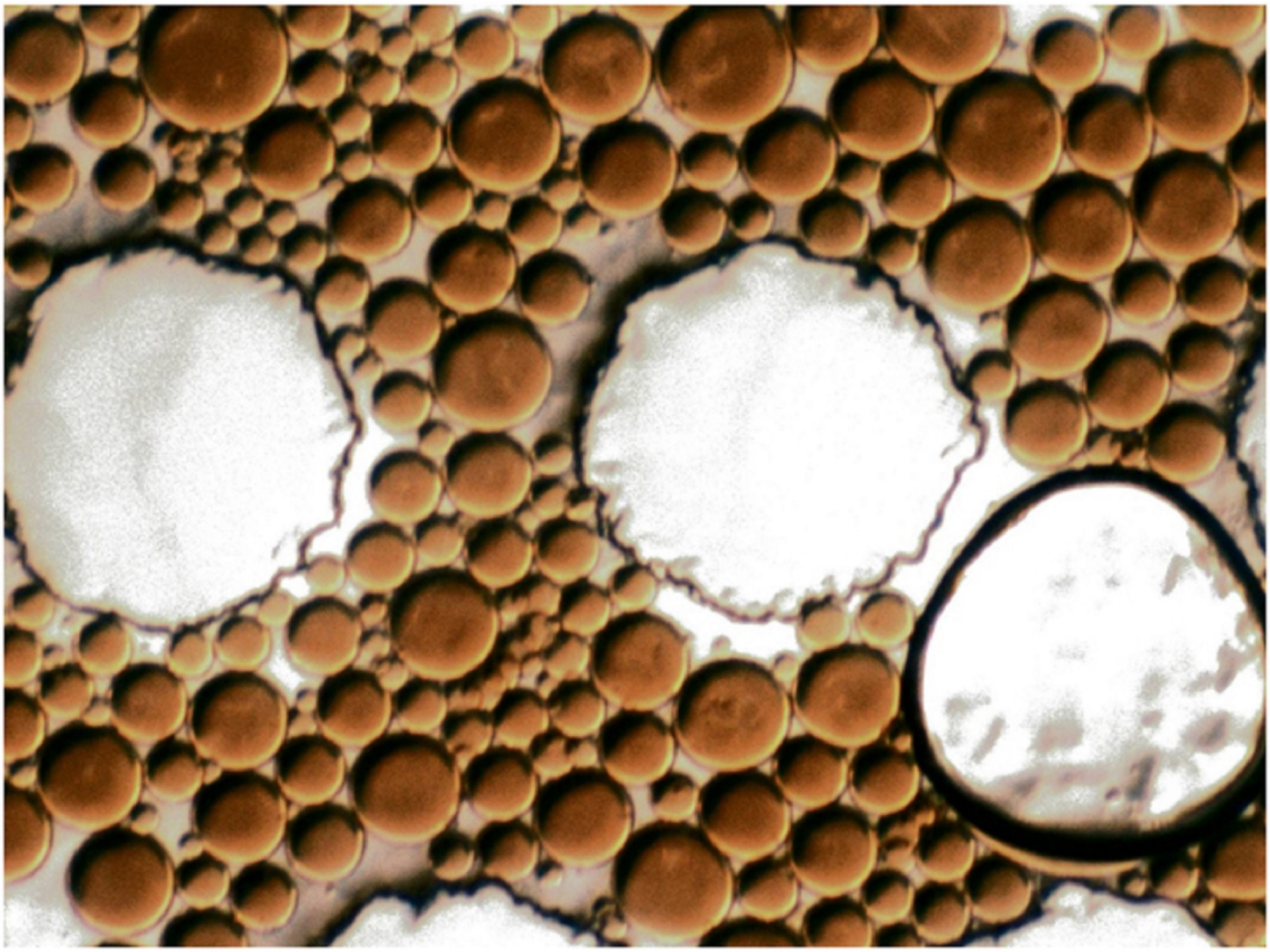


Written on 17 October 2023

10 minutes of reading

News

Fundamental Research

Geology - Sedimentology

Geostatistics - Geological modeling

Petrophysics and transfers in porous media

Chemical engineering and process engineering

Porous media are relevant in **many technological and industrial fields** set to play an important role in the future: energy storage, pollution control, water treatment, renewable energies, biofuels, food-processing and health.

