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News

Fundamental Research

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IFPEN Group’s ambition for the coming years is to consolidate its position as a leading player in the fields of energy transition, circular economy and decarbonization, by developing innovative technologies that are both ecologically-friendly and economically viable. In this context, the mission of the *Process Design and Modeling* division will be to contribute to the scaling-up innovative process concepts, often developed in collaboration with IFPEN’s other divisions and external partners.

This issue contains seven articles presenting a panorama of the expertise deployed in the Division. They illustrate how core Process Engineering skills have made it possible to evolve from traditional hydrocarbon-based activities towards new fields, such as the synthesis of materials for batteries, CO_2 capture and enzymatic conversion of biomass. Some articles also focus on the use of innovative computation tools, such as Computational Fluid Dynamics, Machine Learning and the latest developments in Linear Programming.

In addition, the topics selected cover a broad range of spatial scales (from enzymes to industrial demonstrators) and TRLs (Technology Readiness Levels), and demonstrate the diversity of skills, tools and research required for IFPEN’s future technological developments.

LES BRÈVES

In chemical conversion processes implementing heterogeneous catalysis, the active phase, which accelerates molecular conversions, is often deposited on a porous support. Most of the time, this support has a large internal surface area, making it possible to host a large number of active sites within a small volume. Very often, the porous support is alumina, which needs to have adequate mechanical and thermal resistances and enhance mass and heat transfer. These properties are highly dependent on the texture of the support, which itself stems from its production process.

For alumina supports, this process hinges around a coagulation phenomenon: the assembly of primary boehmite crystallites[a] (between 1 and 5 nm) forms highly stable aggregates (between 10 and 50 nm) which then form agglomerates (between 100 nm and a few tens of ?m) [1]. In practice, the production process begins with a boehmite powder mixed with an acid, in the form of a paste, in order to disperse the grains into small aggregate particles. Subsequently, a base is added to trigger coagulation and form agglomerates. This extremely chaotic agglomeration phenomenon involves an assembly on several size scales, from tens of nanometers to several microns. Its structure determines the final properties of the support.

Better controlling the production of alumina supports requires modeling of their final structure as a function of the physicochemical parameters involved. To this end, a PhD thesis[b] focused on the dynamics of the agglomeration in static conditions (i.e., in the absence of hydrodynamic forces).

To quantify the impact of pH and ionic strength, as well as boehmite concentration, on agglomeration kinetics, three experimental techniques were used: dynamic light scattering (DLS), small-angle x-ray scattering (SAXS) and scanning transmission electron microscopy (STEM). This multi-technique characterization approach made it possible to highlight the structural properties on various scales. This information was exploited via a population balance equation, using a Brownian dynamics model[c]. The population balance results were then used to define the parameters for a morphological agglomeration model, capable of simulating the final porous structure of the solid alumina. A digital twin of the 3D morphology of an agglomerated boehmite grain within a colloidal suspension was thus created. The latter takes into account structural parameters such as size distribution, fractal dimension [d] and assembly order.

The microstructure of the final solid was simulated in several steps using two successive physical models: a Lagrangian Brownian dynamics model and a population balance model.

The first step consisted in building a morphological model of crystallite aggregation (figure 1). Various sticking probabilities were allocated to the concave and non-concave points of an aggregate and associated with physicochemical parameters. The first model provided information about the relationship between the fractal dimension and agglomerate mass, a property confirmed by the results of the SAXS analysis [2].

This relationship was then exploited in a population balance model to enable a realistic simulation of a large-sized colloidal system. The experimental DLS results were used to adjust the model’s parameters.

Lastly, the size distribution and fractal dimension obtained from the population balance were used to define the parameters for the global morphological model and build a 3D aggregate agglomerate.

The morphological model developed integrates the operating conditions required to generate a suitable 3D structure and can be further improved. For example, non-spherical particles could be included in the Brownian model. Moreover, by directly considering boehmite crystallites as primary particles rather than their aggregates, it will eventually be possible to calculate the textural properties of the alumina support, such as pore volume, specific surface area, pore size distribution and tortuosity. Another possible extension to get closer to industrial operating conditions is to consider shear at higher solid concentrations, inducing forced agglomeration and fracture phenomena.

