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News

Fundamental Research

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Doctoral Program Director

"The doctorate suffers from a poor image throughout virtually the whole of French society." This warning, recently delivered by the French National Research and Technology Association (ANRT), is accompanied, in the same report, by another observation: *"The doctorate is strategic, a vital asset within the context of unparalleled international competition for talent."* The combination of these two alarming observations for France gives rise to a powerful appeal *"For a major national plan to support the doctorate"*.

At IFP Energies nouvelles, we have always believed in the vital contribution made by our doctoral students to scientific advances and the expansion of cutting-edge knowledge in our research fields, as well as in the need to thoroughly train our doctoral students and prepare them to take responsibilities

in a broad range of activities and economic sectors. Our doctoral training program, targeting doctoral students as well as their supervisors, reflect this ambition.

The scientific excellence of our doctoral students is recognized via the numerous prizes and awards they are given by their peers for their research, and by the Yves Chauvin Prize for the best IFPEN thesis. In this issue, you can read about the themes submitted to the Scientific Committee for selection this year, starting with that of award winner Alexandre Delarouzée.

LES BRÈVES

Thesis prepared by **Alexandre Delarouzée, winner of the 2023 Yves Chauvin prize**: « ***Ingénierie métabolique de Clostridium acetobutylicum pour l'utilisation de sucres issus de biomasse lignocellulosique*** » ***("Metabolic engineering of Clostridium acetobutylicum for the use of sugars from lignocellulosic biomass")***

Within the context of the energy transition, new bioprocesses are emerging as substitutes for processes using fossil resources. For example, *Clostridium acetobutylicum* is a microorganism capable of converting the large variety of sugars derived from lignocellulosic biomass into a raft of bio-based substances, via fermentation. This makes it a potential candidate for producing biofuels and/or chemical intermediates that can be used by industry.

However, this use of *C. acetobutylicum* comes up against two obstacles. Firstly, the use of different sugars by this microorganism is hierarchized by a mechanism known as “catabolic repression”, meaning that these sugars are assimilated sequentially rather than simultaneously. This characteristic limits the development of an efficient, continuously fed fermentation process. Secondly, the extraction of this mixture of fermentable sugars requires a biomass pre-treatment step that generates chemical compounds that are toxic for the microorganism, thereby having a negative impact on the fermentation process (figure).

This thesis research used various genetic engineering approaches to overcome both these problems. First of all, a series of genetic modifications made it possible to modify the metabolism of *C. acetobutylicum* so that it simultaneously consumes the majority of sugars derived from a reference lignocellulosic biomass [1]. In parallel, adaptive evolution methods in bioreactors made it possible to obtain microorganisms resistant to different growth inhibitors and capable of fermenting pre-treated biomass-type industrial substrates. Lastly, for the third part of the thesis, the doctoral researcher developed a genetic tool making it possible to list all the genes that are essential in the *C. acetobutylicumgenome* [2]. This mapping process results in a crucial database that can be used to determine the priority genetic targets with a view to the rational improvement of this biocatalyst.

The discoveries made in the three areas explored pave the way for the use of *C. acetobutylicum* for the efficient conversion of lignocellulosic substrates in order to produce second-generation bio-based substances in industrial conditions. Future research conducted at IFPEN’s Biotech Department will focus, among other things, on expanding the range of substances that can be produced using this microorganism.

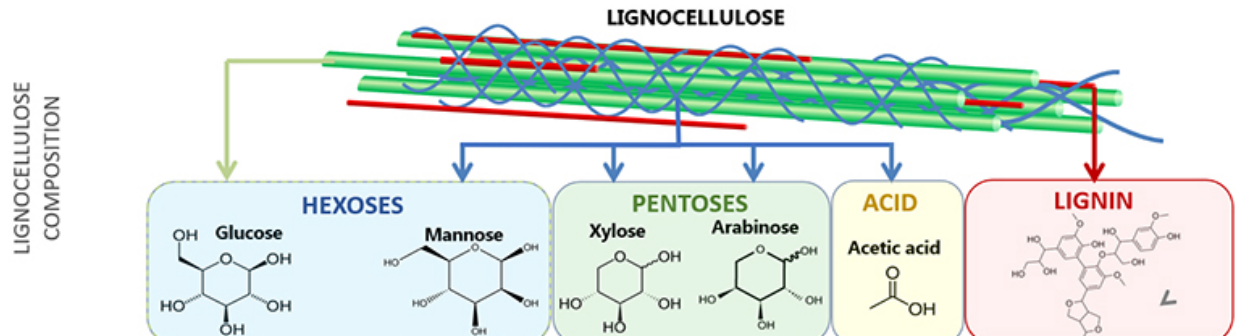

Figure: Composition of lignocellulose and provenance of growth inhibitors resulting from pre-treatment.

