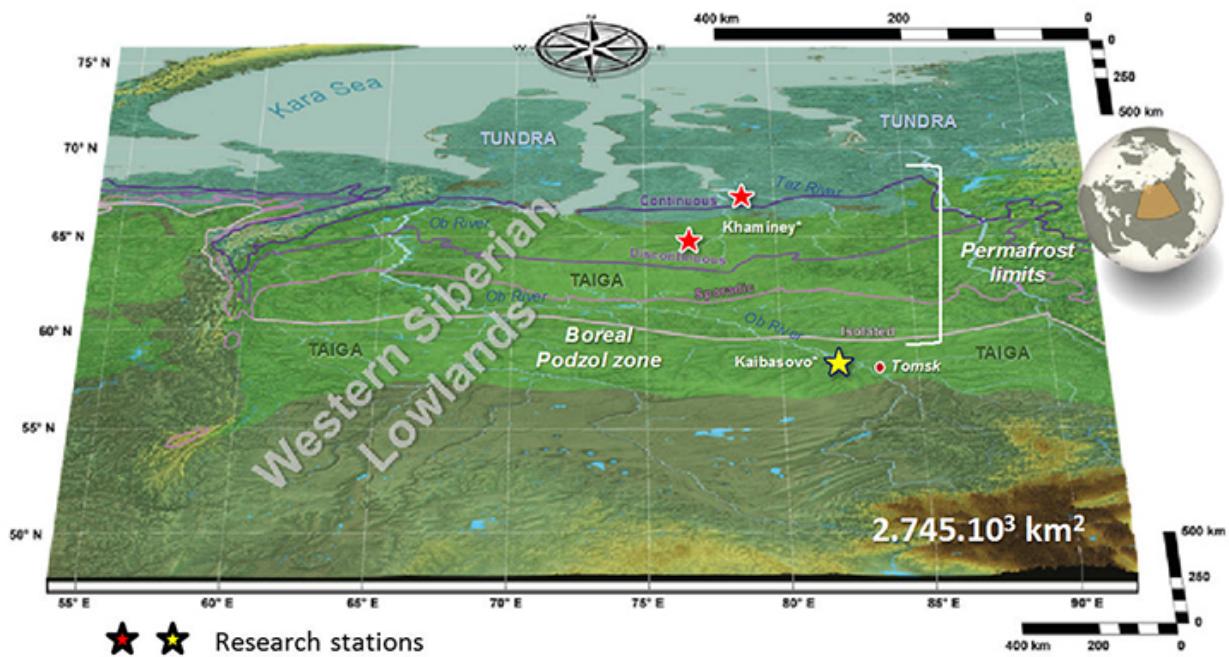
Selected within the framework of the “Towards Sustainability of Soils and Groundwater for Society” call for projects issued by the [Belmont Forum](#), the international VULCAR-FATE project^a ^[3] was launched in June 2021 with two major objectives:

- Study two ecosystems (figure), one in Gabon and one in Siberia, in order to evaluate the impact of recent climate and land use changes on the water balance and sediment and organic matter transport, as well as on soil degradation potentially generating atmospheric carbon emissions;
- Define evolution scenarios for periods ranging from 30-100 years ahead with a view to adapting local policies.

IFPEN's researchers will be responsible, firstly, for modeling geological processes and water and sediment flows using DionisosFlow™ and, secondly, characterizing soil organic matter using the Rock-Eval® method. The models developed will make it possible to integrate all of the data acquired during the project.

Click on pictures to enlarge





VULCAR-FATE project study sites

a- *Global change impact on vulnerable carbon reservoirs: carbon sequestration and emissions in soils and waters From the Arctic To the Equator*: an interdisciplinary project, coordinated by the [IRD](#) (French Research Institute for Development) and bringing together partners from six countries (France, USA, Russia, Gabon, Spain and Switzerland).

Publications:

- [1] Csató I., Catuneanu O., Granjeon D. (2014). *Journal of Sedimentary Research*, 84. <http://dx.doi.org/10.2110/jsr.2014.36>.
- [2] Bremond L., Oslisly R., Sebag D., Bentaleb I., Favier C., Henga-Botsikabobe K., Mvoubou M., Ngomanda A., de Saulieu G., Ecotrop Team (2021). *The Holocene*, 33(7). <https://doi.org/10.1177/09596836211003230>.
- [3] VULCAR-FATE project presentation video: <https://www.youtube.com/watch?v=BOkhcuJocB0>

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Fundamental Research



News

September 2020

Doctor David Sebag joins IFPEN's Soil Science teams

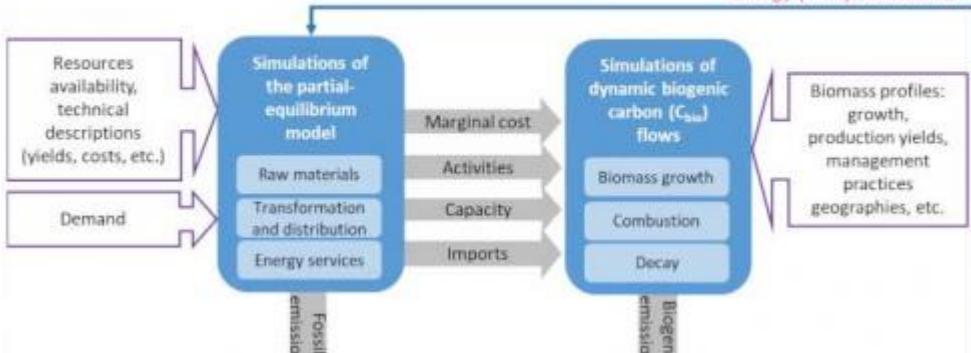
Climate, environment and circular economy

CO2 capture, utilization and storage

Demand model

C_{bio} model

Energy policy constraints



Fundamental Research



News

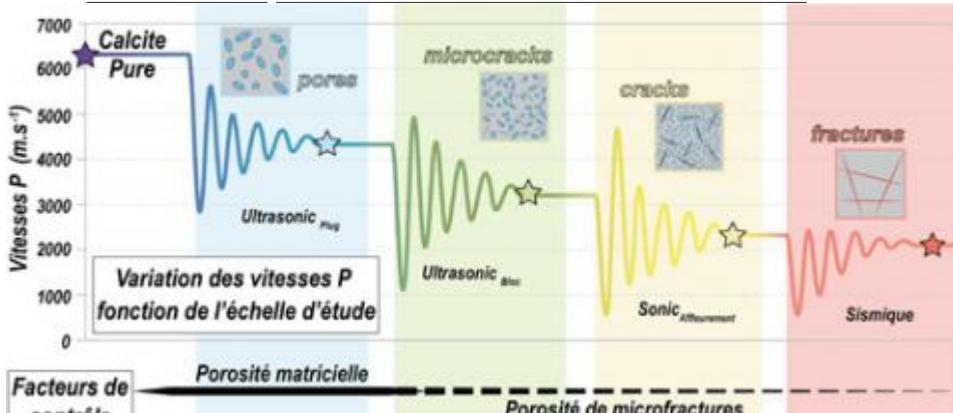
April 2020

Dynamic modeling to help achieve genuine carbon neutrality

Climate, environment and circular economy

Environmental monitoring

Life cycle analysis (LCA)



Characterization and modeling of the facies(a)-eogenesis(b) couple, initial state of carbonate reservoirs (HDR 2017)

Carbonate reservoirs present significant heterogeneities (in terms of types and scales) associated with the biological origin of sediments^C, as well as t

Geosciences

Geology - Sedimentology

Geostatistics - Geological modeling

Petrophysics and transfers in porous media

Global change, impact on landscapes and water resources

Today, air quality is an issue of major concern when it comes to public health. To protect it, it is necessary to reduce emissions but also monitor global chemical changes taking place in the atmosphere. From the economic and safety points of view, it is also important to monitor industrial gas emissions.

