Science @ifpen
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15 minutes of reading

News

Fundamental Research

Cécile Barrère-Tricca
Director of the “Chemistry for Industry” R&I Business Unit

Committed to accelerating the ecological transition, IFPEN's mission is to innovate for a low-carbon, sustainable world, by proposing technological solutions to societal challenges.

These solutions will emerge from structured **fundamental research**, built in line and synergy with applied problems. It is for this reason that our fundamental research activities today are organized around nine scientific challenges (SC) that feed into **IFPEN’s innovation process** while **anticipating future needs**.

In this issue, each of the nine challenges is illustrated by a specific development. Taken together, the articles highlight the scientific pathway to innovation ranging from the understanding of complex physical phenomena (experimentation, data acquisition) to the evaluation of a complete system (economic and environmental impacts), via the modeling and numerical representation (simulation) of these phenomena.

All these scientific results are invaluable for accelerating innovation, with some of them supporting the development of the low-carbon and circular economy:

- The “in situ and/or operando” methodological approaches developed will make it possible to identify the properties of a heterogeneous catalyst and their evolution during its lifecycle, including during operation!

- The identification of a unique control parameter in the laboratory will provide exact knowledge about the mixing operating conditions to be applied in order to produce a paste with a specific porosity. It will also be possible to optimize the design of catalyst supports as a function of each target application.

Enjoy your reading !

Cécile Barrère-Tricca

> List of the nine scientific challenges (SC)

LES BRÈVES

Heterogeneous catalysts are materials that make chemically possible and economically viable countless industrial processes in the service of energy-related and environmental problems, such as fuel production and air quality (vehicle emissions, building interiors). Their implementation involves two major scientific challenges:

1) the identification of the chemical, structural and morphological properties of an optimal catalyst[1],

2) the evolution of these properties over the catalyst's life-cycle (synthesis, preparation, use, recycling).

In order to make progress in overcoming these challenges, the characterization of the material in all its successive states, including during operation, is a key step, but it is also a process that is experimentally demanding.

With this in mind, "in situ[2] and/or operando[3]" methodological approaches make it possible to study the evolution of a material and its fluid environment in physicochemical conditions representative of a manufacturing step or a catalytic reactor. They therefore offer a remarkable advantage over so-called ex situ approaches, which are limited to the final, out-of-context observation of all or part of a complex transformation mechanism.

Within the framework of collaborative research work, IFPEN has contributed to the development and implementation of such approaches, illustrated by the three following examples:

With a view to controlling the synthesis of the catalyst

Hyperspectral synchrotron X-ray absorption imaging in impregnation/maturation/drying conditions was developed on the ROCK beamline of the SOLEIL Synchrotron at Gif-sur-Yvette (figure 1). This made it possible to monitor:

- the mobility and chemical speciation[4] of the different catalytic species (in this case molybdic) of an impregnation solution in mesoporous alumina extrudates (the support),
- the evolution of these species during drying,
- all with relevant time and space resolution vis-à-vis observed phenomena (to the minute and ten or so µm respectively).

This has enabled a better understanding of the heterogeneity of distribution and the nature of active phase precursors due to interaction with the support during these synthesis steps [1].

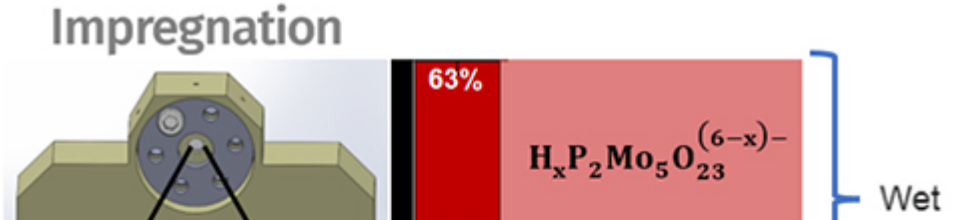

Figure 1: Impregnation/drying system adapted to the ROCK beamline for in situ monitoring by X-ray absorption spectroscopy. The speciation of molybdenum at the end of each step is shown.

Another example[5], the implementation of hydrothermal conditions in environmental cell TEM[6], made it possible to investigate the dealumination, via hydrolysis, of faujasite zeolites for the manufacture of acid catalysts [2]. This development was carried out alongside a study using the same system to dehydrate boehmite, by calcination, for the production of transition aluminas. It was thus possible to observe both these phenomena simultaneously for the first time by TEM (figure 2).

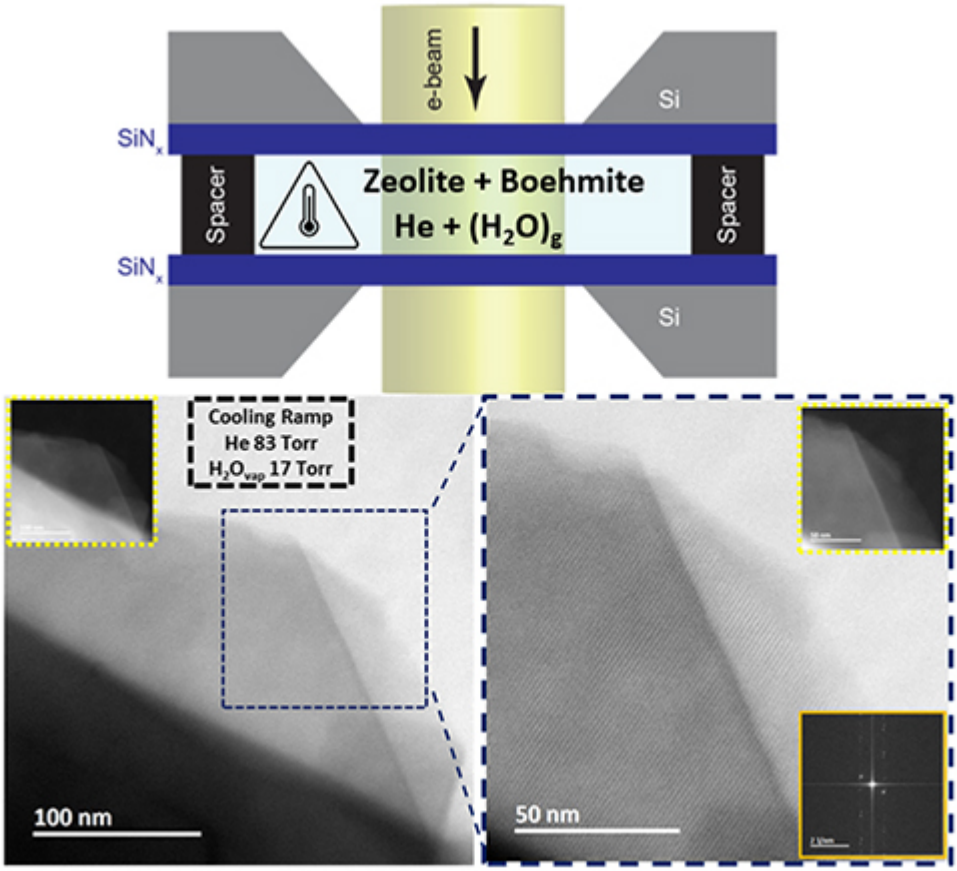

Figure 2: Illustration of the environmental cell used in transmission electron microscopy. The images show, for two magnifications, the morphological and structural evidence of the effects of zeolite dealumination by hydrolysis.

To study a reaction mechanism

Fourier Transform Infrared Spectroscopy (FTIR) was used to study the photoreduction of CO_2 in the presence of water vapor, on a co-catalyst made up of platinum nanoparticles supported on titanium dioxide (figure 3). An operando methodology[7] was used to reveal the impact of carbon impurities on the measured activity and hence the need to control the initial surface state of the photocatalyst. Day/night cycle operando IR measurements also provided an insight into how to improve photocatalyst efficiency, as well as information concerning the reaction mechanisms taking place on the surface of these materials [2]. For example, acetate intermediates were identified by subsequent isotopic measurements, which revealed the presence of Carbon-Carbon coupling reactions.

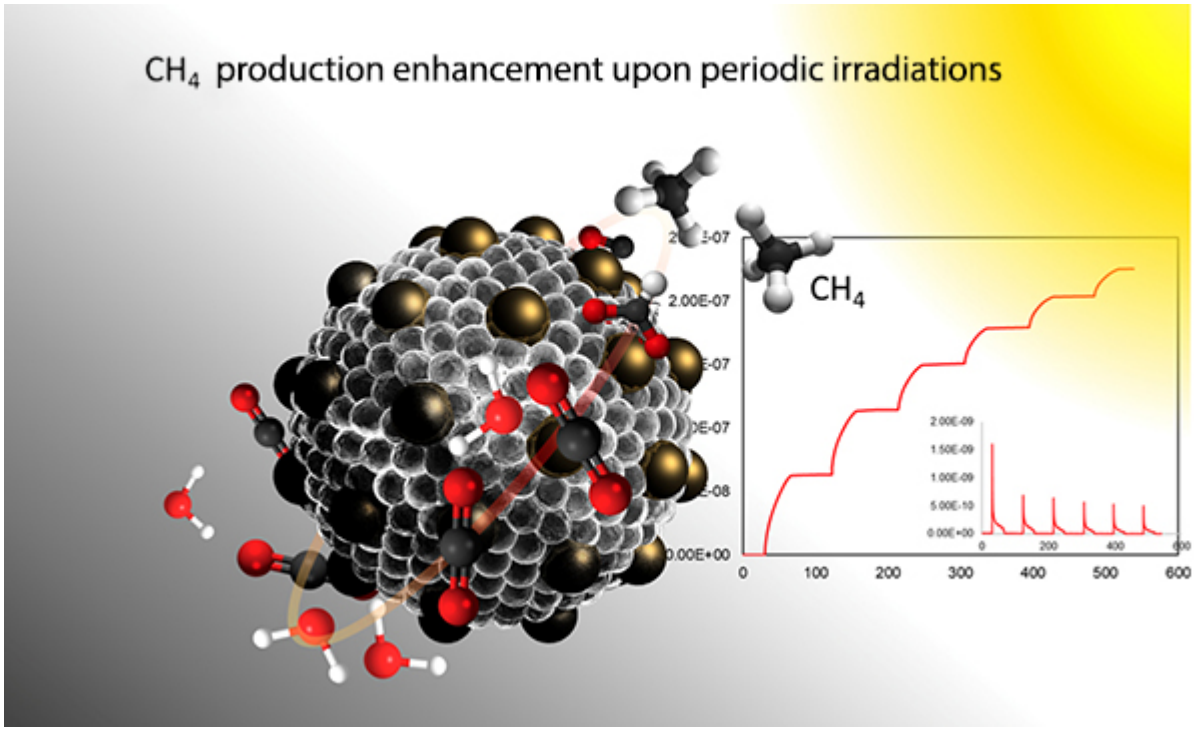

Figure 3: Representation of the platinum-on-TiO2 catalyst, reagents and products of the photoreduction of CO2. The graph illustrates the evolution of the cumulative quantity of CH4 produced and its derivative as function of time.

In all of this research, it became clear that the processing of big and/or noisy data is essential. The development of chemometric and data extraction methods for X-ray absorption and infrared spectroscopies, as well as denoising approaches for electron microscopy, now represent crucial development avenues to be explored alongside instrumentation.

[1]- In terms of properties: activity, selectivity, stability
[2]- In relevant local conditions, without sampling
[3]- In reaction conditions, with monitoring of evolutions and products
[4]- Identification and quantification of the different possible species of an element in a given environment
[5]- Research conducted with the Strasbourg Institute of Materials Physics and Chemistry
[6]- Transmission Electron Microscopy
[7]- Developed in collaboration with the Laboratoire de Catalyse et Spectrochimie de Caen (LCS)

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>> https://doi.org/10.1002/cctc.202201440

2. J. Dankar, V. Rouchon, C. Pagis, M. Rivallan, M. El-Roz, ***Exploring the effect of the reaction conditions on the mechanism of the photocatalytic reduction of CO_2 in the vapor phase over Pt/TiO2: an operando FTIR study***, Inorg. Chem. Front., 2023,10, 7155-7166
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Scientific contacts: christele.legens@ifpen.fr, mickael.rivallan@ifpen.fr and virgile.rouchon@ifpen.fr

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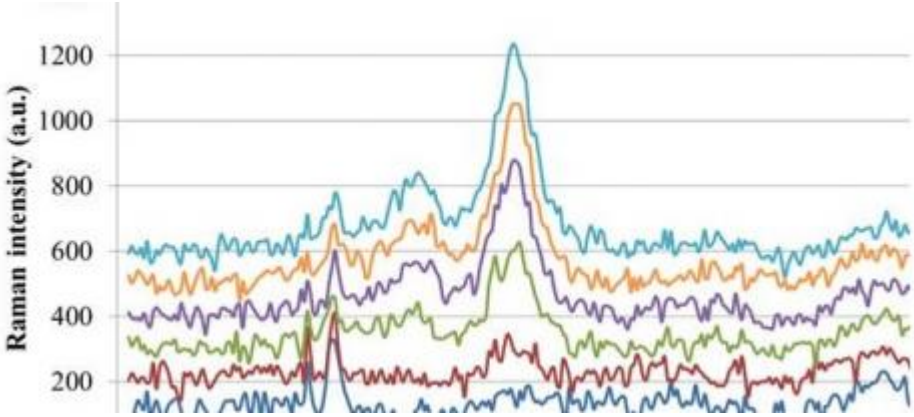
Photocatalysis, a lighted pathway for CO2 conversion

Although the climate crisis makes the reduction of CO2 emissions a matter of urgency, some industries will have difficulty in avoiding them, such as cement plants (where the core process is currently based on the calcination of CaCO3) or refineries, which are currently highly energy-intensive. Hence the huge potential interest in procedures that could capture the CO2 released directly from the plant (...) then recover it at a fraction of the energy cost...