The study of these media requires contributions from numerous different scientific disciplines, including **computational fluid mechanics**, **geosciences** and **process engineering**.

For the 16th edition of JEMP**, the porous media study days event**, hosted by IFPEN from 17 to 19 October 2023, four scientific developments, supported by significant examples, show the variety of fields of application of these porous media and the diversity of approaches deployed by our researchers to study them.

LES BRÈVES

Underground reservoir modeling in essential for many applications: aquifer management, underground compound or energy storage, mineral and energy resource recovery (e.g., geothermal energy). Modeling makes it possible to optimize resource management while minimizing societal and environmental risks. However, in order to be efficient, this modeling must be multiscale, and IFPEN's research teams are therefore guided by this requirement.

Multiscale geoscience modeling

It is easy to understand the multiscale structure of the systems under consideration, for example by observing an underground outcrop, and then extrapolating the underlying underground structure. Observation, as well as drilling and detailed geological/geophysical analysis confirm the existence of **embedded structures with scales varying from that of the pore, typically µm, to multi-kilometric scales**. Geologists, geophysicists and petrophysicists are capable of providing relevant description tools for each of the scales considered, but they remain non-exhaustive.

Ideally, IFPEN's geoscience specialists therefore have to construct models capable of reproducing this complexity, incorporating data observed at different scales, while at the same time taking into account the incomplete nature of the data.
Moreover, these researchers are quickly confronted with models with dozens of input parameters[1]. It is impossible to conduct a detailed exploration of a space of significant dimensions with existing or future calculation tools that soon come up against **the "dimension wall"**. It is this "wall" that justifies approaches such as "experimental design/model reduction" or recourse to artificial intelligence, which are associated with a considerable reduction in calculation cost, but ultimately rely on a very small learning base: at best a few thousand reference simulations to explore **a space with thousands of dimensions**.
A compromise is therefore to be found between these model reduction approaches and the need to maintain good physical coherence.

[1] positions of limits, layer thicknesses, porosities, well positions and trajectories, injection and fluid production flows, etc

Multiscale geoscience modeling

Historically, **the scale change idea** precedes the approaches already outlined while complementing them. The idea is to reduce both the unit cost and the number of degrees of freedom describing the cumulated dimension of the parameters[2]. To do so, the description of the geological model is aggregated by grouping the parameters in order to construct a reduced model that is sufficient to reliably explore the configurations of interest. This approach is justified by the idea that the interest primarily lies in average values (fluid volumes, ore content, etc.) evaluated for the volume of the formation under consideration. This makes it possible to obtain **an averaging effect** similar to a law of large numbers smoothing out the details of the cases under consideration.

[2] parameters qualified as controllable since they are reasonably known, or even chosen (well position, extraction flows) or said to be "uncontrollable" since they are imposed by nature, and therefore known

with a degree of uncertainty.

Research conducted

The approach adopted consisted in tackling a model flow problem in porous media combining **deterministic scaling** with **a stochastic approach**. This involved analyzing simulation results while arbitrarily drawing several “geological reality” scenarios represented in the form of **a random permeability map** using artificially generated structures. This research was reported in the articles referenced below. Some of the principal elements are described here.
Figure 1 illustrates the typical geometry of the simulation of a flow problem in porous media. The real geometry is “meshed” by a fine grid incorporating the details of the form of the boundaries and discontinuities of the domain, and each mesh is described by a set of parameters derived from geological data (porosity, permeability, etc.). An intermediate calculation scale is then used to obtain reliable results, i.e., without any significant degradation in the quality of discontinuity representation or that of geological data. This **optimal quality-cost compromise** can be determined by establishing the characteristic spatial scales of the solutions to the simplified problem.

The approach adopted consisted in tackling a model flow problem in porous media combining deterministic scaling with a stochastic approach. This involved analyzing simulation results while arbitrarily drawing several “geological reality” scenarios represented in the form of a random permeability map using artificially generated structures. This research was reported in the articles referenced below. Some of the principal elements are described here.