It was to tackle these different aspects that IFPEN's researchers began developing a range of technological solutions, within the context of the [Flair Suite™](#) project.

The objective for the multidisciplinary team was to develop tools and models making it possible to geolocate, identify, quantify and understand all sources of greenhouse gas emissions and gas pollutants, of natural or industrial origin. Initially focusing on monitoring CO₂ within the capture-storage context, the project then shifted towards the natural gas, biogas, petrochemicals and waste management industries.

Currently under development are:

- Gas monitoring stations (fixed and mobile) dedicated to monitoring air quality, detecting network gas leaks (Flair box™, Flair car™) and diffuse leaks at ground level (Flair soil™)^[1].



flair box™



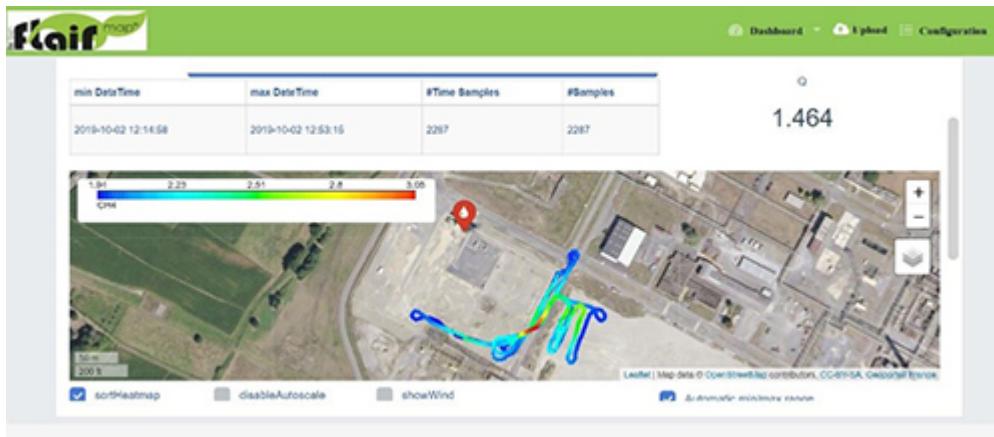
flair car™



flair soil™

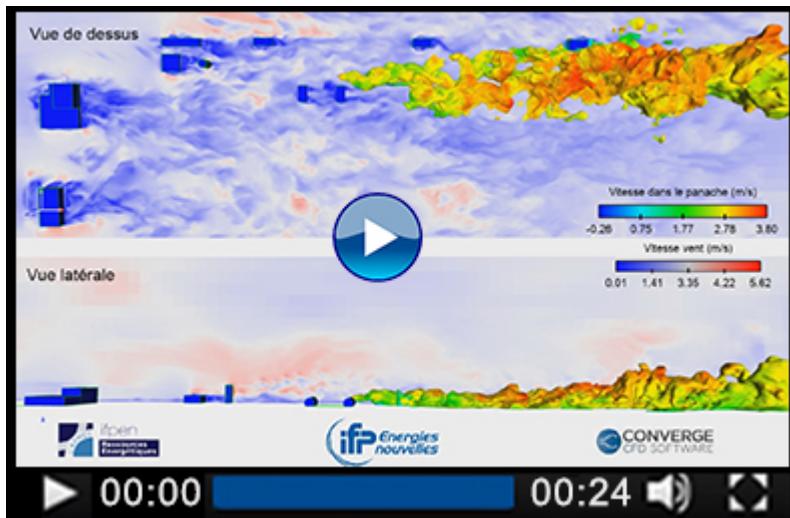
- Software and algorithms for real-time gas concentration mapping (Flair map real time™), leak point calculation (Smog Leak) and plume modeling^[2].

Click on the picture to enlarge



CH4 leak point calculation and 3D CH4 plume simulation

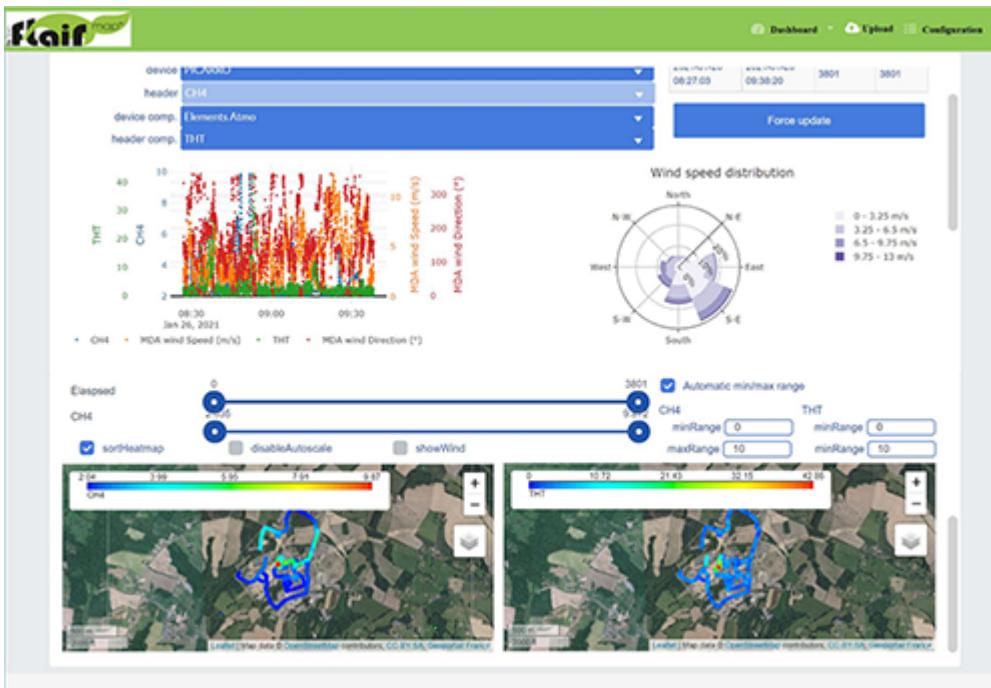
Click on the picture to see the animation



Video: speed of plume and wind, top and side views

- A web application (Flair map™), created with xDash, providing accurate and fun presentation of data[3].

Click on the picture to enlarge



Flair map™ dashboard created with xDash™

New fields of application

Monitoring stations are configured to detect the slightest gas leaks in the ground or surrounding air. In order to characterize the origin of these leaks as accurately as possible, the panel of molecules monitored is constantly being expanded. Some twenty or so molecules can currently be measured in ppb from our monitoring stations. Natural gas emissions (ground gases and those associated with biomass, geothermal energy, permafrost, etc.) are also studied in the Flair Suite™ project, paving the way for potential fields of application.

Olfactory pollution is another major area of focus in the project. The Flair box™ is thus capable of measuring a cocktail of odorous molecules at very low concentrations (ppb) in the atmosphere:

- natural foul-smelling substances (containing ammonia), found in manure, for example;
- synthetic substances, such as tetrahydrothiophene (THT) added to natural gas to facilitate leak detection or pleasant fragrances sprayed to mask industrial site seepages.