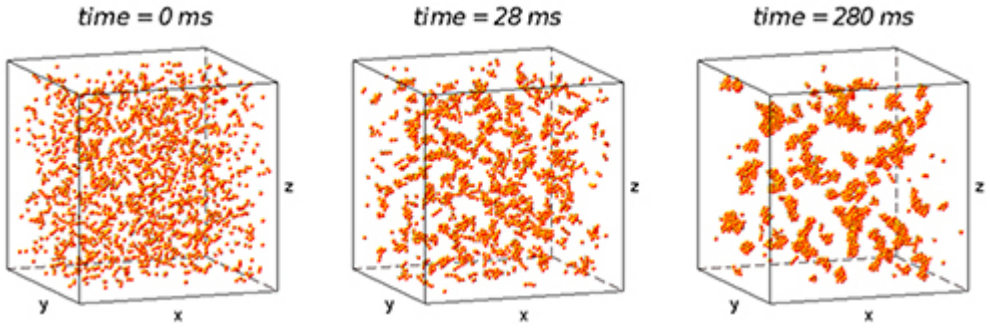

Figure 1: Evolution of a system of agglomerates within a cubic representative elementary volume of 3,800 nm edge length at different times, simulated with a Brownian dynamics model.

[a]- Common name for aluminum hydroxide oxide, a natural hydrated aluminum oxide and constituent of bauxites.
[b]- PhD thesis by G. Ferri: “Identification and study of relevant descriptors of the solid during the synthesis of boehmite”, Paris-Saclay University, 2021.
[c]- Simulation method used to describe the dynamics of particles interacting in a highly damped environment.
[d]- This dimension characterizes the compactness of the structure of a particle assembly. Its value tends to 1, 2 or 3 respectively for linear, planar and spherical clusters. Open structures have a low fractal dimension while compact structures have a high fractal dimension.

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Modeling manufacturing by precipitation - A need for catalyst supports

Building on knowledge acquired relating to alumina precipitation synthesis for heterogeneous catalyst supports, IFPEN's teams set about working on pCAM[a] synthesis for Li-ion batteries. These materials are indeed also obtained by precipitation in stirred tank reactors, which shares similarities with alumina synthesis (nucleation, growth and agglomeration phenomena). Nevertheless, they come with their own challenges and, consequently, with new research opportunities.

For example, this operation involves extremely rapid reactions and very low solubilities, resulting in very high levels and gradients of supersaturation (the driving force behind precipitation) in the reactor. In such conditions, the hydrodynamics and mixing at different scales (macro, meso and micro) become limiting factors in precipitate formation.

For the design and operation of such precipitation reactors, it is essential to understand the various physical phenomena taking place in this synthesis, as well as their interactions. This requires the development of a multiphysics model in which thermodynamics, kinetics, population balances, and hydrodynamics are strongly coupled. This will mobilize expertise in each of the four fields mentioned. The thermodynamic and kinetic models have yet to be optimized and the population balance model is not yet accounted for (simulation example shown in figure 1).

This research will be the focus of two PhD theses, starting at the end of 2024, aimed at characterizing and modeling different particle precursor formation phenomena.

The first thesis, supervised by the *Physics and Analysis* division, aims to capture short-time phenomena (nucleation followed by elementary crystal growth) by developing analytical methods for their detection and quantification.

The second thesis, hosted by the *Process Modeling and Design* division, will focus on understanding and modeling the impact of hydrodynamics on longer-time phenomena (growth, agglomeration, attrition, break-up).

