Science @ifpen
Issue 51 - April 2023

Written on 10 May 2023

15 minutes of reading

News

Fundamental Research

Hélène Olivier-Bourbigou
Coordinator of IFPEN fundamental research

IFPEN is committed to supporting the energy, ecological and digital transition in order to achieve the ambitious but crucial goal of carbon neutrality by 2050.

I am convinced that our **fundamental research**, organized around nine scientific challenges (SC) and in synergy with applied issues, is pivotal to the emergence of **innovative solutions**.

In this issue you will find articles covering a specific aspect of each of these challenges.

This selection gives me an opportunity to highlight the extent to which the structure we have in place promotes cross-functionality and interdisciplinary approaches with:

- **The emergence of new topics associated with the transitions.** Energy with the behaviour of batteries (SC1 and SC6) and wind power (windfarm simulation SC8). Ecological with the vulnerability of peatlands (SC5) and environmental economics (SC9). Digital with the use of advanced approaches (SC2, SC3, SC7) and deep learning for innovation in the field of materials (SC4);

- **Adjacencies with our more long-standing themes.** The research described in the SC1 article draws on our expertise from IC engine studies. The research described in the SC2 article is inspired by an approach previously employed in the field of hydrocarbons. The hydrological study described in the SC5 article is based on DionisosFlow® basin modeling software;

- **The ability to bridge disciplines.** Use of new numerical approaches to characterize phenomena of molecular adsorption and transport in complex media (SC3 article). Use of molecular modeling to analyze degradation phenomena in electrochemical batteries (SC6 article). Combining Lattice-Boltzmann methods with massively parallel computing via GPU (SC8 article) for accelerated real-time simulation of whole windfarms;

- **Scientific cooperation and pooling of skills.** This research is conducted with national and international academic partners (see SC2 and SC8 articles), research bodies (SC5 article), industrial players (SC4 article) and ADEME (SC9 article).

Enjoy your reading !

Hélène Olivier-Bourbigou

LES BRÈVES

The electrification of mobility is a major transformation aimed at reducing greenhouse gas and pollutant emissions by the transport sector. In this context, the Li-ion battery is currently the technology employed by all car manufacturers to provide the energy storage required for the roll-out of electric vehicles.

However, Li-ion batteries can experience incidents with dramatic consequences, associated with a phenomenon known as thermal runaway. This may be the result of abnormal operating conditions: excessive temperature, mechanical deformation, overcharging, internal short circuit. This thermal runaway is characterized by violent combustion that is difficult to control and produces toxic gas emissions. Today, this is a core safety issue that has a significant impact on battery design and control strategies.

Numerical approaches developed over the past 10 years by IFPEN [1] are used to model and simulate battery behavior during thermal runaway. Nevertheless, the models developed depend on reliable experimental data in order to obtain an understanding and detailed quantitative description of the phenomenon.

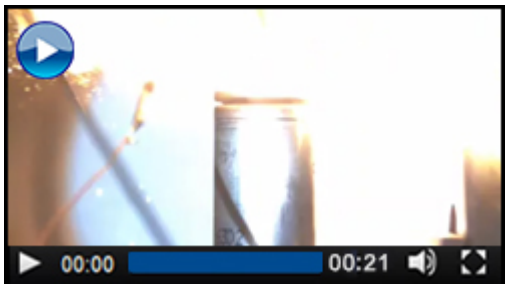
It is for this reason that a new thermal runaway characterization system was developed: it operates in an optically accessible chamber and involves high-speed cameras, pressure and temperature sensors and gas analysis systems. The protocol developed makes it possible to subject a cell (unitary component of the battery) to controlled abuse conditions and combine the different types of available measurements.

The results obtained so far have made it possible to identify the four successive phases leading to the thermal runaway phenomenon [2]:

1. increase in battery temperature associated with internal degradation reactions;
2. voltage decrease in battery terminals;
3. ejection of a liquid and gas mixture via the cell’s safety valve (venting);
4. actual thermal runaway: strong exothermic reactions leading to the appearance of flames coming out of the battery.

In addition, the high-speed color video enables a qualitative understanding of these different phases and the timescale involved. In particular, the observation of a two-phase jet during venting (phase 3) reveals the role of the gas formed inside the cell: this gas is responsible for the expulsion of a significant part of the liquid/solid phase present in the battery. During the last phase, the images acquired provide indications concerning combustion initiation: it seems to occur outside the defective cell due to incandescent particles expelled by it.

Venting phase



Thermal runaway

This system and the associated protocol will be used to acquire the data required to produce numerical models that are both predictive and more precise. In particular, PhD research* underway at IFPEN is aimed at developing a quantitative analysis methodology for the gases emitted and obtaining a detailed understanding of the combustion initiation mechanism.

* Thesis title: *Development d'un protocole de characterization du phénomène d'emballement IC des Li-ion batteries* [*Development of a characterization protocol for the thermal runaway phenomenon in Li-ion batteries*].

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1. Sara Abada, Martin Petit, Amandine Lecocq, Guy Marlair, Valérie Sauvant-Moynot et François Huet, ***Combined experimental and modeling approaches of the thermal runaway of fresh and aged lithium-ion batteries***, Journal of Power Sources, Elsevier, 2018, 399, pp.264-273. >> https://doi.org/10.1016/j.jpowsour.2018.07.094

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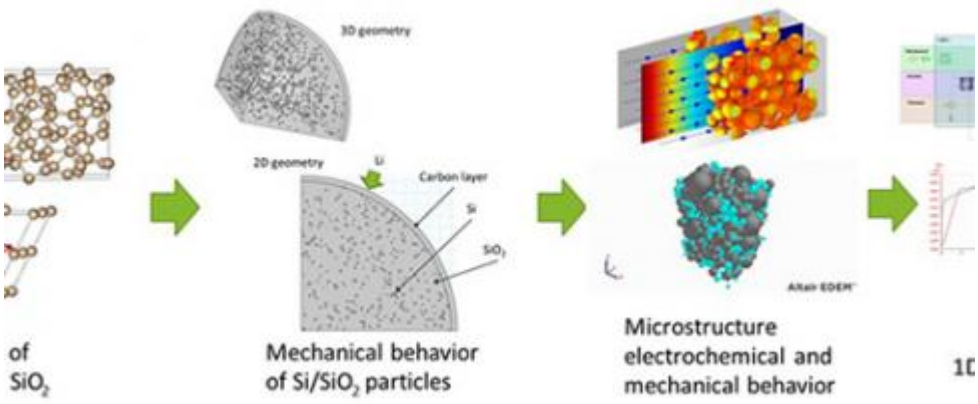
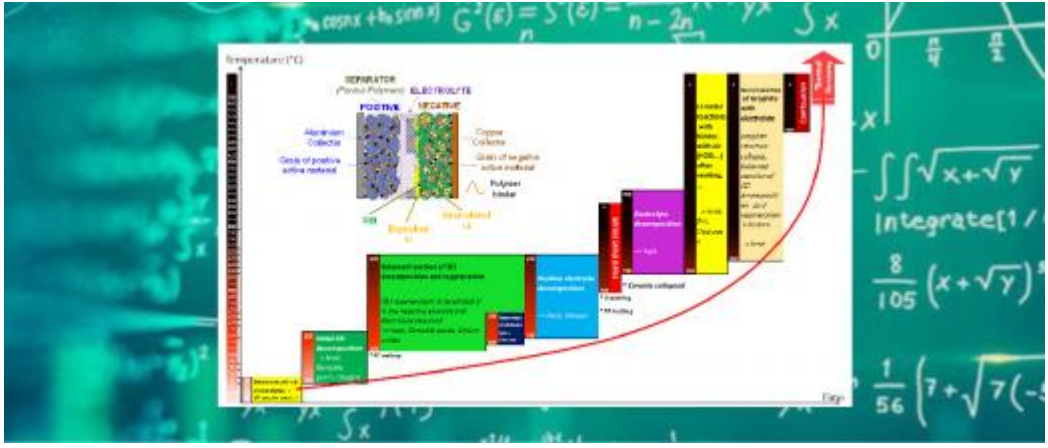


Battery behavior: a complexity best taken into account by modeling

For around fifteen years now, IFPEN has been focusing on modeling conventional batteries to represent their nominal operation (electric and thermal behavior during normal operation), throughout their lifetime (...) and in the event of thermal runaway (failure, improper use)...

Batteries

Electrochemistry and corrosion **Systems modeling and simulation**



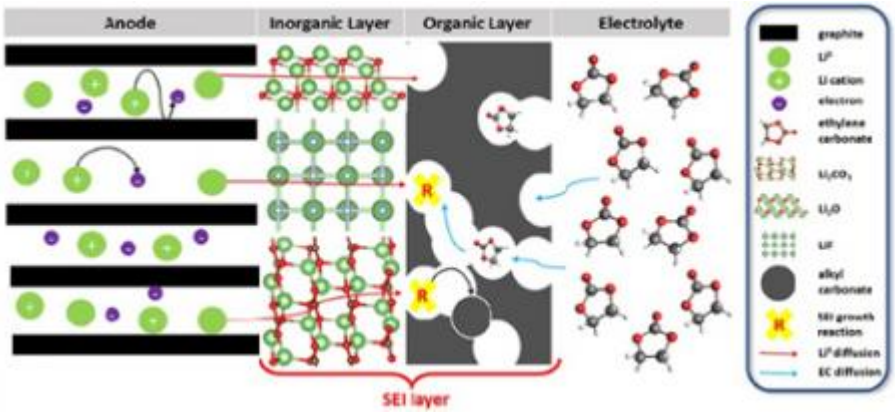
Fundamental Research

News July 2021

Modeling to improve the safety of lithium-ion batteries

Batteries

Physical chemistry | Electrochemistry and corrosion | Engineering sciences



SC6 - How to better control loss of lithium battery capacity

Everybody knows that lithium-ion batteries, used in cell phones, computers, etc., gradually lose capacity and eventually fail. This loss of capacity is primarily due to a layer known as the SEI, which forms between one of the battery's electrodes and the electrolyte (see Figure). This layer already appears after the first battery charge/discharge cycle, and grows over time, consuming lithium ions. The process is irreversible and therefore detrimental to battery capacitye...

Batteries

Thermodynamics/Molecular modeling | Electrochemistry and corrosion

SC1 - New experimental set up to study battery safety

The dehydration of bio-based alcohols to form alkenes is a key reaction to obtain major chemical intermediates from biomass. It is efficiently catalyzed by zeolites presenting Brønsted[1] acid sites and a crucial challenge is the control of its selectivity. Starting, for example, with a branched alcohol like isobutanol, the dehydration reaction does not only produce isobutene (branched isomer from the butene family), as expected by conservation of the molecule's carbon skeleton (Figure 1 (a)). Therefore, despite operating conditions in which isobutene should not be isomerized into linear alkenes, this reaction also produces linear butenes.

Linear alkenes are highly sought-after intermediates in the chemicals industry. As a result, it is important to identify the mechanisms making it possible to produce them via the conversion of isobutanol since this knowledge is required to control the selectivity of these reactions.