Chemical sciences | Catalysis and reaction kinetics | Organic and mineral synthesis | Physical chemistry | Surface, interface and materials science



Operando spectroscopy in full transparency

THESIS OF MARISA DE SOUSA DUARTE

Analysis and characterization | Chemical analysis | Engineering sciences | Chemical engineering and process engineering

Fundamental Research

News December 2022

CARMEN JRL: a breakthrough research for the energy transition

Physical chemistry **Surface, interface and materials science**

SC1 - “Live” heterogeneous catalysts

Biofuels are one of the components of the transition to renewable energies, and their use is an effective way of decarbonizing transport. However, they are produced from feedstocks whose composition can affect the steel equipment used for their conversion. For example, the hydrotreatment of vegetable oils and animal fats leads to the exposure to high concentrations of oxygenated compounds, naturally present in the initial feedstock or resulting from their conversion, which can react with metallic materials. The potential presence of high concentrations of free fatty acids is another factor providing the risks of corrosion.

A PhD study was dedicated to the study of this phenomenon liable to affect the reliability of installations[1]. The research employed corrosion experiments in conditions representative of the process: pressure (up to 80 bar in the presence of hydrogen) and temperature (up to 350°C), with frequent renewal of the corrosve media without opening the autoclave[2]. After exposure tests, analyses conducted on the materials and feedstock made it possible to quantify the corrosion and understand its mechanisms.

Some significant results emerged for different grades of steel:

- at 220°C, generalized corrosion rates of more than 1 mm/year were observed on carbon and low alloy steels with highly acidic feedstocks (TAN > 16)[3];
- in a range between 100 and 290°C, the corrosion kinetics of carbon and low alloy steels follow an Arrhenius-equation-type relationship (Figure 1) and evolve linearly with respect to the TAN (Figure 2);
- in fatty acid distillates (TAN=200), the risk of corrosion requires the use of stainless grades alloyed with molybdenum, such as 316L or 317L.

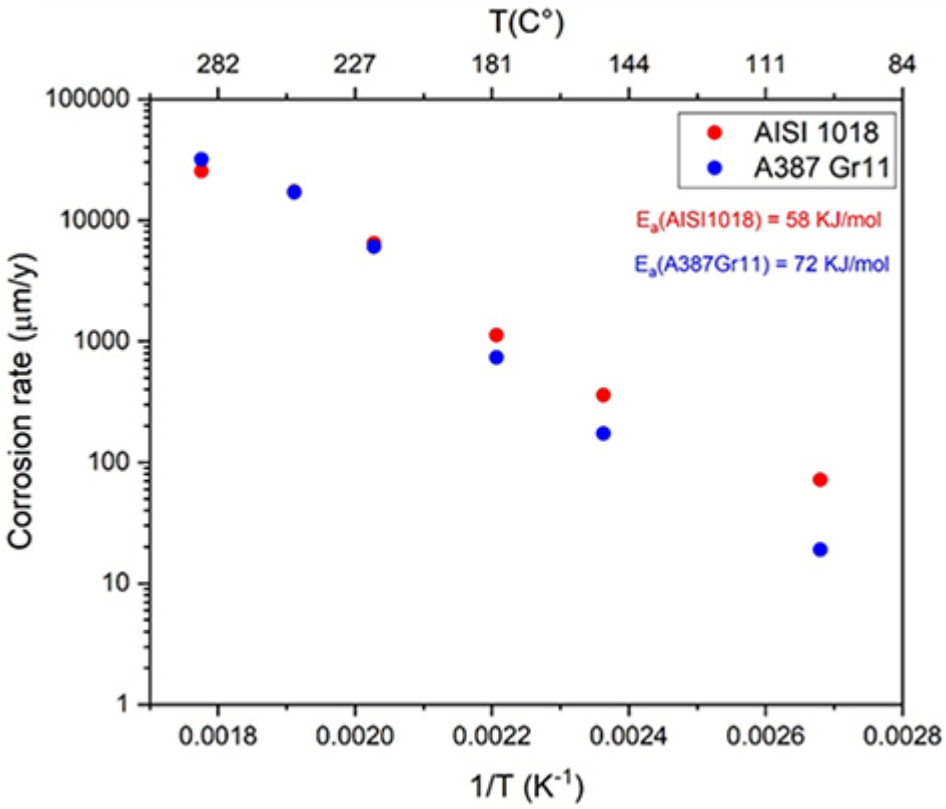


Figure 1: Influence of temperature on the corrosion rate of AISI 1018 carbon steel and A387 Gr11 low alloy steel during DTO (TAN=192) immersion tests

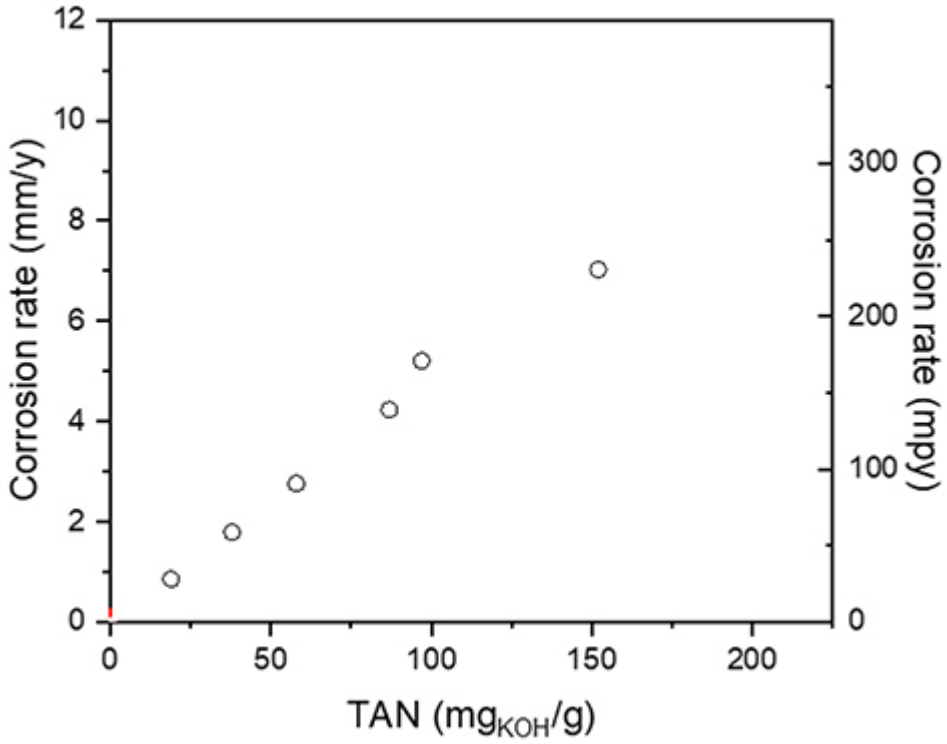


Figure 2: Influence of TAN on the corrosion rate of AISI 1018 carbon steel during immersion tests at 220°C (mixture of rapeseed oil and oleic acid)

The corrosion mechanism was identified through the use of several complementary analysis techniques (potentiometric titration, infrared spectroscopy, simulated distillation). The consumption of free fatty acids with a ratio of 2 moles of acid for 1 mole of dissolved iron is highlighted by the reduction in the characteristic absorption band of the vibration band of the C=O bond at 1711 cm^{-1}, characteristic of oleic acid (Figure 3). In addition, a new IR absorption cluster is observed in the 1567 – 1605 cm^{-1} region, characteristic of the vibrations of the carboxylate function involved in the formation of organometallic complexes. These results prove that steel corrosion in these environments is promoted by the formation of complexes [1-2].

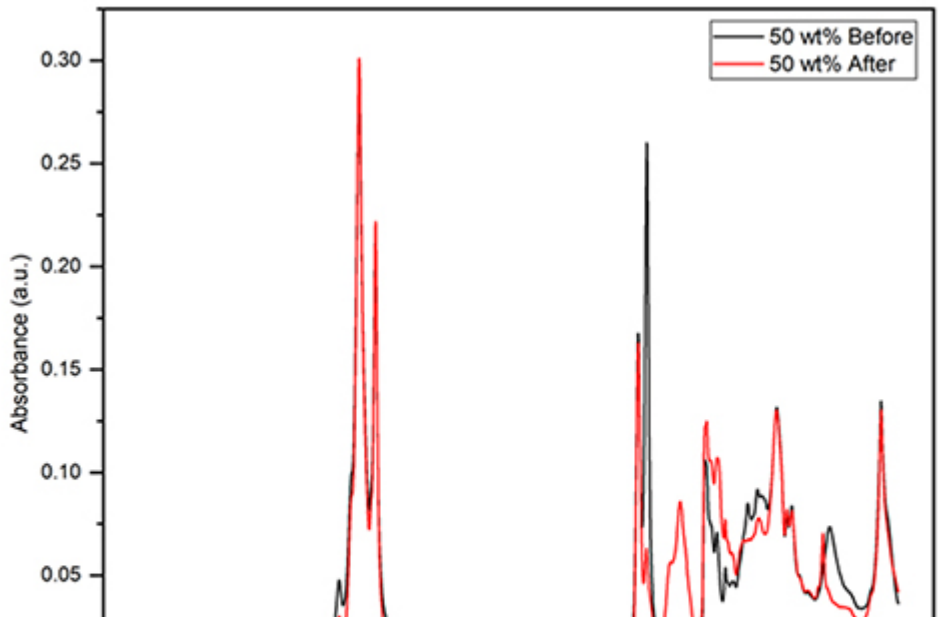


Figure 3: Infrared spectrum of an acidic vegetable oil before and after corrosion test

The methods and knowledge developed during this PhD research are now being used for numerous industrial biomass conversion process developments, as well as for co-processing operations[5]. For the design of new industrial units, safer construction materials can now be chosen, and for revamp of existing units, they provide tools for defining the limits of use of the most corrosive feedstocks.

[1]- [1] Thesis by F. Andari, Impact of biomass composition on corrosion: case of the hydrotreatment of vegetable oils and waste oils to produce biofuels, PhD thesis, Lyon 1 University, 2022.
[2]- Partial renewal of feedstock in semi-batch mode, without opening the test reactor or temperature reduction.
[3]- The TAN (Total Acid Number) is a measurement of the total acidity of an oil, expressed in milligrams of potassium hydroxide required to neutralize one gram of oil (mg KOH/g oil).
[4]- Distilled Tall Oil
[5]- Treatment of a feedstock made up of a mixture of conventional hydrocarbons and an alternative resource (bio-based oil, pyrolyzed plastic waste, etc.)

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1. Andari, J. Kittel, J. Fernandes, N. Godin, B. Ter-Ovanessian, F. Ropital, ***High temperature corrosion in various grades of vegetable and waste oils used for bio-fuel production***, Corrosion Science, 2022, Vol 206, Article 110501
   >> https://doi.org/10.1016/j.corsci.2022.110501

2. F. Andari, J. Kittel, J. Fernandes, L. Dodelin, F. Ropital, ***Corrosion issues in the conversion of vegetable and waste oils to produce biofuels***, NACE/AMPP 2023 Conference paper 19308
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Scientific contacts: Jean Kittel, joanna.fernandes@ifpen.fr and François Ropital

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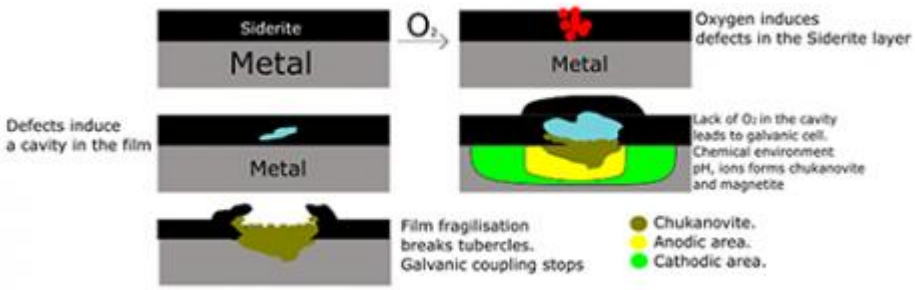


Self-repair against localized corrosion

Due to their low cost and their good mechanical properties, carbon steels are a widely used material, including for equipments in contact with harsh environments, such as aqueous media containing CO2...

