Written on 28 February 2025   15 minutes of reading

News

Fundamental Research

In this special issue of our Science@IFPEN newsletter, we highlight the work of

some of our researchers who have been awarded an accreditation to supervise research (HDR).
An HDR is much more than a title. It is recognition of the holder's capacity to train the next generation of researchers, to lead large-scale projects and to make a significant contribution to removing barriers to knowledge, on a scientific journey that starts with fundamental research and culminates in the development of technological solutions. Every HDR holder within our institute embodies our commitment to finding solutions for the energy and ecological transition. By highlighting the achievements of these researchers, we seek not only to recognize their remarkable contributions, but also to inspire the next generation of scientists, and in particular our PhD students, to continue this quest for innovation and excellence.
The diversity of disciplinary fields and applications reflected in all these texts demonstrates the relevance of the skills of our researchers, who have built on the legacy of the institute's historical activities to develop a complete range of methodologies and scientific concepts that are perfectly aligned with the demands of the energy and ecological transition.

I hope that you enjoy this issue,

Benjamin Herzhaft
Executive vice president, Research and Education

[]

LES BRÈVES

Economic Analysis of Energy Systems :

a large-scale regional approach
(HDR 2021)

Arash Farnoosh

As the title suggests, my research focuses on **the economic analysis of large-scale systems**, i.e. targets such as the energy systems of regions, countries, territories and major cities or vast metropolitan areas. In terms of the economic analysis, it extends beyond pure, autonomous economic elements to include issues related to geopolitical, technical and environmental aspects, as well as energy policies, obviously. The mathematical modeling and economic analysis process deployed throughout my research career therefore integrates all these considerations.

Thus, depending on the nature of the uncertainties existing in the systems studied, **linear programming** [1] and **dynamic programming and optimization** [2] **methods** were selected. However, as this research progressed towards more competitive and eco-friendly systems (due to the greater use of renewable energies), but also more unpredictable ones, the methods used had to factor in an increasing number of uncertainties. It is primarily for this reason that these methods were combined with more innovative approaches such, as distributionally robust optimization[1] and statistical learning (i.e. neural networks). This approach resulted in new models (Figure 1) that were deployed to analyze the energy systems of rapidly developing economies such as India and China [3].
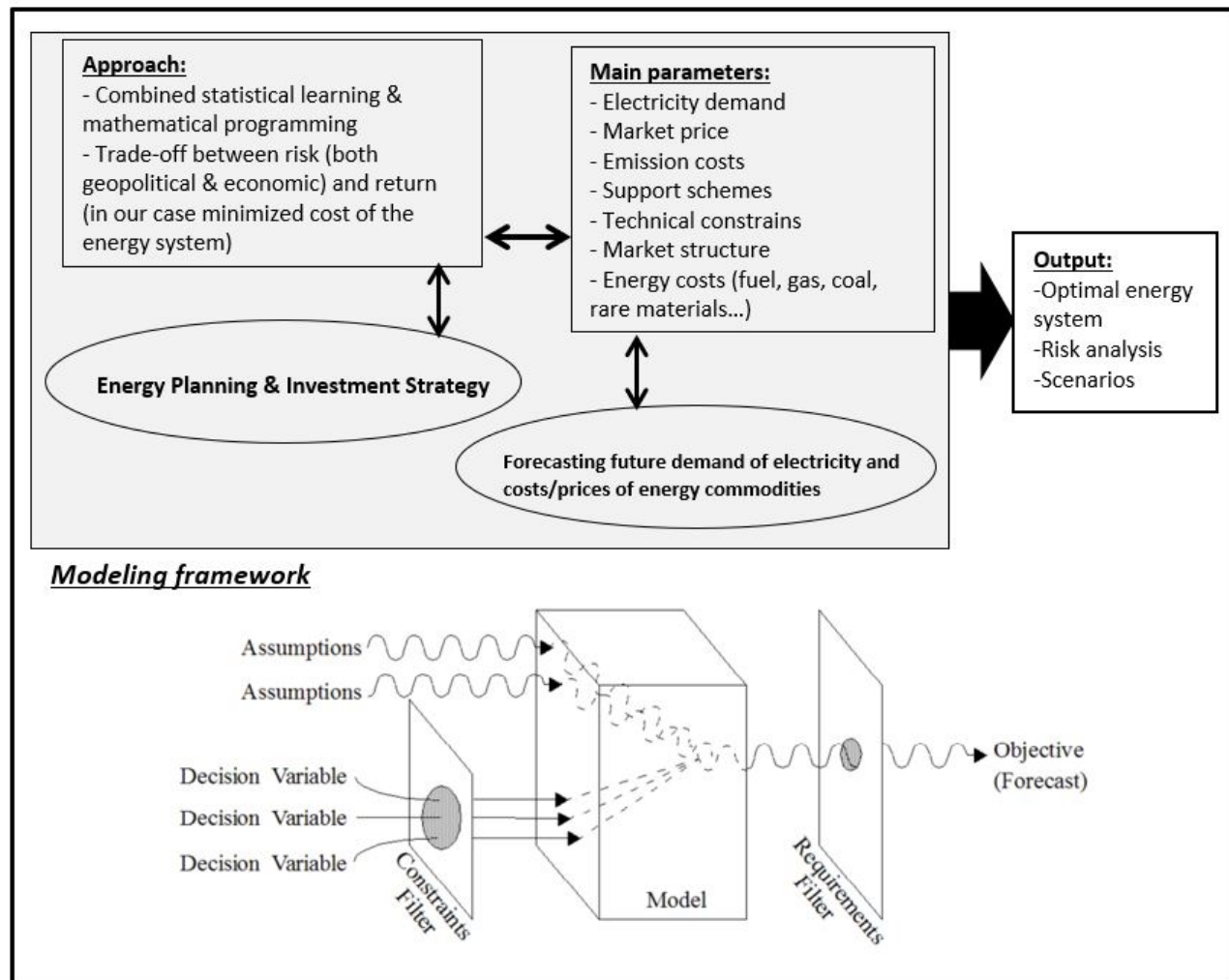
Figure 1– Structure of the techno-economic energy system model