Conducted in collaboration with Comenius University of Bratislava (team led by T. Bu?ko), research focusing on the mechanisms behind the conversion of isobutanol to alkenes used density functional theory (DFT), based on a model zeolite, of the chabazite type. As a result, important transition states were identified, as well as corresponding free energy barriers [1]

This approach made it possible to identify two major families of new mechanisms capable of explaining the formation of linear alkenes from isobutanol:

1. a sequential mechanism of isomerization of isobutanol into other butanols, particularly 2-butanol (Figure 1 (b)), a linear alcohol that can then be dehydrated into linear alkenes,
2. a synchronous isobutanol isomerization and dehydration mechanism making it possible to form linear alkenes directly.

The analysis of free energy profiles made it possible to find the most favorable paths. In typical dehydration conditions, the DFT calculation suggests that the first mechanism represents the fastest reaction route.

These results explain the reaction products observed and pave the way for selectivity control for linear alkene production.

The precise quantification of rate constants is now necessary in order to predict the activity and selectivity of such a catalyst, via a kinetic model. This quantification requires an investigation of these new mechanisms through *ab initio* molecular dynamics, in line with previous research relating to alkene isomerization and cracking.

In addition, the influence of the nature of the zeolite still requires analysis. That is because while the simulation was based on chabazite, it is known experimentally that ferrierite zeolite presents a high degree of linear alkene selectivity. The role of the external surface of zeolite crystallites is thus questioned [2, 3] and research is being conducted within the context of the ongoing collaboration with Bratislava University. This role is being studied *via* the modeling of the reactivity of the external ferrierite surfaces. A visiting PhD student from Bratislava University spent the last quarter of 2022 at IFPEN focusing on this research.

This study will also be continued within the framework of the MAMABIO project (IFPEN, Ecole des Ponts ParisTech, Lorraine University, Caen University collaboration) within the B-BEST Priority

Research Program and Infrastructure (PEPR).

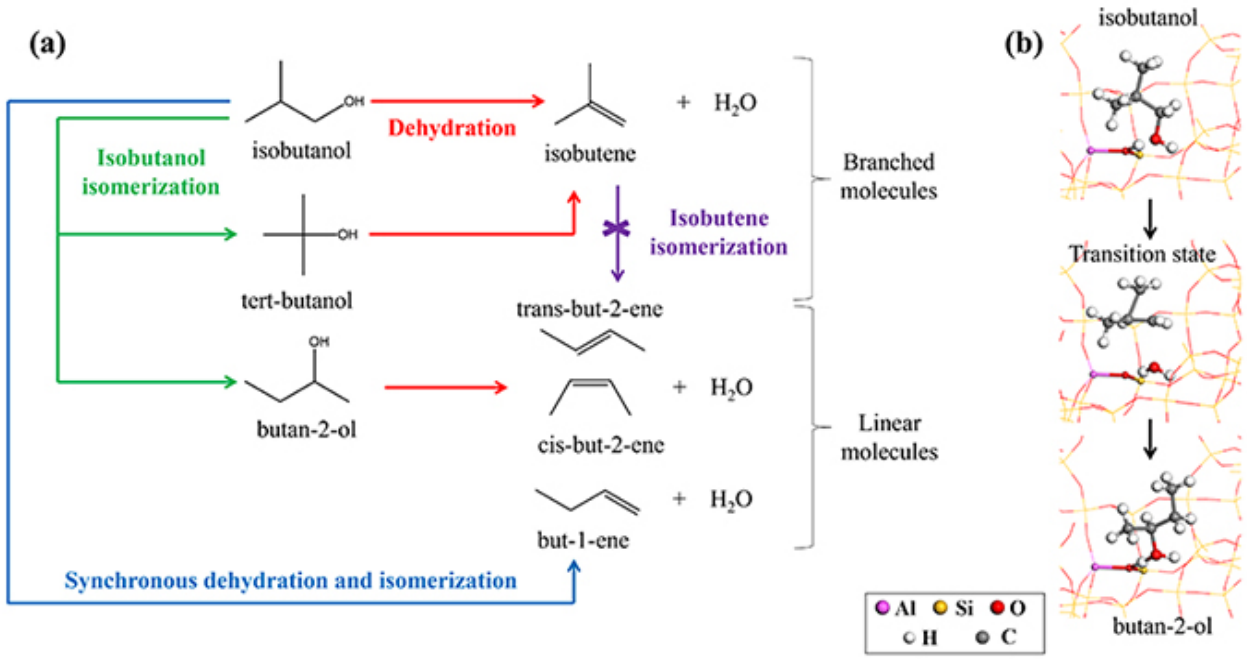


Figure 1: (a) Reaction scheme for the formation of branched (isobutene) and linear (but-1-ene and but-2-enes) alkenes,
(b) structures calculated with DFT concerning the isobutanol isomerization to 2-butanol reaction.

[1]- “Proton donor”-type acid

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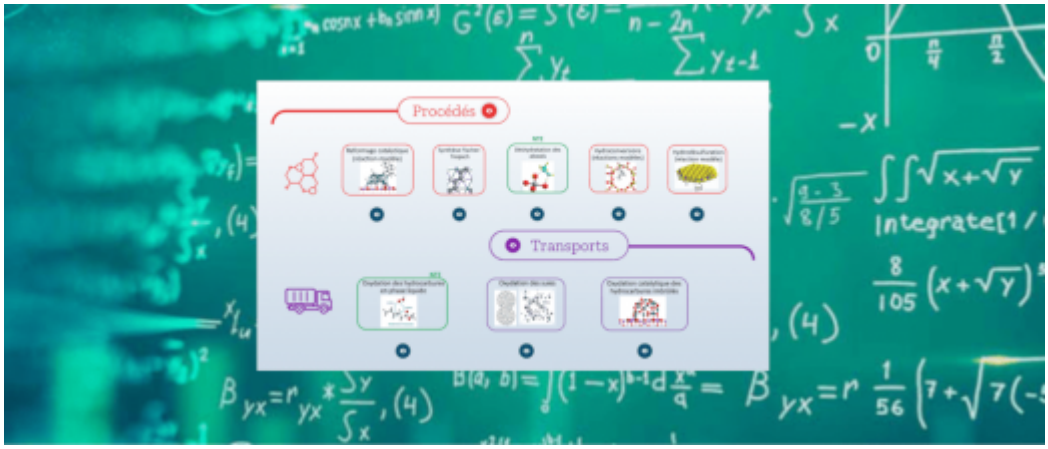
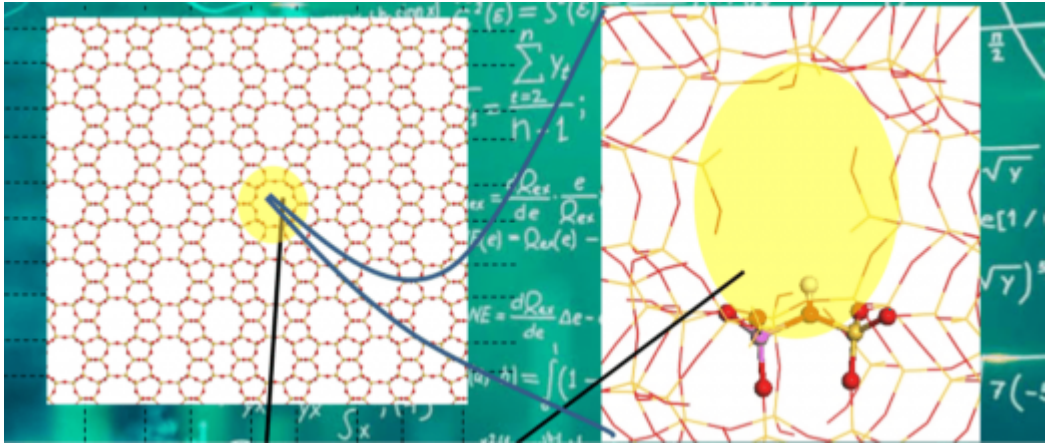


Fundamental Research

News April 2021

Predicting performance from atomic through to reactor scales to improve industrial processes

Chemical sciences | Catalysis and reaction kinetics | Biosciences and biotechnologies | Biocatalysis

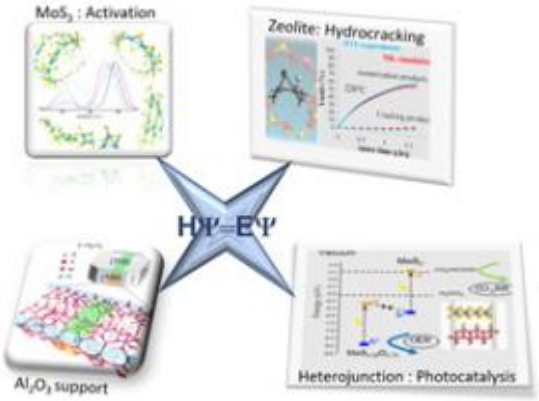


Fundamental Research

News November 2020

Shedding light on the external surface of zeolites by quantum calculation

Chemical sciences | Catalysis and reaction kinetics | Physical Sciences | ce, interface and materials science



Molecular modelling: a key tool for current and future heterogeneous catalysis

Chemical theory at quantum level (density functional theory or DFT) is an essential tool in rationalising the reaction mechanisms involved in the preparation of catalysts, as well as in their use, thanks to the optimisation of their activity [1,2]. IFPEN has carried out a number of projects aiming to shed light on these catalysts, which are of particular interest to industrial processes...

Chemical sciences | Catalysis and reaction kinetics | Theoretical chemistry

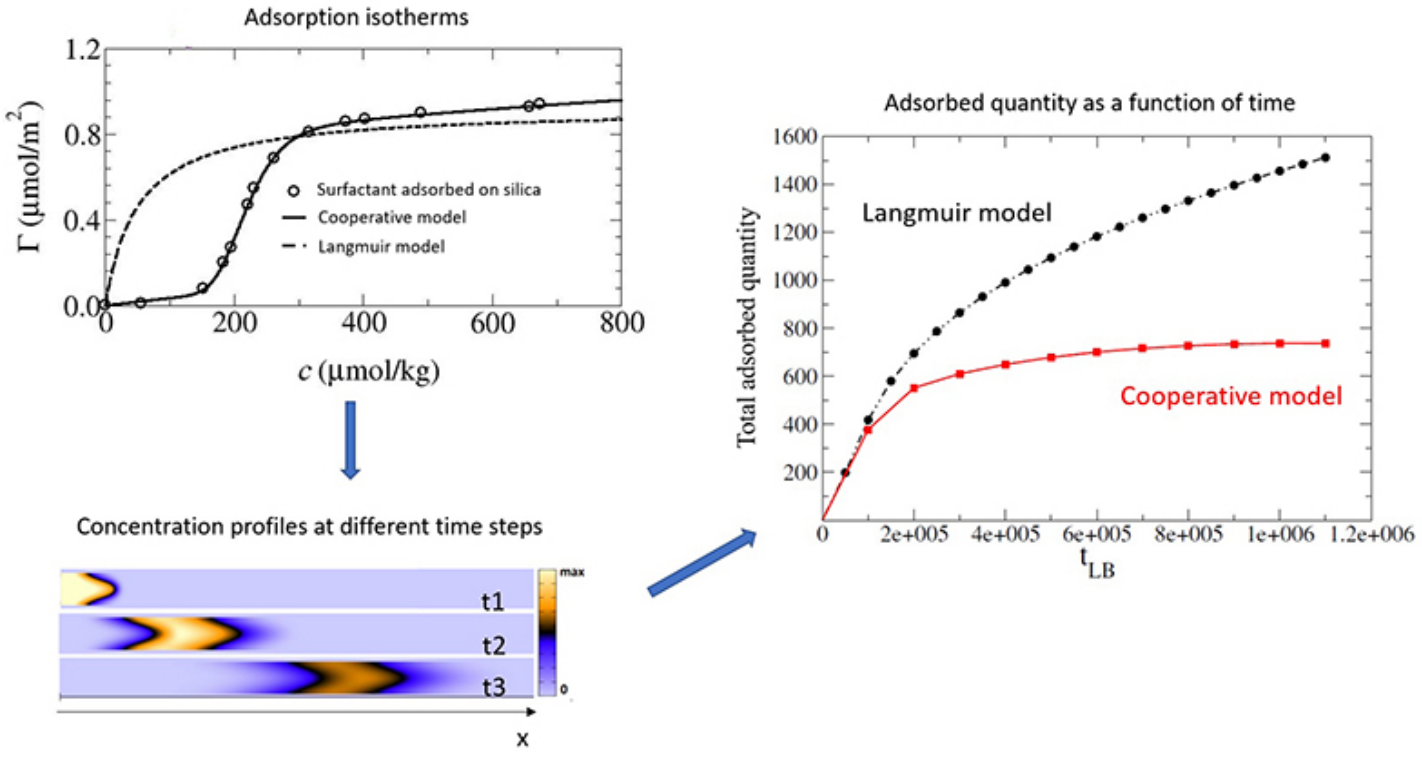
SC2 - Quantum calculation reveals key mechanisms for bio-based chemistry