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>> ISSUE 53 OF SCIENCE@IFPEN

Yves Chauvin Prize: Metabolic engineering at the heart of bio-based processes

Thesis prepared by **Erwan Jézéquel**: « ***Simulations de sillages d'éoliennes en conditions atmosphériques réelles : des simulations aux grandes échelles aux modèles analytiques*** » ***("Wind turbine wake simulations in real atmospheric conditions: from large scale simulations to analytical models")***

In the wake zone located behind each wind turbine, wind velocity is reduced and turbulence increased. This results in a reduction in the lifespan of machines located downstream as well as a decrease in a windfarm's overall electricity production.

To limit these effects and help optimize the siting of turbines on windfarms, analytical wake models exist in the literature but they incorporate numerous simplifying hypotheses concerning wind turbines and their environment. In particular, meandering[1], illustrated in figure 1, is often not explicitly taken into account in stationary flow models and it is merely assumed that it contributes to the evolution of wake in the same way as diffusion. However, these oscillations modify the form and evolution of speed and turbulence profiles in very different ways. Hence, because of meandering, a downstream turbine may alternatively be located inside or outside wake created upstream. Its velocity deficit will be less than is calculated by stationary models. Conversely, actual turbulence, and therefore the fatigue stress, will be higher.

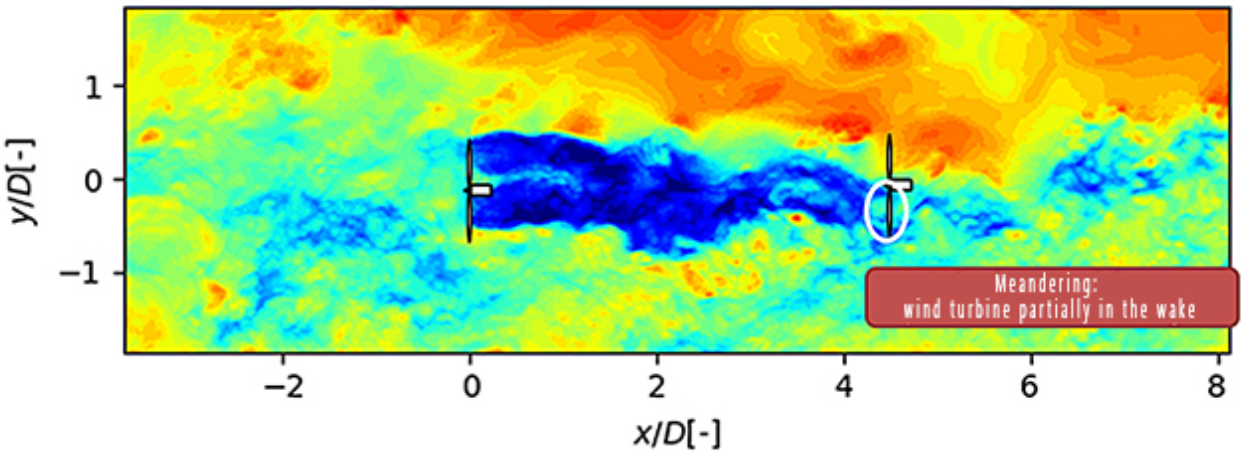

Figure 1: illustration of the effect of non-stationary wake meandering on a simulated case within the framework of the thesis.
Blue: low velocities
Red: high velocities
Distances scaled by the diameter of the wind turbine.

Meandering is caused by the large atmospheric vortices and is directly related to the state of the atmospheric boundary layer[2] (ABL). ABL instability increases with the extent of thermal and mechanical phenomena, with a direct impact on the development of meandering.

In order to directly simulate the effect of the ABL on meandering (wind and turbulence profiles), IFPEN researchers use a numerical code (Meso-NH) developed by the French Meteorological Research Center and the French Aerology Laboratory. This high-fidelity code, based on Navier-Stokes equations, was specifically created to model phenomena within the ABL and we were thus able to use

its results as a reference. We were able to precisely simulate the wake generated by a single turbine for a stable, unstable and intermediate case. This enabled us to demonstrate commonly accepted results in the literature, while at the same time clarifying certain underlying assumptions that are rarely detailed [1].