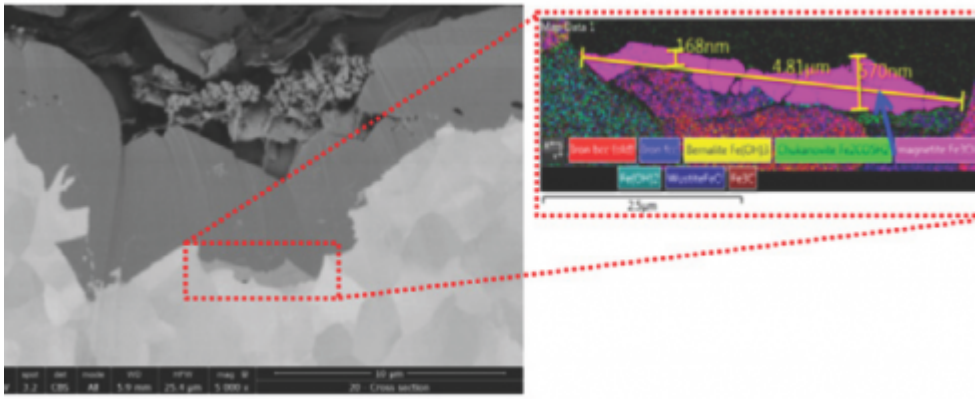
Electrochemistry and corrosion

IFPEN

News April 2021

Corrosion, one of the major challenges of the energy transition, has been the focus of significant research at IFPEN

Renewable energies | Responsible oil and gas



Carbon steel in self-defense mode against corrosion

Carbon or low-alloy steel corrosion, by aqueous media containing CO_2, hampers the development of numerous technologies[a] f

Physical chemistry | Surface, interface and materials science | Electrochemistry and corrosion

SC2 - Biofuel production: understanding and controlling corrosion by renewable feedstocks

Injectivity in geological formations has long been an important factor in oil production (enhanced recovery) but it is now just as important in fields related to new energies and the climate (geothermal energy, CO_2 storage, etc.). Injectivity losses, which result from the clogging of geological formations, are a recurrent problem associated with the fact that reinjected water often carries a high concentration of organic and mineral elements in suspension, in the form of colloidal particles.

To remedy this clogging, or at least minimize it, it is important to clearly understand the mechanisms involved.

The phenomenon of particle transport and deposition in porous media has been extensively studied in the past, particularly through coreflood permeability measurements. Its quantitative impact on this property is thus well established but, due to rock opacity, less has been known about the mechanisms taking place at pore scale.

In recent years, advances in imaging and visualization tools have enabled researchers to study phenomena at the pore scale. Coupled to microfluidics, a methodology allowing the control and use of very small volumes of fluids[1] in confined microstructures, key results on clogging dynamics have been obtained. Moreover, recent developments in engraving techniques enable researchers to reproduce the complexity of real porous media in these microstructures. By combining all these techniques, it is possible to directly visualize the flow in order to more accurately describe the phenomena involved on a local scale.

During thesis research carried out at IFPEN[2] in partnership with ICMCB[3], the problem of deposition and clogging was studied using a microfluidic approach combining two visualization techniques: optical imaging [1] and laser-induced fluorescence [2]. The micromodels used (Fig. 1(a)) feature geometries inspired by images of real rock pore networks. A model suspension of micrometric particles with repulsive charges[4] was used. Combining multi-scale observations (Fig. 1(b), (d)) and macroscopic measurements (pressure and concentration) (fig. 1(c)) has enabled to characterize in detail the mechanisms acting at the pore scale and to gain a better understanding of the phenomena at play, depending on both hydrodynamics (velocity, pore geometry) and particle-particle and particle-solid matrix interactions (DLVO forces[5]).

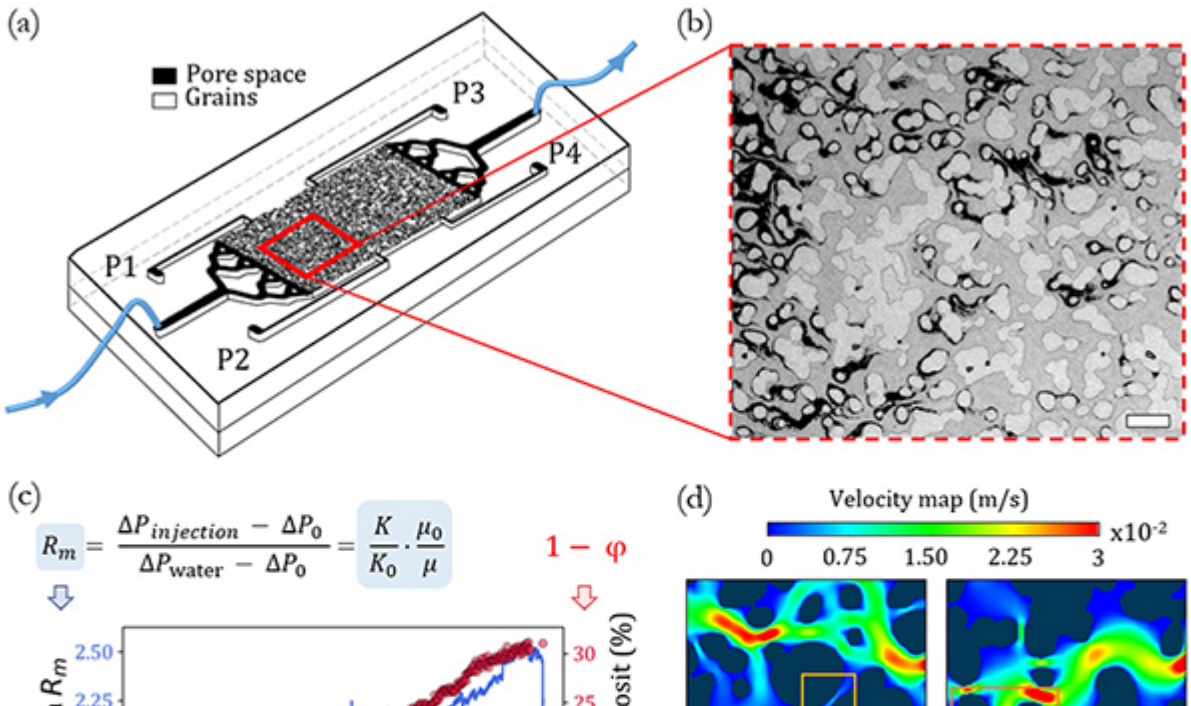


Figure 1 - (a) Illustration of the micromodel used. P1/P2/P3 and P4 correspond to pressure measurements.
(b) Example of observation based on traditional imaging of particle transport in porous media. Deposits, the porous space and grains are shown in black, dark gray and light gray respectively.
(c) Characteristic evolution of the mobility reduction coefficient Rm during injection of a particulate suspension and of the associated porosity reduction, obtained via image processing.
(d) Local observations of deposition sites and nature as a function of location in the porous medium and local flow velocity obtained by numerical simulation. G and PS correspond to a grain and the porous space respectively. The deposit is shown in black.

By cross-referencing the characteristics of the deposits obtained experimentally with the velocity fields determined by numerical simulation, this study, carried out under geothermal fluid reinjection conditions (small particles, high flow rate, permeable porous media), enabled the identification of the various deposition sites and regimes, as well as the description of clogging mechanisms. One of the most significant results obtained was the demonstration of a shear-induced aggregation phenomenon [3]. Deposition sites, which represent traps primarily governed by streamlines in the porous medium, generate a local overconcentration of particles according to five configurations: in the wake of a solid grain, at stagnation points, in flow-free regions, at the confluence of two local flows or at the entrance to a narrow pore. This local over-concentration of particles, when combined with significant local shear [6], induces formation of aggregates.

The phenomenon of hydrodynamic aggregation is closely correlated with high injection rates and presents a major risk that needs to be anticipated and controlled. In fact, these irreversible aggregates can form even when fluids are finely filtered and contain very few particles. They are easily carried along in the flow, without breaking up, leading to clogging at pore thresholds via geometric exclusion, the aggregates being too large to circulate.

The kinetics of this damage were studied as a function of particle concentration, particle size and injection rate. Interpretations based on local observations and highlighted mechanisms were then proposed. Finally, the main results obtained using microfluidics were validated for more real systems (for example, a suspension of polystyrene particles in reconstituted sand beds or clay particles in micromodels) and paved the way for potential solutions to the phenomenon.

[1]- Order of magnitude of a microliter or even a picoliter.
[2]- **Anne-Sophie Esneu**, ***Etude des mécanismes d'endommagement des formations lors de la réinjection des fluides géothermiques* (*Study of formation damage mechanisms during geothermal fluid reinjection*),** Bordeaux University, 2024.
[3]- Bordeaux Institute for condensed matter chemistry - UMR CNRS 5026
[4]- To avoid aggregation prior to injection.
[5]- Derjaguin, Landau, Verwey, Overbeek.
[6]- Shear consecutive to fluid flow in the presence of a random arrangement of grains.

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Scientific contacts: anne-sophie.esneu@ifpen.fr and jalila.boujlel@ifpen.fr

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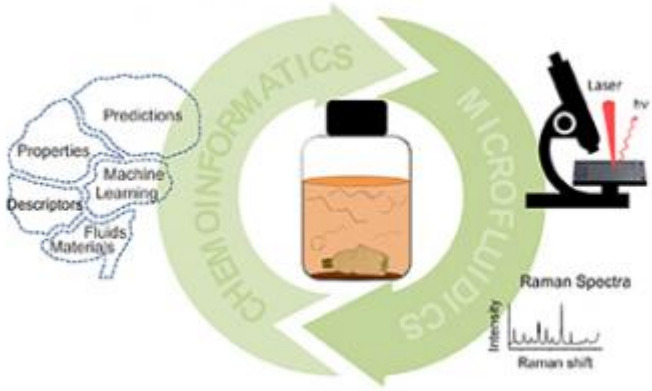


Microfluidics and Chemoinformatics: a highly complementary approach to studying material/fluid compatibility

Pour de nombreuses applications industrielles, comme le recyclage chimique des plastiques, ou encore pour assurer la compatibilité entre polymères et nouveaux carburants, il est essentiel d’anticiper les interactions entre matériaux et fluides...

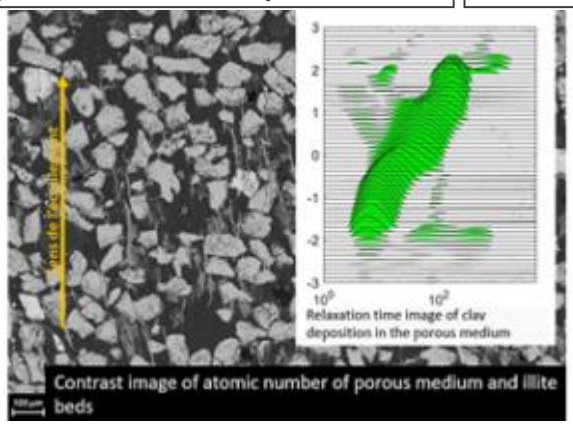
Chemical analysis **Microfluidics** **High-throughput experimentation (HTE)**
Signal processing/Data science

Fundamental Research

News September 2023

Geothermal plugging: what are the mechanisms and what are the levers for action?

Petrophysics and transfers in porous media | Structural analysis and Imaging



Clogging is a major challenge for geothermal energy

In a porous geological structure, the flow of a geothermal fluid carries along solid particles for which the rock acts as a filter. The capture of these particles causes the permeability of the porous medium to gradually decrease, which can lead to a drastic reduction in injectivity and eventual failure of the industrial operation...

SC3 - Microfluidics supporting preserved injectivity

Data from NIRS[1] are processed mathematically, via chemometric approaches[2], generally using a Partial Least Squares (PLS)-type model. This linear methodology is aimed at establishing a statistical relationship, represented by the maximum covariance, between an explanatory variable X and a response variable y. It has been successfully used at IFPEN to predict the properties of oil products and, in recent years, it has mirrored the evolution of new energy technologies (NET) for applications in fields such as bio-fuels and the chemical recycling of plastics.

The approach is based on signal pre-processing operations aimed at correcting analytical artefacts impacting the relevance of models from the use of experimental data. However, in a constantly evolving field requiring more regular model updating, this solution is no longer considered satisfactory.

Deep learning, a promising alternative for the development of experimental models, is the focus of PhD research currently underway[3]. In this approach, a neural network extracts information from data without the need to explicitly specify how to do so. An error calculated[4] between the prediction of the model and the expected value for the response variable makes it possible to optimize the internal parameters of the neural network. This is a complete paradigm shift from chemometrics where it is necessary to develop an experimental design and test different signal processing combinations.

Research at IFPEN has focused on deep convolutional networks, with the goal of developing its own - Inception for Petroleum Analysis (IPA) - to better meet the day-to-day needs of NIRS [1] analysis . This is inspired by the state of the art in deep learning for computer vision and is based on several computational blocks whose architecture is described in Figure 1.