Transport of molecules within porous structures that adsorb on the surfaces plays an important role in numerous contexts and very different applications. These include pollutant transport in soils, industrial catalytic conversion and purification processes, and chromatographic techniques. In all these situations, adsorption effects are known to strongly influence the circulation and transport of the fluids moving through confined geometries.

In view of this adsorption effect, particular attention must be paid to the behavior of complex molecules, such as surfactants, for example. These molecules are characterized by physico-chemical behavior at the fluid-solid interface that -most of the time - cannot be described using a classical adsorption model (for example the Langmuir model, which is a single-layer adsorption model). Often, since their behavior at the interface is characterized by aggregate formation, their adsorption may be dominated by cooperative effects and this interfacial behavior may have a specific and not insignificant influence on their transport properties. A better understanding of the transport of this type of molecule compared to conventional molecules is therefore necessary.

Within the context of PhD research* conducted in partnership with the CNRS and Grenoble University, we looked at adsorption kinetics and surfactant transport in combination *via* a generalized Lattice-Boltzmann approach, incorporating this adsorption effect [1]. To do so, we simulated the transport of molecules between two parallel planes, with adsorption isotherms from experimental data (anionic surfactant adsorbed on silica: see figure 1.a). The simulations were conducted on the basis of two different adsorption hypotheses in terms of thermodynamics: firstly, a conventional Langmuir model and, secondly, a surfactant adsorption model developed by us to include cooperative effects [2].

We showed that the total expected quantity adsorbed with the Langmuir model is far greater than that estimated by the new thermodynamic model, which accurately reproduces experimental data [3]. In addition, with the Langmuir model, this quantity increases more significantly over time (figure 1.b) due to its thermodynamics, which cannot correctly describe the specific interface behavior of complex molecules.



These results show that in transport models, obtaining physically coherent adsorption/transport behavior requires the development and inclusion of modeling specific to each type of adsorption, based on experimental data. This is particularly true for a better prediction of the transport of complex pollutants (nanoplastics, PFAS[1], heavy metals, cosmetic products, etc.), the specific behavior of which in terms of adsorption must be taken into account by the modeling.

Future research will consist in examining transport and adsorption in combination in geometries that are representative of more complex structures, such as porous media. The challenge here relates to the heterogeneity of the porous medium, resulting in a specific velocity field, marked by significant disparities.

[1]- Perfluoroalkyl substances

* Thesis by Zaineb Zaafouri: ***Modeling surfactant adsorption and transport in porous media: influence of adsorption thermodynamics and kinetics***.
>> https://theses.hal.science/tel-03187740

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   >> https://doi.org/10.1016/j.advwatres.2022.104143

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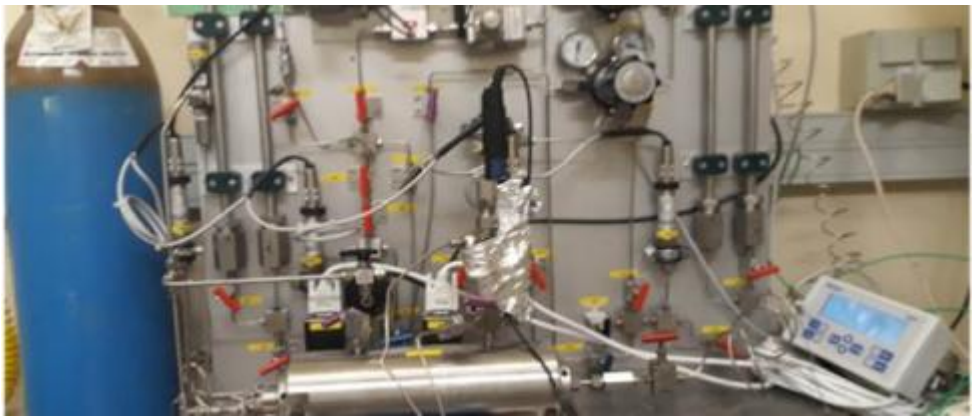

Adsorption, a key factor for geological storage

Low permeability geological layers, already known within the context of oil exploration, are once again becoming a focus of inter

Geosciences | Petrophysics and transfers in porous media | Physical Sciences | Transfer and transport physics | Physical chemistry | Surface, interface and materials science

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

Recherche fondamentale

Actualités January 2018

Mieux comprendre les phénomènes de diffusion au cœur des catalyseurs

Hydrocarbures responsables | Carburants | Pétrochimie

Analyse et caractérisation | Sciences physiques | Physique du transfert et du transport | Chimie physique | Science des surfaces, des interfaces et des matériaux

SC3 - Simulation of the adsorption/transport combination via a generalized lattice-boltzmann approach

Inside porous materials, physico-chemical phenomena such as matter transport, catalytic reactions and capillary effects are strongly influenced by the geometry of the pore networks, i.e., the degree of porosity, the distribution of pore sizes and their connectivity. These characteristics are usually obtained *via* macroscopic models applied to experimental characterization results. Additionally, a reliable estimation of these properties on a smaller scale can come from so-called microscopic approaches, via statistical mechanics.

IFPEN and Saint Gobain Research Provence decided to tackle the problem differently, by exploring a new numerical approach. This approach directly combines realistic numerical modeling of microstructures with a novel simulation framework of gas physisorption from a morphological point of view.

The approach was hinged around three components:

- random models to realistically represent complex microstructures;
- mathematical morphology to reproduce the various physical processes involved in physisorption [1];
- and deep learning to accelerate simulation results [2].

Since the new approach consists in artificially reproducing physical phenomena using mathematical morphology operators, it paves the way for physisorption simulations, with results directly comparable to experimental results. The calculation of these operations can be estimated via deep learning, using convolutional neural networks , leading to a considerable reduction in calculation time.

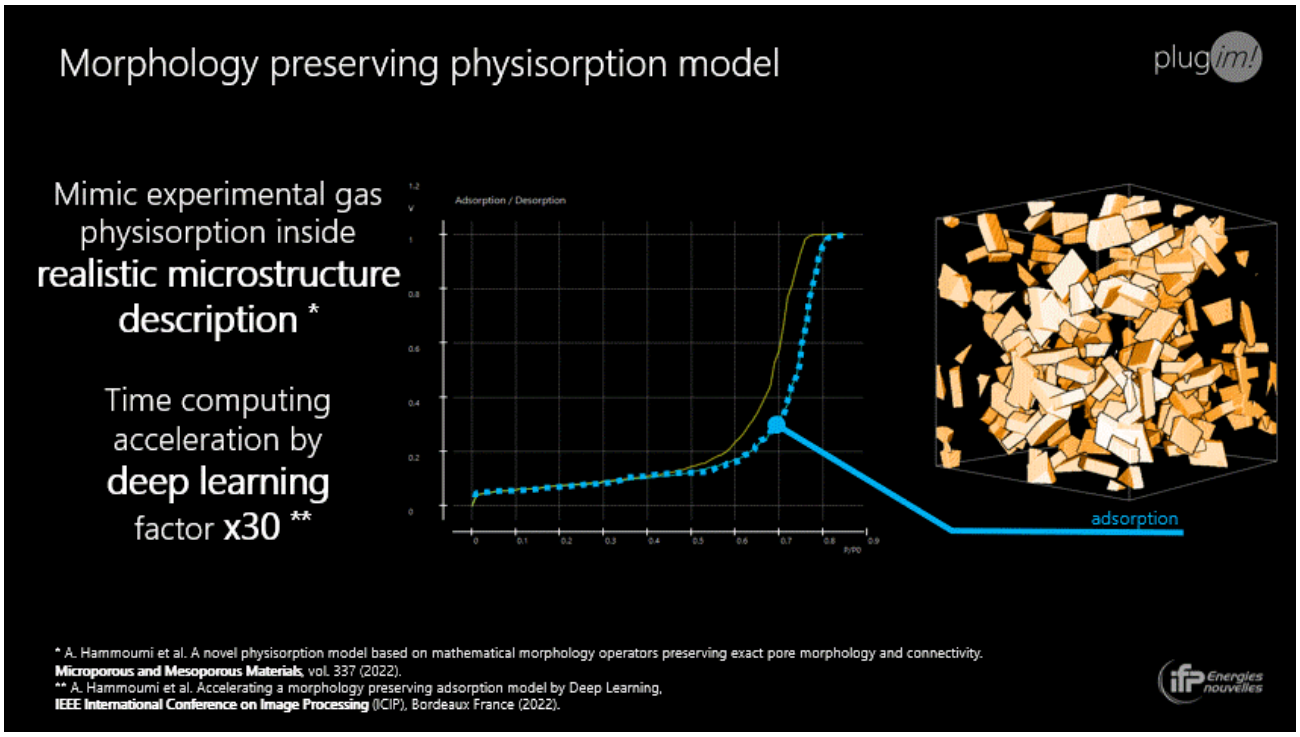

Illustration of an adsorption and desorption simulation using our new numerical approach.

This original methodology was successfully applied to ordered structures such as SBA-15 and KIT-5 aluminas, leading to numerical isotherms close to experimental isotherms (figure). Comparable results were obtained for more complex aluminas, with controlled multi-scale porosity specifically synthesized for this research [3].

Extending the approach to other experimental techniques for the characterization of porous materials is the next step in the continuation of this research, the ultimate objective of which is to obtain innovative materials designed directly on the basis of the targeted usage properties.