The long-term planning and sustainable expansion of large-scale energy systems in highly unpredictable contexts present significant challenges due to the presence of various types of uncertainties. The application of these models improves the robustness of our analysis to help overcome this issue.

[1] Distributionally robust optimization (DRO) assumes that the probability distribution governing uncertain parameters is unknown but belongs to an ambiguous set of probability distributions

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>> ISSUE 57 OF SCIENCE@IFPEN

Modeling of major energy systems

Maria Romero-Sarmiento

Analytical Methodologies for Organic Matter Characterization:

Application to the characterization of complex source-reservoir rocks, microplastics and solid deposits in geothermal installations (HDR 2021)

The scope of my HDR (accreditation to direct research) covers ten years of research at IFPEN, initially focusing on topics related to hydrocarbons:
- Characterization of **the nanostructure of sedimentary organic matter** as a function of **thermal maturity**;
- Development of **the Rock-Eval® Shale Play^{TM} method** to enhance **the characterization of liquid-rich source rocks**;
- Development of an analytical methodology to better estimate the free hydrocarbons among those adsorbed within a source rock containing liquid hydrocarbons

Subsequently, my research shifted other issues, particularly those related to new energy sources and the environment. This led to the development of experimental procedures to characterize: solid deposits present in geothermal power stations [1], corrosion inhibitors, lubricants and, more recently, polymers (issues related to microplastic pollution) [2] and textile microfibers [3].

These contributions have supported various IFPEN developments, including:
-   the TemisFlow^{TM} **basin modeling software solution**, commercialized by BeicipFranlab, by integrating new models involving **organic geochemical concepts** (e.g., modules for calculating organic porosity and methane adsorption potential;
-   Rock-Eval® **technology** (figure 1), commercialized by Vinci Technologies, via the development of new analytical methods to improve the characterization of various types of samples.
My research trajectory reflects the shift undertaken by IFPEN in recent years to address the challenges of the energy and ecological transition.
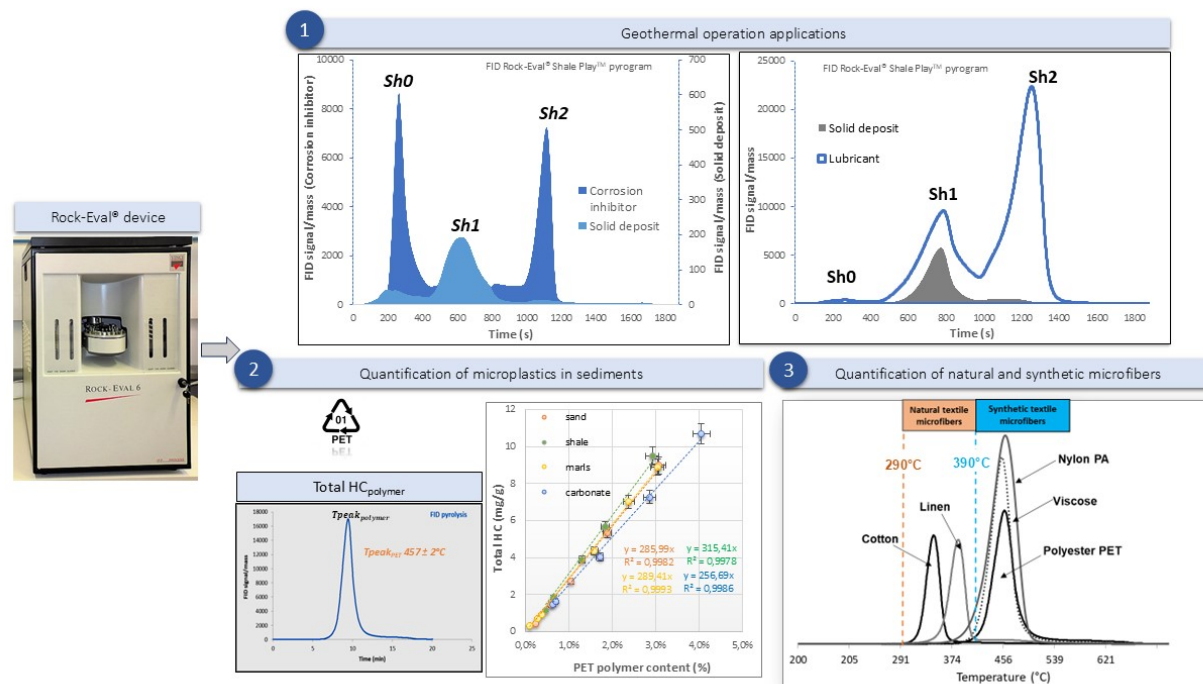
Figure 1 : Rock-Eval® application examples covering new themes in the fields of Earth Sciences and environment technologies.