The solution has been used in real conditions to differentiate between the smells emanating from two industrial sites: a natural gas storage facility (rotten egg smell: THT) and a household waste storage facility (fermented cabbage smell: thiols).

Evolution of Flair: nose, eyes and ears

Researchers are now working to enhance Flair with new sensory functionalities to add to those already provided by gas monitoring stations (figure). For example, the processing of images from monitoring station onboard cameras (fixed and mobile) will optimize gas concentration maps: an

algorithm will make it possible to display a 360° photo of the environment in the event of an abnormal gas reading. Similarly, the study of sound frequencies around monitoring stations will be combined with atmospheric data, in order to characterize recorded gas reading anomalies (leak noise, passing vehicles, etc.).

Lastly, for reasons relating to the accessibility of sites to be studied, it is necessary to be able to place monitoring stations onboard different modes of travel: on foot, car, drone, bicycle, etc. Technological research is therefore under way to reduce the size and weight of stations.

Publications:

- [1] Patent: France (NP) - 23 April 2020 - 20/04.067 "Système et procédé pour la surveillance de fuites de gaz au moyen d'une mesure optique" (System and process for monitoring gas leaks using optical measurement methodologies).
- [2] Kumar P., Broquet G., Yver-Kwok C., Laurent O., Gichuki S., Caldow C., Cropley F., Lauvaux T., Ramonet M., Berthe G., Martin F., Duclaux O., Juery C., Bouchet C., Ciais P., Atmos. Meas. Tech. Discuss. [preprint], in review, 2020. <https://doi.org/10.5194/amt-2020-226>.
- [3] Berthe G., Rouchon V., Ben Gaid M., El Feki A., Int. Arch. Photogramm. Remote Sens. Spatial Inf. Sci., XLIII-B4-2020, 775–779, 2020. <https://doi.org/10.5194/isprs-archives-XLIII-B4-2020-775-2020>.

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Innovation and Industry

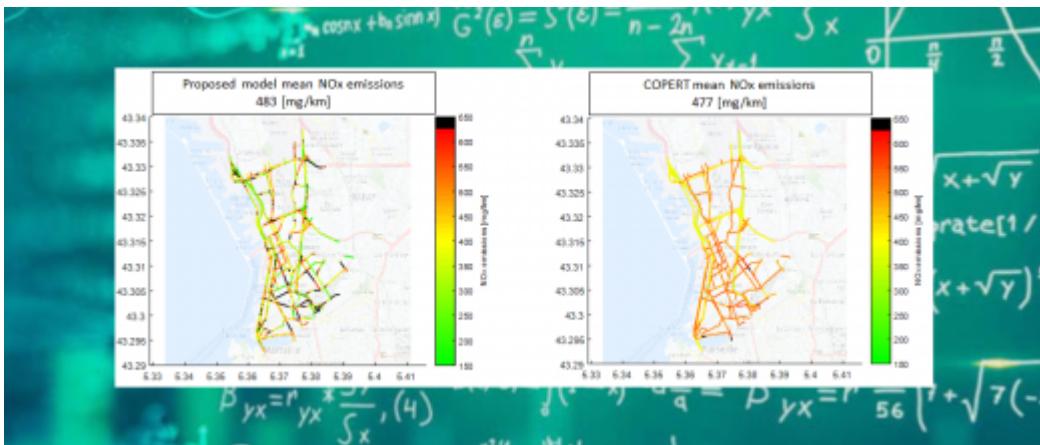


News

June 2021

Air quality: the Geco air clean mobility barometer adapt ours journeys to the weather

Press release



Fundamental Research



News

March 2021

“Floating Car Data” to improve air quality

Engineering sciences

Combustion and engine technologies

Systems modeling and simulation

Mathematics and IT

Numerical methods and optimization

Flair Suite™: supporting environmental and industrial gas monitoring

To address the challenges of the energy transition, the subsurface has an important role to play, both in terms of providing resources and offering storage solutions. For example, the subsoil is necessary to produce heat from geothermal drilling, to recover rare earths such as lithium, present in dissolved form in some underground water, and to identify geological conditions favorable to hydrogen formation. It is also of interest in terms of storage, either temporary or permanent, as significant volumes may be available in porous underground media to temporarily store energy or, in the longer term, to trap CO₂ captured from industrial facilities.

Numerical models can help gain a better understanding of the subsurface with a view to its long-term management and optimal use. Developed for a number of years now at IFPEN, [initially for the petroleum industry](#), such models cover scales ranging from the sedimentary basin to the reservoir:

- basin models^b are designed for modeling the stratigraphic environments (DionisosFlowTM) or modeling the entire geological history of the basin considered, with a view to deducing its properties and the location of the fluids it contains (TemisFlowTM);
- for smaller time and space scales, reservoir models predict the dynamic behavior of fluids and fractures present in the underground environment (PumaFlowTM, FracaFlowTM, TightFlowTM).

These tools also form an excellent basis for addressing problems relating to the production and storage of non-fossil energy or gas. Adaptation research is thus underway at IFPEN to add new functionalities to the models to address these emerging needs. Examples of this research include:

- consideration with TemisFlowTM of heat transfer via the faults present in a basin, in order to better estimate and locate its geothermal potential;
- modeling movements of CO₂ injected into the underground environment, as well as the resulting geochemical interactions with the rock, via the development of the CooresFlowTM software based on elements from PumaFlowTM.

It has also appeared necessary to integrate several scales and/or several types of physical analyses within the same model, as is already done when:

- combining “basin” and “reservoir” tools in order to identify the location of potential CO₂ storage zones in little-explored regions;
- integrating geomechanical aspects in such a way as to better represent tectonic and mechanical effects in the underground environment.

The risks associated with these new uses of the underground can be studied using approaches, either currently available or under development, in the field of uncertainty quantification (CougarFlowTM).

This research is being conducted on a partnership basis, within the context of the Ademe Aquifer- CO_2 Leak project^[1] or the European SENSE project^[2], for example. In the former project, the use of CooresFlowTM was validated to predict CO_2 flow in the underground environment, comparing numerical results with data from an experimental site in Saint-Emilion. In the latter, a reservoir model has been combined with a geomechanical model to monitor CO_2 storage sites from satellite measurements of surface deformation.

Other collaborative projects, based on multi-scale and multi-physical modeling, are under way with TotalEnergies. One of these is examining approaches combining small and large scales with a view to better predicting some underground properties during CO_2 storage (figure 1). Another is aimed at combining, for the first time in an industrial setting, a basin model and a geomechanical model^[3] to better predict natural sedimentary rock fracturing under the effect of tectonic stress (figure 2).

This research illustrates the evolution of underground modeling deployed by IFPEN to address the technological challenges of the energy transition, as well as the mobilization of its researchers as they seek to make progress in this field.