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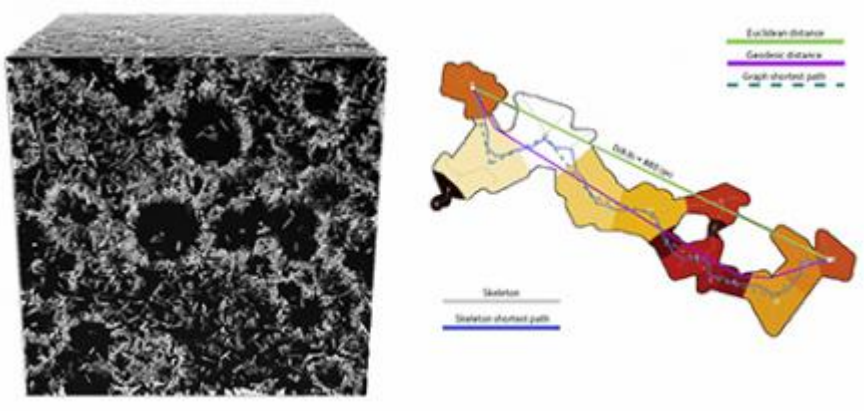
Diffusion in catalysts: an often tortuous path!

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...

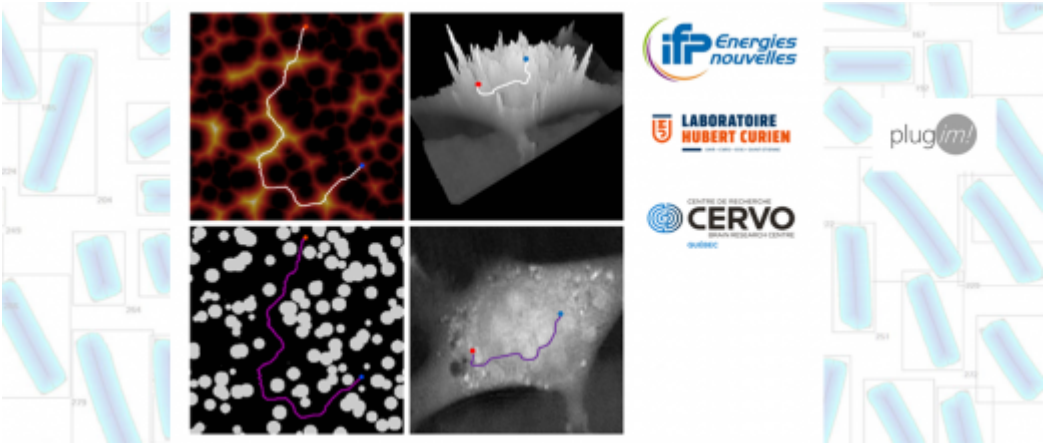
Structural analysis and Imaging | Chemical engineering and process engineering | Systems modeling and simulation



Numerical design based on the analysis of multi-scale porous material microstructures

The design of high-quality porous materials is a major challenge for the energy efficiency of industrial processes in the fields of catalysis and biocatalysis and separation and purification operations. For such applications, these materials derive their properties of interest from their specific microstructure, incorporating a large quantity of empty spaces that are organized and connected on a nanometric scale. IFPEN and Saint Gobain Research Provence (SGRP) joined forces to acquire a tool that will ultimately facilitate the development of porous materials optimized for given usages.

Analysis and characterization | **Structural analysis and Imaging** | **Physical chemistry**
Surface, interface and materials science | **Mathematics and IT** | **Signal processing/Data science**



Fundamental Research

News December 2019

New porous microstructure descriptors based on tortuosity and accessibility

Geosciences | Petrophysics and transfers in porous media | Analysis and characterization | Structural analysis and Imaging | Mathematics and IT | Signal processing/Data science

SC4 - New numerical approach for the characterization of virtual porous materials

Peatlands only occupy 3% of the earth's surface but contain more than 25% of the organic carbon stored in the surface layers of the subsoil. Plant matter accumulates slowly there and undergoes a slow decomposition process under the effect of a water-saturated, oxygen-poor environment. Therefore the peat can still decompose and is particularly vulnerable to environmental changes. Hence, the exposure of these organic carbon stores to the effects of climate change (increase in temperatures, drought, fires) and human activities (drainage and destruction of wet zones) can lead to the release of significant quantities of greenhouse gases.

In order to better understand and characterize these carbon storage/release phenomena, an international team recently turned their attention to the "Cuvette Centrale" peatlands of the Central Congo Basin[1] (figure 1.a). Researchers from CEREGE (European Center for Research and Education in Environmental Geosciences) and MARUM (Center for Marine Environmental Sciences) successfully reproduced the evolution of the regional environment and climate over the course of the past 22,000 years by studying biomarkers (figure 1.b).

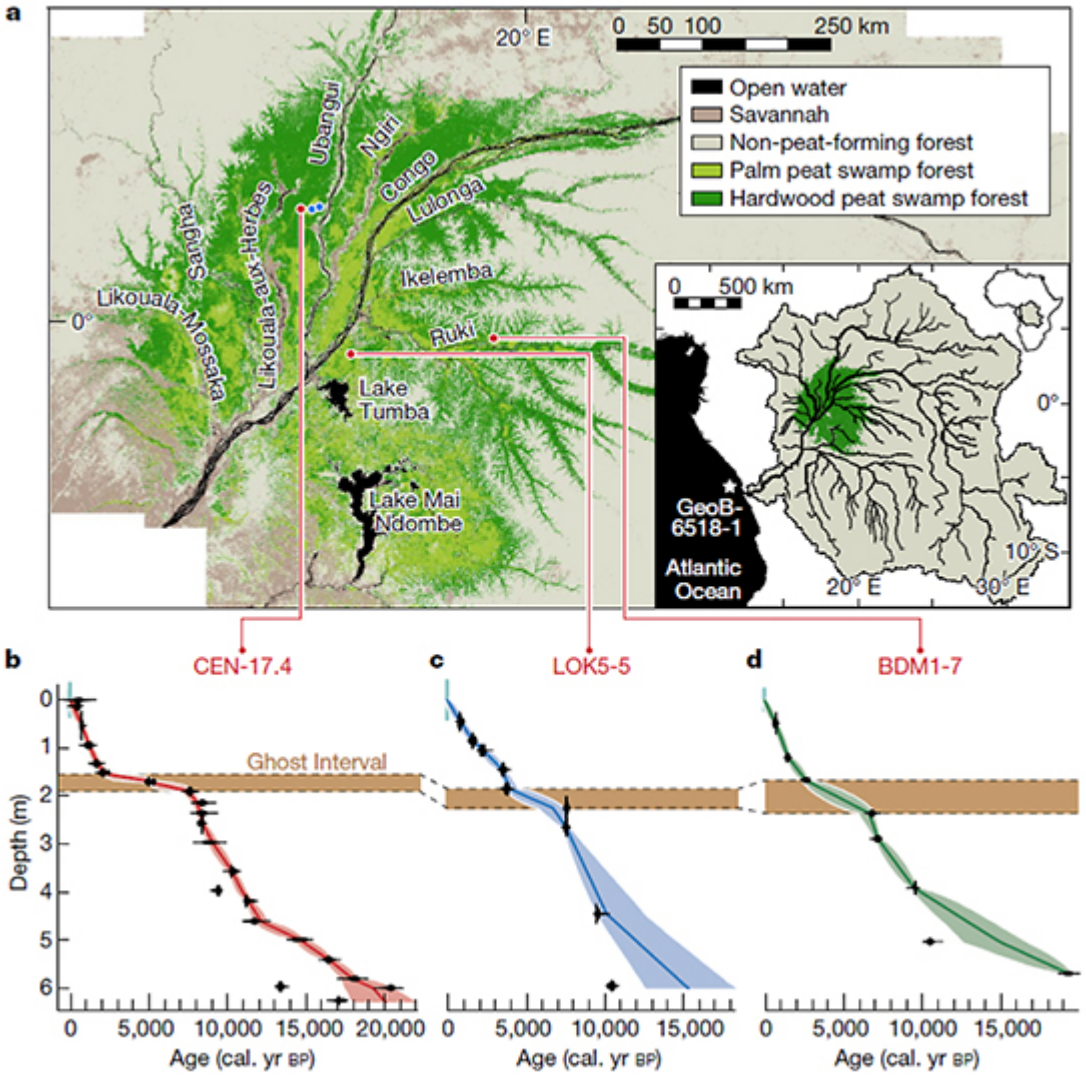


Figure 1: Peatlands of the Central Congo Basin [1]:
a) Map of the Cuvette Centrale showing the spatial distribution of the swamp forests and the location of peat cores;
b) Radiocarbon dating of the peat cores studied.

The break in the modeled age-depth profiles, highlighted by a horizontal brown band, indicates the “Ghost Interval” of very little peat build up. The dotted lines show the stratigraphic correlations.

In addition, researchers from IFPEN, UNIL[2] and the British Geological Survey measured the degree of peat decomposition using Rock-Eval® analyses. The global study, published in *Nature* [1], showed that between 5,000 and 2,000 years BP, the region experienced a drought responsible for the decomposition of several meters of peat, which necessarily led to the emission of considerable quantities of greenhouse gases.

While the hydroclimatic conditions enabling the formation of peat gradually became re-established around 2,000 years ago, this study showed that this peat remained extremely vulnerable to hydroclimatic changes. Such changes, like a variation in rainfall and/or seasonality, may once again cause the release of a quantity of carbon dioxide equivalent to three years of global emissions currently.

In order to avoid the flow of greenhouse gases into the atmosphere, under the effect of a further degradation of this peat, it is necessary to have access to tools to predict the effect of these environmental changes (climate, impact of human activities) on the regional water balance. Topogenic peatlands[3], like those studied, are primarily controlled by the quantity and distribution of rainfall in the catchment area. In order to understand their formation and dynamics over time, it is necessary to describe hydrologic changes on the surface and in the groundwater of the catchment area.

To do so, hydrological and stratigraphic modeling was conducted within the context of the VULCARFATE project [2, 3]. From the map showing the Congo’s topography (figure 2a) and climate data, surface and subsurface water flows (figure 2b) were determined using DionisosFlow® software. This modeling was then combined with sediment transport laws in order to determine the location of certain sedimentary environments (figure 2c).

Concerning peatlands, we thus have a tool that can be used to anticipate the effect of climate change and human activities on their carbon stocks, which could then be used as a basis for better managing their vulnerability.