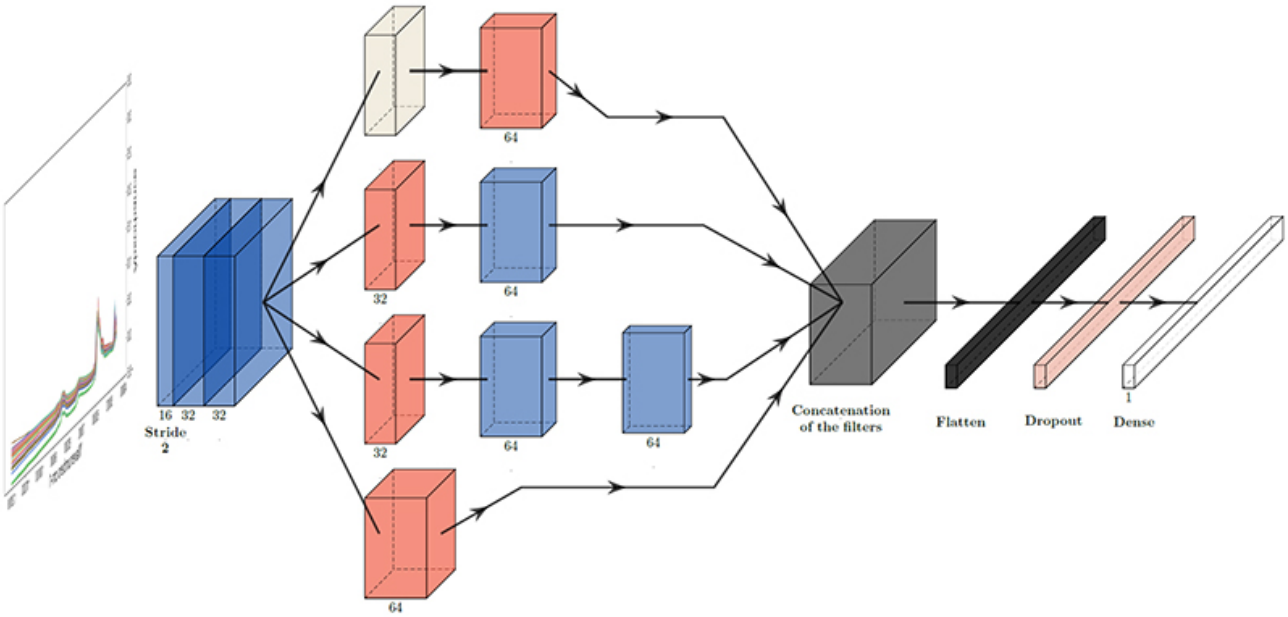


Figure 1: IPA (Inception for Petroleum Analysis) architecture

Through comparison with a traditional chemometric model (PLS) and with a deep learning model, DeepSpectra [2] taken as a reference, the IPA model was tested for its capacity to predict the cetane number[5] of middle distillates produced using a variety of industrial processes. All three were first of all trained on a set of 174 NIRS spectra, recorded in the 4,000-12,000 cm^{-1} spectral range and then

tested for validation on another base of 75 spectra. In these bases, the cetane number varied between 19.0 and 71.1, with an average of 43.3 and a standard deviation of 11.1. The spectral range was initially reduced to remove NIR bands between 4,000-4,500 cm^{-1}, saturated and affected by problems of non-linearity. The PLS model required a signal pre-processing step prior to calibration incorporating a baseline correction, in contrast to calibration of the IPA model, which is done directly on the data without the need for pre-processing.

Model quality is generally assessed using several distances, particularly the square root of the mean quadratic error, calculated between model predictions and measured values. For the reduced spectral range, between 4,500 and 12,000 cm^{-1}, the IPA model presented an error 40% lower than the PLS model, and was 20% more accurate than the DeepSpectra deep learning model. Moreover, in two cetane number zones with little information in terms of calibration[6], a significant prediction difference between the different models was observed (Figure 2): these are the outermost parts of the validation base parity plot, where IPA proposes relevant predictors while the PLS model lacks precision (as does DeepSpectra, not shown here). Finally, for the same set of data, taking into account the complete 4,000-12,000 cm^{-1} spectral range, IPA was 50% more precise than PLS and 21% more precise than DeepSpectra.

The superior performances of the IPA model demonstrate its ability to capture more relevant information than the PLS and DeepSpectra models, particularly in the complete spectral range and it can do so without being affected by the saturated part. Similarly, within the range of extreme values considered, IPA performed well at generalizing information across a wide range of predicted property values, unlike the PLS and DeepSpectra models.

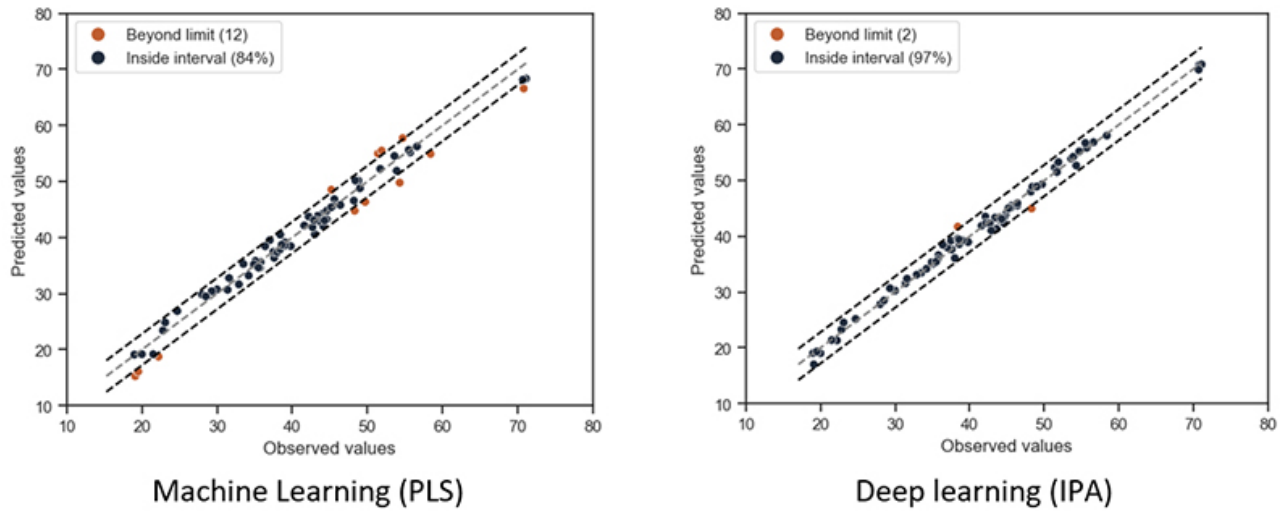


Figure 2: Parity plot – Middle distillates (reduced spectral range of 4,500-1,200 cm-1)

[1]- Abbreviation for Near Infrared Spectroscopy
[2]- Chemometrics is the application of mathematical tools, particularly statistical ones, to obtain maximum information from physicochemical analysis data.
[3]- Thesis by **F. Haffner**, ***Apprentissage profond et proche infrarouge pour intensifier l'usage des méthodes spectroscopiques (Deep learning and near infrared to intensify the use of***

spectroscopic methods).
4- Based on a loss function.
5- Number used to precisely evaluate a diesel's ignition delay.
6- Cetane numbers of 18 to 20 and 70 to 72.

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   >> DOI: 10.1016/j.aca.2019.01.002

Scientific contacts: Maxime Moreaud (deep learning) and marion.lacoue-negre@ifpen.fr (near infrared, chemometrics)

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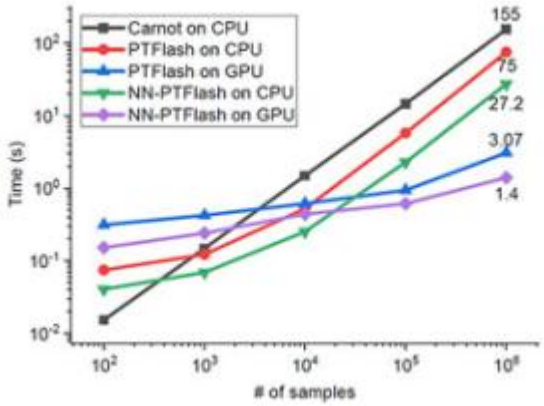
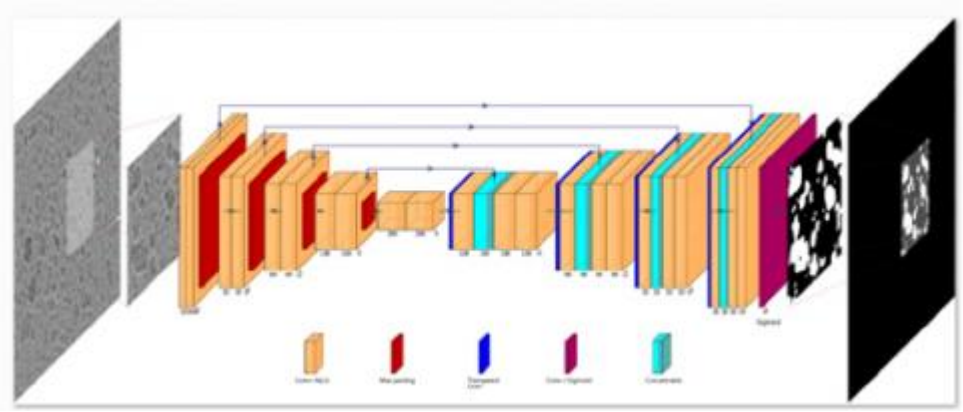


Deep learning in the field of thermodynamics

Reactive fluid transport simulation has multiple applications - flows in porous media, combustion, process engineering - and requires thermodynamic equilibrium calculations (also knows as “flash” calculations). However, these calculations can take a long time and, as they are involved in large numbers in the simulations carried out, in practice they limit the latter to systems containing few chemical species or to restricted time and space scales...

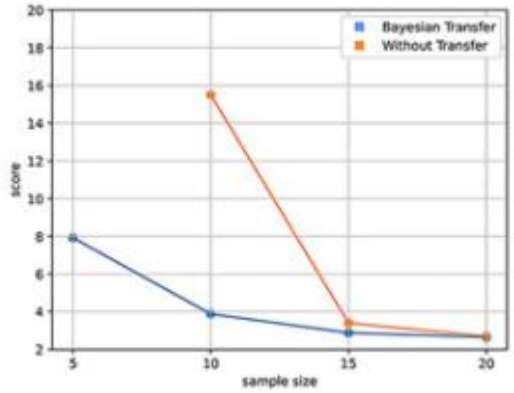
Thermodynamics/Molecular modeling **Signal processing/Data science**



Semantic segmentation through deep learning in materials sciences

Semantic segmentation conducted on microscopy images is a processing operation carried out to quantify a material’s porosity and its heterogeneity. It is aimed at classifying every pixel within the image (on the basis of degree of heterogeneity and porosity). However, for some materials (such as aluminas employed for catalysis), it is very difficult or even impossible using a traditional image processing approach, since porosity differences are characterized by small contrasts and complex textural variations. One way of overcoming this obstacle is to tackle semantic segmentation via deep learning, using a convolutional neural network.

Chemical sciences | **Organic and mineral synthesis** | **Analysis and characterization**
Structural analysis and Imaging | **Mathematics and IT** | **Signal processing/Data science**



Transfer learning for process optimization

IFPEN is a global leader in the development of catalysts and processes for clean fuel production. For these processes themselves to be eco-efficient1, it is necessary to optimize the coupling of catalysts with the operating conditions, as a function of the feedstocks used and the target specifications for the refined products. It is therefore useful to be able to draw on predictive models for the performance achieved, and machine learning can help improving these models...

Chemical engineering and process engineering | **Signal processing/Data science**

SC4 - Deep learning for fluid characterization

Processes using heterogeneous catalysis[1] require the design and development of innovative materials, with controlled mechanical and textural properties, to produce effective catalyst supports. The porous microstructure of these supports has a significant impact on the performance of the supported catalyst, since it strongly affects the support's mechanical resistance and transport phenomena. The industrial manufacture of alumina extrudates is conducted using a kneading-extrusion process, aimed at converting a powdered alumina precursor (boehmite) into micrometric solids.

This preparation process makes it possible to optimize the support's properties of interest by adjusting the conditions of each of the two individual operations.

An experimental study conducted as part of ongoing PhD research[2] related exclusively to the kneading operation, with a view to characterizing its effects on the properties of boehmite pastes [1, 2]. To do this, several pastes were prepared in a pilot mixer (illustrated in Figure 1), mixing boehmite powder and acidic and basic aqueous solutions. The textural and mechanical properties of the pastes obtained were studied as a function of kneading time (from 3 min to 4 h), blade rotation speed (from 10 to 100 rpm) and paste composition (resulting pH between 5 and 9, modified by the addition of different concentrations of basic solutions). The distribution of pore sizes, the specific surface area and pore volume were analyzed via nitrogen physisorption and mercury porosimetry on dry samples, while the mechanical properties were characterized in situ in the mixer by measurement of the mixing torque.

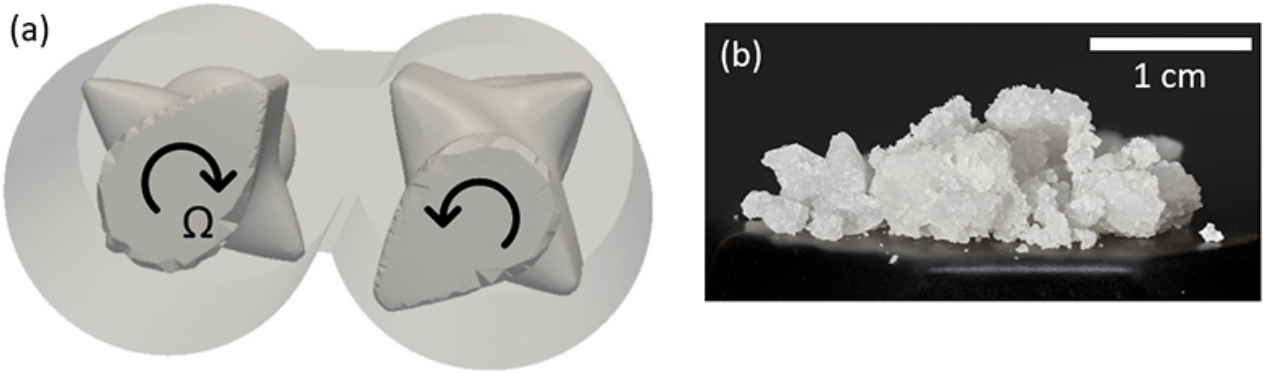


Figure 1: (a) Illustration of mixing tank (volume of 80 cm3).
(b) Photo of a boehmite paste with pH = 6.2, taken outside the mixer.