The results obtained firstly confirmed that the form of the turbulence profile in a turbine's wake is influenced by meandering and that, compared to a neutral situation, ABL instability causes the profile to rapidly evolve from a bimodal form to a unimodal form.

These findings then formed the basis for the proposal of a new analytical model to describe turbulence in a turbine's wake taking into account meandering [2]. This is the first analytical model based on physics rather than on an entirely empirical approach to predict an added turbulence profile.

Figure 2 illustrates the fact that the analytical model developed during this research (in blue) makes it possible to find different simulated profiles with Meso-NH, unlike the models found in the literature (example in red), which systematically predict a bimodal form due to calibration with respect to neutral cases.

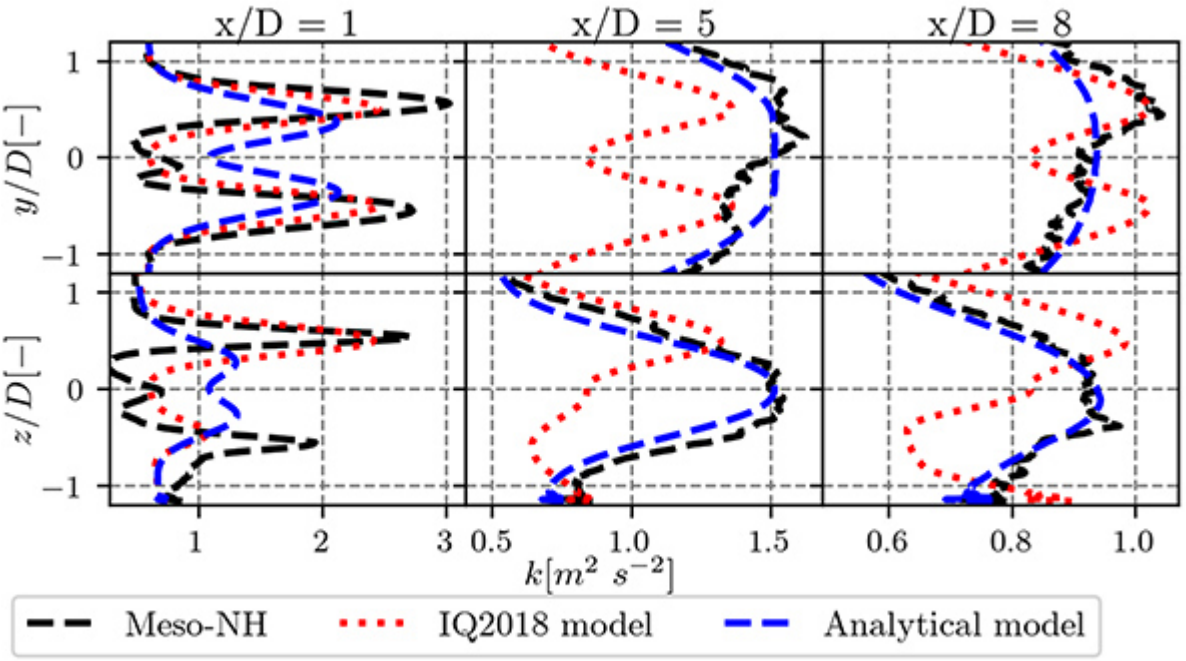

Figure 2: Horizontal (top) and vertical (bottom) turbulence profiles for three positions behind the wind turbine (distance x scaled to the diameter D of the machine).
Black: Meso-NH
Red: analytical literature model
Blue: proposed analytical model

To continue this research, a calibration of the model will be proposed, based on other high-fidelity Meso-NH simulations. This will make it possible to precisely predict turbulence profiles as a function of atmospheric conditions while keeping calculation costs very low.

1- Wake oscillations.
2- The lowest part of the atmosphere, in contact with the planet's surface, the behavior of which is directly influenced by friction with the latter.

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>> ISSUE 53 OF SCIENCE@IFPEN

Modeling wind turbine wake: a question of atmosphere!