Click on pictures to enlarge

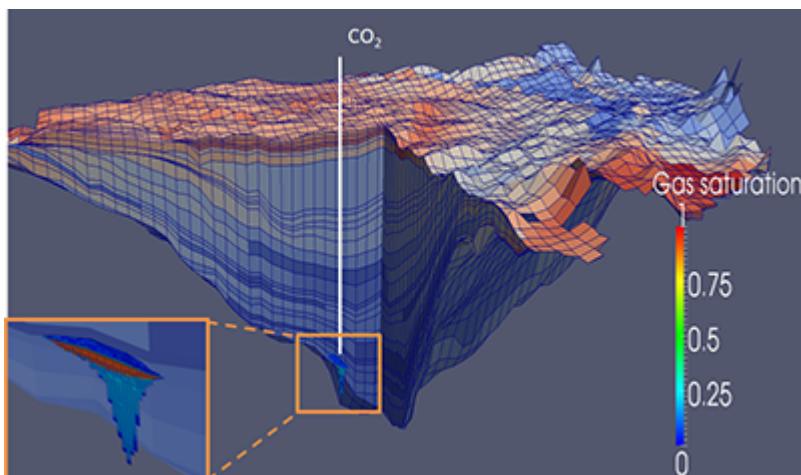


Figure 1: CO_2 injection modeling in a potential basin – combination of basin and reservoir modeling tools

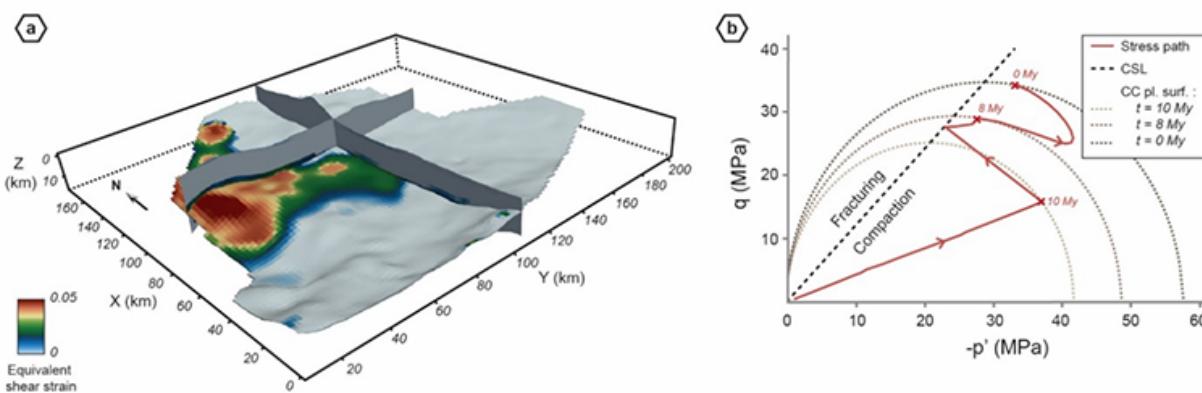


Figure 2: Mechanical stress modeling on a basin scale in the Vaca-Muerta formation in Argentina.

a) combined 3D model and b) evolution of stresses in a cell

a- For example natural gas, compressed air or hydrogen.

b- Between 10,000 and 100,000 km².

c- Succession of different geological layers or strata.

Publications:

[1] O. Gassara et al, ***The Aquifer-CO₂Leak project: Numerical modeling for the design of a CO₂ injection experiment in the saturated zone of the Saint-Emilion (France) site, International Journal of Greenhouse Gas Control***, 2021. <https://doi.org/10.1016/j.ijggc.2020.103196>.

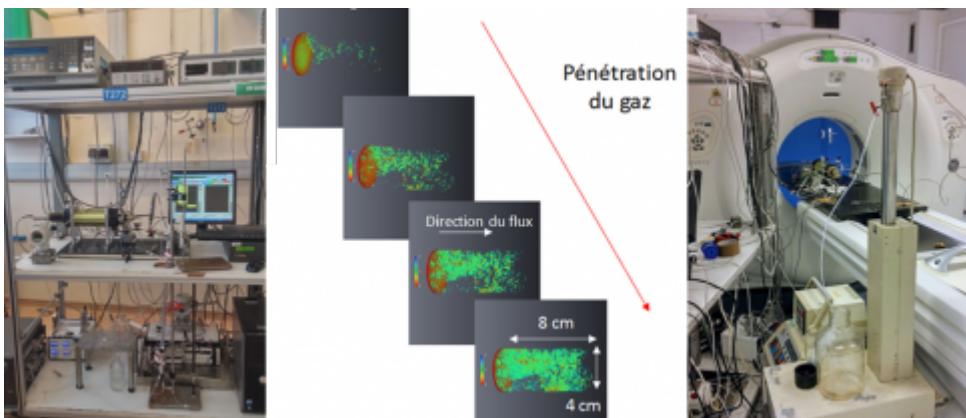
[2] S. Bouquet et al., ***Analysis of surface movement through conceptual and coupled flow-geomechanics models, an example of surface monitoring assessment for CCS project, Trondheim Conference on CO₂ Capture, Transport and Storage***, 2021.

[3] J. Berthelon, A. Brüch, D. Colombo, J. Frey, R. Traby, A. Bouziat, M.C. Cacas-Stentz, T. Cornu, ***Impact of tectonic shortening on fluid overpressure: Insights from the Neuquén basin, Argentina, Marine and Petroleum Geology, Volume 127, 2021.*** <https://doi.org/10.1016/j.marpetgeo.2021.104933>.

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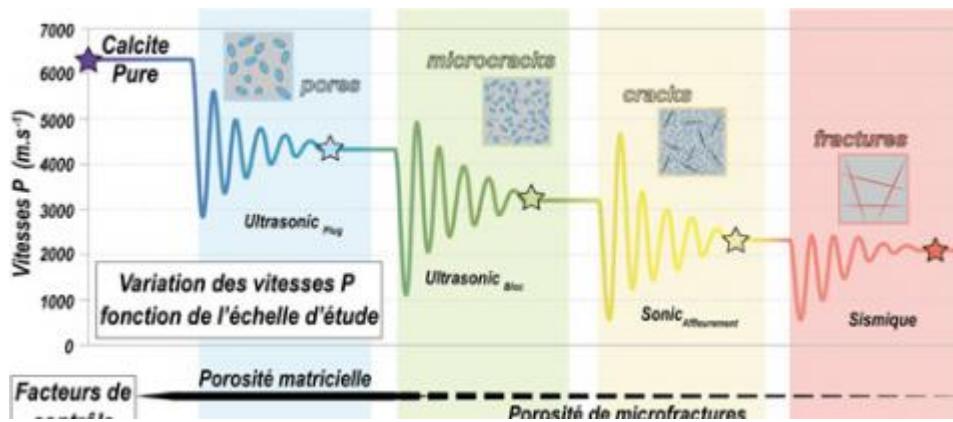
A scientific visitor helps improve the monitoring of CO₂ storage facilities

Over the past ten years, IFPEN has been conducting research on the **geochemical monitoring of the geological storage of CO₂**, in order to gain a better understanding of the

