

# LGPM, EA 4038

## LABORATOIRE DE GÉNIE DES PROCÉDÉS & MATÉRIAUX



**T**he LGPM research department works on two fields of investigation in close interaction: chemical and biochemical engineering and materials. Modelling, simulation and experimentation are the common pillars of the different research themes addressed.

### **Sustainable industrial production as a key challenge for the Twenty-First Century**

This complementarity makes possible to start from the understanding of microscopic phenomena to the intensification of transformation and elaboration processes through the simulation and optimisation. Scaling-up and multi-scale approaches are therefore often at the heart of its actions and are the preferred means of moving from academic studies to industrial applications. Our know-how, firmly anchored in process engineering, is applied to the sustainable aspects of material transformation processes (material and energy savings, optimisation and intensification), bioprocesses (use of living organisms to consume and transform biomass into added value products) and the development of bio-materials.

These Departmental competences have been strengthened by the participation of the LGPM in the creation of a Centre of Excellence for Industrial Biotechnology (CEBB) at the end of 2010 in Pomacle (close to Reims/Grand-East Area). Altogether 75 researchers, post-doctorate and PhD students located on both sites (campus Paris-Saclay and campus Reims-Pomacle) are deeply involved in the promising fields of the bio-economy and decarbonisation of the industry.

The Department is organised in three Teams:

#### **MATERIALS & BIOMATERIALS**

- Liquid metals, wetting and reactivity at high temperature
- Wood, bioproducts, bio-based materials, building materials
- Coupled heat and mass transfer
- Elaboration and transformation processes
- Characterisation, upscaling, multiscale modelling

#### **CHEMISTRY & SEPARATIVE PROCESSES**

- Separation and purification by liquid-liquid extraction, membranes, electro-chemistry, preparative chromatography, crystallization
- Multiphase flows (liquid films, drops, bubbles, particles), deposition
- Process intensification
- Trace analysis and sample preparation - Exobiology

#### **BIOPROCESSES**

- Biological processes (suspended and immobilised cultures)
- Multi-scale modelling and bioreactors control
- Cell/community characterization (biofilm structure, microalgae characterization on *lab-on-chip* systems,...)
- Use of microorganisms to treat wastewater/ produce biofuels (lipids from microalgae, methane generation,...)
- Production and purification of high value molecules

# REMARKABLE EQUIPMENT/SKILLS

## 2D and 3D imaging:

Confocal Laser Scanning Microscope (CLSM), Environmental SEM + EDS, Interferometric microscope, Nano-tomography, Optical Coherence Tomography (OCT), Particle Image Velocimetry, Raman microscope, Image processing tools.

## Analysis/characterisation:

ATG/DSC coupled with GS-MS, BET, CHNSO, DMA, triple quadrupole ICP-MS Spectroscopy (UV, IR, MS, Raman, fluorescence X), UHPLC-Orbitrap (HRMS), UHPLC-IMS-QToF (TIMS-ToF), laser and morphological size analysers, flow cytometry, liquid and gas chromatographs, mass diffusion, mineralizer, Motorized MicroProfiling System for O<sub>2</sub> and pH measurements permeability, rheometer, sorption isotherms, tensiometer, wetting measurements at high temperature, chromatic confocal measurement of film thickness.

## Processes and pilot devices:

Bioreactors, Drying, Dispensed metal drop device, Electrodialysis, twin-screw extruder, Liquid-liquid extraction, Photo-bioreactors, Preparative chromatography, Reverse osmosis, Powder flowability tests (rotating drum), Thermal treatment, Ultra- and nano-filtration, Versatile annealing device.

## Modelling/simulation:

CFD (OpenFOAM), Discrete modeling of particles (LIGGGHTS), Discrete and continuous modeling of Bioprocess, Machine learning, Chemometrics, Image-based representation, Meshless methods (LB, MPM...), Multiscale modeling of reactive and bio-active transfer in heterogeneous media, Up-scaling. Access to HPC computers (Ruche, Romeo).