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>> ISSUE 57 OF SCIENCE@IFPEN

Organic matter characterization

Emmanuel Hache

Emmanuel
Hache

Price, cycle and scarcity on the raw materials markets:
from oil to energy transition materials

A historical, economic and geopolitical perspective
(HDR, 2021)

The scope of my accreditation to direct research (HDR) covered fifteen years of research at IFPEN on **raw materials and market prices formation mechanisms**, with a specific focus on **the short-, medium- and long-term dynamics**. This work was partly informed by research conducted within the framework of the ANR **Generate** (Geopolitics of renewable energies and prospective analysis of the energy transition) project, which I led between 2018 and 2020.

Trois contributions illustrent la démarche que j'ai adoptée.

Three contributions illustrate the approach I adopted.

Against a backdrop of global economic and geopolitical transformations, the first of these focused on revisiting the long-term factors that can influence **oil prices** and **the principles of coordination between players**. To this end, it examined **the influence of the Organization of the Petroleum Exporting Countries** (**OPEC**) on markets as a function of the different price regimes observed since 1970, using various econometric methodologies (co-integration, Granger causality, panel data analysis, etc.) [1].

The second contribution focused on **the relationships between financial markets and short-term price dynamics** by estimating **a Markov Switching Vectorial Error Correction model (MS-VECM) with two distinct states (standard state and crisis state)**[1]. The analysis specifically related to the relationships between the Spot and Futures prices of WTI[2] in the USA and highlighted the role of speculation, particularly during the financial crisis of 2007-2008 [2].

The third contribution covered **the evaluation of the criticality of raw materials** present in low-carbon technologies using the TIAM-IFPEN model. This research highlighted **the soaring demand for these resources**, and **the importance of water**, through the modeling of value chains for materials such as bauxite, cobalt, copper, lithium, nickel and rare earths. Taking lithium, for example (figure), for a scenario of +2°C with business as usual mobility, an increase in consumption of this element representing 47% of resources over the period 2005-2050 can be observed, i.e., a reduction of the safety margin to 53%, compared to 63% with new mobility standards [3].
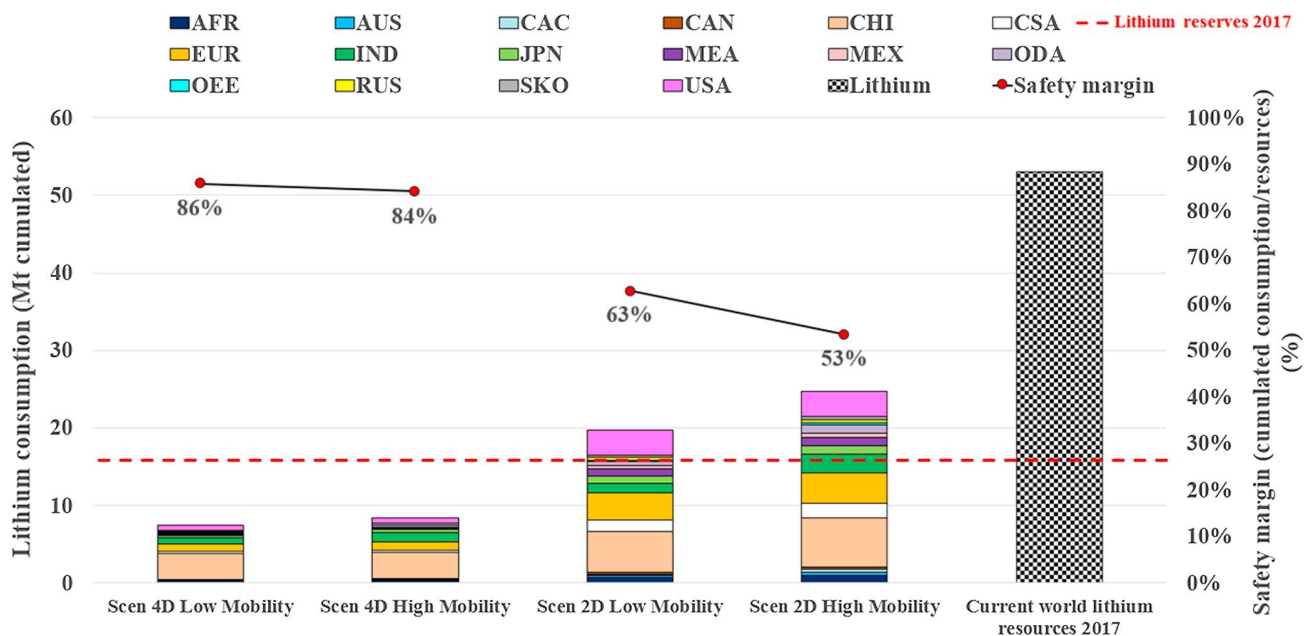
Lithium safety margin calculated based on consumption between 2005 and 2050 and available resources in 2017