Geosciences

Geochemistry

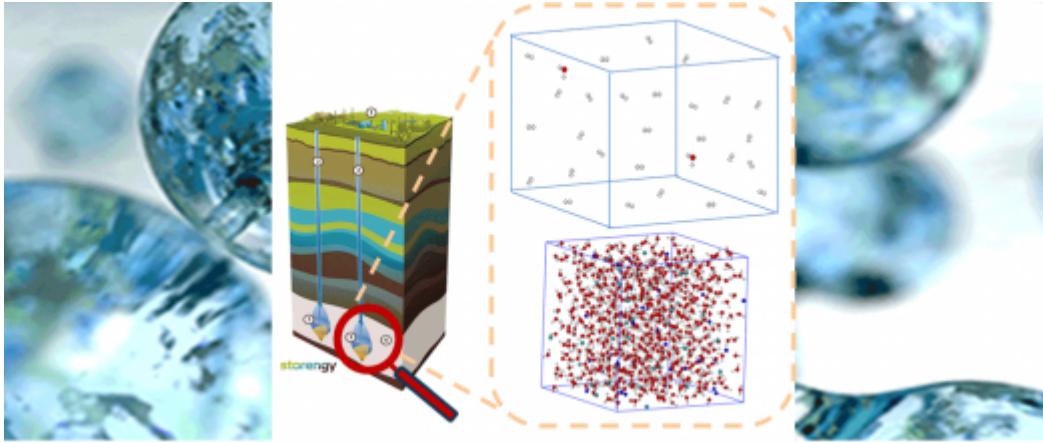
Petrophysics and transfers in porous media



Characterization and modeling of the facies(a)-eogenesis(b) couple, initial state of carbonate reservoirs (HDR 2017)

Carbonate reservoirs present significant heterogeneities (in terms of types and scales) associated with the biological origin of sediments^C, as well as t

Geosciences	Geology - Sedimentology	Geostatistics - Geological modeling
Petrophysics and transfers in porous media		



Fundamental Research



News

February 2020

Molecular simulation to support geological hydrogen storage

Renewable energies

Hydrogen

Energy storage

Physical Sciences

Thermodynamics/Molecular modeling

Underground modeling: an essential step for the energy transition

Salt precipitation in permeable rocks is a risk faced by some energy sectors, particularly for gas storage in geological formations during operational phases (injection and extraction), when there is contact with saline aquifers. This is because the circulation of a gas phase in a partially brine-saturated porous medium induces salt crystallization and precipitation within the porous space. This precipitation reduces the space where fluids can circulate, altering rock permeability, or even leading to plugging under certain conditions.

In order to understand the underlying mechanisms behind this damaging phenomenon, experiments examining gas flow in a brine-saturated porous medium were conducted on IFPEN's CAL-X flow test bench^[1]. These experiments made it possible to observe the dynamics of salt migration in 2D, through X-ray radiography. However, the use of X-rays alone is not sufficient to both measure local water saturation and differentiate the states in which the salt is found.

To overcome this limitation, these experiments were replicated on the D50T neutron line at the [Laue-Langevin Institute](#) (UGA-77 proposal)^[2], within the framework of a partnership with the [NeXT-Grenoble](#) laboratory^[3] and Equinor. This line also has an X-ray source, thereby making it possible to simultaneously produce X-ray imaging and neutron imaging observations. The complementary nature of these two methods thus makes it possible to monitor local water saturation and salt quantity, both dissolved and precipitated.

Figure 1 shows a series of neutron and X-ray radiographies during the injection of a dry gas (N_2) into a rock, in contact with brine at 100 g/l of KBr in its lower part. The neutron radiography clearly shows the presence of water at the base of the sample, while the X-ray radiography reveals salt migration.

Figure 2 illustrates the evolution over time (a) and space (b) of different magnitudes of interest (quantity of water, dissolved salt and precipitated salt). These observations have shown that salt precipitation results from the interaction of different parameters, i.e., the pressure gradient, brine concentration, capillary forces and water vapor partial pressure. Moreover, observations reveal that the injection of dry gas systematically cause salt to precipitate but permeability alteration is only observed if capillary contact is maintained with the brine.

This experimental work led to the construction of a 2D flow model incorporating the various physical and physicochemical mechanisms observed. Once calibrated, the model demonstrated good experiment predictability on a laboratory scale. Researchers will be able to use this model as part of a parametric study, with the possibility of scaling up through well simulation.

Click on pictures to enlarge

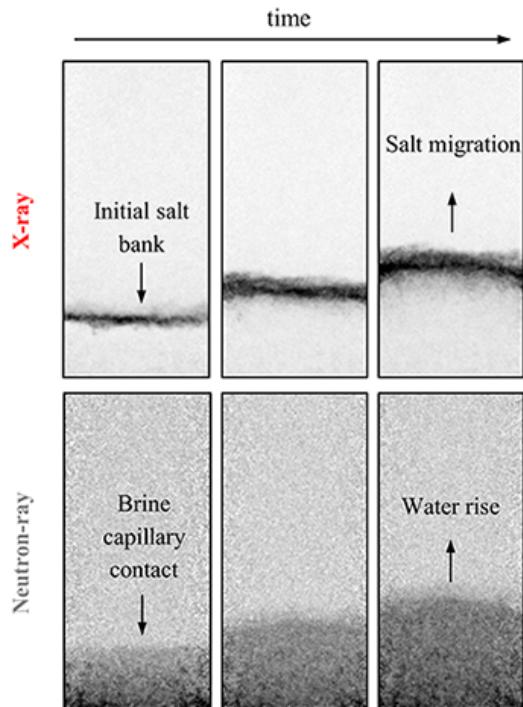


Figure 1: 2D radiographies during salt precipitation, taken at 100 min, 120 min and 140 min from left to right. The gas is injected from top to bottom, capillary contact is maintained at the bottom of the sample

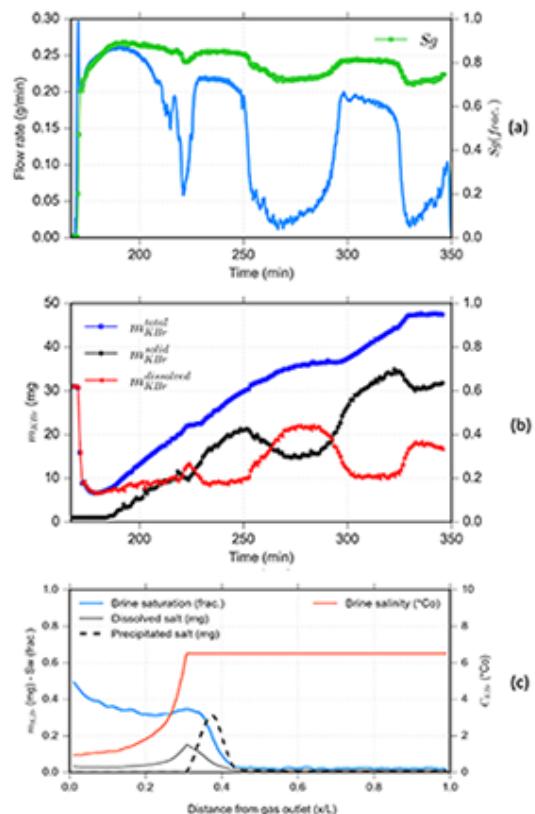


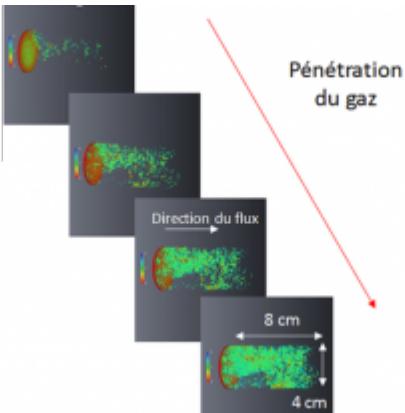
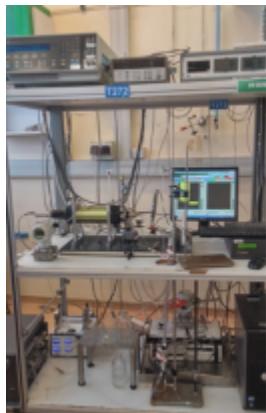
Figure 2: Nitrogen injection test with 100 g/l KBr brine capillary contact maintained at the exit. a) gas saturation and flow, b) evolution over time of salt quantity and c) distribution of salt in the different phases ($t = 150$ min).