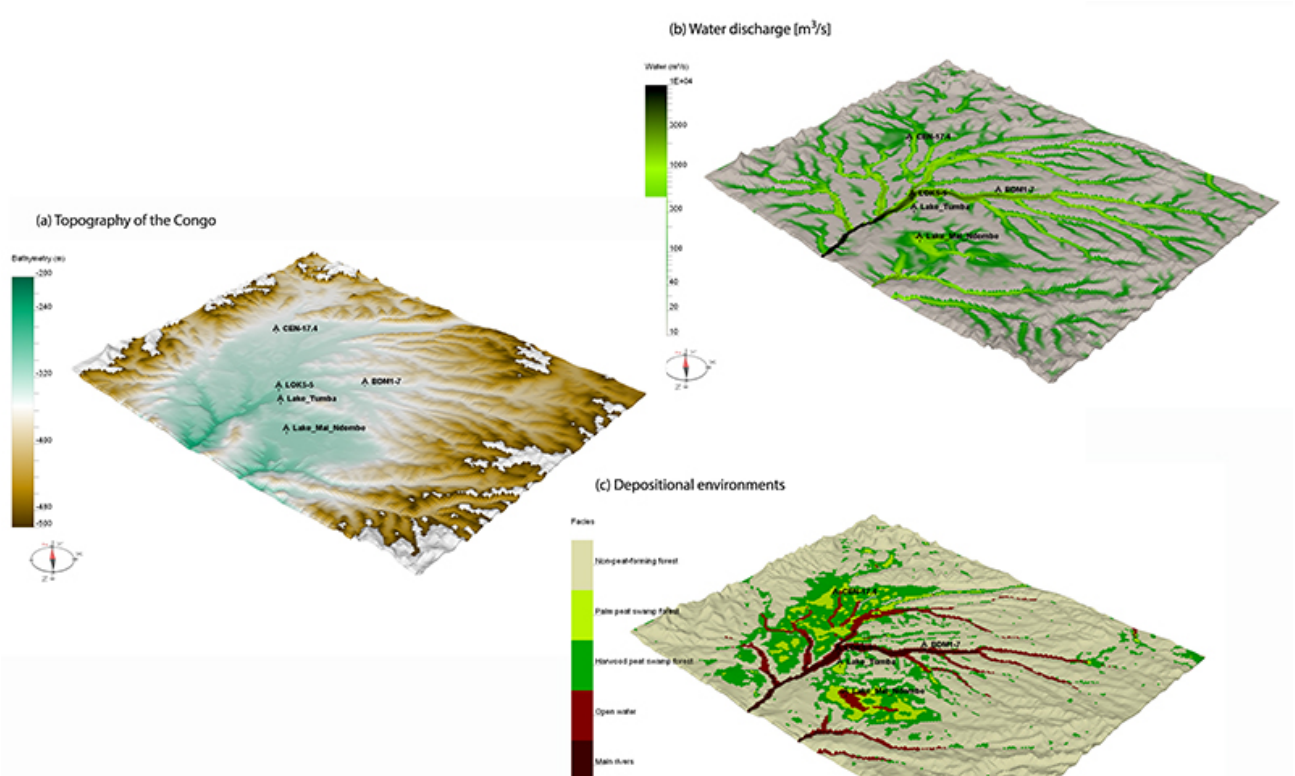


Figure 2: Hydrological and stratigraphic modeling of the “cuvette centrale” of the Congo using DionisosFlow®.
a) map of current topography;
b) simulation of surface water flow;
c) simulation of the distribution of different types of swamp forests and peat.

[1]- Extending over 16.7 million hectares and representing 28% of the carbon of tropical peatlands.
[2]- Lausanne University.
[3]- Peatland in which water is trapped in depressions, called “cuvettes”.

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   >> https://vulcar-fate.obs-mip.fr/en/homepage

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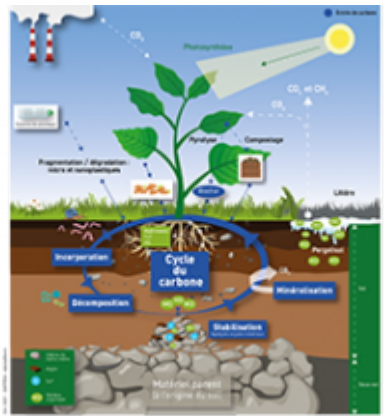

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One way to decrease the amount of atmospheric CO2 is to reduce greenhouse gas emissions of fossil origin, but it is also possible to increase the quantities of carbon stored in the soil. (...) In the current context of climate change, understanding 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...

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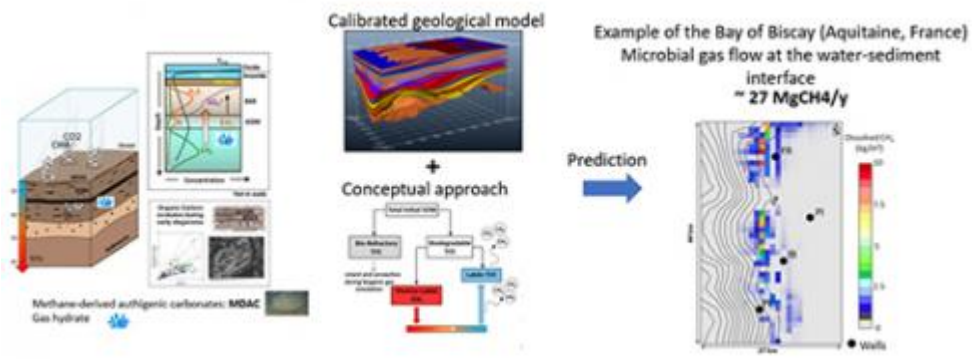

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Just like carbon dioxide (CO2), but with a much higher GWPa, methane CH4) is a gas which, according to the IEAb, is responsible for around 30% of the increase in global temperatures since the industrial revolution...

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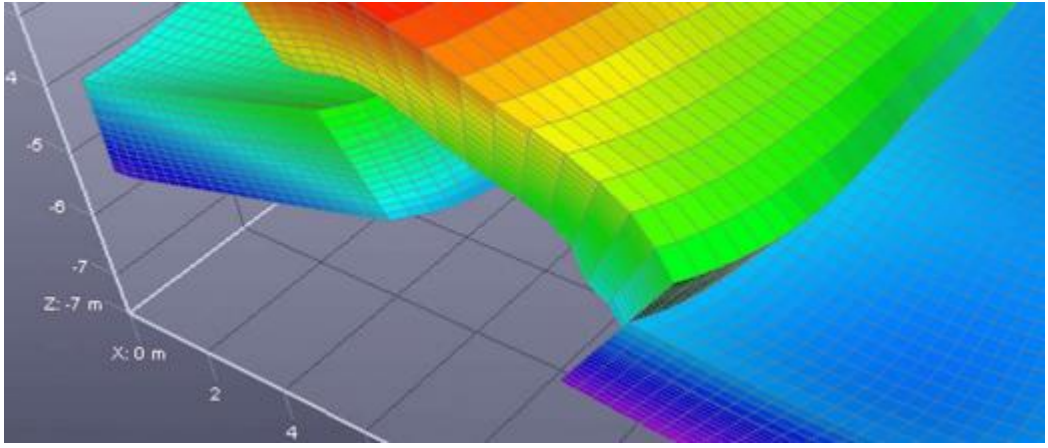

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Géosciences | Pétrophysique et transferts en milieux poreux | Sciences physiques | Mathématiques et informatique | Maillage et visualisation

SC5 - Vulnerability of peatlands to climate change

Everybody knows that lithium-ion batteries, used in cell phones, computers, etc., gradually lose capacity and eventually fail. This loss of capacity is primarily due to a layer known as the SEI[1], which forms between one of the battery's electrodes and the electrolyte (see Figure). This layer already appears after the first battery charge/discharge cycle, and grows over time, consuming lithium ions. The process is irreversible and therefore detrimental to battery capacity [1].

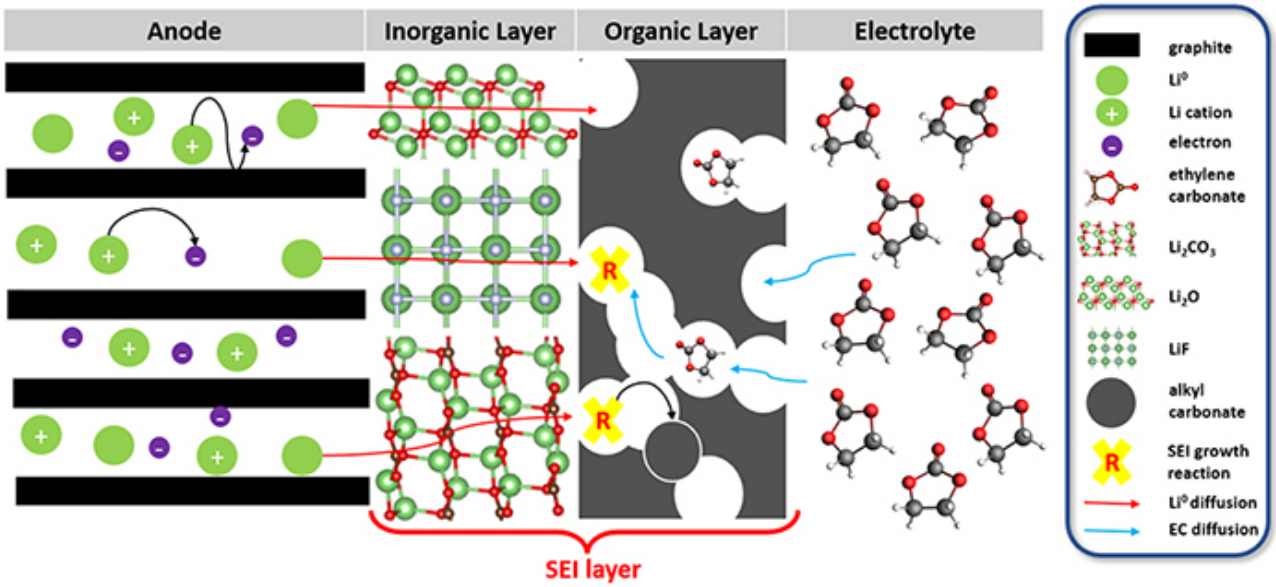

Figure: Illustration of the graphite/lithium anode, inorganic and organic layers forming the SEI layer and the electrolyte

While the chemical composition of this SEI layer can be determined through experimental analysis, other aspects concerning its formation, such as the thermodynamic conditions of its appearance and its growth kinetics, are more advantageously studied using theoretical approaches, such as molecular modeling. Methods based on quantum chemistry (QM) are well adapted to this need, since they explicitly take into account electrons, which play a key role in the solvent (electrolyte component) reduction reactions at the negative electrode interface, and it is this set of reactions that initiates and fuels the formation of the SEI layer.

However, QM based methods require too many IT resources to be applied to a system the size of a battery. A multi-scale approach therefore appears to be a suitable alternative, enabling a detailed description of the chemical reactions involved in the solvent degradation over periods of time ranging from the picosecond to a second (or more). The QM approach can then be extended by use of the Kinetic Monte Carlo (kMC[2]) simulations.

The first stage of this PhD research involved establishing a database of the chemical reactions involved, with their reaction energies and their activation energies [2], measurements that have a direct influence on the reaction rate. These energies were calculated with methods based on DFT[3].

The kMC simulations subsequently conducted showed that salts such as Li_2CO_3 ou Li_2O, resulting from electrolyte reduction, played a significant role in the formation of the SEI [2]. These salts promoted the appearance of various organic degradation species, whose presence corroborated analytical observations and result in a multi-layered SEI structure.

kMC simulations were also used to predict the loss of battery capacity as a function of the composition of the SEI layer initially formed (Figure 2). It turns out that in the absence of Li_2CO_3 ou Li_2O, this capacity reduction is non-linear, and that it is slower in their presence. These results tally with other experimental and theoretical studies [3] and encourage further research taking into account the appearance of other salts resulting from the degradation reactions, such as LiF. In the future, the aim is to expand the reference library of degradation reactions that can take place in the presence of these salts, and to use methods that require fewer CPU resources than DFT.