Thesis prepared by **Flavia Domingues de Souza**: « ***Étude et modélisation d'une Machine à Mémoire de Flux Variable à base des aimants Fe-Cr-Co pour son alimentation et sa commande sans capteur mécanique à haute vitesse.*** » ***("Study and modeling of a Variable Flux Memory Motor fitted with Fe-Cr-Co magnets for its power supply and sensorless high-speed mechanical control").***

Permanent magnet synchronous motors (PMSM) are a reference technology for electric vehicle propulsion. However, their large-scale deployment is subject to the constraints associated with magnets:

- **the capacity to obtain resources** (particularly rare earths), since 40% of the raw materials required for their production are located in China;
- **as well as the environmental challenges related to mining, recycling and refining.**

In addition, PMSMs often require flux-weakening[1] strategies in order to operate at high speeds, which can result in energy losses and, consequently, a reduction in the efficiency of the overall system.

Variable Flux Memory Motors (VFMM) represent an alternative technology that uses Fe-Cr-Co-based "reduced coercive field" magnets. Still little used for these applications, this alloy is advantageous due to its low cobalt content (critical metal) and its good mechanical resistance. Moreover, the control of VFMMs presents an additional degree of freedom since their magnetic flows can be regulated via very short pulses of magnetizing current.

The research conducted for this thesis was aimed at characterizing and understanding the behavior of the Fe-Cr-Co in the target operating conditions. To do so, the configuration studied was that of a PMSM, where the permanent magnet rotor was replaced by a solid cylinder of this alloy, a simple geometry and adapted to high-speed applications. The experimental study was conducted in two stages:

1. standstill magnetization, via injection of currents in the stator windings at zero speed, with the aim of characterizing the magnet inserted into the machine environment;
2. dynamic magnetization (rotating motor) in which the magnetization state is adjusted as the electric motor is driven, and which is used to control its electromagnetic torque.

The first step was based on equations describing operating points in the hysteresis loop and relating the magnetic field strength H to the magnetic flow density B [1]. Two methodologies were proposed and deployed to describe the magnetization profile of the Fe-Cr-Co at a standstill, as a function of being located either in the easy or difficult magnetization axis. The magnetic characteristics of the cylinder were deduced from standstill tests, as well as from finite element simulations and the results were compared to the references provided by ideal measurement equipment (Hysteresis Graph),

which characterizes the magnet outside the machine environment. Figure 1 presents the differences observed, discussed in [2], for which the studies conducted via numerical simulation led to the conclusion that they are linked to the geometry and saturation of the material making up the stator.