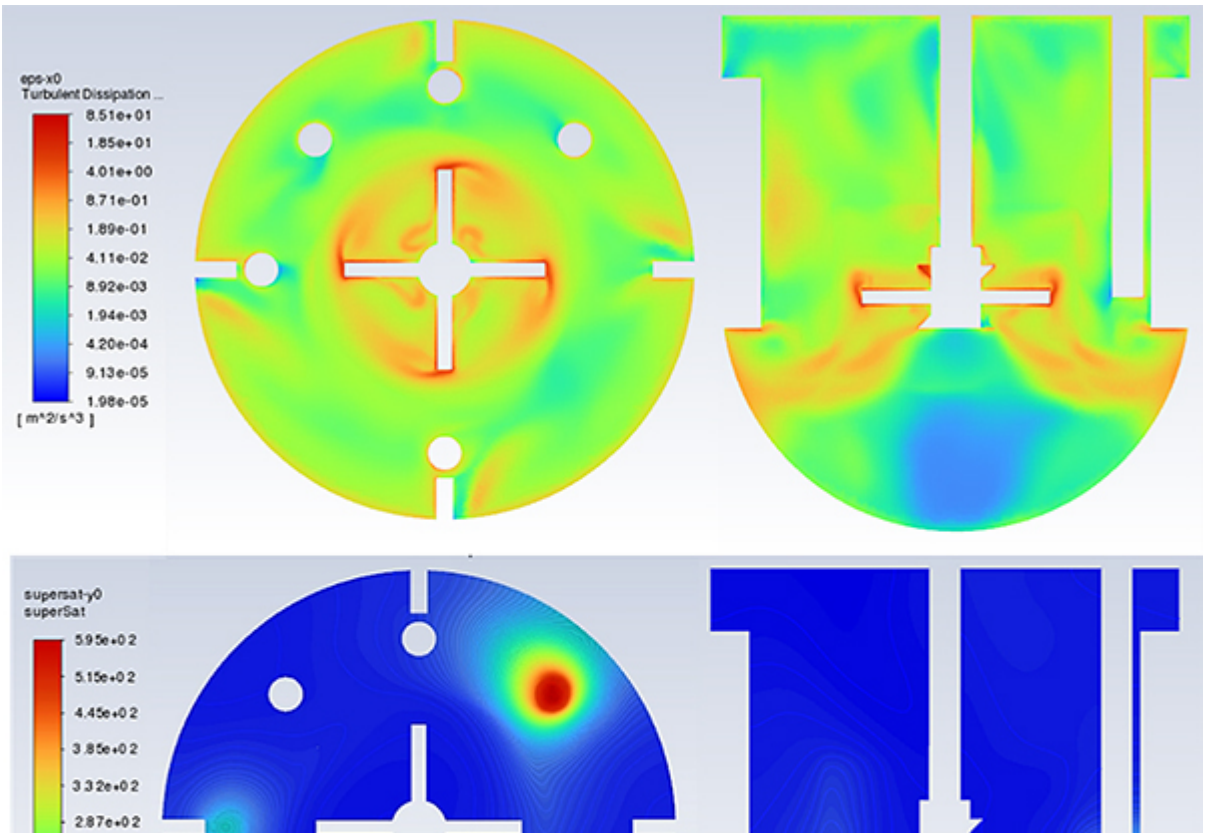

Figure 1: Turbulent energy dissipation (top) and supersaturation (bottom) rates in a 2L pCAM synthesis reactor (CFD RANS model with integrated micro-mixture model)

a- Precursors of Cathode Active Materials

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Modeling manufacturing by precipitation - A skill set for the production of battery cathode materials

Metal- and ceramic-based solid foams are porous structures that have begun to be used relatively recently in the field of chemical processes although they have been the focus of research at IFPEN for a few years already.

Due to their 3D texture, made up of a multitude of juxtaposed spherical cavities (familiar in the field of heterogeneous catalysis), these structures are highly porous (around 70-80%) and have a large specific surface area. On the face of it, this is associated with good external transfer performances, in terms of both heat and matter. Therefore, they seemed to be suitable for rapid, highly exothermic chemical reactions, such as selective hydrogenations or methane oxidation reactions. This was thus the focus of specific research conducted in partnership with the Polytechnic University of Turin [1], which characterized matter transfer in open cell foams (OCFs).

The use of OCFs was subsequently considered for particle trapping at the top of hydrotreatment reactors for non-conventional feedstocks (vegetable oils, recycled plastics) and was the subject of PhD research[a] carried out in partnership with the same university. The filtration mechanism inside foam pebbles was simulated via the Euler-Lagrange CFD method, using OpenFoam® and Ansys Fluent codes (Figure 1 left) [2], making it possible to precisely determine which morphological foam descriptors impact filtration efficiency.

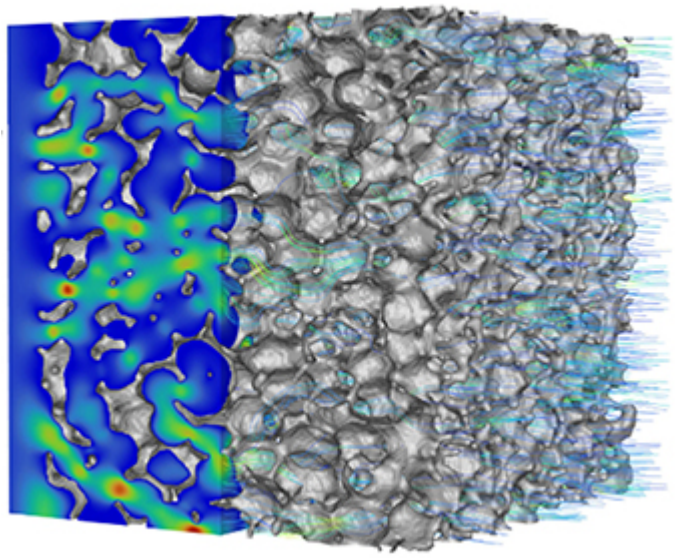

Figure 1: Digital twin of a ceramic foam;

In parallel, capture tests were conducted using a dedicated experimental set-up, in order to quantify filtration efficiency (characteristic filtration height) in representative gas-liquid hydrodynamic conditions on vrac-packing of foam pieces.