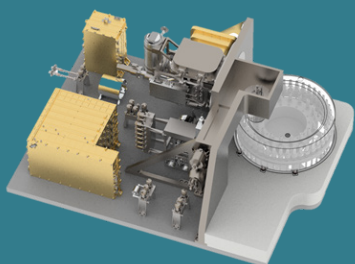
(a) Twin screw extruder enables the elaboration of new biomaterials, the extraction of molecules of interest from biomasses and reactive extrusion to be carried out by adding various reagents and enzymes. It's a versatile tool calibrated for research and scale-up. (b) example of a new biocomposite produced with agro-industrial by-products to substitute traditional plastics.

## APPLICATION DOMAINS

- 2G/3G biofuels,
- Astrobiology,
- Biogas purification,
- Bioprocessing design and evaluation,
- Biotechnologies,
- Developing innovative bio-sourced materials,
- Digital twins applied to sustainable development,
- Exobiology,
- Hydrogen production from biomass,
- Instrumental development for space application and search for trace of life in the universe,
- Iron coating,
- Liquid metal heat exchanger,
- Mould/ yeast / bacteria / microalgae production,
- Tissue scaffold for bone regeneration.

# HIGHLIGHTS 2022

- **Purification processes of H<sub>2</sub>** obtained from solid biomass were developed following an approach based on the digital twin concept (patent FR3106284).
- LGPM, in collaboration with LATMOS and NASA, is involved in the instrumental development of the future **DraMS instrument** aboard NASA's Dragonfly mission, which will explore Saturn's largest moon, Titan.
- **Drug bioproduction:** bioprocess modeling with metabolic shifts and recent results on new bioreactor sensors (Calipso project).
- **Patrick Perré**, Professor and head of CentraleSupélec Biotechnology Chair, received the Gold Medal from the *Académie d'Agriculture de France* (AAF) for "his work in physics and biotechnology, linking theory and industrial applications".
- **Manasa Periyapattana-Iyer** (Cifre thesis supported by Air Liquide) received the first Prize in the CentraleSupélec Foundation's Impact Thesis Award in the category "Impact Innovation", for her comprehensive study of distillation packing hydrodynamics.



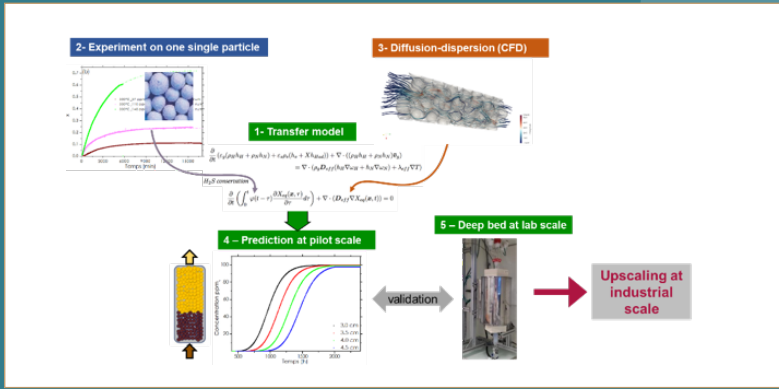


Fig.1.1 Scientific approach used to design and optimise the process for eliminating  $H_2S$  and  $CO$  from  $H_2$  on an industrial scale using numerical simulation, supported by lab measurements and validated by a lab pilot

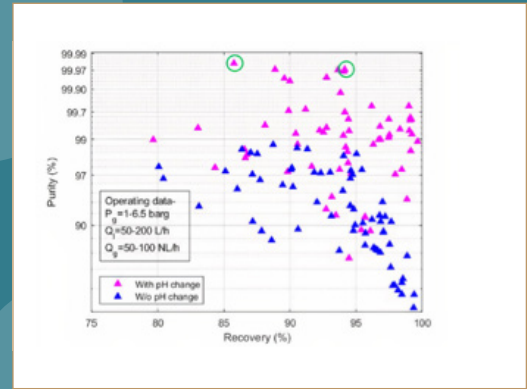


Fig.1.2  $H_2$  purity and yield with the new patented process (with pH swing) and the previous one (without pH swing)