Obtaining the HDR has enabled me to consolidate my academic credentials and develop new research projects, including **the ANR Get More H2 project** (Energy Transition Geopolitics and Global Economic and Social Modeling of Hydrogen Production Technologies), which runs from 2023-2027, in partnership with the CEA (French Alternative Energies and Atomic Energy Commission), Paris-Nanterre University and IRIS (the French Institute for International and Strategic Relations), and which I am coordinating.

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>> ISSUE 57 OF SCIENCE@IFPEN
Raw materials markets: at the heart of energy challenges

Sedimentary budgets :
concept, methods and integration in basin analysis
on a land-sea continuum
(HDR 2022)

Sébastien
Rohais

In a given sediment compartment[1], **the sedimentary budget consists in evaluating sedimentary inputs, transfers and exports, and equating them to the net gain or loss over a specified period of time** (figure).

Sedimentary budgets are very widely used in geosciences:
-    they have been used for many years in the field of oil exploration to predict the occurrence and quality of oil reservoirs or source rocks;
-    and more recently in the environmental field, as a component of risk assessments, in order to anticipate coastal erosion and adjust land-use planning in a context of climate change.
Often deployed on a sediment compartment scale, **these budgets, when integrated on a larger scale, offer the possibility of acquiring a global vision of sedimentary systems**. Thus, through the development and implementation of numerical methods and tools, my HDR research was aimed at quantifying these budgets on a sedimentary basin[2] scale across the land-sea continuum (see figure). The approach adopted helped determine the relevant boundary conditions and gain a better understanding of the interactions between the various compartments, based on global balances.

SYSTEM
Sediment budget

SOURCE
Inputs

SINK
Outputs
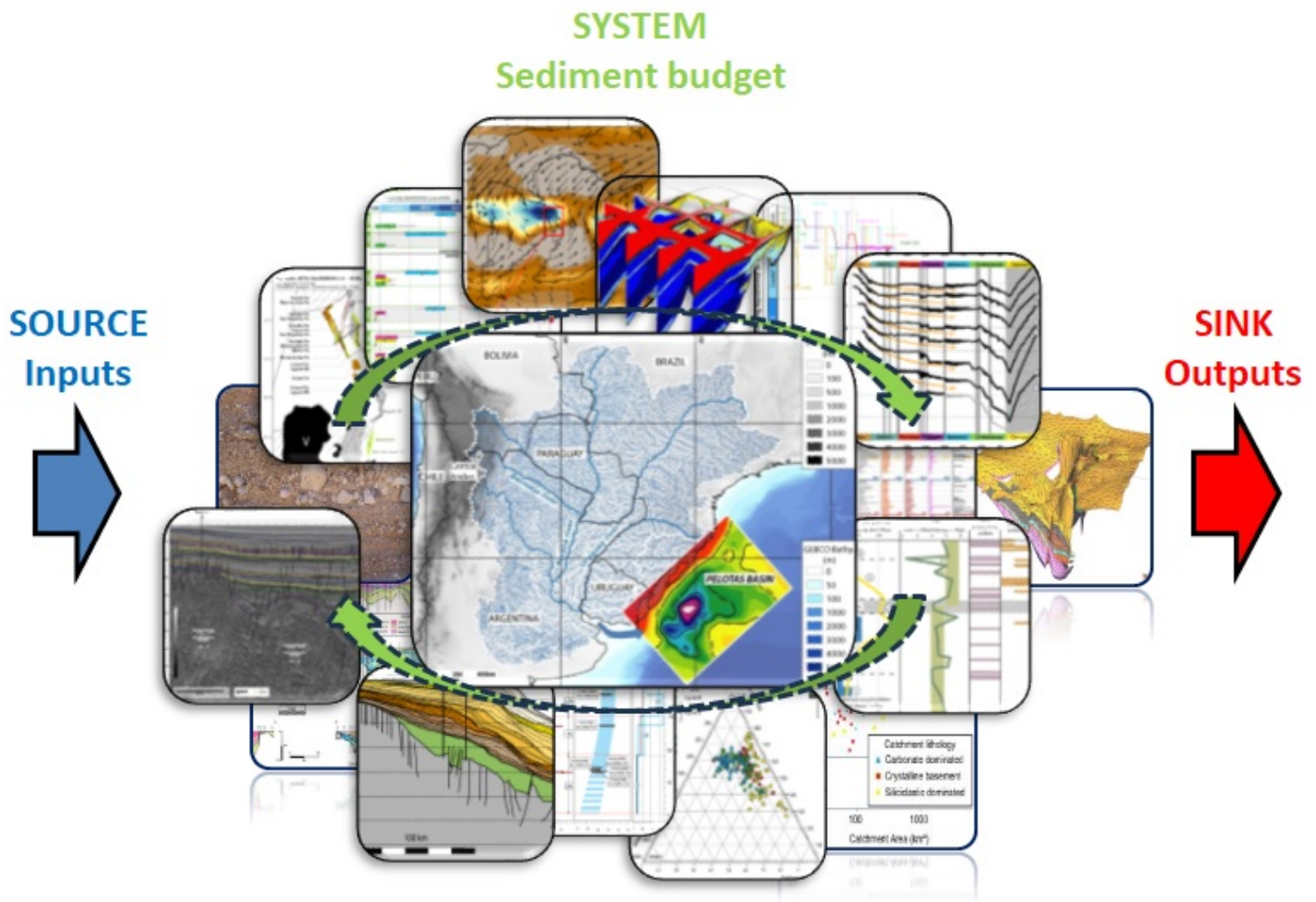
[1] A sediment compartment is a distinct geological zone characterized by specific deposit conditions
[2] A sedimentary basin is a depression of the Earth's crust, often very extensive, where sediments accumulate over a long period of time. They may contain several types of sedimentary rocks