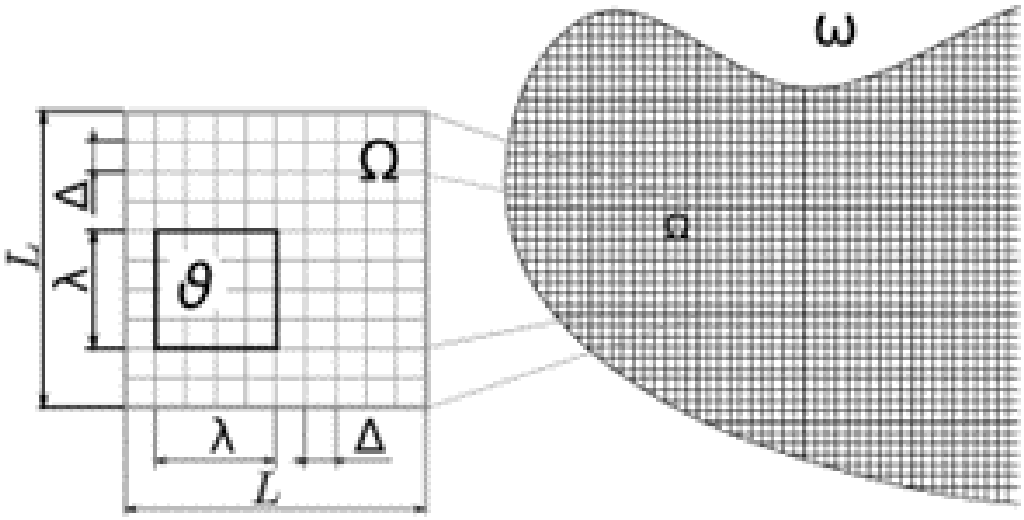


Figure 1 : the fine model is simplified by aggregating the fine mesh size ? into meshes of size ?>?. To keep control, the simulation is conducted for sub-volumes ? and by varying ? the evolution of the conductivity distribution can be quantified as a function of the averaging scale. This makes it possible to identify behaviors on a large scale: percolating, non-percolating, capable of being homogenized or otherwise, etc.

Figure 2 illustrates the post-treatment results obtained via a rapid resolution of the flow for a random medium. The histograms of the permeability distributions obtained via post-treatment of the solution at

different scales are shown on the figure on the right. Convergence of the distributions towards the Gaussian distribution illustrates the role of the size of the representative elementary volume. It can be noted that convergence toward a limiting distribution is slower when a bimodal permeability distribution is taken into account. At the connectivity (percolation) threshold, the bimodal character persists on a large scale and convergence towards “the equivalent homogeneous” becomes very slow, since the medium can hardly be homogenized anymore.