Contribution to the design and optimisation of  $H_2$  purification from syngas, as part of the PIA3 "Vitrhydrogène" project led by Haffner Energy (2018-2022) and funded by ADEME ("Démonstrateur de la Transition Ecologique et Energétique" programme). LGPM worked to eliminate pollutants: (Fig 1.1) For  $H_2S$  and  $CO$ , experiments were carried out first on a grain scale (by TGA), then on a fixed bed scale, which made it possible to estimate the capacity of the solid phases, the reaction kinetics and any equilibria. This information was used to produce two numerical tools for estimating performance depending on the operating conditions, with the aim of optimising and sizing this purification system. (Fig 1.2) For  $CO_2$ , using a digital twin, an "in silico" solution was obtained for reducing the residual  $CO_2$  to below 10 ppm. After validation in a laboratory pilot, the process was patented (FR3106284), then optimised, in order to follow the evolution of the syngas enrichment and purification chain.

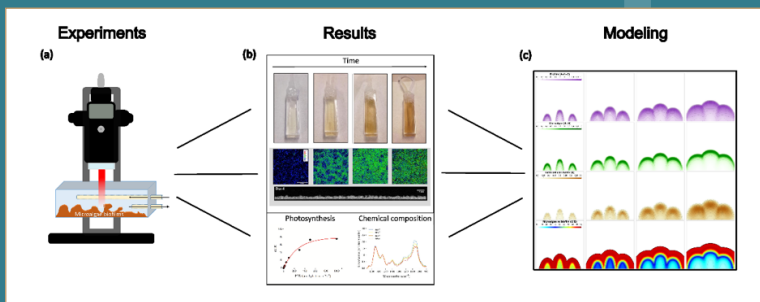


Fig 2. Microalgae biofilms are spatially organized communities with a great biotechnological potential, and the coupling of experimental and computational strategies represents a robust approach to finely characterize these complex biological systems. A fluidic device was developed to cultivate and characterize microalgae biofilms using optical methods, such as confocal laser scanning microscopy (CLSM) and optical coherence tomography (OCT) (a). Metabolism was also monitored by measuring cells photosynthesis and biochemical composition (b). This experimental setup allowed to show that cell physiology is more affected in thicker biofilms as a consequence of alterations in local environmental conditions (Fanesi et al., *Biotechnology and*

*Bioengineering* <https://doi.org/10.1002/bit.28147>). Computational approaches can be used to investigate hypothesis that are too complex for experimental strategies. Using a spatial 2D-model, microalgae biofilm development was simulated and it was found to be inhibited by oxygen accumulation and water limitation (c) (Polizzi et al., *PLoS Computational Biology* <https://doi.org/10.1371/journal.pcbi.1009904>). These works suggest that biofilm 3D architecture and metabolism are key traits that must be fully understood to optimise their utilisation in bioprocesses.

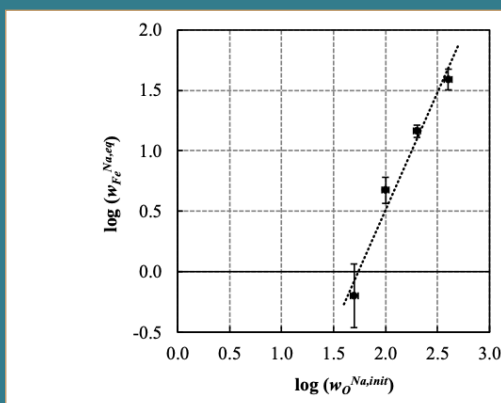


Fig. 3.1. Variation in the mass fraction of iron in liquid sodium at equilibrium as a function of the dissolved oxygen content at 550 °C.

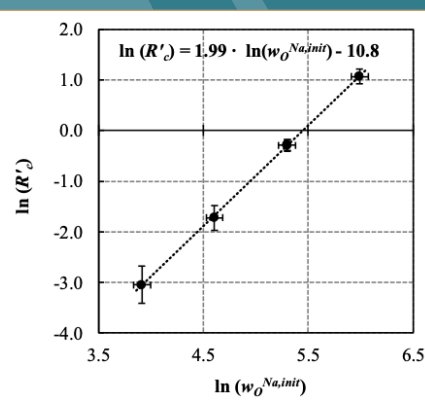


Fig. 3.2. Thickness loss rates  $R'_2$  of iron in  $\mu m/year$ , at 550 °C as a function of dissolved oxygen content in ppm (50, 100, 200, 400 ppm).