The results obtained demonstrate that the paste composition had a significant effect on sample properties. For example, an increase in the torque measured in the mixer was observed, as well as in the porosity of the dried paste (Figure 2), for compositions with a higher pH. Moreover, the evolution over time of the torque as well as of the textural properties of the paste are governed by the cumulative deformation, a quantity calculated as the product of rotation speed and mixing time and homogeneous to the number of revolutions undergone by the paste. Lastly, it turns out that a relevant parameter to rationalize the evolution of these textural properties - as measured for a broad range of pH values, mixing times and rotation speeds - is the product of this cumulative deformation by paste pH.

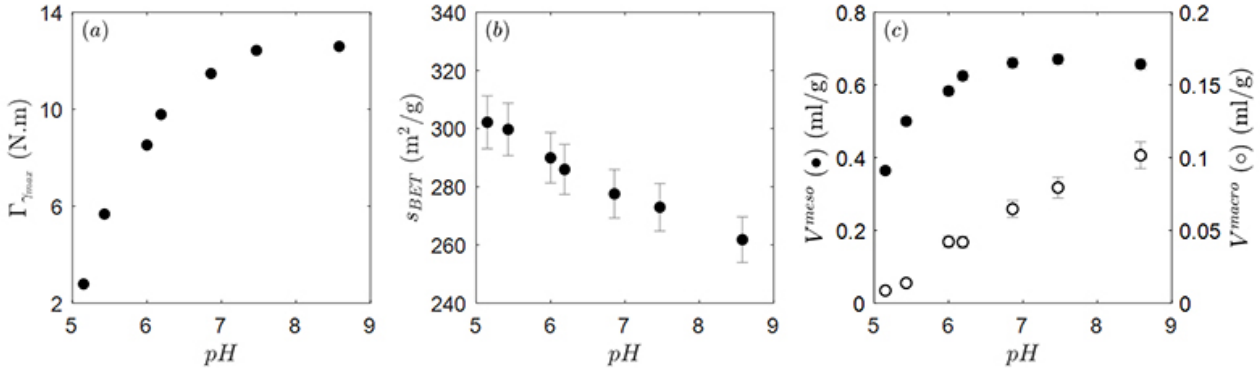


Figure 2: Influence of paste pH on (a) torque measured in situ after 2h40 of mixing at 50 rpm, (b) the specific surface area (nitrogen physisorption on dry pastes) and (c) pore volumes (mercury intrusion on dry pastes).

This study, dedicated to the characterization of the effects of kneading on the textural and mechanical properties of boehmite pastes, made it possible to separately identify the acidic-basic influence of their composition and the mechanical contribution of the mixer. Identifying a unique control parameter (product of paste deformation and pH) will make it possible, in the laboratory, to determine exactly what operating conditions should be applied at the mixing stage to manufacture a paste with a specific porosity. Consequently, this result is of interest for the development of new innovative heterogeneous catalysts. Finally, the next stage of this research will involve ex situ determination of the mechanical properties of pastes, using techniques such as rheometric analysis, indentation and compression, in order to obtain a more rigorous characterization of the effect of kneading on the mechanical properties of boehmite pastes.

[1]- Such as hydrotreatment and catalytic reforming processes.
[2]- Thesis by **Mathilde Auxois**, ***Identification et étude de descripteurs du malaxage d'une pâte de boehmite pour la conception de nouveaux solides. (Identification and study of boehmite paste kneading descriptors for the design of new solids)***

References:

1. Mathilde Auxois, Marine Minière, Chloé Bertrand-Drira, Fabien Salvatori, Jan Verstraete, Sébastien Manneville, Thibaut Divoux, ***Tuning properties of catalysts supports via kneading conditions of colloidal pastes***, European Colloid and Interface Society congres, 2023

2. Mathilde Auxois, Marine Minière, Chloé Bertrand-Drira, Fabien Salvatori, Jan Verstraete, Sébastien Manneville, Thibaut Divoux, ***Textural properties of dense granular pastes produced by kneading***, arXiv:2402.09220

Scientific contacts: mathilde.auxois@ifpen.fr and marine.miniere@ifpen.fr

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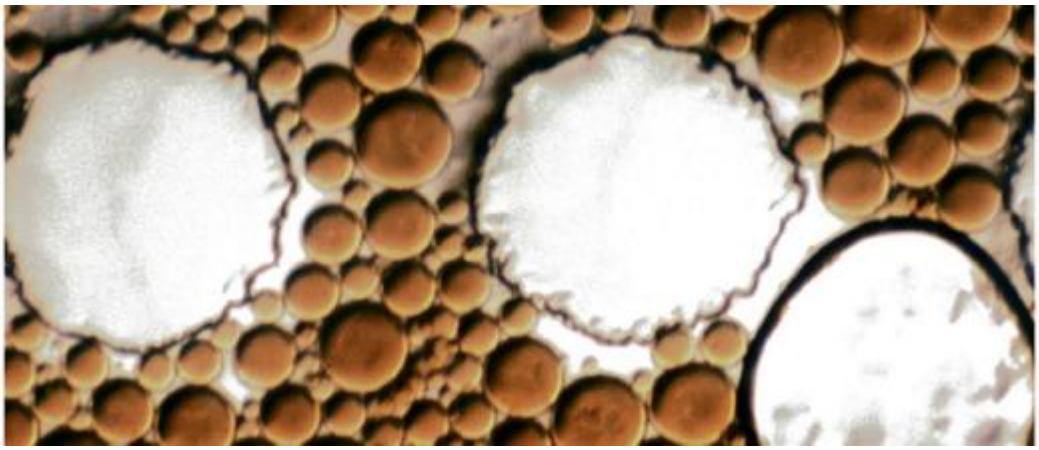


Fundamental Research

News October 2023

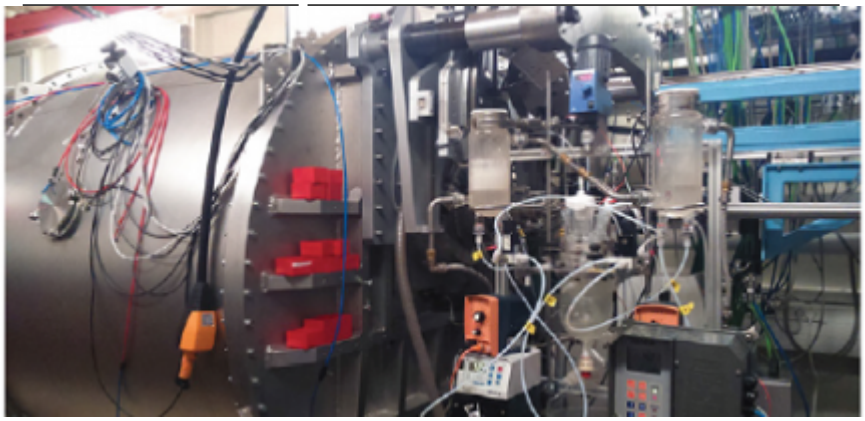
Porous media challenge scientists

Geology - Sedimentology | Geostatistics - Geological modeling | Petrophysics and transfers in porous media | Chemical engineering and process engineering

Fundamental Research

News December 2022

CARMEN JRL: a breakthrough research for the energy transition



Boehmite rhapsody! Controlled precipitation

Transition aluminas[a], widely used as catalyst supports, play a key role in numerous refining processes.

Responsible oil and gas | Fuels

Chemical sciences | Organic and mineral synthesis | Analysis and characterization | Structural analysis and Imaging

Diffusion in catalysts: an often tortuous path!

In catalytic processes, an active phase is necessary to accelerate the transformation of the molecules in the fluid treated. Most of the time, this catalytic agent is placed on a porous support with a large internal surface area, making it possible to host a large number of active sites within a small volume...

Structural analysis and Imaging | **Chemical engineering and process engineering** | **Systems modeling and simulation**

SC5 - Manufacture of catalytic supports: a new parameter for controlling the kneading of boehmite pastes

Mooring lines are essential components for the stability of offshore floating structures, such as those supporting wind turbines. They often consist of steel spiral ropes linked by a chain to the platform (also known as the "floater"). New solutions are currently being studied, in which the rope is directly connected to the floater, thereby removing the need for the chain - which has proved to be a mechanical weak point - and simplifying the connection. But, in such configurations, the rope is subject to a load combined with cyclical tension and bending for which it has not been designed. Spiral ropes have a single-strand[1] and are optimized for use under tension only.

Rather than perform representative fatigue tests[2], which are expensive and difficult to interpret, IFPEN adopted an approach based on multi-scale numerical simulation. In this approach, detailed modeling of the rope makes it possible to calculate local loads on the metal wires from global loads - tension and bending - at floater level [1, 2]. These calculated loads can then be reproduced in the laboratory on a test bench designed to test numerous applications[3].

The cyclical tension and bending of the rope are shown to generate fretting fatigue[4] in the wires, a phenomenon that is absent with cyclical tension alone, for which friction-induced damage is negligible. In this combined load scenario, the most critical local stress is partial slip, characterized by the fact that the center of the contact remains fixed while its periphery slips (Figure 1).

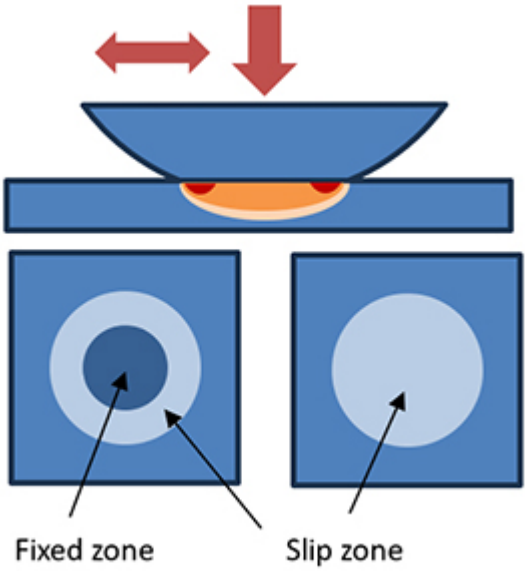


Figure 1: illustration of fretting stress with two possible slip scenarios: partial slip on the left and total slip on the right.

However, in an offshore anchor cable, the wires are not bare since they are protected from corrosion by a zinc coating[5] and grease, in addition to a waterproof polymer sheath around the cable. Fretting fatigue tests helped to elucidate the mechanical effects of these protections. They were conducted for one form of protection only (zinc or grease) or for both.

Taken individually, galvanization and grease have no notable effect [3]. The zinc layer is quickly removed from the contact area by wear and tear, and the grease, which is thick enough not to run down the rope but is quickly removed from the contact area, has limited lubricating power in the event

of partial slip.

However, the two protections taken together lead to a significant improvement in wire fretting fatigue [4]. The removal of zinc from the contact area (Figure 2) creates a trough that limits the loss of grease and improves its lubricating power, even in the event of partial slip.

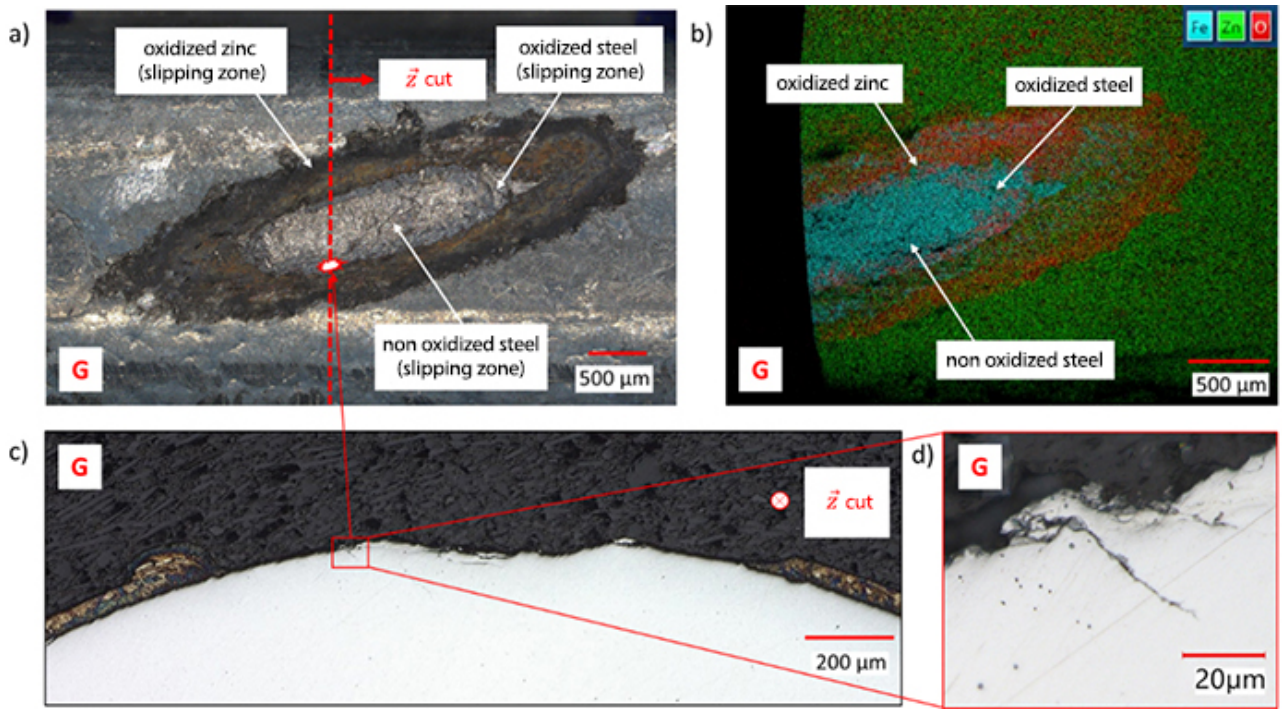


Figure 2: single interrupted fretting test on galvanized wires
a) optical view of trace,
b) EDX view of trace (display of oxygen, zinc and iron),
c, d) optical views of the axial section.