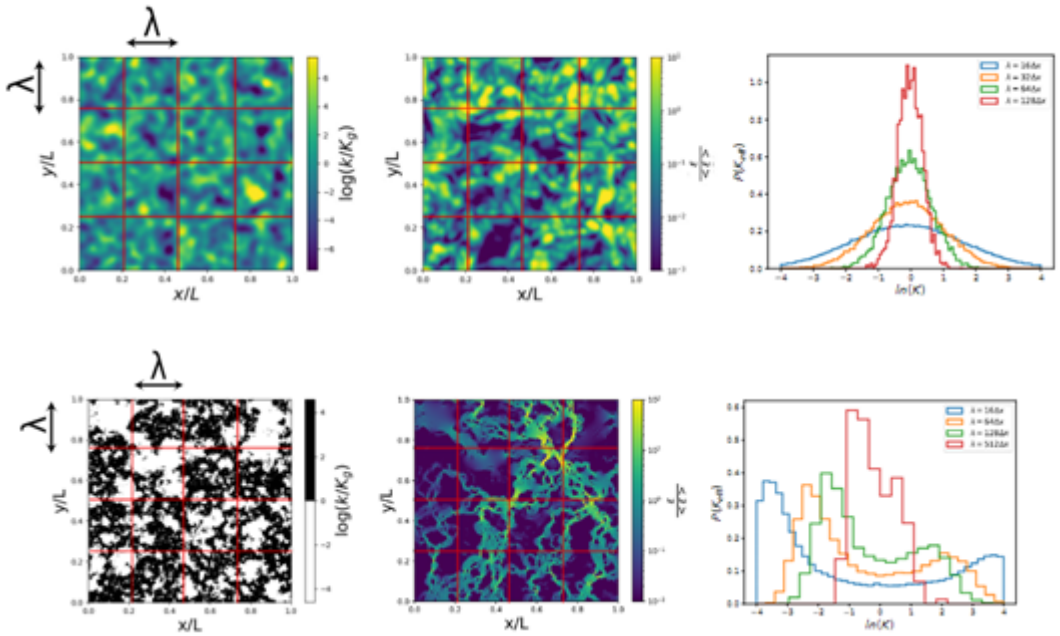


Figure 2 : Depending on the scale value ?, for a continuous distribution (top figure) or discrete distribution (bottom figure), local dissipation maps are observed that, suitably processed, can give access to the distributions of hydraulic conductivities in a single calculation. The flow localization phenomenon is clearly visible and can sometimes explain the limitations of experimental design-type approaches that neglect this phenomenon.

Figure 3 presents the permeability variance evolution (in Log) as a function of the distance to the percolation threshold, for various discrete image generation techniques (bottom of figure 2). The grouping of the curves can make it possible to rapidly anticipate the macroscopic flow regime for a specific case, and the relevant scales of a problem.

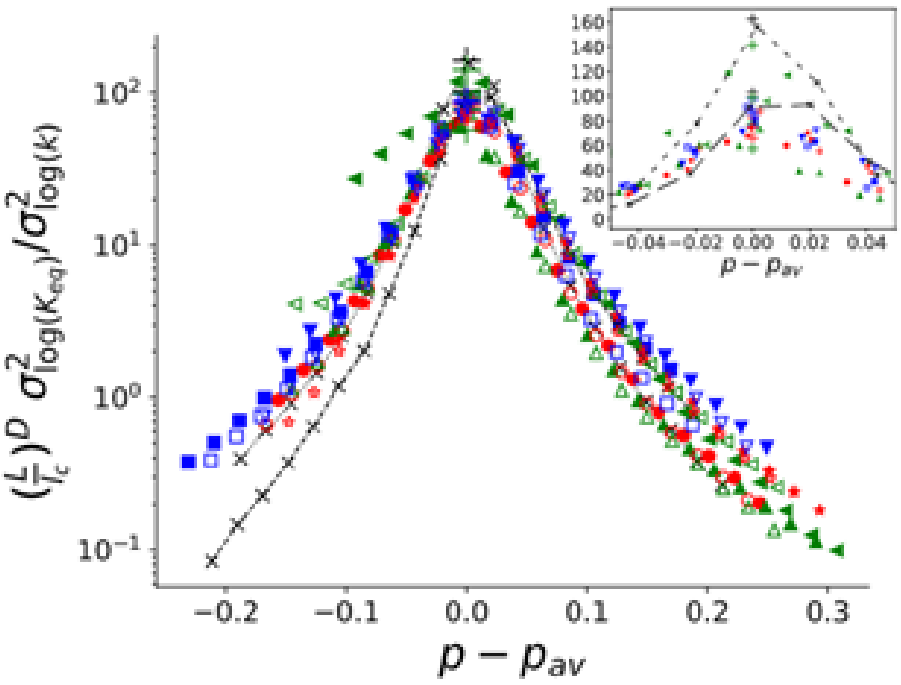


Figure 3 : Variance re-normalized by the number of correlated volumes and normalized by the small-scale variance, as a function of distance to the percolation threshold. The emergence of a “universal” curve can be observed (the colors represent heterogeneous media “manufactured” in different ways). This curve can be used to anticipate, with minimal calculation, the large-scale behavior of the case under consideration, and help to set up an experimental design strategy based on physics.