This research has resulted in direct applications at IFPEN for:
•   **basin modeling**: in order to characterize the deformation dynamics of sedimentary basins (such as burial or uplift rates, for example), with implications for the determination of thermicity[3]), the timing of deformation[4] and/or sand generation periods, all information that is essential in basin and reservoir exploration [1, 2];
•   **reservoir modeling**: to link the stratigraphic architecture of sedimentary basins to climate forcing, with a view to better constraining the distribution, heterogeneities and quality of a source rock or reservoir [3];
•   **impact analysis**: to anticipate the response of landscapes and landforms to climate-related, catastrophic and extreme events, with a particular focus on the issue of erosion [4];
•   **the environment**: to track and trace pollutants, such as plastics and microplastics, with a view to defining environmental monitoring tools and proposing remediation solutions [5, 6].
With respect to the latter aspect, which represents a major challenge for our societies, my research represents an important step forward in terms of **identifying and characterizing areas where**

microplastics accumulate, with a view to applying appropriate solutions. The three PhD theses I have been co-supervising since 2023 all fit squarely with this crucial area of research for the environment.

[3] Time and space evolution of underground temperature
[4] i.e., a chronological timeline of major events affecting basin structures

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>> ISSUE 57 OF SCIENCE@IFPEN

Elodie Devers

The life cycle of hydrotreatment catalysts: from active phase genesis to catalyst recycling (HDR 2023)

Catalysts are essential products for numerous industrial processes, including **the hydrotreatment of oil feeds or bio-based feeds**. Their properties stem from the active metal materials they contain, the value and criticality[1] of which justify efforts to recover them from waste products. Accordingly, as **a major producer of catalysts**, one of IFPEN 's key priorities is to apply **the principles of the circular economy** to them. To improve their recycling, it is essential to have a thorough understanding of the life cycle of these catalysts - made up of transition metal sulfides on a porous alumina-type oxide (figure 1) - and this was the focus of my national accreditation to direct research (HDR).

The results presented summarize research conducted within the framework of some ten PhD theses and post-doctoral projects that I supervised in partnership with academic laboratories. From a fundamental point of view, this research was aimed at acquiring **a better understanding of the link between the genesis of these materials and their catalytic performances,** drawing on innovative synthesis and advanced characterization methods (ASAXS[2], in-situ XAS[3]).
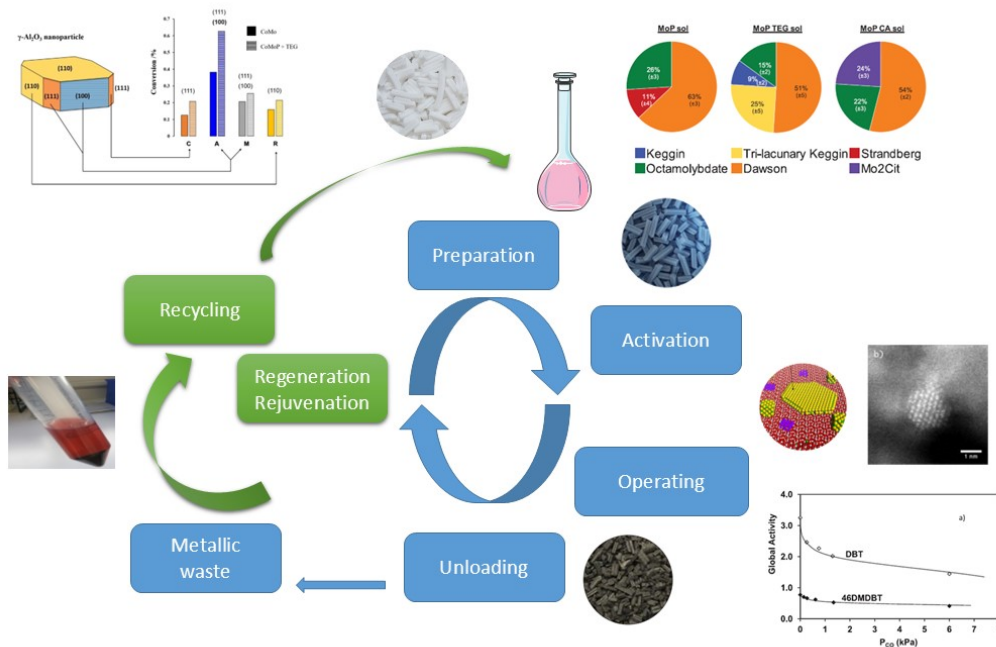
Figure 1: Diagram illustrating the life cycle of refining catalysts