This unexpected synergy is beneficial to the service life of metallic materials exposed to fretting fatigue, as demonstrated by our experimental results (Figure 3).

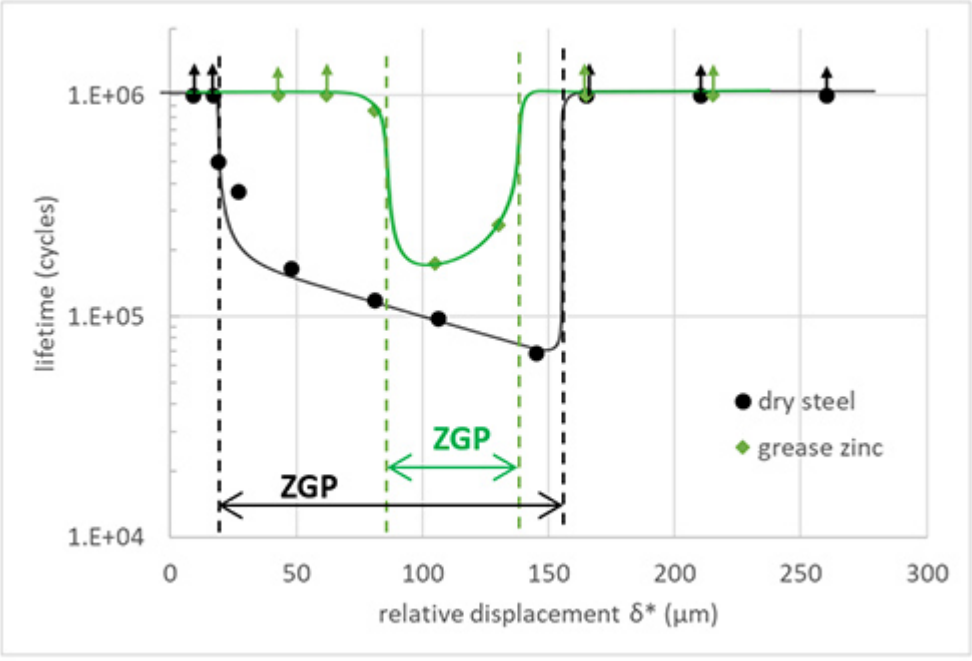


Figure 3: Fretting fatigue curves for dry contact between steel wires (black) and greased contact between galvanized wires (green). Load under constant fatigue and force conditions Relative slip between wires on the x-axis and lifespan on the y-axis. The combination of zinc and grease significantly increases lifespan. ZGP: critical damage zone in partial slip conditions

Combining numerical simulation with mechanical tests representative of local wire loads made it possible to reproduce the mechanisms at play on a small scale, in order to better elucidate them . This understanding of fretting fatigue damage and the favorable synergy between protective elements not designed for this problem opens up new opportunities for improving the design and use of steel anchor cables for floating offshore supports.

[1]- A strand is an assembly of metal (or textile) wires coiled around a longitudinal axis. A rope may be made up of one or several strands.
[2]- Reproducing the real full-scale configuration.
[3]- Located at the Laboratoire de Tribologie et Dynamique des Systèmes (Tribology and System Dynamics Laboratory, Ecole Centrale de Lyon).
[4]- Phenomenon of crack initiation and propagation due to a combination of fatigue and friction.
[5]- Galvanic protection.

Thesis by **Sébastien Montalvo**, ***Étude de l'endommagement par fretting-fatigue de fils de câbles d'ancrage offshore : influence de la galvanisation, de la graisse et de l'eau de mer (Study of damage induced by fretting fatigue of wires in offshore anchor cables: influence of galvanization, grease and seawater)*** defended on 8 November 2023.

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1. F. Bussolati, M. Guiton, P.-A. Guidault, O. Allix, and P. Wriggers: ***Lecture Notes in Application and Computational Mechanics***, vol. 93 (2019)

2. S. Montalvo, S. Fouvry, M. Martinez, ***A hybrid analytical-FEM 3D approach including wear effects to simulate fretting fatigue endurance: Application to steel wires in crossed contact***, Tribology International 187 (2023) 108713
   >> https://doi.org/10.1016/j.triboint.2023.108713

3. S. Montalvo, S. Fouvry, M. Martinez, ***Effect of zinc coating on the fretting fatigue endurance of crossed steel wires, submitted to Wear in December 2023***, submitted to Wear in December 2023

4. S. Montalvo, M. Martinez, S. Fouvry, ***Effect of zinc coating and grease on the fretting fatigue life of steel wires used in spiral steel ropes***, OIPEEC Conference, Lake Garda, Italy, 2024

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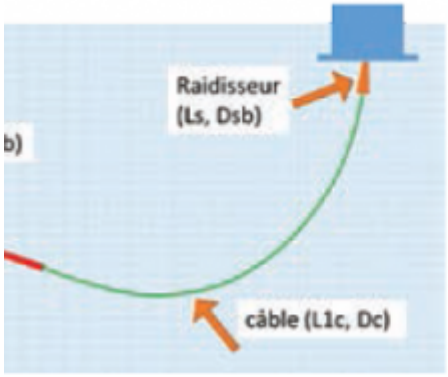
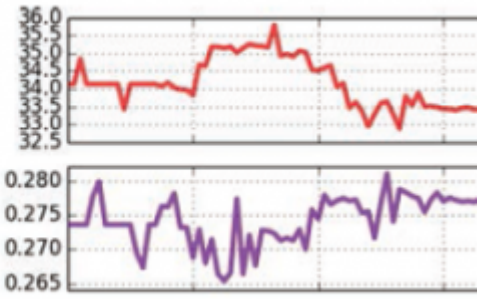


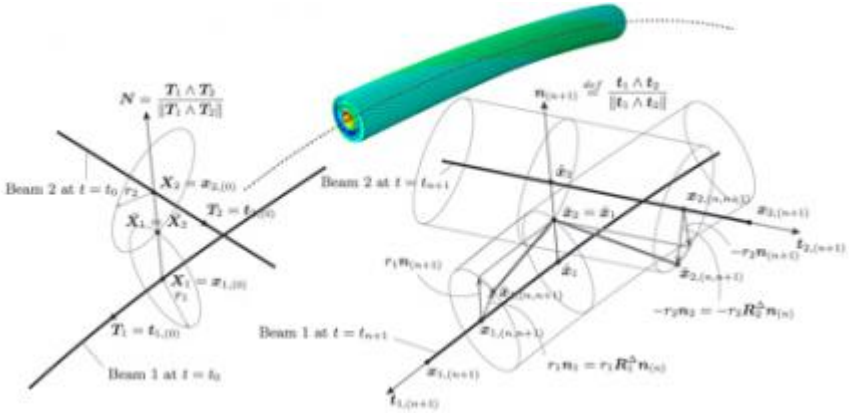


Optimizing the electric cable of a floating wind turbine

Floating wind turbine technologies, such as those co-developed by SBM and IFPEN[a] , are designed to **optimize the recovery of offshore wind energy**

Renewable energies | **Wind Energy**

Engineering sciences | **Systems modeling and simulation** | **Mathematics and IT** | **Numerical methods and optimization**



“From material to structure” modeling: the case of anchor cables for offshore wind, in corrosive environment

Anchor lines, the majority of which are carbon steel cables, are essential components for the stability of offshore floating structures, such as those supporting wind turbines. To overcome the risk of breakage during service, redundant lines are generally incorporated at the design stage, which adds significantly to the cost...

Mechanical and thermal testing | Solid mechanics | Numerical methods and optimization

SC6 - Floating wind turbines: gaining a better understanding of the behavior of steel mooring ropes

Urban road traffic is a significant source of pollutant emissions that impacts air quality. Being able to predict the dispersion of these emissions is of major importance for evaluating real exposure and planning traffic flows.

To this end, a PhD research project[1] proposed a modeling chain making it possible to simulate highly turbulent flows on a local urban scale and obtain two-dimensional spatial maps of pollutant concentration (figure 1) [1].

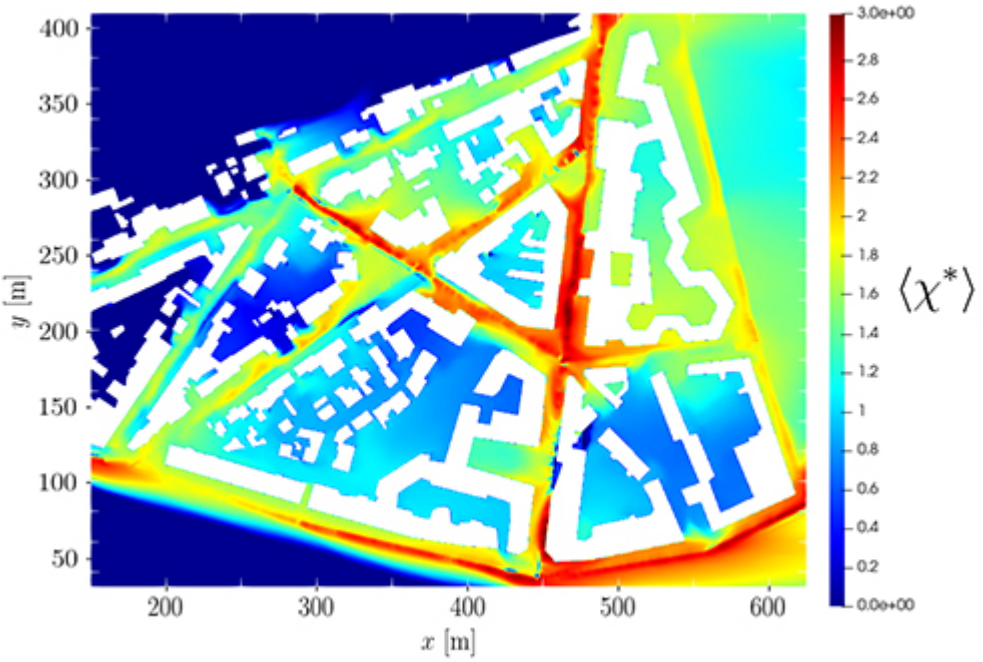


Figure 1: Example of pollutant concentration map simulated by the calculation chain described in [1] for a neighborhood in Issy-les-Moulineaux, near Paris.

Drawing up these maps involves different uncertain variables (i.e., variables that are either unknown or little known in advance): weather-related variables (wind direction ? and strength "U" _"?") and traffic-related variables (traffic volume q, speed limit v_{max} and proportion of diesel and gasoline vehicles ?). Some have a greater impact than others on the outputs predicted by the model and these are identified using sensitivity methods, one of the themes tackled within the CIROQUO consortium[2].

Concerning these methods, the traditional approach consists in calculating a usual sensitivity index (such as Sobol indices[3]) on a discretized space to obtain sensitivity maps. Within the framework of another CIROQUO/IFPEN thesis[4], a new family of sensitivity indices adapted to model outputs, which are not scalars but sets, was proposed [2] and implemented for this application [3]. Instead of producing sensitivity maps, this new approach characterizes the influence of different input parameters on a random set. Here, the set considered is three-dimensional, with spatial coordinates on the one hand (x,y) and the pollutant concentration level on the other, as calculated from various values of uncertain variables. Its performance was compared with methods taken from the literature: Sobol indices (following adaptation to sets) and so-called universal indices that can be applied to all types of variables.

The results of this comparison are presented in figure 2 and show, firstly, that the different approaches deliver similar results in terms of ranking the influence of input variables. However, the new, more sophisticated method also makes it possible to determine whether or not variables are negligible in nature via a statistical test (screening). The result is a potential reduction in the number of variables to be studied. Moreover, the confidence intervals obtained on index predictions are globally lower than with the other approaches [3].

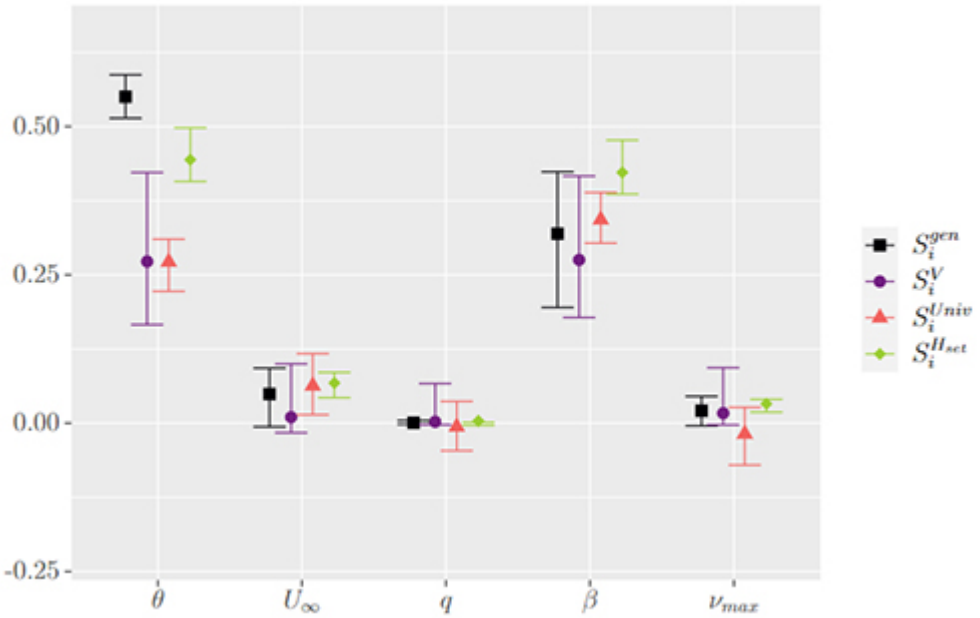


Figure 2: Different global sensitivity indices of 5 uncertain variables used for calculating the pollutant concentration map. The new index proposed is shown in green (see [3]).