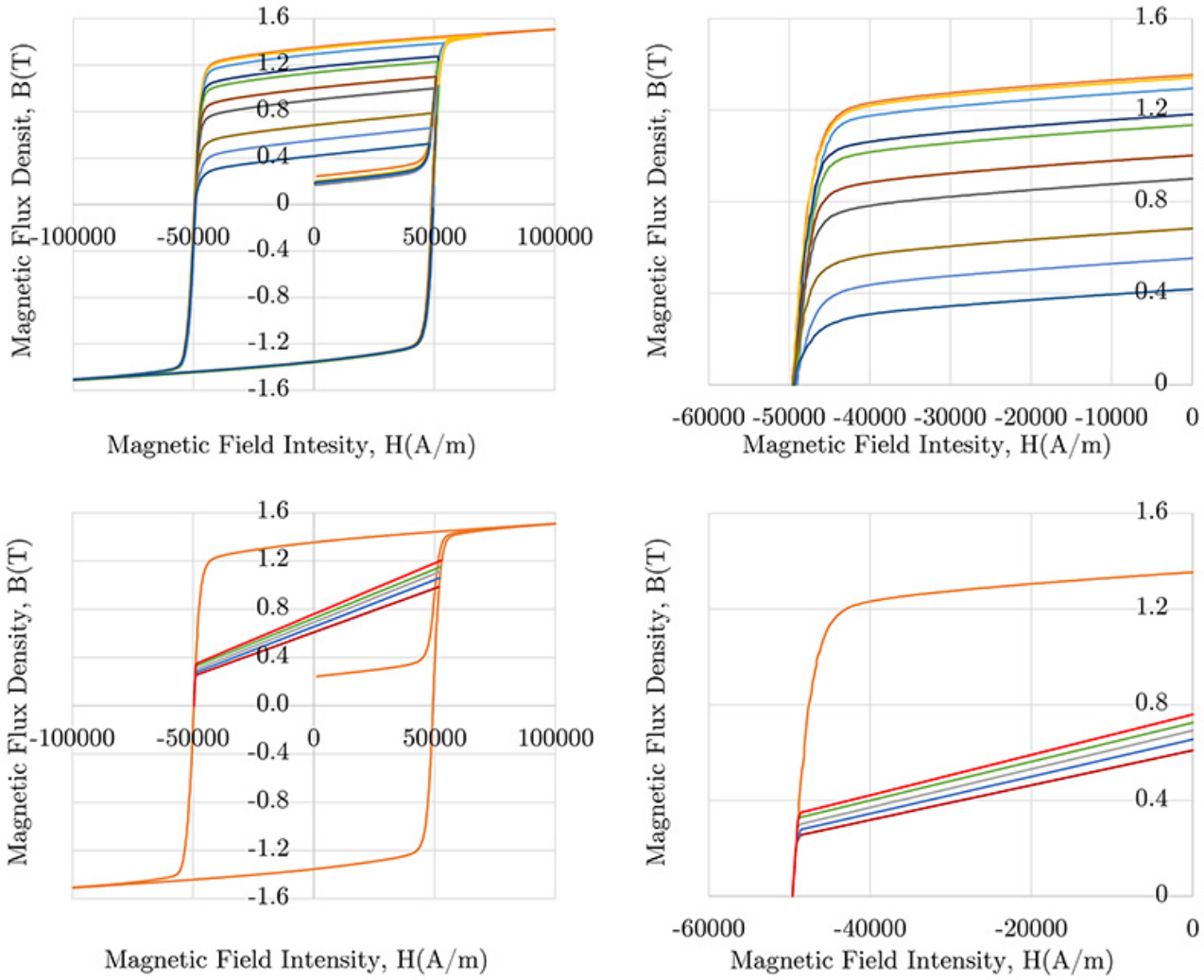

Figure 1: Hysteresis cycles obtained
Line 1 graphs: from hysteresis graph measurements
Line 2 graphs: from experimental tests and finite element simulations

The second part, focusing on the dynamic magnetization and control of the motor's electromagnetic torque, resulted in the development of a command algorithm without a rotor position sensor, adapted from previous research [3]. This system estimates the position and speed of the rotor using the measured output voltages, taking into account phase delay compensation. These are strongly influenced by the inductances of the direct and quadrature axes (dq axes)[2]. A methodology using FEA simulations was proposed to estimate them, and also considering the anisotropic effects of the magnet and stator iron saturation.

An important result of this work relates to the partial magnetization states of the magnet, which were derived from the standstill magnetization tests, and were then used to predict the expected dynamic operating points. The magnet's magnetic model resulting from the tests was also used as a basis for the analysis of machine inductances, information that is required to optimize the control of the system aimed at maximizing the torque generated by the machine.

Another conclusion concerns the demonstration of the influence of electric machine geometry (slot design, magnet length, etc.) on the magnetization state expected by a magnet inserted in an VFMM.

This research paves the way for further scientific studies aimed at improving the geometric design of a stator adapted and optimized for Fe-Cr-Co magnet properties.

[1-] Flux weakening of an operating machine consists in reducing the inductor flux in order to increase its speed beyond its nominal value without increasing the supply voltage.
[2-] Axes associated with changing the machine's real three-phase frame of reference to a rotating frame of reference fixed to the rotor, in order to align the model of an AC machine with that of a DC machine, allowing independent control of the flux and torque in the machine (vector command).

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>> ISSUE 53 OF SCIENCE@IFPEN

Magnets for future generations of electric vehicles

Thesis prepared by **Adam Hammoumi**: *"Analysis-Driven Design of Digital Multi-scale Microstructures of Materials"*

While macroscopic models combined with experimental analysis of porosity are well established for geometrically simple pores, hierarchized and disordered microstructures defy existing frameworks and call into question conventional interpretations. We proposed a digital framework to help overcome this challenge, taking into account morphology, connectivity and pore size distribution.

On the basis of realistic digital twins, our strategy firstly made it possible to faithfully reproduce the results of porosity characterization techniques [1]. New numerical simulation models also made it possible to associate physicochemical phenomena with the geometric properties of microstructures [2]. Lastly, calculations conducted on the basis of these models were accelerated by a factor of 30 via deep learning (example in figure 1), thanks to our auto-encoding model enabling, for large volumes, precise simulation of mesoporosity down to the nearest nanometer [3].