[1] The majority can be found on the European Union's list of critical metals
[2] Anomalous Small-Angle X-Ray Scattering
[3] X-ray Absorption Spectroscopy

For example, with regard to **the effect of the support (alumina, titanium oxide and silica)**, groundbreaking results were obtained concerning the influence of the crystallographic nature of alumina, leading to the proposal of an original approach in the field of surface science. Thus, the effects of alumina face orientation on interactions with the active phase, the rate of sulfidation, the promotion ratio of MoS_2 by Co and ultimately on **HDS performance**[4] were demonstrated as a function of the presence of a dopant, such as phosphorus and/or organic additives [1].

The study of the catalyst activation stage revealed differences in the sulfidation mechanism depending on whether it is carried out in the gas phase, as is standard practice in laboratories, or in the liquid phase, as is the case in the refinery setting. In addition, a novel combination of Raman spectroscopy and XAS enabled the first ever speciation of molybdenum-based substances, firstly in an aqueous solution, and secondly supported on an alumina surface. This paves the way for **new insights into catalyst oxide precursors and their link with catalytic performance** [2].

Lastly, **the operational function of catalysts** was studied, with a specific focus on **the impact of inhibitors on their deactivation and regeneration**. The inhibitors chosen for this were the oxygenated compounds H_2O and CO, particularly representative as by-products of the oxygenated substances contained in large quantities in the new biomass-derived streams now entering refineries in the context of co-processing [3]. This research highlighted the challenges of meeting refined product specifications while coping with increasingly heterogeneous feedstocks, in particular the search for new, more efficient and resistant catalysts.

The solid foundation of knowledge resulting from this research can be used to generate proposals for future catalyst recycling strategies and processes.

4 Hydrodesulfurization

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>> ISSUE 57 OF SCIENCE@IFPEN

Catalysts and the circular economy

Laurent Cangémi

Contribution to the study of couplings in interfaces, polymers and porous materials (HDR 2023)

The work conduced within the context of my HDR (accreditation to direct research) relates to the field of modeling and concerns **the formulation of multiphysical couplings in materials**. The starting point for this research related to an industrial damage problem: cavitation caused by the explosive decompression of dissolved gases in the polymers used to seal flexible underwater pipes. By extension, it applies to all **porous media** exposed to **the effects of mass transfer, heat, plasticity or damage**, such as catalyst supports or natural underground environments.

Within this context, some couplings between plasticity and damage were also examined from different angles: a two-phase viscoplastic approach and cohesive zones[1].

The general approach I followed consisted in adopting the theoretical framework of the **Thermodynamics of Irreversible Processes** (TIP)[2] in order to deduce coupled behavior laws that are consistent with the fundamental principles of thermodynamics. The findings are the result of close collaboration with academic partners[3].

This approach shed light on existing coupling processes between **mass transfers and deformation and damage phenomena in semi-crystalline polymers**[4] [1,2]. More specifically, the mixed Fickian and Darcean nature of these transfers induces internal stresses that can generate localized cavitation phenomena that are seemingly counter-intuitive (the material being in a state of compression). Figure 1 illustrates an example of cavitation obtained in a Polyvynilidene fluoride (PVDF) polymer exposed to high external water pressure.

Beyond this example, the theoretical framework obtained makes it possible to propose an explicit form for a chemo-mechanical constraint, by introducing **chemical potential as the main driving force behind the couplings**. This formulation can, for example, be extended to **the description of sorption laws in nano-confined porous media** (such as zeolites[5]) or to **dendrite growth in solid electrolyte batteries**. On this latter theme, research is underway to adapt the model's formalism to

the presence of electric fields and electrochemical phenomena.