Numerous analyses were also conducted by X-ray tomography[b] to characterize the fouling by measuring the rate of cell plugging in waste foams, recovered from industrial reactors (figure 2).

In parallel, experiments of fouling were conducted at the laboratory,involving a fluid containing iron particles flowing through foam pieces.

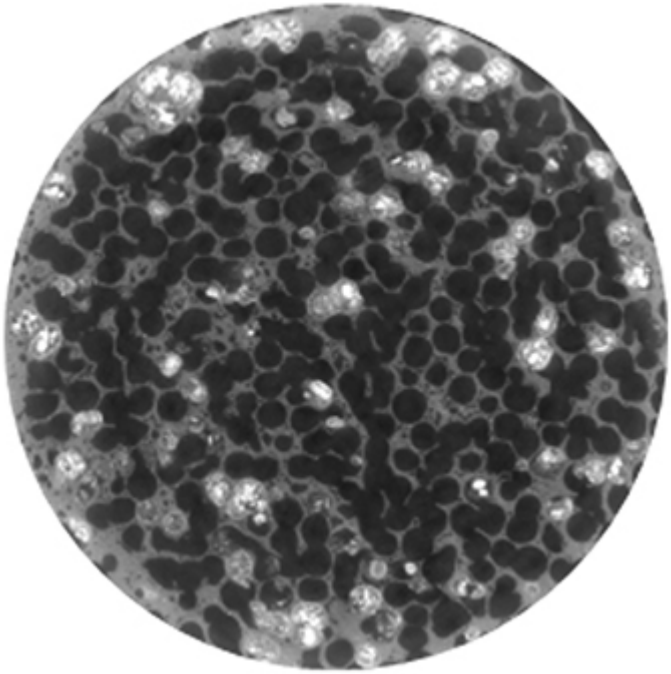

Figure 2: X-ray Tomography observation of a partially fouled foam piece after use in a trickle-bed reactor

The results of capture and foam fouling experiments were modeled and integrated in a macroscopic 1D simulator to predict capture performances applicable to industrial catalytic reactors. This global capture model was successfully validated, through comparisons with cold-model experiments and data and matter analyses from industrial units.

All of the work carried out at IFPEN on ceramic or metallic foams has demonstrated the value of these structures both as catalytic supports with high transfer performances and for very high-capacity capture. The expertise acquired in the course of this research paves the way for the intensification of certain rapid reactions, and also for innovation in the field of filtration materials (OCF) with optimized geometries.

[a]- Thesis by Enrico Agostini, *Fluid dynamics and mass transfer in porous media: Modelling fluid flow and filtration inside open-cell foams*, 2023.
[b]- In partnership with IFPEN's *Physics and Analysis* Division

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Foaming processes

In the energy and chemicals sectors, the conversion of raw materials into finished or semi-finished products is conducted via a succession of processes in dedicated units. Each of these processes comprises input conversion steps and output separation steps (Figure 1).