The results of this research provide a better understanding of **the scaling process** through **the sparing** (post-treatment) **use of simulation results**. By using this method, during the calculation process it becomes possible to identify relevant scales and parameter aggregates controlling end results of interest for applications. In particular, approaches of this type will be put to good use in the ERC Karst project.

References:

[1] Colecchio, I., Boschan, A., Otero, A. D., & Noetinger, B. (2020). On the multiscale characterization of effective hydraulic conductivity in random heterogeneous media: a historical survey and some new perspectives. Advances in Water Resources, 140, 103594, https://doi.org/10.1016/j.advwatres.2020.103594.
[2] Noetinger, B. (2020). Statistical physics and applied geosciences: some results and perspectives. Comptes Rendus. Physique, 21(6), 539-560, DOI:10.5802/crphys.40.
[3] Colecchio, I., Otero, A. D., Noetinger, B., & Boschan, A. (2021). Equivalent hydraulic conductivity, connectivity and percolation in 2D and 3D random binary media. Advances in Water Resources, 158, 104040, https://doi.org/10.1016/j.advwatres.2021.104040.

Scientific contact : B. Noetinger

YOU MAY ALSO BE INTERESTED IN

Fundamental Research

News December 2022

KARST research project : IFPEN recipient of an ERC Synergy Grant

Press release

Fundamental Research

News May 2023

Karst aquifers: IFPEN launches a research project in hydrogeology

Water cycle management

Geosciences | Geology - Sedimentology | Structural analysis and Imaging

Fundamental Research

News November 2019

Adrien Constantin De Magny Prize awarded to Benoît Noetinger

Geosciences

Modeling transfer in porous underground media: a multiscale approach

Pollutant transport in soils is directly dependent on the heterogeneity of the media present (topology, structure, etc.), which itself is heavily impacted by certain human activities, such as agriculture, industrial operations and mining. The precise description of this phenomenon, across all time scales, can thus prove complex. Yet it is important when it comes to tackling major challenges, such as efficient waste water treatment, or providing access to high-quality drinking water to as many people as possible. In this context, IFPEN's researchers have been working on methods to gain a better understanding of how pollutants are transported in the underground environment.

Pollutant transport impacted by the heterogeneity of the media

Pollutant transport regimes (transient or asymptotic), as well as the time taken to reach a critical location (for example, an aquifer or a well) are significantly dependent on **the underlying heterogeneity of the permeability field**. Moreover, in the case of pollutant retention, transport is also characterized by exchange kinetics that depend on local soil properties. This explains why retention times too are spatially heterogeneous.

Two approaches for solute transport modeling

In this research, IFPEN's researchers focused on the influence of heterogeneous permeability and retention times for transient and asymptotic species transport regimes. Transient regime transport cannot be described by a standard transport equation (Advection-Diffusion equation). This equation only becomes valid in the asymptotic regime.
Researchers began by simulating this transport in **a two-dimensional, heterogeneous porous medium**. A Mobile-Immobile model[1] was used to describe the impact on global solute transfer of mass transfer between the mobile and immobile parts of the medium. This problem was solved using a Lattice Boltzmann method[2] [1].

[1] This model differs from the classic transport model in that, within the same simulation mesh, it separates the fluid region into **mobile** (flow and diffusion) and **immobile** (stagnant) regions with transfer between the mobile part and the immobile part. This transfer follows a first-order kinetics equation.
[2] Numerical method employed to solve the Navier-Stokes equation and the advection-diffusion equation using a collision-propagation scheme.

Next, **a new one-dimensional random walk model** (continuous time random walk, CTRW) was implemented by researchers to determine these transport behaviors on a large scale. The model is based on **a spatial Markov model[3] for particle speeds**, which combines advective-dispersive transport and heterogeneous mass transfer via a Poisson process[4]. This model, which is on a larger spatial and temporal scale, can be fully parameterized by permeability and flow statistics (without any adjustment parameters) and enables longer numerical simulations to be carried out to reach asymptotic regimes.

[3] Stochastic process describing the transition from one state to another.
[4] Stochastic process used to describe random events with a certain probability over time.