Publications:

- [1] O. Lopez, S. Youssef, A. Estublier, J. Alvestad et C. Weierholt Strandli. 3S Web Conf., 146 (2020) 03001. <https://doi.org/10.1051/e3sconf/202014603001>.
- [2] M. Mascle, O. Lopez, H. Deschamps, L. Rennan, N. Lenoir, A. Tengattini et S. Youssef. Int. Sym. of the Society of Core virtual, SCA 2021-06.
- [3] A. Tengattini, N. Lenoir, E. Andò, B. Giroud, D. Atkins, J. Beaucour et G. Viggiani. Nuclear Instruments and Methods in Physics Research Section. Volume 968, 2020. <https://doi.org/10.1016/j.nima.2020.163939>.

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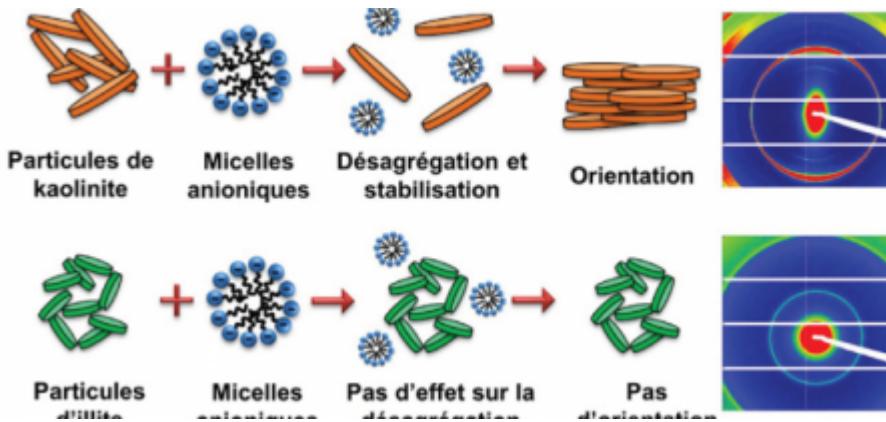
A scientific visitor helps improve the monitoring of CO2 storage facilities

Over the past ten years, IFPEN has been conducting research on the **geochemical monitoring of the geological storage of CO₂**, in order to gain a better understanding of the

Geosciences

Geochemistry

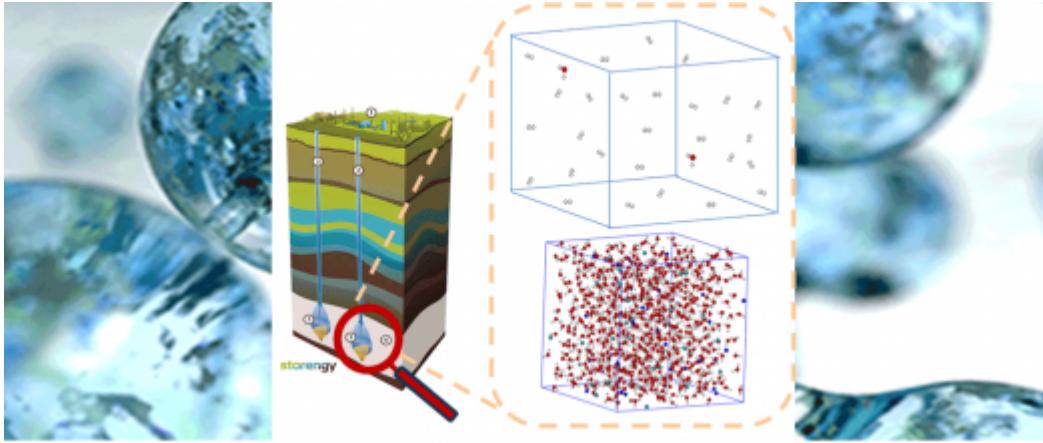
Petrophysics and transfers in porous media



Interactions between clay minerals and anionic surfactants

THESIS OF ARIANE SUZZONI

Physical Sciences	Rheology and behavior of materials	Physical chemistry
Complex fluids, colloids and condensed matter		Surface, interface and materials science



Fundamental Research



News

February 2020

Molecular simulation to support geological hydrogen storage

Renewable energies

Hydrogen

Energy storage

Physical Sciences

Thermodynamics/Molecular modeling

X-rays and Neutrons for imaging salt migration

Emerging in the 1990s, the notions of geoheritage and geodiversity have been receiving growing attention from academic communities, international organizations and public authorities. The concept of geoheritage notably incorporates the idea that certain geological sites represent precious windows onto past natural events and the way the planet works. As such they need to be protected and promoted in the same way as historical heritage sites are. As for the concept of geodiversity, it is based on a parallel between the variety of geological objects and that of living beings. The idea is thus to implement identification and conservation initiatives comparable to those used for biodiversity.

It was in this context that, in 2020, IFPEN signed a partnership agreement with UNESCO, one of the objectives of which is to share digital tools facilitating the promotion of geoheritage and geodiversity to the general public^[1]. These tools are constructed in synergy with the R&D initiatives conducted for industry, revisiting underlying technologies as part of a society-focused approach.

One example is the use of virtual reality enabling people to visit geological outcrops^a. This research is hinged around DOM (*Digital Outcrop Models*) methodology: from a series of photos acquired using the principles of photogrammetry^b, it is possible to produce a virtual 3D geometric representation of an outcrop, with its original texture and colors. Initially developed to meet the needs of the oil industry^[2] and increasingly used in the teaching of “Earth Sciences”, DOM methodology is also ideal for disseminating knowledge related to geoheritage to the general public, enabling people to discover sites without having to actually travel to them.

IFPEN’s researchers took advantage of the increasing accessibility to immersive technologies in 2020 within the framework of a partnership with an SME. The result was a demonstrator integrating a DOM model in a virtual immersive environment, focusing on the Annot sandstone formation, a reference site for the understanding of deep-water sedimentary systems (figure 1). Non-expert users can interactively learn about the geology of the outcrop and access educational content (texts, photos, videos) directly integrated in the visualization of the natural site.

A second example is the use of artificial intelligence to raise public awareness of geodiversity. IFPEN’s researchers trained a deep learning model to recognize different types of rocks from photos of samples. This model was then integrated into a mobile application enabling non-experts to derive information from photographs of the rocks around them about their nature, their characteristics and their different uses (figure 2). Currently at the prototype stage, this application, called RockNetTM, is designed to promote a citizen science type approach. Accordingly, all of the photos taken by users will be used to build a common atlas and a database, thereby gradually improving the accuracy and quality of the results provided^[3].

Both these examples illustrate how digital technology can potentially help promote geological knowledge to the general public^[4], one of the keys to ensuring more and more citizens become active players in debates about the protection of the environment, the sustainable use of resources and the evolution of the planet.

Click on pictures to enlarge

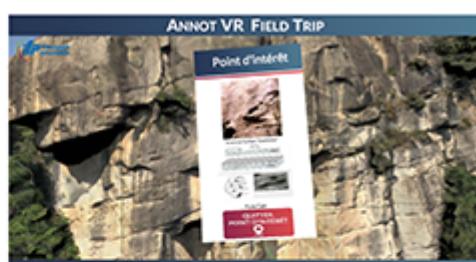


Figure 1: Illustration of the integration of the Annot sandstone outcrop in a virtual and immersive environment.