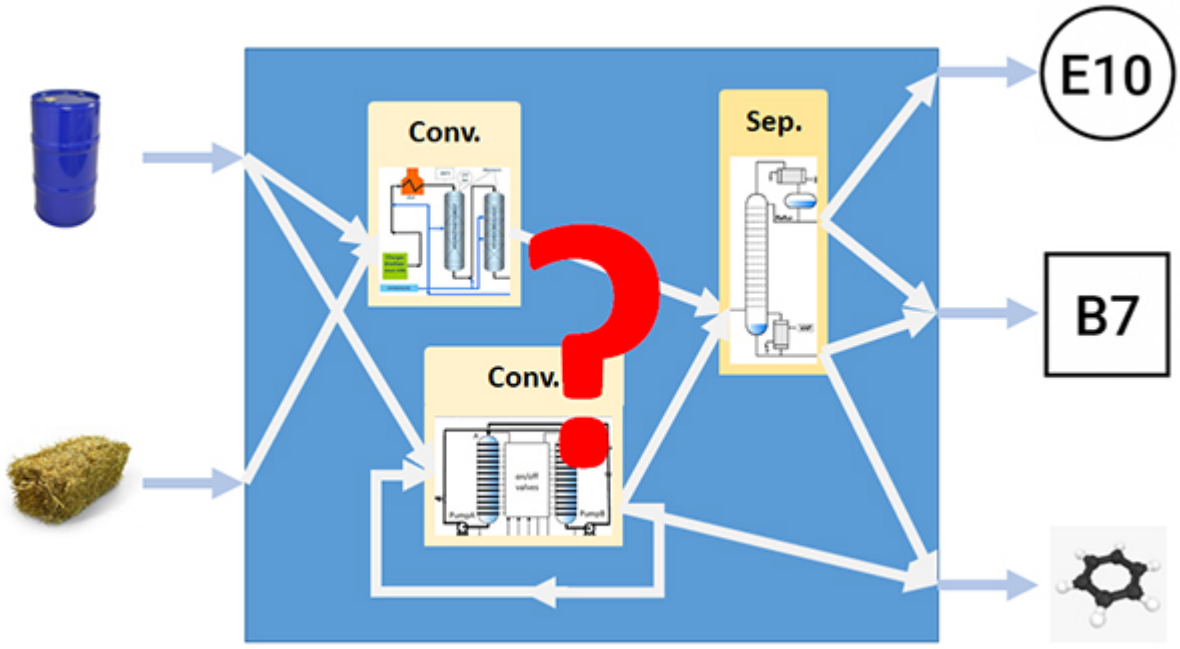


Figure 1: The challenge of optimizing the arrangement of units

In an industrial context where the focus is on optimizing the use of resources and reducing the environmental footprint, the capacity to redefine and optimize the arrangement of units appeared essential at IFPEN. So its teams developed a tool for the purpose.

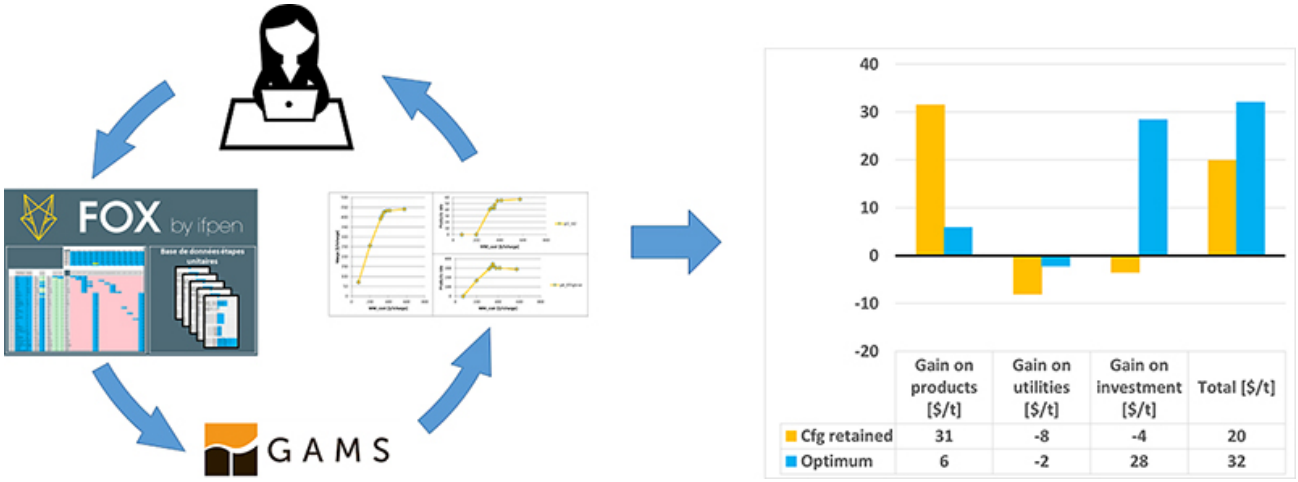
In the literature, the first mathematical approaches to the subject emerged at the end of the 1970s. They consisted in choosing the individual conversion and separation steps to be implemented, along with the routing of flows between feeds, individual steps and products. The most efficient solutions to emerge are based on MINLP (Mixed Integer Non Linear Programming) solvers enabling the use of both continuous and Boolean variables. The latter are required in terms of the mathematical formulation to manage the notion of unit and flow existence [1].

Despite research conducted to improve these solvers as well as problem formulation, tackling real industrial cases with existing MINLP solvers remains complex. The difficulty lies not only in calculation times but also in the capacity of the solvers to find solutions.

The need to take into account multiple variables - representing products, energy consumption and costs - led us to adopt a linear approach making it possible to use solvers that are far more efficient and robust. In this case, each individual step needs to be described by a meta-model[a] [2]. As well as obtaining representative linear meta-models, we developed a generic platform - FOX-Prod - enabling the deployment of the calculation tool and the maintenance of a database of meta-models of individual steps. The database used is the result of several years of capitalization in the refining and petrochemicals sectors. The platform is interfaced with GAMS software for algebraic modeling and optimization.

Initially, this platform was tested for a reduced, well controlled perimeter[b] after years of process development [3]. Thereafter, it successfully generated innovative unit configurations for a mature domain where the optimization margin was low. With meta-models obtained by learning from experimental design data, it was possible to propose the recycling of some flows and the pooling of separation steps.