The approach was recently used to develop **new porous material architectures via topological optimization** [3] and we plan to deploy it for the case of concentrating solar heat exchangers for energy-intensive processes or for solar fuel production (see Figure 1). A further future application involves the design of optimized magnets to increase the efficiency of electric machines.
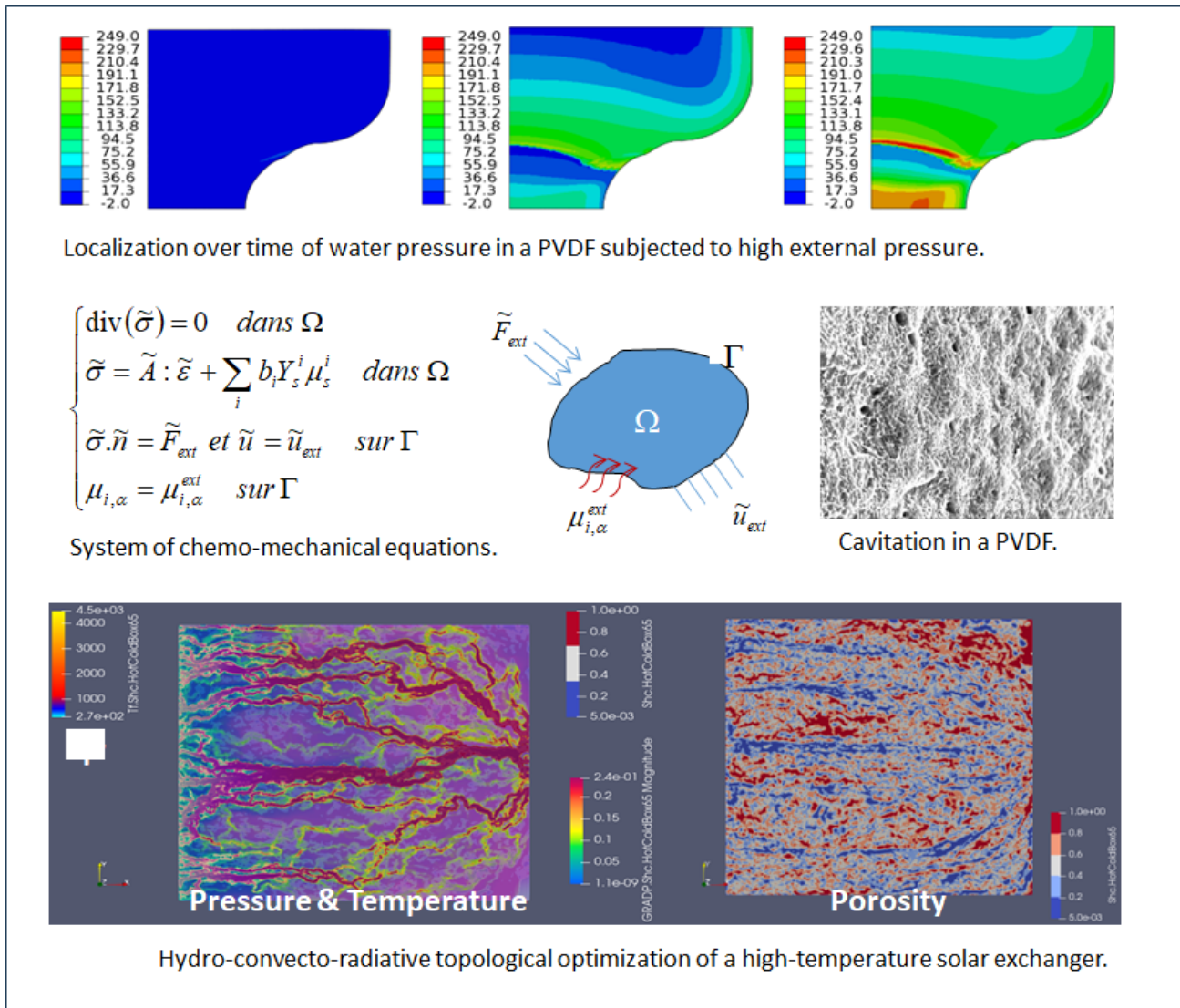

Localization over time of water pressure in a PVDF subjected to high external pressure.

$$\begin{cases} \mathrm{div}(\tilde{\sigma}) = 0 \quad dans\ \Omega \\ \tilde{\sigma} = \tilde{A} : \tilde{\varepsilon} + \sum_i b_i Y_s^i \mu_s^i \quad dans\ \Omega \\ \tilde{\sigma}.\tilde{n} = \tilde{F}_{ext}\ et\ \tilde{u} = \tilde{u}_{ext} \quad sur\ \Gamma \\ \mu_{i,\alpha} = \mu_{i,\alpha}^{ext} \quad sur\ \Gamma \end{cases}$$

System of chemo-mechanical equations.

Cavitation in a PVDF.

Pressure & Temperature

Porosity

Hydro-convecto-radiative topological optimization of a high-temperature solar exchanger.