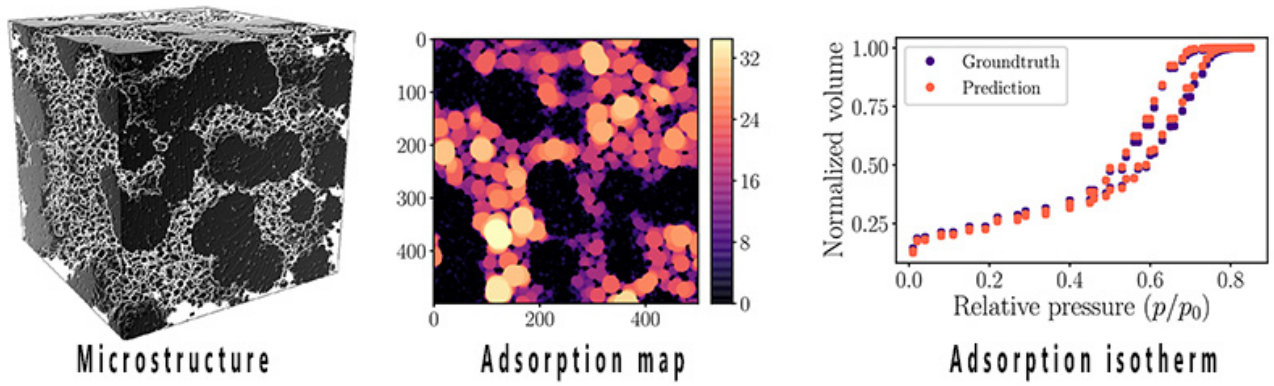

Figure 1: Illustration of a simulated microstructure and its adsorption map derived from the morphological model, and comparison between the real isotherm (Groundtruth) and the isotherm obtained through Deep Learning (Prediction).

The results of this PhD research are very encouraging and the simulation platform developed also paves the way for virtual tests to reproduce operations on materials, such as grinding, and provide access to a unique vision of the internal transformations undergone by microstructures during them.

Beyond the usual processes of microscopic modeling and the experimental characterization of porous material microstructures, the approach employed is also aimed at establishing a new rapid and adaptive digital framework, with a view to:

- understanding the relationships between the textural and usage properties of complex porous materials;
- being able to obtain a “rapid flow” of simulated experimental results.

[a]- https://www.ifpenergiesnouvelles.com/brief/numerical-design-based-analysis-multi-scale-porous-material-microstructures
[b]- https://www.ifpenergiesnouvelles.com/brief/sc4-new-numerical-approach-characterization-virtual-porous-materials
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>> ISSUE 53 OF SCIENCE@IFPEN

Digital porous materials: from the virtual to very real interest!

Thesis prepared by **Loïc Iapteff**: *"Transfer Learning for Smart Predictive Analytics"*

IFPEN is a global leader in the development of catalysts and processes for clean fuel production. For these processes themselves to be eco-efficient[1], 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.

For each new process and each new catalyst, the model has to be trained with experimental data acquired on pilot facilities. The operation of these facilities is time-consuming and costly, which is why it is important to drastically reduce the volume of experimental data needed to develop new generations of catalysts, while maintaining the quality of the predictive models. This is where transfer learning comes in, an approach consisting in pre-training a model in a similar field, and then adapting it to a specific problem so as to take advantage of knowledge already acquired.

Bayesian[2]-type techniques were implemented within the framework of this thesis to transfer different model types [1, 2], the main advantage being the reduction in the number of observations needed to obtain a new efficient modeling process. This is illustrated in Figure 1 relating to the nitrogen content for the hydrocracking pretreatment process: the effectiveness of Bayesian transfer compared with simple data addition can be seen, especially when the volume of data added is low.

This transfer learning methodology made it possible to significantly reduce (by 30%) the number of experimental points needed to optimize models relative to the hydrotreatment process for new generations of catalysts. This research has already been extended to other applications and no fewer than five research projects have from this methodology. This has contributed to accelerate the development of new models while reducing the associated costs.

For the development or improvement of predictive models in the industrial sector, it is necessary to have access to large volumes of data. The current trend is to produce more data. Our work will help to counteract this trend using an innovative and efficient method. With this method, it will be possible to model a phenomenon on the basis of a reduced quantity of experimental data, exploiting prior knowledge to the full.