Assuming a non-linear relationship between local permeability K and local exchange time ?, researchers studied the impact of the Damköhler number (Da, ratio of advection and retention time scales) on the spatial evolution of the solute concentration field.
Fig. 1 shows concentration fields for different Da values [2]. The two mobile concentration fields are very similar, while significant differences can be observed in the immobile concentration fields. In the case of a reliable Da, there are a greater number of depleted regions (dark blue) at the front. In addition, other regions of higher concentration can still be observed a long way behind the front. These two effects result from the heterogeneity in retention time and these regions correspond to high values of this parameter.

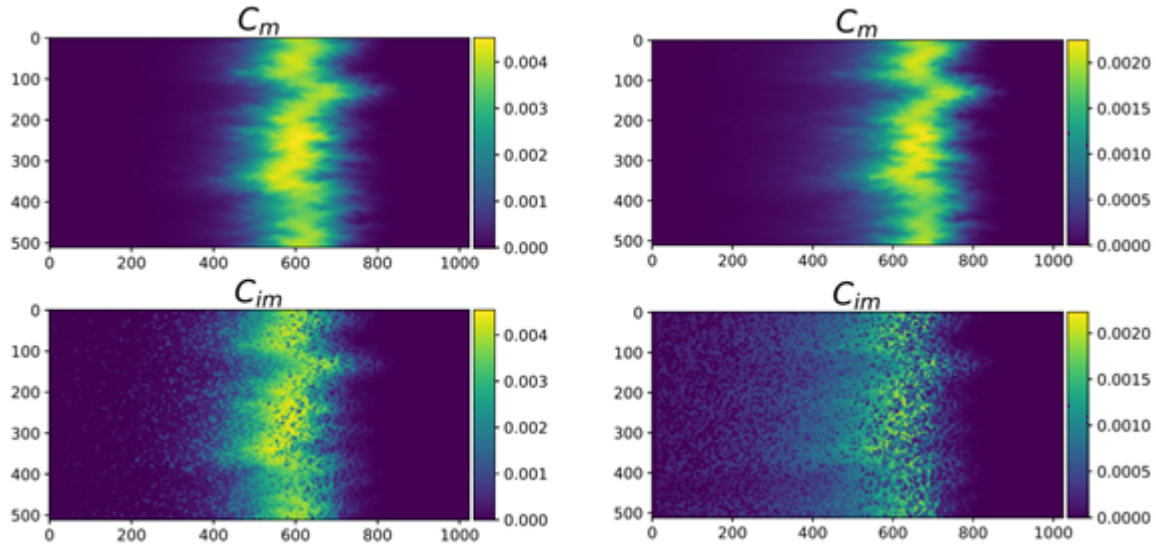


Figure 1: Concentration fields for Da=1/8 (left) and Da=1/40 (right). Cm represents the concentration in the mobile zone and Ci the concentration in the immobile zone.

Using CTRW numerical simulations, the researchers also showed that the time required to reach asymptotic regimes in heterogeneous media is, on average, twice as long as for the case of a homogeneous porous medium.

Significant pollutant retention time variability

In conclusion, on the basis of numerical simulations, the researchers showed that **pollutant concentrations can sometimes remain in soils for a very long time**. This can be explained by the existence of stagnant zones (blue regions, Fig. 1) with high retention times. These zones store and release pollutants over extremely long periods of time.

Moreover, CTRW simulations showed that **transient transport regimes may be important**, but their correct description requires more sophisticated models. Finally, the results potentially make it possible to explain specific behaviors observed experimentally that cannot be modeled by a standard transport equation.