In conclusion, the new approach proposed makes it possible to determine whether or not a variable is negligible, and then to rank the remaining variables by degree of importance. Finally, this new method potentially opens up interesting avenues for other applications requiring knowledge of the influence of uncertain variables during robust optimization[5] [2].

[1]- Thesis by **Mathis Pasquier**, ***Quantification d'incertitudes pour la dispersion turbulente de polluants liés au trafic routier à l'échelle micro-urbaine (Uncertainty quantification for the turbulent dispersal of road traffic pollutants on a local urban scale)***, Aix Marseille University, defended on 21 December 2023.
[2]- Consortium Industrie et Recherche pour l'Optimisation et la Quantification d'incertitude pour les données onéreuses (Industrial Research Consortium dedicated to the Optimization and Quantification of Uncertainties for Expensive Data): https://ciroquo.ec-lyon.fr/
[3]- Sensitivity index of an output variable with respect to an input variable (based on variance decomposition).
[4]- Thesis by **Noé Fellmann**, A***nalyse de sensibilité des problèmes d'optimisation sous incertitudes (Sensitivity analysis of optimization problems under uncertainties)***, Ecole Centrale Lyon (ongoing).
[5]- i.e., optimization for which all admissible solutions are defined by constraints dependent on uncertain variables.

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   >> 10.1016/j.buildenv.2023.110562

2. Noé Fellmann, Christophette Blanchet-Scalliet, Céline Helbert, Adrien Spagnol, Delphine Sinoquet. ***Kernel-based sensitivity analysis for (excursion) sets***, *Technometrics*, 2024, 1–13
   >> 10.1080/00401706.2024.2336537

3. Noé Fellmann, Mathis Pasquier, Céline Helbert, Adrien Spagnol, Delphine Sinoquet, Christophette Blanchet-Scalliet, ***Sensitivity analysis for sets: application to pollutant concentration maps***. 2023
   >> hal-04312097

Scientific contacts: adrien.spagnol@ifpen.fr and Delphine Sinoquet

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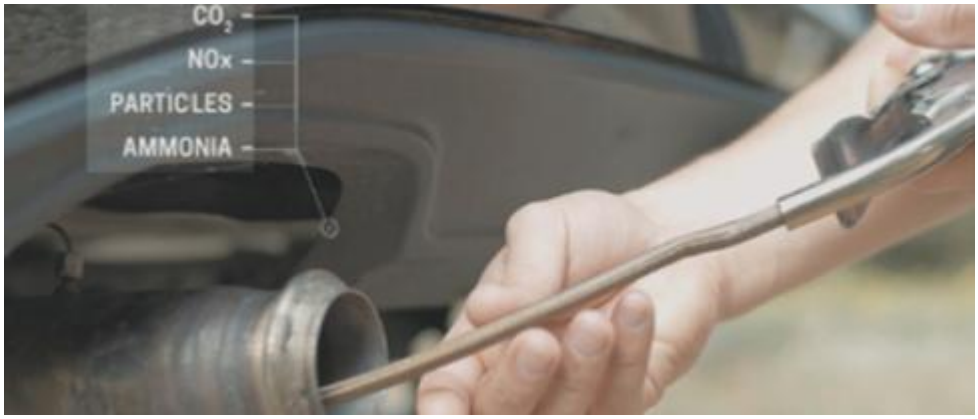
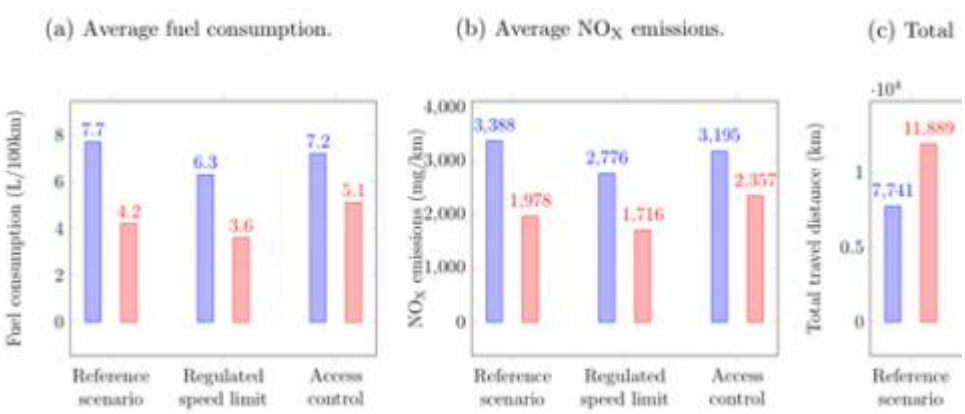


Road transport emissions: integrated research for air quality!

According to the WHO, 7 million premature deaths worldwide each year are linked to poor air quality, a problem to which road transport makes a significant contribution. Thanks to regulatory and technological developments, as well as the renewal of the vehicle fleet, emissions from this sector have certainly been falling in recent years. However, it remains a major contributor to the deterioration of air quality...

Combustion and engine technologies | **Systems modeling and simulation**



SC7 - Variable speed limits: for more eco-friendly urban traffic management

Driven by environmental and energy frugality challenges, there is growing interest in vehicle fuel efficiency and a reduction in the impact of mobility. While the promotion of alternative transport modes to cars remains the principal lever for change, much can still be done in terms of road traffic management. An IFPEN team worked on this subject as part of a thesis in collaboration with Gipsa-lab...

Systems modeling and simulation | **Numerical methods and optimization**

Fundamental Research

News February 2023

The benefits of speed regulation in urban areas are demonstrated in terms of air quality, fuel consumption and traffic flow

Systems modeling and simulation | Numerical methods and optimization

SC7 - Sensitivity analysis of pollutant concentration maps to weather conditions and traffic parameters

High-Performance Computing (HPC) is a scientific field involving both mathematics applied and computer science, with applications in numerous fields, including climate, energy, sustainable mobility, etc. In all of these fields, we often need to simulate large-scale physical phenomena with mathematical models that require a lot of computing time and storage space.

The aim of HPC is therefore to optimize the use of resources - machines, software, algorithms, development methodologies, etc. - to process large and complex problems from a wide variety of applications, accurately and in reasonable time.

These simulations are performed using supercomputers[1] that have CPUs[2] with a large number of cores[3] (for example 18 for Ener440 from IFPEN, or 64 for Irene from TGCC or 96 for Adastra from GENCI-CINES).

Despite their intrinsic power, the question now is how to calculate more efficiently with these machines, their multi-core processors, their complex memory hierarchy and the sophisticated computing units. In particular, this concerns fast and efficient core synchronization.

Shared-memory synchronization has been around for a long time and numerous models have been proposed, which can be found in different compilers used in HPC. For the traditional parallelization of a shared-memory code, core synchronization is aimed, firstly, at organizing calculations in the right order (via the insertion of barriers[4]) and, secondly, at guaranteeing the capacity to combine the results produced by all of the cores (in order to reduce them to a scalar result). In all cases, the time required should be kept to a minimum, but for processors with a large number of cores, the extra cost in computing time associated with the intensive use of these standard compiler synchronization mechanisms (such as GCC or Intel) is significantly high. They can even become performance bottlenecks for massively parallel codes.

Figure 1 illustrates the Extended Butterfly synchronization barrier, proposed within the framework of a thesis[5] conducted at IFPEN, for shared-memory parallel codes in order to address this problem. Its originality lies in the implementation of group synchronization[6] on two levels: intra-group then inter-group synchronization [1]. The number of steps required for synchronization depends on the log of the number of groups, which means that for seven cores, four steps are sufficient to synchronize them.

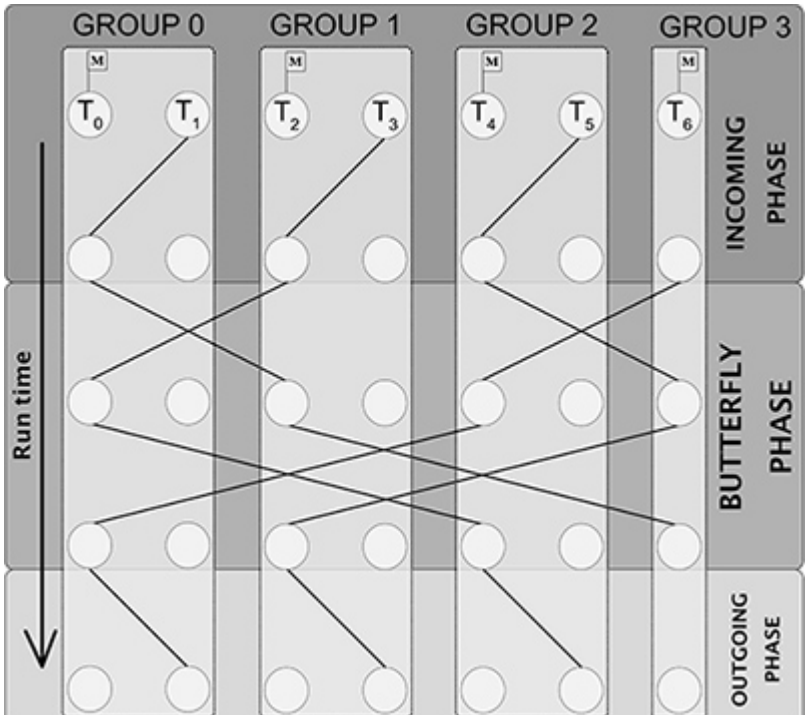


Figure 1: Illustration of notification exchanges between cores in the Extended Butterfly barrier with 7 cores or threads. The dark lines symbolize the sending of notifications from one core to another. The barrier consists of 3 steps: an input step, a step in Butterfly and an output step. Only the cores represented with a flag are authorized to enter in the Butterfly phase while their partner waits for their output phase notification.

The results of the performance tests conducted (figure 2) show that this barrier (light blue histogram) requires a shorter synchronization time (or latency) than the OpenMP programming interface barrier with GCC compilers (dark blue histograms).

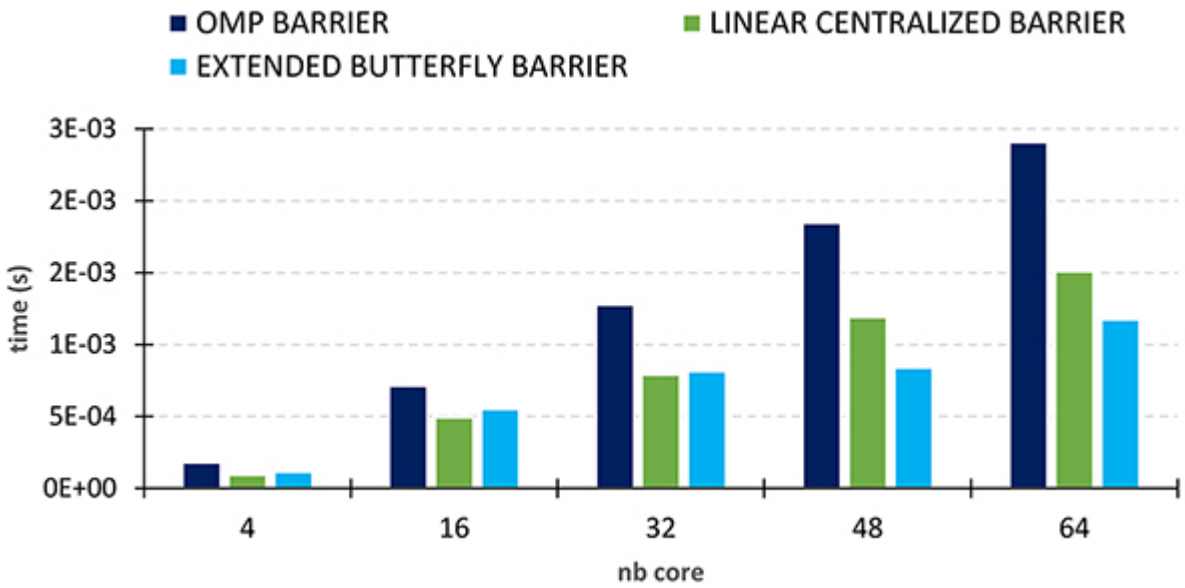


Figure 2: Result of barrier synchronization times on the AMD Milan processor.

Our Extended Butterfly barrier was then used as a support for reduction operations. Our Extended Butterfly Reduction method is up to four times faster (for 64 cores) than the OpenMP reduction with GCC on the AMD Milan processor (figure 3).