Liquid sodium can be used as a heat transfer fluid in heat exchangers. Under isothermal conditions at 550 °C, the equilibrium iron concentration  $W_{Fe}^{Na,eq}$  follows a power law of order 2 as a function of the dissolved oxygen content  $W_O^{Na,init}$  in liquid sodium (Fig. 3.1), due to the formation of a soluble complex  $NaFeO_2$ . An equilibrium law of this complex in liquid sodium was developed as a function of temperature and dissolved oxygen content (S. Meddeb et al. *J. Nucl. Mater.* (2022) <https://doi.org/10.1016/j.jnucmat.2022.153785>). The rate of pure iron dissolution in liquid sodium  $R'_2$  follows a power law of order 2 as a function of the dissolved oxygen content (50-400 ppm) (Fig. 3.2). The corrosion kinetics measured is limited by the transfer of the soluble complex through the mass transfer boundary layer [S. Meddeb et al. *J. Nucl. Mater.* (2023) <https://doi.org/10.1016/j.jnucmat.2023.154541>).

## Industrial Partners

- AIR LIQUIDE
- ARCELORMITTAL
- ARD
- BIOREA
- CEA
- CHENE et Cie
- CNES
- CRISTAL UNION
- DRY4GOOD
- EDF R&D
- ECOTECNILIN
- EUROPEENNE DE BIOMASSE
- GENOMINES
- GIVAUDAN
- GRT gaz
- HAFFNER Energy
- IFPEN
- INALVE
- INEVO
- INTERNATIONAL ZINC ASSOCIATION
- LESAFFRE
- Metha'groupe
- MIYOSHI
- NUTROPY
- OLYGOSE
- PROCESSION
- PRONOE
- PROSNY NC
- SANOFI
- STH Biotech
- SYNOVANCE
- TIPEE
- THALES ALENIA SPACE
- TMA Process
- VEOLIA
- V.E.R.A. SAS
- VICAT
- VITO
- WIGWAM
- YPSO-FACTO

## Academic Partners

**International:** School of Mathematical Sciences QUT (Australia), University of São Paulo (Brazil), São Paulo State University (Brazil), EMBRAPA (Brazil), ITAL (Brazil), Federal University of Rio de Janeiro (Brazil), Université du Québec in Abitibi-Témiscamingue (Canada), Danish Technological Institute (Denmark), Gottingen University (Germany), Institut Von Karman (Germany), Max Planck Institute for Solar System Research (Germany), Technical University of Dresden (Germany), University of Hannover (Germany), University of Padova (Italy), TU Delft (Netherlands), Wageningen University (Netherlands), University of Almeria (Spain), Engineering school of Monastir (Tunisia), Engineering School of Sfax (Tunisia), Higher Institute of Biotechnology of Beja (Tunisia), University of Carthage (Tunisia), Imperial College London (UK), GSFC-NASA (Maryland, USA), JPL-NASA (Pasadena, USA), Ohio State University (USA).

**France:** AgroParisTech, ENS Paris Saclay, ESIEE (Noisy-le-Grand), GEPEA (Nantes), IFREMER, INRAE (Antony, Jouy en Josas, Narbonne), IMFT (Toulouse), INRIA, INSERM, IS2M (Mulhouse), Institut de Matériaux Microélectronique, LRGP (Nancy), Nanosciences de Provence, SMS (Université de Rouen), Sorbonne Université (UPMC), Unilasalle Beauvais, Université Picardie Jules Verne, Université Reims-Champagne Ardenne, Université de technologie de Compiègne, Université de Lorraine, Université la Rochelle, Université Savoie Mont Blanc.

## Key figures

- Professors, Associate Professors & Scientists 30
- Engineers & Administrative staff 20
- PhD Students 20
- PostDocs 7
- Publications of the year (WoS) 31

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