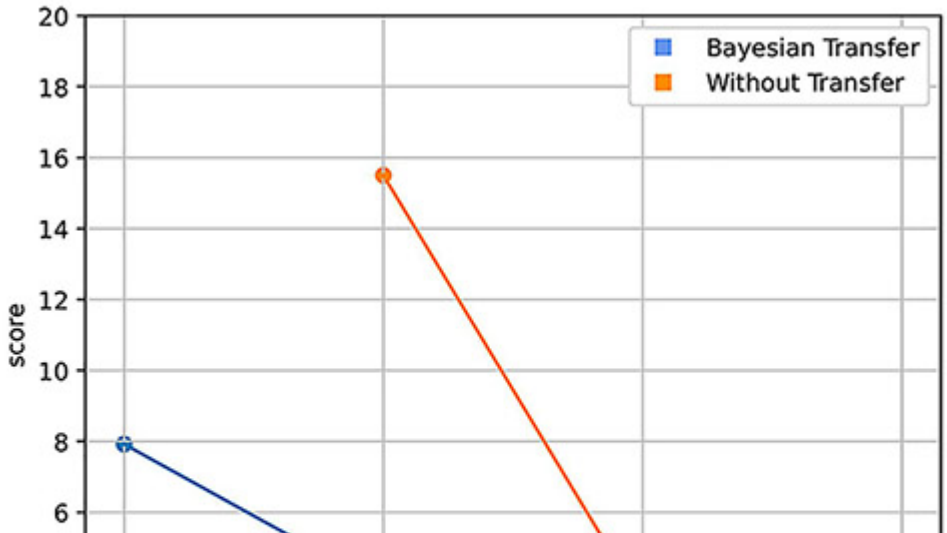

Figure 1: Evolution of the quality of the prediction of nitrogen content (score = mean absolute error) as a function of the number of points used (sample size) with Bayesian transfer (blue) and without transfer (orange).

1- Eco-efficiency expresses the relationship between economic benefit and the environmental impact caused.
2- Statistical approaches based on Bayesian inference, whereby the probability expresses a degree of belief in an event.

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>> ISSUE 53 OF SCIENCE@IFPEN

Transfer learning for process optimization

Thesis prepared by **Jingang Qu**: *"Acceleration of Numerical Simulations with Deep Learning: Application to Thermodynamic Equilibrium Calculations"*

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.

The research conducted for this thesis consisted in accelerating the two-phase flash calculations, integrating deep learning models in the existing flash algorithm [1]. The idea was to accelerate the convergence of the algorithm, thereby reducing the calculation time, without compromising the accuracy of the solution.

The objective was met, with a six-fold acceleration on existing single-core computing architectures [2, 3]. Moreover, the provision of a parallel algorithm able to function on GPU[1] -type hardware architectures led to a 100-fold time saving (figure 1).

There are numerous prospects for further research since implementation in industrial reactive transport simulators requires significant developments to adapt codes to the hardware architectures used. Moreover, extending this research to three-phase flash calculations, as well as to more complex equation of state models, is under consideration. This will make it possible to model a broader range of chemical interactions, particularly concerning aqueous systems.