In addition to being able to view the outcrop from various angles and zoom in and out, users can interact with the geological data and accompanying educational content (stratigraphic interpretations, sedimentary logs, sample photos, texts and videos, etc.).

>> More images of the technology in the following **video clip**:

<https://www.youtube.com/watch?v=QOPX0wwUE0>.

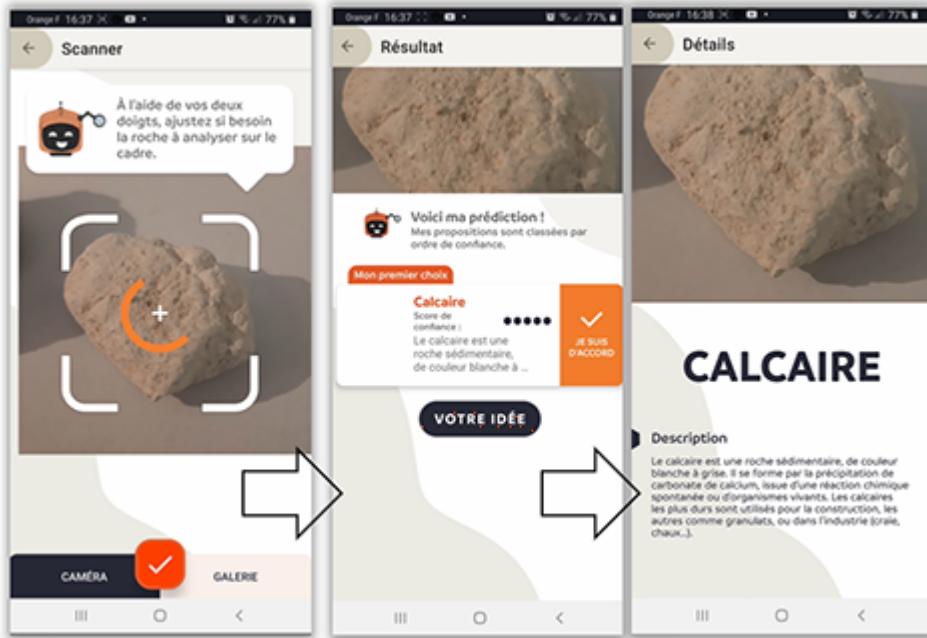


Figure 2: Illustration of the interface and operation of the RockNetTM application.

From a photo taken by the user with their smartphone, the artificial intelligence model identifies the corresponding rock type and provides the public with some basic information. More details on www.rocknet.fr (in French).

- a- Exposed solid rock formations, often dozens of meters long, directly visible on the Earth's surface. They are extremely useful for geologists because they offer a direct picture of the nature of the underground environment.
- b- Technique used to reproduce a scene in 3D from images acquired from different angles and viewpoints.

Publications:

[1] "[IFPEN and UNESCO join forces in the field of geoscience](#)" press release, 6 October 2020.

[2] Deschamps R., Joseph P., Lerat O., Schmitz J., Doligez B. et Jardin A. (2015). AAPG Search and Discovery, Art. no 41696.

http://www.searchanddiscovery.com/documents/2015/41696deschamps/ndx_deschamps.pdf.

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[4] Bouziat A., Schmitz J., Deschamps R. et Labat K. (2020). *European Geologist*, 50. <http://doi.org/10.5281/zenodo.4311379>.

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Fundamental Research



News

October 2020

IFPEN and UNESCO join forces in the field of geoscience

Press release

Renewable energies

Geosciences



Artificial Intelligence-assisted interpretation of geological images

Over the last decade, deep learning applied to image analysis has rapidly developed in scope to cover numerous fields. However, its potential remains underexploited in geology, despite the fact that it is a discipline that relies to a large extent on visual interpretation. To contribute to the digital transformation of industries related to the underground environment, researchers at IFPEN have implemented deep learning in three “profession-specific contexts”, each involving different types of geological images.

Geosciences

Geology - Sedimentology

Mathematics and IT

Signal processing/Data science



IFPEN



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Geoheritage and geodiversity accessible to all thanks to digital technology

The transport of colloidal particles in porous media is relevant to a number of fields, including geosciences and environmental engineering. Particle-matrix interactions can lead to deposit formation and accumulation, potentially damaging the medium and altering its permeability.

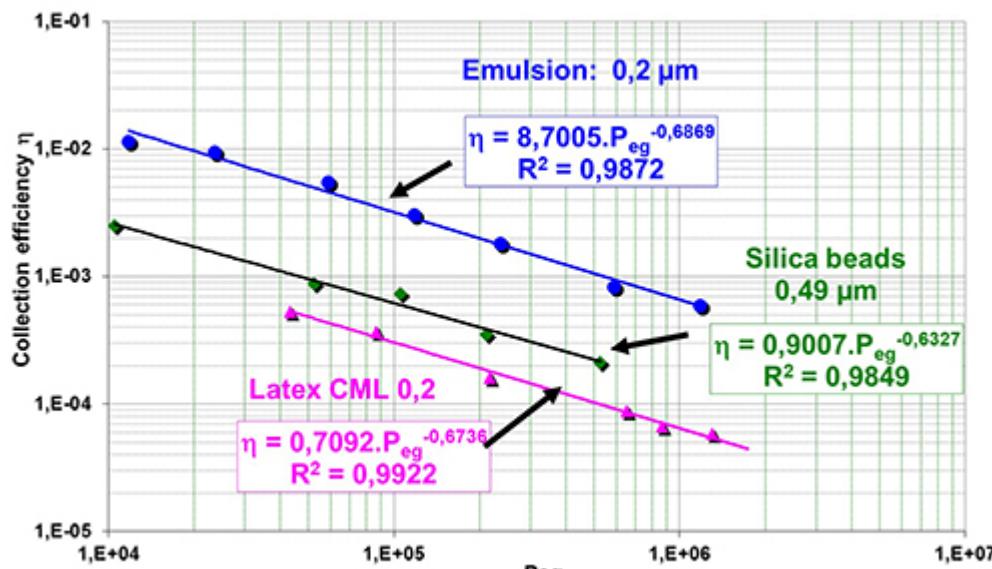
This phenomenon is particularly frequent in numerous natural and industrial systems where matter is present in a finely divided state: examples include the fields of oil production (solid particles, emulsions, asphaltene, etc.), geothermal energy and water and soil pollution remediation. During fluid production and reinjection operations, for example, fine particles (endogenous and/or exogenous) can plug pores in the well column under the effect of major physicochemical and hydrodynamic changes, significantly reducing injectivity and productivity, sometimes to the point that the well has to be decommissioned. Controlling these phenomena in porous media thus represents a major challenge for the industries concerned.

At IFPEN, the problem was originally studied for oil and gas production, but research has now been extended to include the fields of geothermal energy and geological storage of CO₂. To understand and carry out experimental characterization of these deposit/plugging phenomena and their consequences on the petrophysical properties of media, dedicated tools have been developed:

- Coreflood systems^a with intermediate pressure readings enabling Darcy^b scale deposit formation characterization.
- A high-pressure membrane filtration system equipped with a camera to monitor the evolution of cake thickness (particle accumulation at the entrance to the medium)^c.
- Micro-models^d enabling the direct observation of these flow phenomena at pore level, as well as the characterization of deposits and mechanisms involved at this scale.