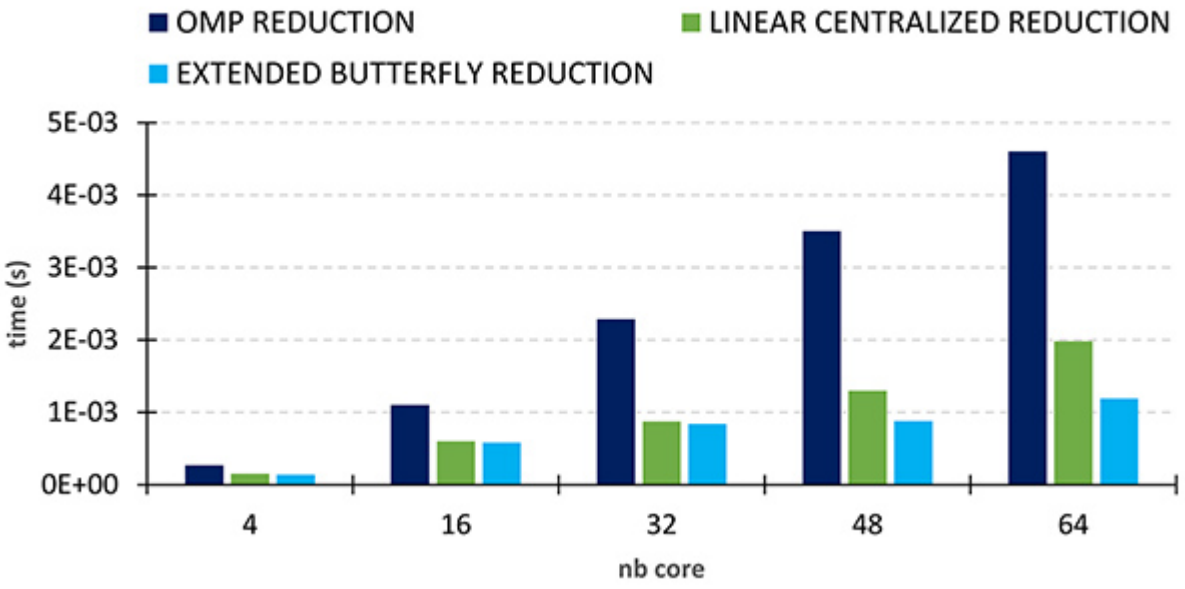


Figure 3: Result of reduction times on the AMD Milan processor.

The barrier and Linear Centralized reduction (green histograms) represent old methods implemented in MCGSolver[7], IFPEN's massively parallel library of linear solvers. Once again, the new methods Extended Butterfly lead to significantly better performances when the number of cores exceeds 40.

In summary, the computing power provided by new processors, thanks in particular to the large number of cores embedded, raises the issue of their optimal exploitation. Our new Extended Butterfly method proposes an effective approach to address this problem, with several benefits in terms of core synchronization. These methods have been integrated in the MCGSolver library.

[1]- Like Adastra (GENCI-CINES), the most recent machine that is in the top 3 of the 2022 Green500 rankings of supercomputers.
[2]- Central Processing Unit.
[3]- A core is a set of circuits capable of independently running programs.
[4]- Action designed to suspend the calculation of some cores while waiting for the others.
[5]- **A. Mohamed El Maarouf**, ***Factorisation incomplète et résolution de systèmes triangulaires pour des machines exploitant un parallélisme à grain fin (Incomplete factorization and resolution of triangular systems for machines exploiting fine-grained parallelism).*** Bordeaux University, 2023. HAL : tel-04429547 >> https://theses.hal.science/tel-04429547
[6]- Algorithmic notion introduced as part of this research.
[7]- Multi-Core multi-Gpu Solver.

Reference:

1. A. Mohamed El Maarouf, L. Giraud, A. Guermouche, T. Guignon, ***Combining reduction with synchronization barrier on multi-core processors***, CCPE Journal, 2023.
   >> DOI : 10.1002/cpe.7402

Scientific contacts: aboul-karim.mohamed-el-maarouf@ifpen.fr and thomas.guignon@ifpen.fr

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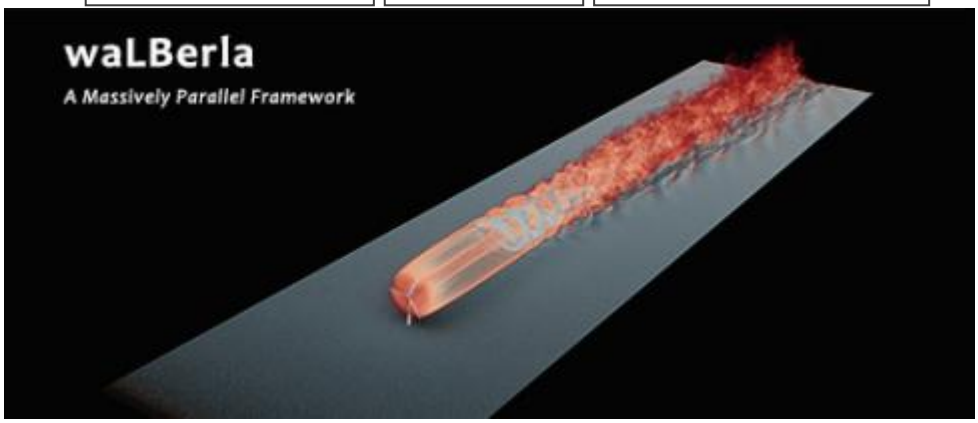

SC8 - “Massively” accelerated windfarm simulation

In the field of wind energy, Large Eddy Simulations (LES) are widely used to gain a better understanding of wind flow within wind farms. On a wind farm scale, they are also used to establish analytical wake models, and are useful for studying the interactions between individual wind turbines as well as with the atmospheric boundary layer (ABL)...

Fluid mechanics | **Numerical methods and optimization** | **High performance computing**

SC8 - Synchronizing cores rapidly: a matter of efficiency

At a time when the European Union is targeting carbon neutrality by 2050 (i.e., net zero greenhouse gas emissions), global CO_2 emissions from the transport sector, which represent a quarter of the total, are continuing to increase. To overcome this and address the climate emergency, technological improvements and carbon taxes do not appear to be enough. There also needs to be a change in behavior.

The FRAME[1] project relates to the incorporation of environmental considerations in the travel decisions of private individuals and focuses on new, less interventionist approaches as recommended in the literature, such as information and communication policies. The introduction of these "nudges", the direct effect of which remains marginal, can have a significant impact in terms of both raising environmental awareness and complementing more interventionist policies (prices, taxes, regulations, etc.). One of the most well-known types of nudges is the framing effect which seeks to make communication campaigns more effective by associating with them with a suggestion to alter the perception of some aspects of the problem under consideration and influence the decision accordingly. For example, the consequences of a given type of behavior can be presented either in terms of expected gains, by adopting a change, or in terms of losses suffered as a result of not adopting it.

As part of the FRAME project, the effect of attribute valence framing,- *i.e.* a description of the same object (or characteristic) positively or negatively - was tested on individuals' preferences to promote pro-environmental transport behavior *via* a DCE[2] [1], specifically designed for the purpose. Various analyses were conducted to determine whether this type of framing may or may not have an impact in terms of reducing transport-related CO_2 emissions. Easier to implement than traditional levers, such as taxes, nudges like this are not based on the strong assumption that individuals are entirely rational.

The DCE was conducted on a representative sample of the French population (age, gender, occupation: in total, 1,032 people aged between 18 and 75 living in mainland France). A hypothetical scenario was presented to participants, asking them to travel for a private purpose using public transit (domestic haul). The origin and destination of the trip were assigned, and two travel alternatives by means of public transit were proposed (see Table 1).

	Option 1	Option 2
Duration	6h35	3h00
Price	50 €	175 €
Sanitary (One seat gap)	Oui	Non
CO2	39 kg	51 kg

Table 1: Example of choice card

Ten choice cards were presented to each respondent, with various combinations of travel time, cost, sanitary distancing and CO_2 emissions (see. Table 2).

Attribute	Levels			
Price (€)	50	75	125	175
Duration (min)	180	235	305	395
CO2 (kg)	30	39	51	66
Sanitary (One seat gap)	Yes	No	_	_

Table 2: Attribute levels proposed in choice cards.

The main framing effects studied were the gains and losses of two distinct attributes, namely travel time and CO_2 emissions.

Respondents were asked to make successive choices from the choice cards proposed with a view to having them reveal their preferences for the different attributes. The results were obtained using dedicated econometric and statistical methods associated with discrete choice models (see. [2] for more details). The coherence of the attribute coefficients was verified by analyzing their signs[3] and relative values.

Firstly, it emerged from the analysis that respondents focused above all on trying to minimize the price and duration of their trip, with price being twice as important as duration, and then on maximizing the sanitary measures on offer. Even if the CO_2 criterion was ranked last, a negative coefficient has been observed, meaning that in general transit users do care about their emissions and seek to minimize them.

Secondly, results indicated that a loss framing on travel duration or CO_2 emissions was significant and increased the weight of the framed attribute in the individual's decision. On the contrary, this effect was not observed for gain framing. The loss framing effect is larger when applied to CO2 than to duration, which is a more familiar attribute.

In terms of public policies, two aspects emerge from this research. Firstly, we demonstrated that a loss framing on CO_2 emissions significantly increases the respondents' choice of pro-environmental behavior, while a loss framing on duration increases the average preference for shorter trip duration; gain framing has no significant effect. This result needs further confirmation but, by providing a better understanding of travelers' choice priorities, it could serve as a basis for the design of more appropriate pro-environmental policies. Secondly, we showed that the effect of loss framing was greater for CO_2 than for duration. One possible explanation for this finding is that framing on a more distant or complex attribute (e.g. kg of CO_2 emissions) has a greater effect than framing on an already well-known and typical attribute (e.g. duration). If so, it would be beneficial to find a way to communicate on CO_2 emissions with a more understandable unit of measurement.

[1]- Project financed by ADEME (2021 - 2024): cadrage de l'inFoRmAtion pour la promotion d'une Mobilité durablE (framing of information for the promotion of sustainable mobility) In partnership with Gustave Eiffel University, Nantes University and Rennes University.
[2]- Discrete Choice Experiment
[3]- Relevance and statistical significance.

References:

1. Collet C., Gastineau P., Chèze B., Mahieu P-A., Martinez F. (2023), ***Combining economics and psychology: Does CO_2 framing strengthen pro-environmental behaviors ?***, Ecological Economics, Volume 214.
   >> https://doi.org/10.1016/j.ecolecon.2023.107984

2. Chèze, B., Collet, C., Paris, A. (2021), ***Estimating discrete choice experiments: theoretical Fundamentals***,
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Scientific contact: Benoît Chèze

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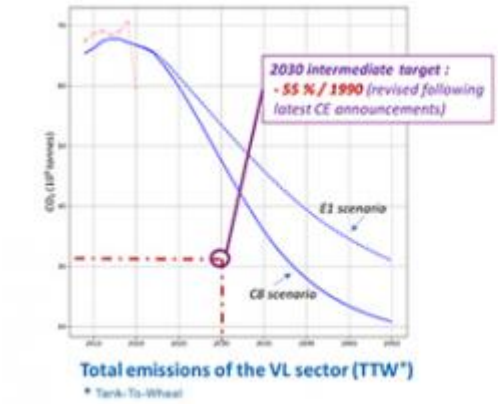
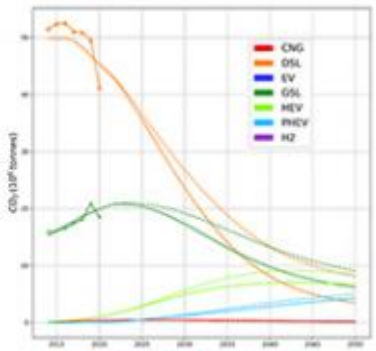


Total emissions of the VL sector (TTW*)

* Tank-To-Wheel



Contribution by technology

SC9 - New resources for the prospective analysis of french road transport

Cutting CO2 emissions from road vehicles is essential and necessary to reduce long-term greenhouse gas (GHG) emissions in France. The transport sector is still responsible for more than 30% of national emissions, making it the sector with the highest level of emissions. The development of new low-carbon powertrains may also result in an improvement in air quality and help reduce our reliance on imported fossil fuels.

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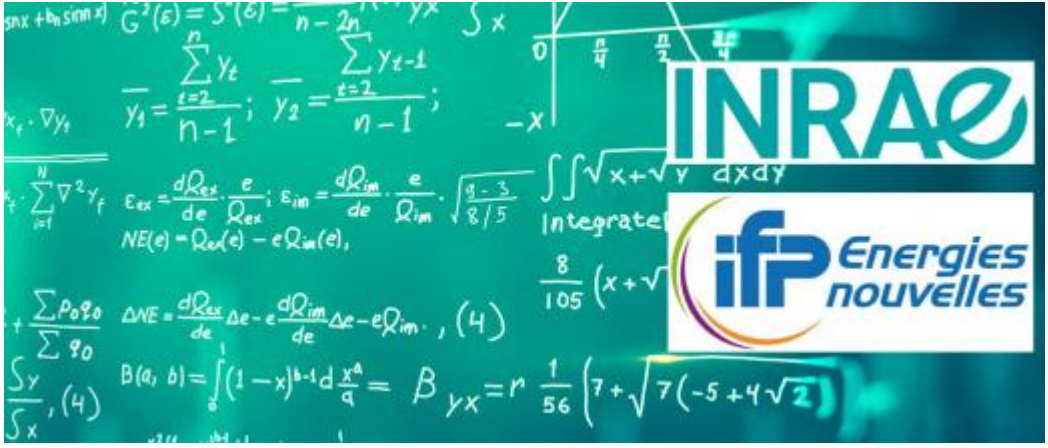

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