[1]- Solid Electrolyte Interphase.
[2]- Method used to simulate the behavior of systems evolving as a function of a master equation, using kinetic data relating to elementary chemical reactions.
[3]- Density Functional Theory.

* Thesis title: ***Gaining a better understanding of the formation and growth of the Solid Electrolyte Interphase in Li-ion batteries via a molecular modeling approach.***

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News December 2021

EleTher JIP: an industrial community to better understand thermodynamic electrolyte models

Fundamental Research

News March 2021

Molecular simulation methods contribute to the understanding of the early stages of zeolite synthesis

Chemical sciences | Catalysis and reaction kinetics | Physical Sciences | Thermodynamics/Molecular modeling

SC6 - How to better control loss of lithium battery capacity

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[1] , and developed a dynamic tool for regulating speed limits zone by zone.

A first step in the study consisted in establishing, for different speed limits, the effect of traffic congestion on fuel overconsumption, by coupling:

- an open-access traffic simulator to reproduce vehicle dynamics at various levels of congestion;
- and a model developed by IFPEN to characterize the operation of an engine and estimate the consumption and pollutant emissions of a vehicle, with a high level of precision, depending on a variety of factors: powertrain technologies, the road conditions, driving style and network configuration, etc. [1, 2].

Figure 1 shows the average fuel consumption of vehicles at steady speeds for various traffic densities, for speed limits of 20 km/h and 50 km/h. It is obtained by simulating road traffic at steady speeds (case of a ringroad).
Where traffic density is low, a speed limit of 50 km/h is more energy efficient due to the more favorable engine speed, as long as traffic remains free-flowing. Conversely, above a certain density, a speed limit of 20 km/h becomes less energy-consuming. That is because the “accordion effect” kicks in later, and the associated accelerations, which are largely to blame for overconsumption, are more moderate..

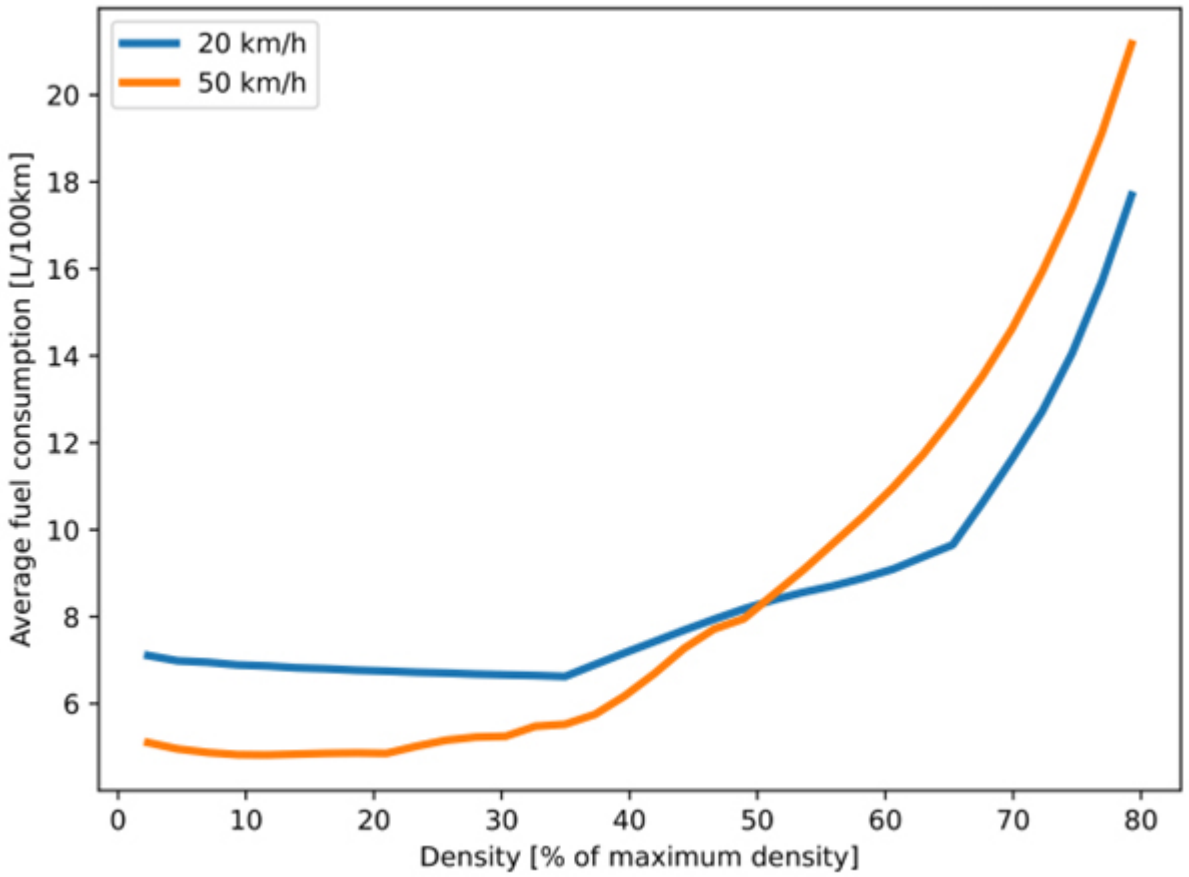

Figure 1: Average fuel consumption as a function of traffic density for two speed limits.

Following these observations, the idea for a regulator emerged, in order to adjust the speed limits of an urban zone in real time [3, 4] and thus reduce overall traffic fuel consumption.

The impact of this regulation was evaluated via numerical simulation on a road network covering a distance of around 28 km, comprising an urban area and a suburban area, at rush hour. Its effect was compared to that of two other scenarios:

- a reference scenario: with constant speed limit zones;
- and a scenario known as "access control": with regulated green light timeframes.

The study shows that regulating speed limits makes it possible to:

- reduce fuel consumption (figure 2.a);
- reduce pollutant emissions (figure 2.b);
- improve traffic flow, increasing the distance covered (figure 2.c).

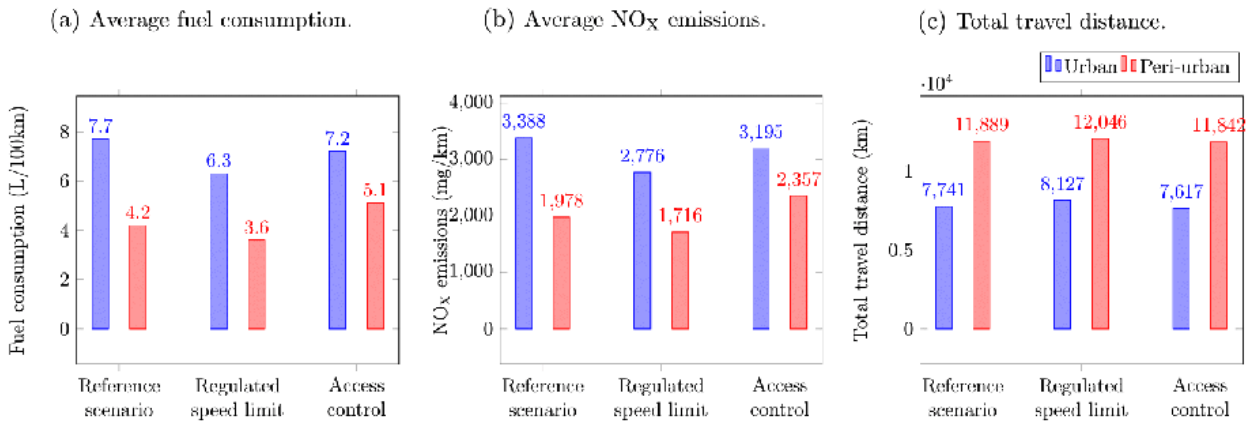

Figure 2: Fuel consumption, NOx emissions and traffic flow for each of the three control strategies.

In practice, the regulator slightly lowers the speed limits of road sections leading to zones that are about to become congested. This preemptive action makes it possible to reduce congestion as well as the resulting overconsumption and excessive emissions. It should also be noted that traffic flow is improved as a result.

Furthermore, it turns out that this method is more advantageous than traffic light control, both in terms of fuel efficiency and traffic flow, due to more moderate acceleration and less frequent stops [5].

To realize its full potential, speed limit regulation will need to be evaluated on more complex urban road networks and potentially combined with practices such as eco-driving.

[1]- Grenoble Images Parole Signal Automatique.
[2]- SUMO (Simulation of Urban Mobility) software.

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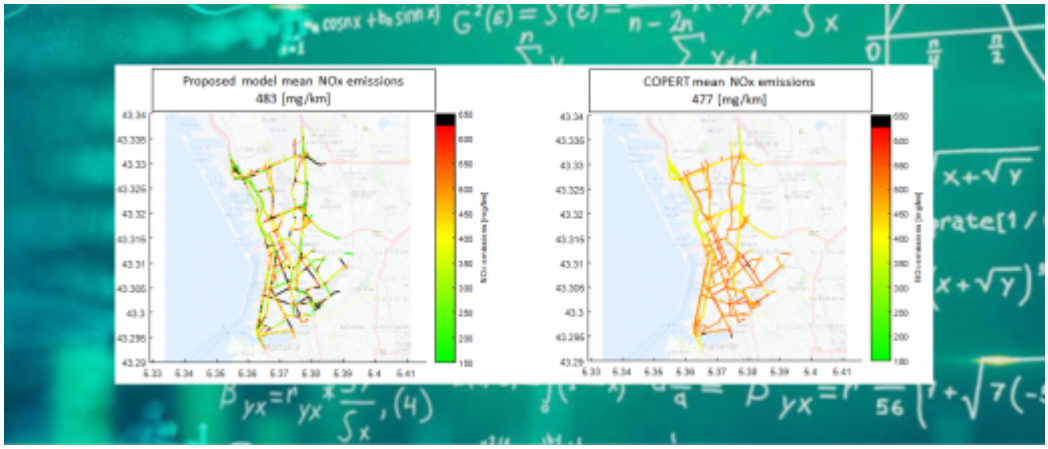

Fundamental Research

News March 2021

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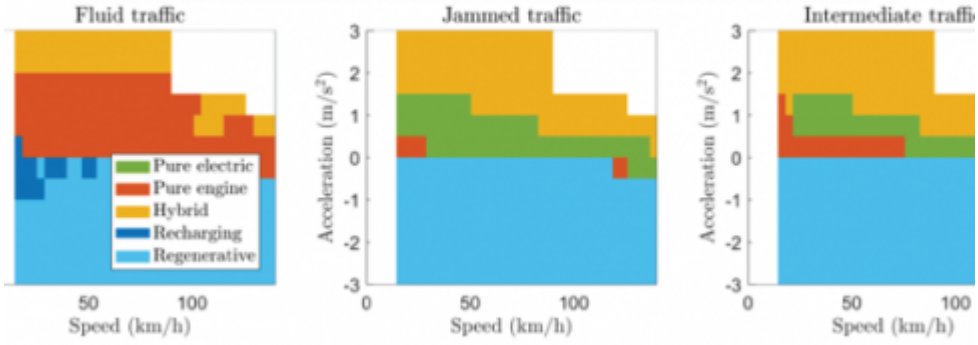
Engineering sciences | Combustion and engine technologies | Systems modeling and simulation



Hybrid vehicle energy management optimization within the framework of the partnership with INRIA

The scientific cooperation agreement signed with INRIA in 2015 covers two fields: the “**digital and IT performance of simulato**rs” and the “**control and optimization of comple**

Engineering sciences | **Automation and control systems** | **Systems modeling and simulation**

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

In the field of wind energy, Large Eddy Simulations (LES[1]) 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). However, existing computing resources do not enable a sufficiently detailed resolution of these models[2] while carrying out associated simulations within acceptable periods of time.