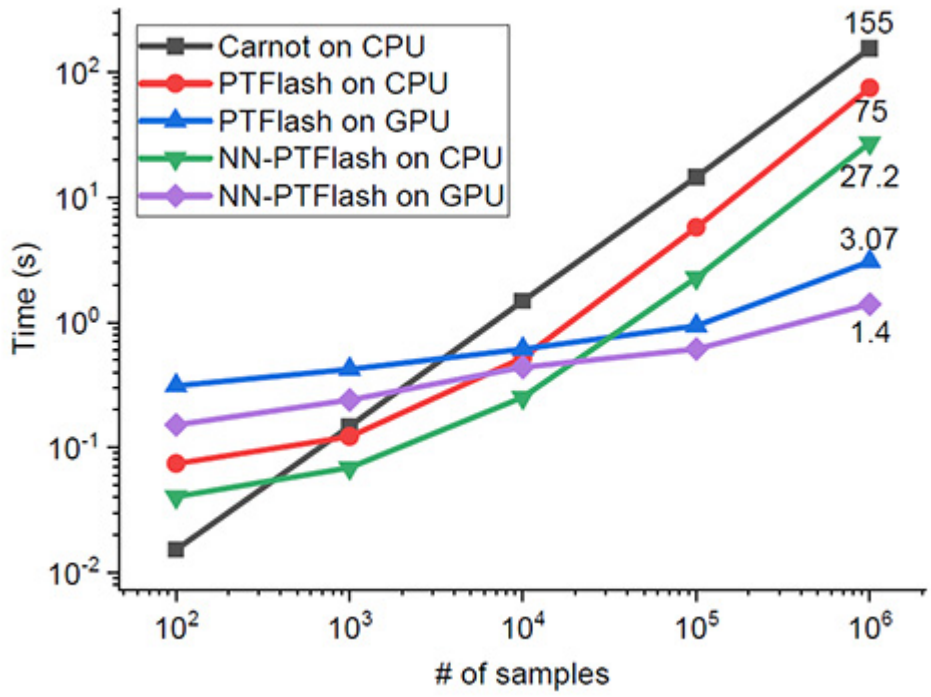

Figure 1: Comparison of calculation times between CARNOT[2] and the PTFlash algorithm incorporating learning models for a mixture of nine chemical species.

1- Graphics Processing Unit
2- IFPEN library implementing the conventional algorithm

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>> ISSUE 53 OF SCIENCE@IFPEN

Deep learning in the field of thermodynamics

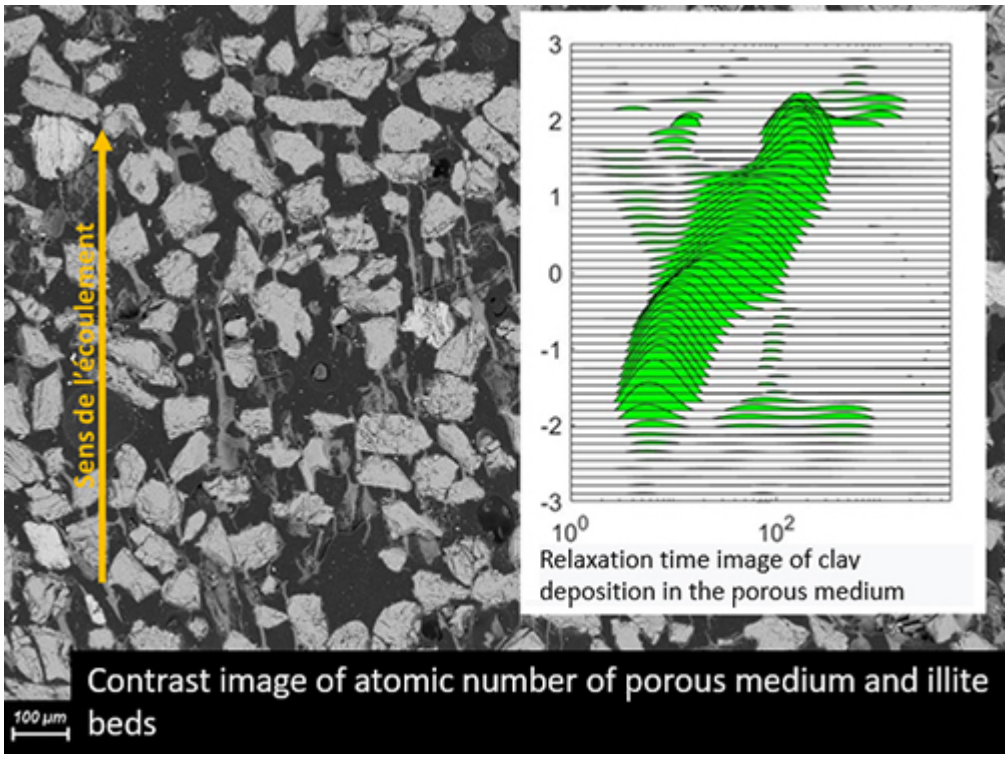
Thesis prepared by **Inès Raies**: « ***Identification et compréhension des mécanismes de déstabilisation colloïdale dans les procédés géothermiques*** » ***("Identification and understanding of colloidal destabilization mechanisms in geothermal processes")***

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.

In order to gain a more detailed understanding of the mechanisms at work, the PhD research was structured around three priority areas [1, 2]:

1. Identification of the clays that cause clogging;
2. Study of clay stability under geothermal conditions;
3. Study of the drop in injectivity caused by the deposition of clay particles in porous media.

A combined NMR and SEM approach was employed to better qualify the micrometric-scale alteration of the porous network and obtain the information required to interpret measured flow pressure losses, thereby improving the accuracy of the predictive numerical modeling of the phenomenon.



>> More information

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Clogging is a major challenge for geothermal energy

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