Figure 1. Examples of applications of the coupled mechanical approach developed

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[1] Cohesive zone formalism enables the mechanical behavior of interface discontinuities between two media with different properties to be considered through displacement jumps
[2] Unlike "conventional" thermodynamics (reversible transformations), the framework makes it possible to describe out-of-equilibrium systems that evolve through a sequence of equilibrium states.
[3] Particularly Institut P' and Poitiers University
[4] Crystalline aluminosilicates of interest for the manufacture of catalyst supports

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>> ISSUE 57 OF SCIENCE@IFPEN

Multiphysical couplings in materials modeling

Senta
Blanquet

The degradation of plant biomass by the Trichoderma reesei enzyme cocktail:
composition, interactions and improvement avenues (HDR 2024)

The development of alternative, low-carbon energies is essential in order to reduce greenhouse gas emissions and tackle climate change. One example is **second-generation bioethanol**, produced from lignocellulosic biomass and used as a fuel in the mobility sector.

My research, conducted over a period of more than 15 years at IFPEN and summarized in my HDR (accreditation to direct research), has focused on a crucial step in the production process for this biofuel: **enzymatic hydrolysis**[1]. Biomass degradation is carried out by **a complex cocktail of enzymes produced by the filamentous fungus Trichoderma reesei**. However, for industrial purposes, it is necessary to enhance the performance of this cocktail. It was to this end that I studied various aspects of its production, composition and improvement:

- Conditions for cellulase[2] gene induction;
- Regulation of the secretion of these enzymes and identification of target genes to increase the fungus' secretion capacity.
- Enzyme interaction with the lignocellulosic substrate at various stages of hydrolysis;
- Using a mathematical model, identification of limiting enzymes for a given substrate (limitation being due to their inadequate proportion in the cocktail and/or their insufficient activity). For the hydrolysis of wheat straw, the composition of a cocktail leading to   maximized yield could be predicted;
- **Improvement of the cocktail** via the addition of **enzymes obtained from microbial biodiversity** (see figure).

With respect to the latter point, the enzymes secreted (known as **the "secretome"**) by different **filamentous fungi**, such as Podospora anserina and Aspergillus japonicus, were analyzed. From the secretomes providing the biggest boost of activity when incorporated in the T. reesei cocktail, the enzymes potentially responsible for this improvement were identified using mass spectrometry. In one of these secretomes, AA16s, a new family of enzymes capable of boosting cellulases was discovered and characterized [1].

I also explored bacterial biodiversity within a metagenomic approach[3]. Initially, a functional screening of a gene library resulted in the identification of about forty enzymes acting on lignocellulosic biomass. Four enzymes belonging to a family of endoglucanases were then characterized and their mechanism of action on cellulose was described [2].
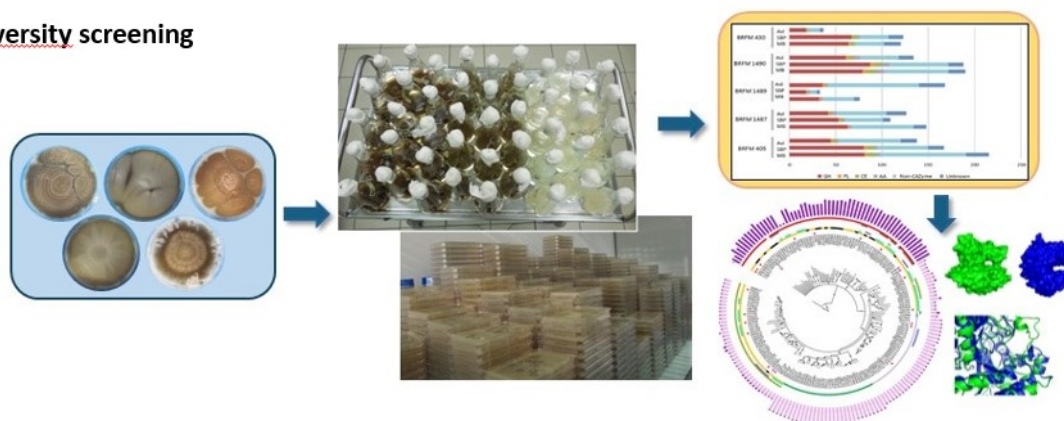
[1] Degradation of a compound in the presence of enzymes following its reaction with water
[2] Enzyme that hydrolyses cellulose
[3] A method for studying the genetic content of samples taken from complex environments

This research opened up new avenues for progress, through the identification of limiting enzymes and targets for improving the secretion system in T. reesei. As a result, I demonstrated the potential of biodiversity exploration for the discovery of new efficient enzymes, and it is in this vein that I am currently pursuing my research.

Biodiversity screening workflow: Fungal secretomes (top photo) or metagenomic library clones (bottom photo) are tested for their activity on a representative substrate. The best samples then undergo further analysis (biochemical, phylogenetic, structural modeling, etc.)

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>> ISSUE 57 OF SCIENCE@IFPEN

Biochemical conversion of biomass

Issue 57 of Science@ifpen - French accreditation to supervise research
28 February 2025

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