To reduce this calculation cost, researchers already use actuator methods [1], for example, to model blades using the body forces[3] technique (actuator lines and actuator disks). This makes it possible to limit the mesh size while not explicitly representing blade geometry. However, while significant, the reduction in calculation time associated with LES is not yet sufficient for the detailed numerical simulation of a windfarm.

In practice, such simulation needs to consider the interaction between phenomena occurring on a kilometer scale (atmospheric phenomena) and a meter scale (effects of wake turbulence). It is this constraint that leads to costly simulations, particularly with traditional LES solvers[4].

As an alternative to these solvers, IFPEN decided to study the use of the Lattice-Boltzmann Method (LBM), accelerated by using graphics cards (GPU[5]). Indeed, while founded on theoretical bases different from LES, LBM can solve equivalent problems and solvers based on this method are more efficient and particularly suited to massively parallel heterogeneous computing architectures.

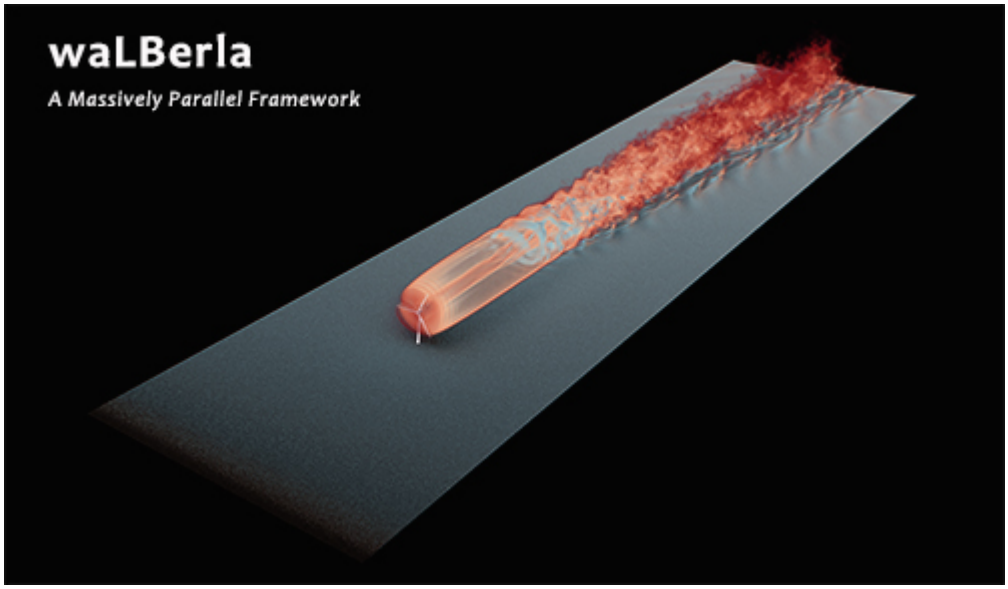
This research was conducted within the framework of the European EoCoE-II project, completed at the end of 2022, in collaboration with the developers of the massively parallel solver waLBerla[6], at Erlangen University. On this basis, IFPEN developed the waLBerla-wind solver for two microprocessor architectures (x86 and ARM). Due to its unique software design, which provides a common code base for CPU and GPU, the portability of the different target architectures is ensured, with a reduced maintenance cost. Moreover, this solver is compatible with NVIDIA's GPUDirect® technology for efficient data transfer between several GPUs.

As with LES, the physical models deployed in waLBerla-wind to simulate wind turbines use actuator methods, with optional end-of-blade load loss corrections. This solver can also be used to simulate different wind turbine configurations, both horizontally and vertically.

The numerical results and calculation performance of waLBerla-wind were compared [2] with those of SOWFA, the most widely used LES solver in wind energy research, and Meso-NH, a tool co-developed by IFPEN and Meteo France, based on a meteorological solver developed by the CNRM[7].

The comparison is related to a relatively simple test case, with a single turbine, applying the same time step and the same mesh size for the three solvers.

It turned out that with CPUs alone, and for the same number of compute nodes, the waLBerla-wind LBM solver was 70 times faster than SOWFA and 40 times faster than Meso-NH. Using GPUs as well for the LBM solver (Figure 1), the ratios were even more remarkable: 470 and 290 respectively, while producing comparable results (Figure 2).



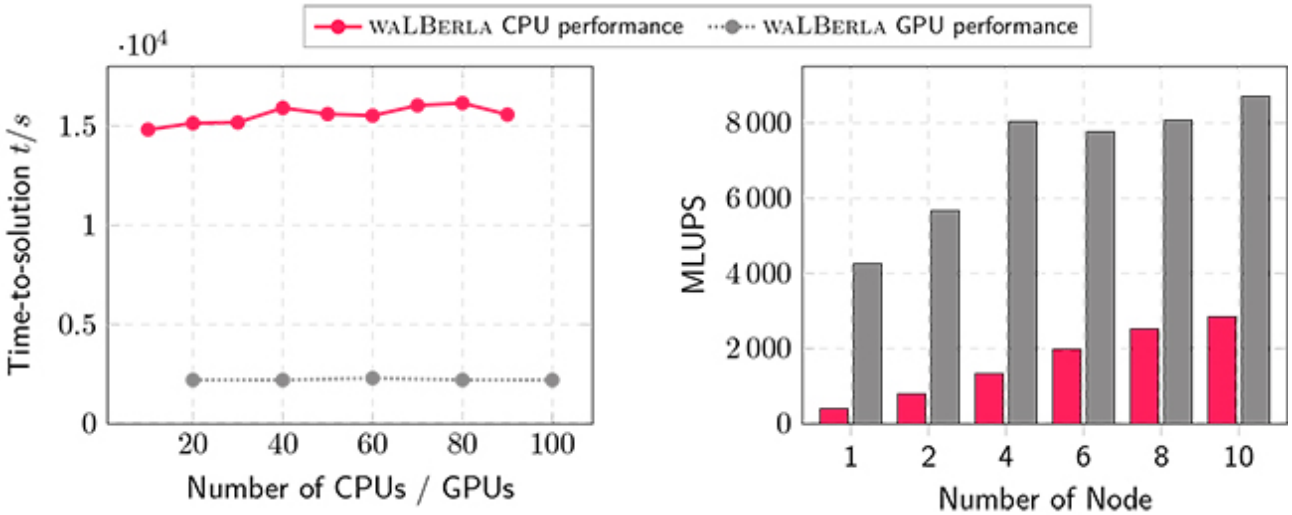


Figure 1: Velocity field in the wake of a horizontal turbine (waLBerla image) and influence of parallel computing on the computing performance at this scale (graphs above)

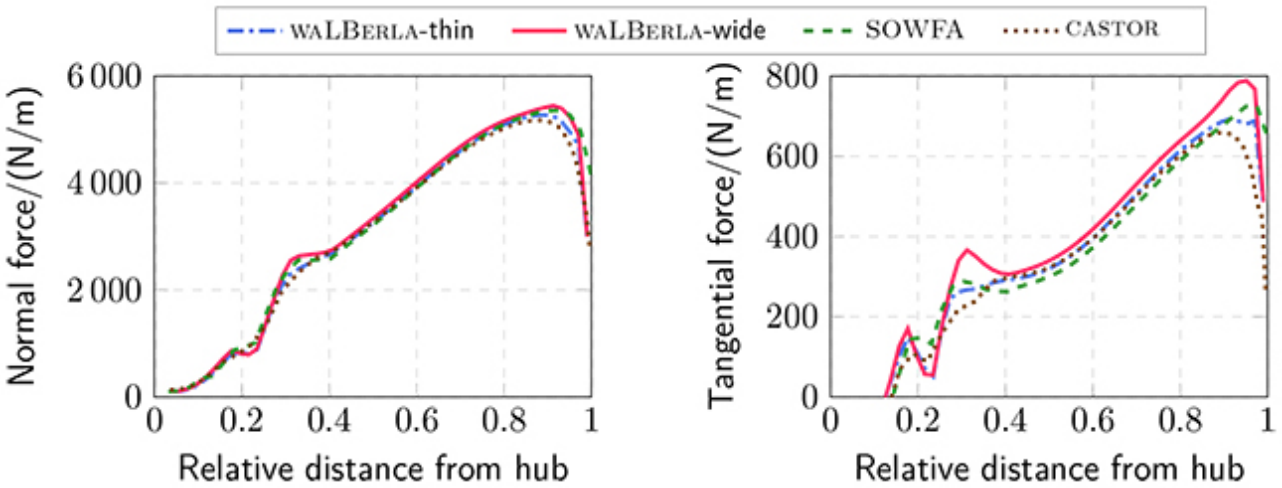


Figure 2: Distribution of normal (left) and tangential (right) forces along the blade.

The massive parallelism deployed in waLBerla-wind gives this code the capacity to efficiently simulate not only individual turbines but also entire wind farms. The most remarkable aspect is that combining the use of the LBM method with massively parallel computing on GPUs makes it possible to envisage real-time simulations.

Work to enhance the software to consider the atmospheric boundary layer (ABL) phenomenon is currently underway in the context of PhD research* aimed at simulating wind farms in even more realistic conditions.

[1]- Mathematical turbulence model used in numerical fluid dynamics.
[2]- See Science@ifpen issue 49.
[3]- Forces acting throughout the entire volume of a body.
[4]- Based on Navier-Stokes equations.
[5]- Graphics Processing Unit, vs Central Processing Unit (CPU).
[6]- This open-source solver is currently one of the most efficient that exists thanks, in particular, to the use of high-performance code generation techniques.
[7]- *Centre National de Recherches Météorologiques* (French Meteorological Research Center, *Météo France*).