The platform also enables optimization under constraints. Hence, Figure 2 represents differences for a reference industrial case with, firstly, the absolute optimum scenario and, secondly, an optimized scenario taking into account flow circulation constraints ("cfg retained"). The calculated gain, amounting to several tens of dollars per ton of feed processed and representing a substantial improvement (several percentage points), was then validated by simulations of the identified architecture.



	Gain on products [$/t]	Gain on utilities [$/t]	Gain on investment [$/t]	Total [$/t]
Cfg retained	31	-8	-4	20
Optimum	6	-2	28	32

Figure 2: Illustration of the use of the FOX-Prod platform – left: user environment, right: detail of marginal gains for a petrochemicals complex (difference in $/t compared with the reference industrial scenario)

Subsequent research is aimed at extending the platform's scope of application, particularly for plastics recycling and the production of a bio-based substance, and the meta-model database has been enriched for the purpose. Specific developments (consideration of azeotropic mixtures[c], solvent management, etc.) were necessary to overcome limitations that emerged during the work. In the short term, the goal is to exploit these new developments in order to optimize configurations and thereby improve industrial unit performance for renewable fuel production (production of aviation fuel via the alcohol-to-jet or e-Fuel process).

[a]- Correlation-type mathematical model in which the available data are used to estimate parameter values.
[b]- Gasoline production from naphtha.
[c]- Liquid mixture that has a constant boiling point while retaining a fixed composition.

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Fox-Prod: effectively combining units for optimized processes

Driven by the quest for innovative transport technologies, IFPEN has spent many years developing and helping to market new biofuel production processes (Vegan®, Futurol®, BioTfueL®). Among the various process options studied, the bioethanol production chain based on lignocellulosic resources offers numerous advantages, particularly in terms of resource availability and operating conditions for their conversion, which are gentle compared with a thermochemical process.

Bioethanol production consists of three key conversion steps: pre-treatment of lignocellulosic biomass, enzymatic hydrolysis of cellulose and fermentation of the sugars obtained[a]. The main role of enzymatic hydrolysis is to depolymerize cellulose into glucose, and to do so it uses a mixture of specialized enzymes (endoglucanases, cellobiohydrolases, ?-glucosidases, etc.) that act in synergy to catalyze the reaction.

The characteristic duration of this hydrolysis is several days, which is a long time compared to the pre-treatment and fermentation steps, and reducing this duration would go a long way towards improving the economic viability of the overall process. Notable progress has been made in recent years in terms of understanding the reaction mechanisms [1] but without shedding light on the deactivation phenomena that affect the enzymatic hydrolysis reaction by significantly reducing enzyme activity (by 50% every 24 hours). Among the phenomena considered, the loss of activity at the air-liquid interface through enzyme denaturation, the loss of activity through adsorption on the inert lignin surfaces and the loss of activity by non-productive adsorption on the cellulosic surfaces (enzymes blocked on the cellulose and no longer acting) was studied within the context of PhD research[b].

The experimental study of the loss of activity in the presence of contact with air revealed that the phenomenon was extremely marked for high Surface/Volume ratios (air-liquid surface to solution volume ranging from 0.3 to 1.7 cm^2/cm^3) and could lead to activity losses of up to 40% (figure 1 - left). It was then followed up with a kinetic modeling approach to predict activity losses associated with this particular phenomenon [2]. Since the model required knowledge of the air-liquid surfaces produced by agitation, these were determined using CFD numerical simulation[c] (figure 1 - right).

Concerning activity losses associated with enzyme adsorption on different lignocellulosic biomass surfaces, other research conducted during the PhD thesis made it possible to evaluate the distribution of enzymes adsorbed on the cellulose and lignin surfaces during enzymatic hydrolysis. Since enzymes adsorbed on lignin play no role in the reaction, this study showed, from adsorption isotherm calculations, that enzyme activity losses associated with adsorption on lignin may represent up to 25% of initial activity (publication pending).

All of these results will be combined with mechanistic models already available at IFPEN [1] to improve the prediction of enzymatic hydrolysis performances, optimize reaction time and reduce reactor volumes.