Their use in a number of research projects has made it possible to identify and characterize different porous medium deposit regimes and kinetics, and propose physical modeling, both generic and original. This takes the form of a scale law, of the Peclet (P_{eg})^e number power law type, with a universal exponent equal to -2/3 and a prefactor that depends on the nature of the particle, as illustrated by the figure for three types of colloids.

Click on the picture to enlarge



Deposit kinetics for different particle types

A pragmatic approach was then proposed for injectivity loss modeling. This is based, firstly, on the physical modeling described above concerning internal damage (deposit formation) and, secondly, on empirical correlations for external damage (external filtration cake). These models have recently been integrated into a reactive transport simulation tool^f [3], one use of which is to model CO₂ injection in the underground environment during sequestration operations.

This work once again illustrates IFPEN's capacity to exploit its experimental resources, models, and multidisciplinary expertise to support progress in fields of vital importance to the ecological transition^[4]

a- Fluid injection experiment in a rock core.

b- 1 Darcy = 0.97.10⁻¹² m².

c- Combined with measurement of pressure loss, this information makes it possible to characterize the external cake (in terms of permeability, k_c , and density, ρ_c) and the relationship between water quality, ρ ($\rho = C_{\text{particles}} / k_c \cdot \rho_c$) and C concentration.

d- Glass chip engraved with a 2D porous network.

e- Number comparing convective forces with diffusive forces ($Pe = v \cdot Lc / D$, where v represents fluid speed, Lc the system's characteristic dimension and D the particle diffusion coefficient.

f- CooresFlowTM simulator.

Publications:

[1] D. Rousseau, L. Hadi et L. Nabzar, *SPE Production & Operation*, novembre 2008, 525-532.

[2] S. Buret, L. Nabzar et A. Jada, *SPE Journal*, 15(2), June 2010, 557-568. SPE-122060-PA.
<https://doi.org/10.2118/122060-PA>.

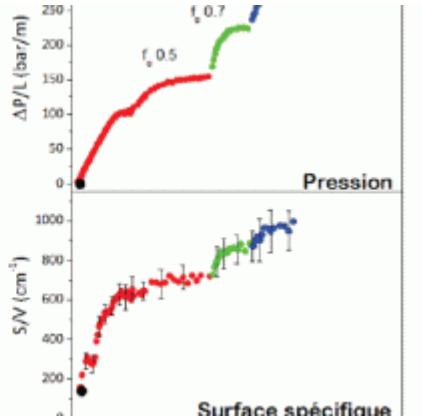
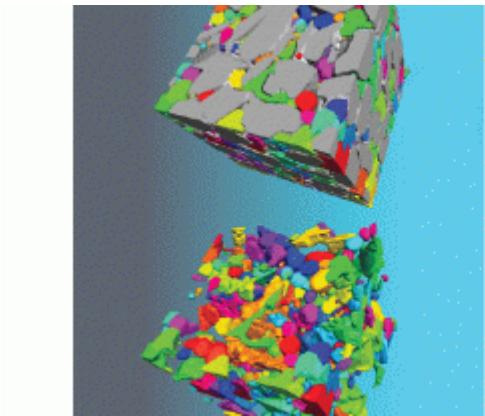
[3] Petrobras-IFPEN R&D collaborative project on Reactive transport simulation – CooresFlowTM Phase 2, 2020-2021.

[4] Collaboration with Geofluid: “Problématique de l'injection en milieu poreux non consolidés. Processus d'endommagements et remédiations. Mesures sur sites (l'Albien) et essais en laboratoire” (Problem of injection in unconsolidated porous media. Damage processes and remediations. On-site (Albien) measurements and laboratory tests), Ademe project on geothermal energy, 2020-2022.

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In situ study of the detailed structure of a foam flowing in a real porous medium

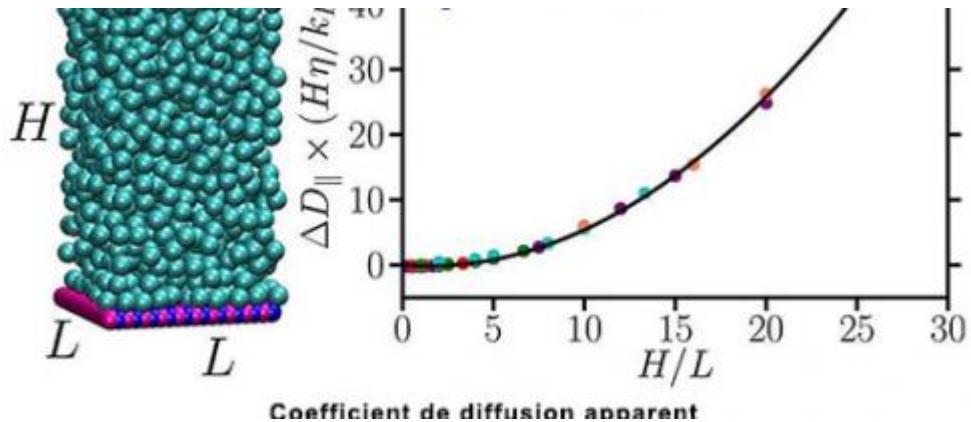
Foam injection during oil production or ground remediation is aimed at overcoming problems of gravity segregation and viscous fingering^a created by

Geosciences

Petrophysics and transfers in porous media

Analysis and characterization

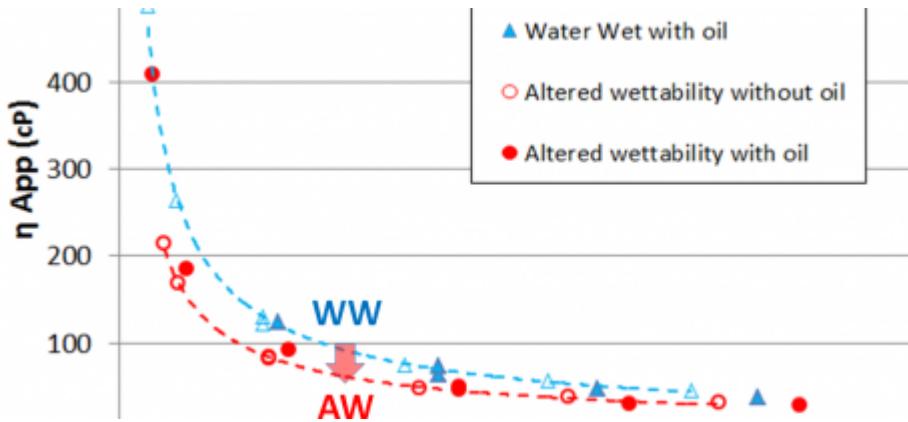
Structural analysis and Imaging



Improving the simulation of the transport process in nanopores using molecular dynamics

THESIS BY PAULINE SIMONNIN

Geosciences	Petrophysics and transfers in porous media	Physical Sciences
Thermodynamics/Molecular modeling	Mathematics and IT	Numerical methods and optimization



Foam rheology in porous media

For processes involving gas injection, such as enhanced oil recovery (EOR^a) and CO₂ storage operations, the

Geosciences	Petrophysics and transfers in porous media	Physical Sciences
Rheology and behavior of materials	Physical chemistry	
Complex fluids, colloids and condensed matter		

Colloid transport in porous media: deposits and plugging

Link to the web page :