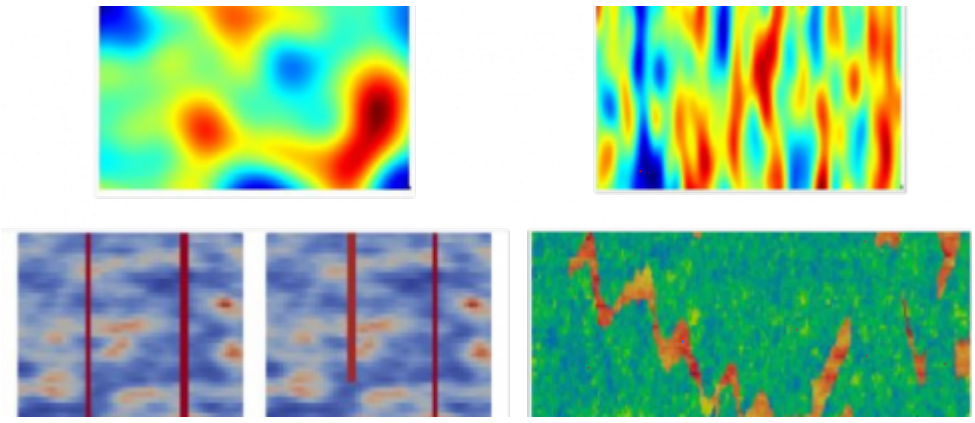
Consideration of more complex media

As a follow-on from this study, a difficult and ambitious task remains: to simulate pollutant transport in more complex structures, particularly anisotropic or stratified, in order to take into account the highly heterogeneous nature of geological media.

[1] Talon L., Martin J., Rakotomalala N., Salin D. and Yortsos Y., 2003, Lattice BGK simulations of macrodispersion in heterogeneous porous media, Water Resources Research. https://doi.org/10.1029/2002WR001392
[2] Talon, L., Ollivier-Triquet, E., Dentz, M., Bauer, D., 2023. Transient dispersion regimes in heterogeneous porous media: On the impact of spatial heterogeneity in permeability and exchange kinetics in mobile–immobile transport. Advances in Water Ressources. https://doi.org/10.1016/j.advwatres.2023.104425

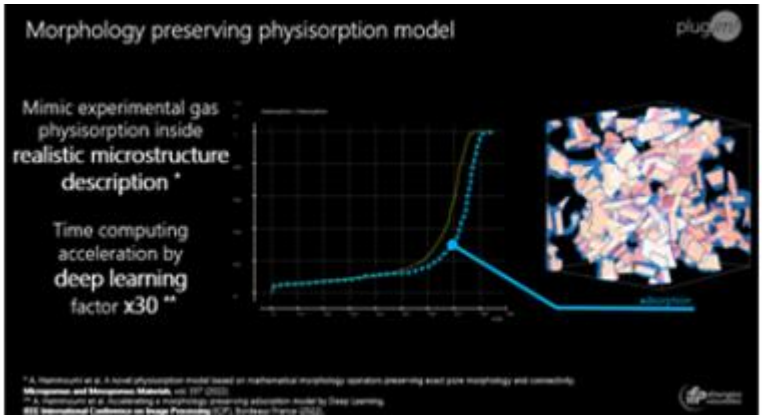
Scientific contact : daniela.bauer@ifpen.fr

YOU MAY ALSO BE INTERESTED IN



Adaptive model for flow simulation in heterogeneous porous media

The calculation of water and gas flows in complex and heterogeneous media is central to technological solutions aimed at tackling current climate and energy challenges.



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

Inside porous materials, physico-chemical phenomena such as matter transport, catalytic reactions and capillary effects are strongly influenced by the geometry of the pore networks, i.e., the degree of porosity, the distribution of pore sizes and their connectivity. (....) IFPEN and Saint Gobain Research Provence decided to tackle the problem differently, by exploring a new numerical approach...

Separation and adsorption techniques | **Numerical methods and optimization** | **Signal processing/Data science**

Fundamental Research

News January 2023

Dual-porosity and dual-fracture model for fractured geothermal reservoir simulation

Geothermal energy

Petrophysics and transfers in porous media | Transfer and transport physics

Numerical methods and optimization

A better understanding of pollutant transport in the subsoil

High-throughput experimentation (HTE) reactors are more and more used in chemical engineering for catalyst screening. The reduction in the size of these fixed-bed catalytic reactors has many advantages, with lower quantities of catalyst and reagents used, better temperature control, minimized safety risks and reduced waste products. Moreover, these reactors can easily be set up in parallel (usually 16 reactors, or more). But despite the many advantages, the behavior of these reactors varies significantly depending on certain parameters (such as the ratio between the diameter of the reactors and that of the particles). It is important to fully understand this type of dependence to ensure optimal operation of the catalytic processes. A PhD thesis led to the definition of a calculation chain capable of accounting for the behavior of these catalysts.