* Thesis entitled: ***Lattice Boltzmann methods for windfarm application: aeroelastic wind turbine modeling in an atmospheric boundary layer.***

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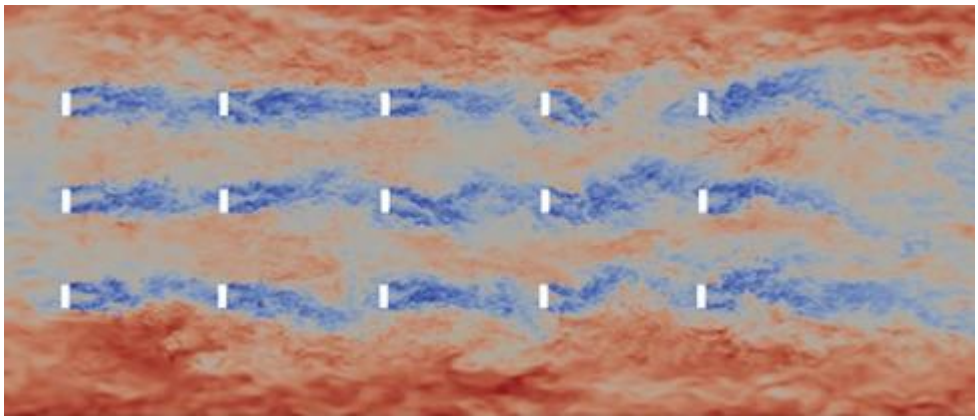
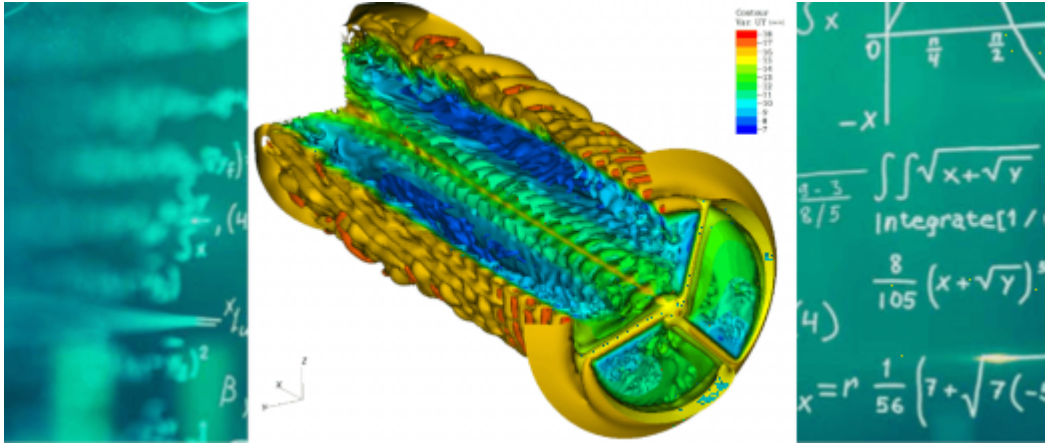


Wind farm optimization: in the wake of modeling advances

Wind energy accounts for an increasing share of the energy mix thank to the construction of wind farms designed to reduce investment and operating costs. However, within a farm, downstream wind turbines are exposed to the wakes of upstream rotors, leading to a reduction in their production and an increase in their fatigue stresses...

Fluid mechanics | Systems modeling and simulation

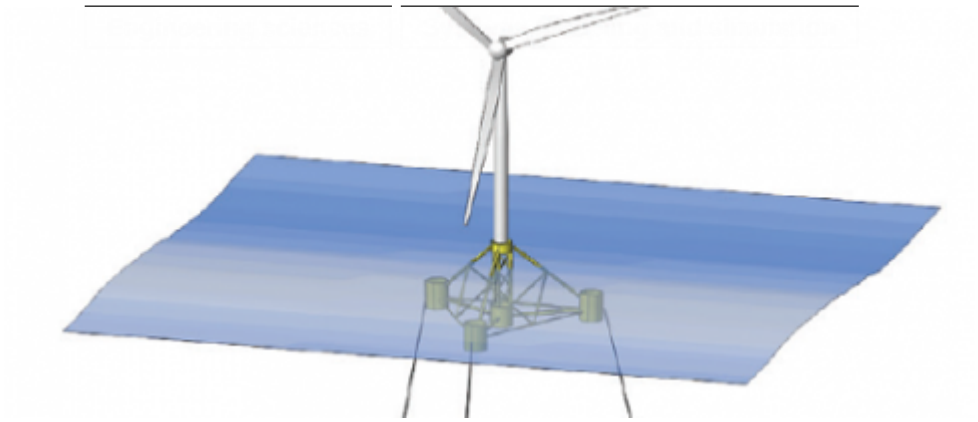


Fundamental Research

News September 2020

Wind energy: a new numerical tool to support the sector’s future

Renewable energies | Wind Energy



Wind turbines have the wind in their sails, thanks to GPUs

IFPEN has been carrying out research in the field of **floating wind turbines** for a number of years, developing, for this purpose, the **DeepLines Wind™**

Renewable energies | Wind Energy

Mathematics and IT | Numerical methods and optimization | Software design | High performance computing

SC8 - “Massively” accelerated windfarm simulation

Cutting CO_2 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.

In order to compare the various technologies available for road transport, both mature and future, IFPEN joined forces with ADEME to conduct the E4T 2040 prospective economic and environmental study of the sector [1]. To do so, it developed methods and tools making it possible to conduct the analyses required following a multi-scale approach.

These analyses were initially conducted on a vehicle scale, studying a multitude of segments, ranging from urban cars to heavy articulated trucks, as a function of several operating conditions combining urban and extra-urban journeys. Starting from hypotheses relating to the evolution of propulsion technologies, the consumption and emission results for each type of vehicle were determined and forecast to the year 2040.

These economic and environmental results were then fed into a discrete choice model[1], DRIVERS (DiscRete choIce modeling for low-carbon VEhicles fleet scenaRioS), in order to transpose these analyses to the scale of the global vehicle fleet on the road. The DRIVERS model can be used to produce different road transport demand forecasts, global or by technology type, as a function of several public policy scenarios, and to deduce the associated pollutant emissions.

This methodology, deployed for the E4T 2040 study, was developed by IFPEN within the framework of a dedicated research project. For the environmental part, methodological developments related more particularly to vehicle Life Cycle Analysis (LCA) indicators [2]. As for the new DRIVERS prospective model, its utility function[2] incorporates a first component related to the costs of vehicle ownership and a second component related to the behavior of economic agents. This second component was the focus of more fundamental research in behavioral economics [3].

The results obtained using these new approaches show that technical progress combined with the fall in the cost of electric solutions (particularly batteries) will enable them to penetrate the market. The LCA results show that with the French electric mix the shift to battery electric vehicles produces significant benefits in terms of reduce GHG emissions, with emissions associated with battery production tending to reduce between now and 2040 due in part to the relocation of this production to Europe during the timeframe (Figure 1).

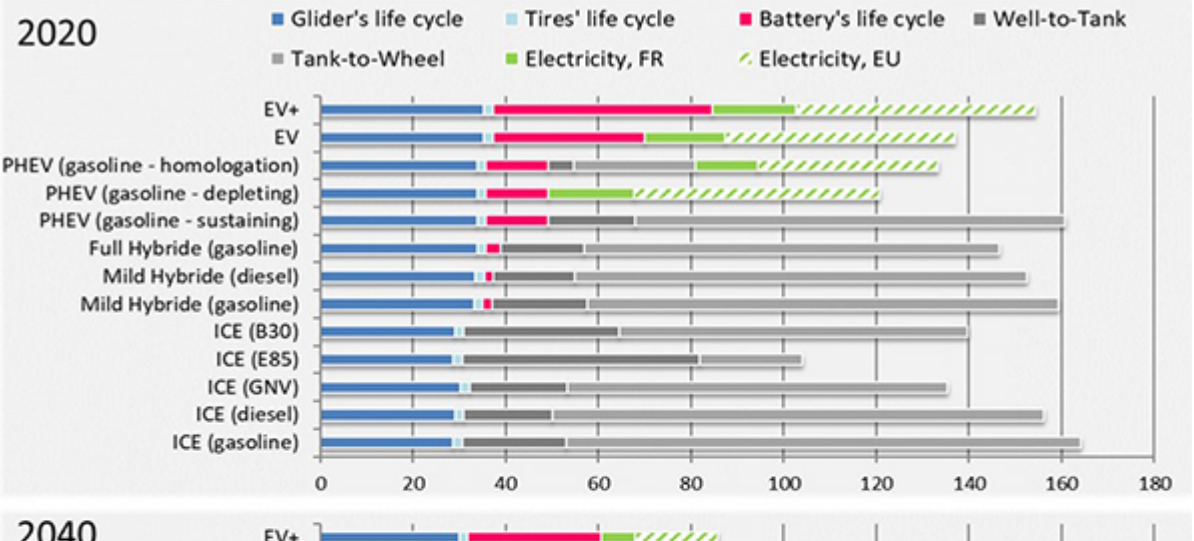


Figure 1: Potential impacts on climate change for segment C vehicles. WLTC. Timescales 2020 and 2040 (12,500 km/year)

Lastly, looking towards 2050, the prospective analysis of the evolution of the French vehicle fleet indicates that, even in the most favorable scenario for the sale of battery electric vehicles, the ***Green Deal*** objectives (90% cut in transport sector CO_2 emissions by 2050 compared to 1990) are not met (Figure 2). These projections show that, without an increase in the use of biofuels and a fundamental change in mobility behavior *via* suitable public policy support measures[3], the stated decarbonization objective for the transport sector will be difficult to achieve.

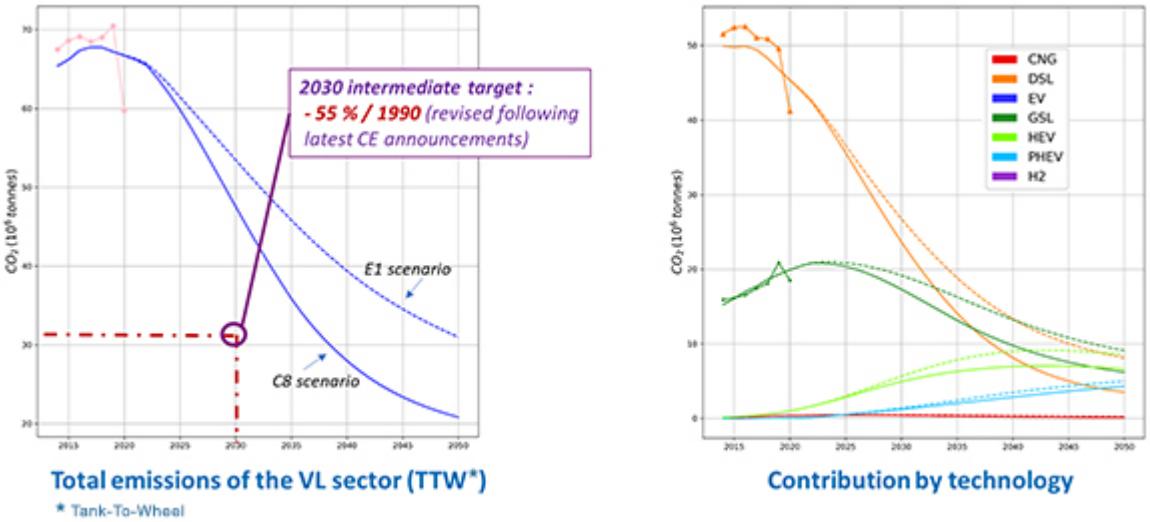


Figure 2: Evolution over time of CO2 emissions for the light vehicle fleet (left), and for each technology (right) for C8 scenarios (pro-electric) with and without a ban on the sale of IC vehicles after 2035.

[1]- Type of model widely used in transport economics to determine the probability of users adopting alternatives, drawing on utility functions.
[2]- Mathematical function aimed at quantitatively translating the utility concept in order to incorporate it in a choice model.
[3]- Car-sharing, development of public transport and inter-modal transport options, soft mobility, etc.

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