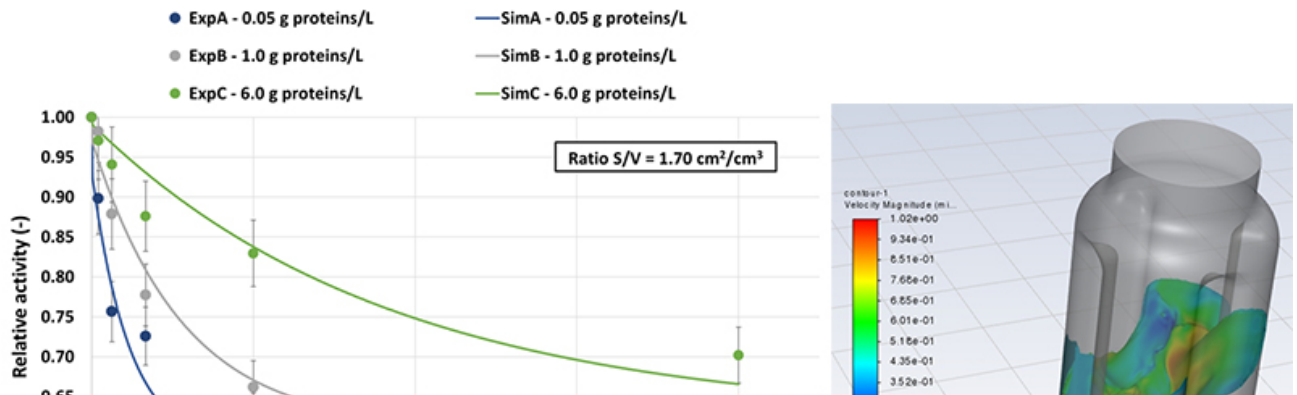

Figure 1: Impact of air-liquid surfaces on enzyme deactivation: Experimental study conducted on an orbital agitation table (left) – Numerical study conducted by CFD-Numerics (right)

[a]- Glucose, xylose, galactose, arabinose, mannose.
[b]- Thesis by Laura Cachafeiro, "*Hydrolyse enzymatique de la biomasse lignocellulosique : étude de l'adsorption et de la désactivation des cellulases*" (*Enzymatic hydrolysis of lignocellulosic biomass: cellulase adsorption and deactivation study*), Lyon 1 University, 2023 (supervised by D. Hudebine - IFPEN).
[c]- *Computational Fluid Dynamics.*

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Improving the understanding of enzyme deactivation during lignocellulosic biomass hydrolysis

IFPEN is a global leader in the development of fossil feedstocks hydrotreating[a] for clean fuel production. Processes from the same family now apply to a broader diversity of feedstocks: plastic and tire pyrolysis oil, in the context of chemical recycling, vegetable oils for biofuel production, etc. For these processes themselves to be eco-efficient[b], beyond the targeted environmental benefit, their operating conditions need to be optimized by the use of kinetic or hybrid models[c], as a function of the feedstocks employed and the specifications sought for the target products.

In a competitive context, new processes have to be developed fast and it is necessary to minimize the experimental phase, which is always time-consuming and costly, without undermining the quality of the models it feeds into. This is where the TL[d] approach comes in, 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.

At the end of a thesis conducted in partnership with the “Process Experimentation” Division [1], Bayesian[e] and Monte Carlo Markov Chain[f] methodologies were implemented to transfer information from the “fossil world”, such as the development of old catalysts, to new catalysts and new processes [2, 3].

This approach produced two main benefits:

1. Concerning a new catalyst, a model was trained using old data relating to pilot and industrial facilities. The model was then transferred to the new catalyst and turned out to be of far better quality than that obtained using traditional techniques (RMSE[g] = 4.8°C for the old method, 2.9°C for the new).

2. Concerning new feedstocks, and particularly the Rewind Mix[h] process for purifying plastic waste pyrolysis oils, a new model was very quickly developed with a reduced number of experimental points (see Figure 1). The transfer learning approach also increases the model’s robustness..

This research has also been extended to more traditional hydrotreatment fields and no fewer than five research projects have benefited to date, to accelerate the availability of new models and the reduction in their access costs.

In the context of the ecological transition and the associated need to treat new feedstocks, either bio-based or recycled, this research is an important contribution to the development of new processes. By building on previous knowledge, it helps accelerate development, representing a significant competitive advantage in these emerging markets.

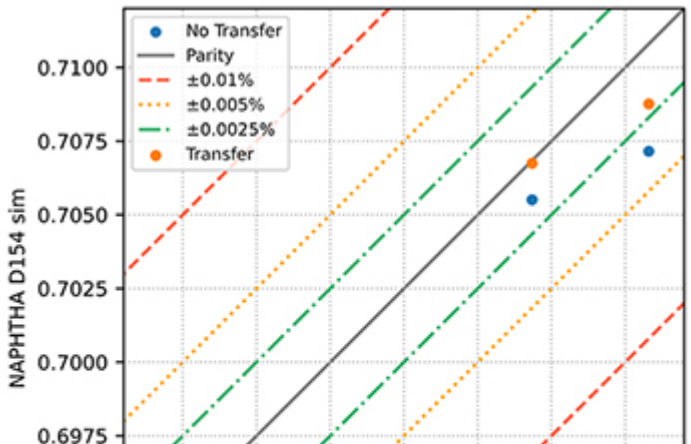

Figure 1: Prediction of the density of the Naphtha cut on a validation base (blue: traditional approach, orange: Transfer Learning approach)

[a]- This process consists in removing heteroatoms (N, S, etc.) and cracking the molecules to produce fuels. To achieve the required specifications, the use of hydrogen is essential.
[b]- Eco-efficiency expresses the relationship between economic benefit and the environmental impact caused.
[c]- Combining traditional chemical approaches and the latest advances in the field of data science.
[d]- Or transfer learning.
[e]- Statistical approaches based on Bayesian inference, whereby the probability expresses a degree of belief in an event.???????
[f]- https://www.lemonde.fr/blog/binaire/files/2016/06/MCMC.pdf
g- Root mean square error.???????
h- https://www.axens.net/markets/plastic-recycling
i- Light hydrocarbons recovered from the top of the distillation column

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Drawing on lessons from the "fossil world" for the benefit of greener processes.

Testimony of Li Zhang, process engineer at IFPEN

According to the NZE (Net Zero Emission) scenario of the IEA[a], the deployment of CCUS (Carbon Capture, Utilization and Storage) needs to accelerate and increase from around 40 Mt of CO_2 captured globally in 2022 to 1 Gt in 2030 [1]. Among the solutions developed, post-combustion capture using solvents is, so far, considered to be one of the most robust, efficient and appropriate [2].

The DMX^{TM} solution, which addresses the need to have access to effective and economical technologies, is one such option. The fruit of more than 10 years research at IFPEN, this technology, now entering the final development phase, had to be demonstrated in a real industrial setting [3] [4].

Hence the launch of the 3D[b] (DMX Demonstration in Dunkirk) project in 2019 to build an industrial demonstrator. And where better to build it than at one of Europe's biggest industrial sites, thereby contributing to the decarbonization roadmap of one of France's leading emitters, the ArcelorMittal's steelworks in Dunkirk (Image 1)?

Image 1: DMX(TM) demonstrator on site of ArcelorMittal in Dunkirk. Acknowledgements: IFPEN

This project required input from a dedicated IFPEN team based at the industrial site, to monitor the construction and conduct tests, with remote support from the IFPEN team at the Solaize site. For the very first time, IFPEN was responsible for an operation on an outside industrial site!

Modules more than 26 meters in height arrived at the site in November 2021, following months of workshop studies and construction.

Once the demonstrator had been connected to the steelworks site's blast furnace gas pipes, unit start-up operations began in March 2022 with technical coordination provided by partner AXENS (Image 2).

Image 2: IFPEN/AXENS team members on site. Acknowledgements: IFPEN

In my capacity as a process engineer at IFPEN, I monitored the tests from their launch through to the end of the test campaign at the Dunkirk site. Before going there, I had worked as a process design engineer, using an early version of the numerical DMX™ simulator. This time, I found myself "on the other side", contributing to the acquisition of experimental data used to improve the simulation model, which will be used for sizing future equipment!

I was also exposed to the reality on the ground and the unexpected events that can occur during a demonstration, occurrences that make each experimental aspect unique and invaluable. Industrial demonstration and process design are two sides of the same coin in this respect!

Now, just over two years after the completion of on-site construction, the demonstration of the DMX™ process has ended. After evaluation of the composition of the gases representative of different applications[c] (steelworks, cement works or electric power plant), the performances of the capture process have been validated, highlighting various benefits:

- a significant reduction in energy penalty (30% lower compared to MEA or CESAR1[d] solvents),
- the solvent's considerable capture capacity, high quality of the CO_2 captured[e],
- good solvent stability, etc.

In addition to the success of the demonstration, the data obtained during the test campaign formed the foundation to produce a new version of the simulator that partner AXENS[f] will benefit from.

Although the demonstration phase for the DMX^{TM} process has now been completed, the Dunkirk facility is going to be used for a further few months to test a new solvent formulation. This time, I will follow the tests from my base at IFPEN but it will be an opportunity for other colleagues to go and be part of this unique experience: to see the culmination of years of research supporting the decarbonization of industry and thereby help to combat climate change.

[a]- International Energy Agency.
[b]- Project partners: ArcelorMittal France, TotalEnergies and AXENS. Demonstrator capacity: 0.5t CO_2 captured per hour.
[c]- Blast furnace gas was used as the unit's base feedstock gas, but other compositions were deliberately produced via the unit's recycling operations, in order to validate the DMX^{TM} process for different applications.
[d]- MEA: aqueous solution with monoethanolamine, CESAR1: aqueous solution with aminomethyl propanol (AMP) and piperazine (PZ).
[e]- Purity of CO_2 above 99% (dry CO_2).
[f]- Software development led by P. Bachaud and V. Carlier.

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