Hydrodynamics governed by preferential paths

The **extremely small ? ratio between the diameter of HTE reactors and that of the particles** makes it **difficult to extrapolate results to bigger scales**. In the catalytic beds of these millimetric reactors, particles are arranged non-randomly, resulting in **non-uniform radial distributions** and **higher void fractions**. Preferential paths are preponderant and govern the hydrodynamics. The axial behavior of the flow in the reactor is modeled by a 1D convection-dispersion equation. For the latter, the dispersion coefficient with respect to a piston-type flow can be introduced as an axial Péclet[1] number.

[1] Number comparing convective and diffusive forces

A modeling-based approach

Within the framework of a PhD thesis [1], **a fully numerical approach** was employed to study the case of **single-phase flows in fixed beds of spherical particles** with low reactor-sphere diameter ratios (? < 4). The packing of particles was calculated using the internal Grains3D DEM tool and the OpenFOAM library was used[2] to calculate flows and deduce a local Péclet number from the moments of age[3].

[2] Using the simpleFoam stationary solver, augmented by solving moment of age equations to the second order (See Liu and Tilton, AIChE J. 56, 2010)
[3] i.e., from the residence time of fluid particles (first moment), and their variance (second moment)

Possible impacts on process performance

Figure 1 illustrates an important result of this research, namely **the reduction in the Péclet number for certain values in the range of low ? ratios**, with **possible consequences on the catalytic process conversion rate** [3]. This can be explained by the formation of ordered arrangements of particles, leading to preferential passages for the fluid and hence less contact time between the fluid and the catalyst.

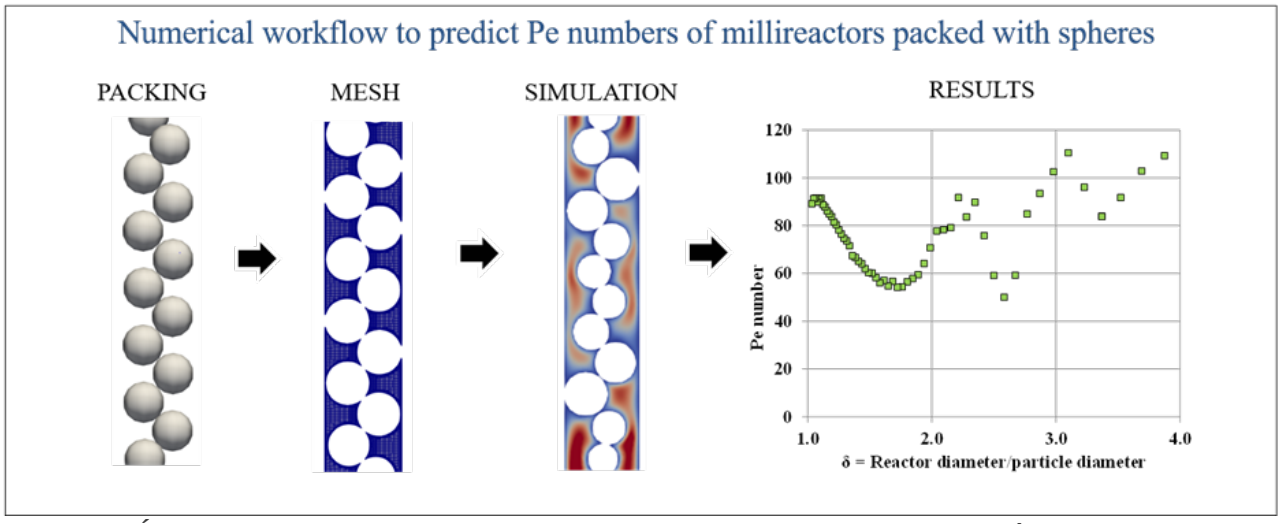


Figure 1: Évolution du nombre de Peclet en fonction du rapport de diamètre entre le réacteur et les particules.

Simulation results that match reality

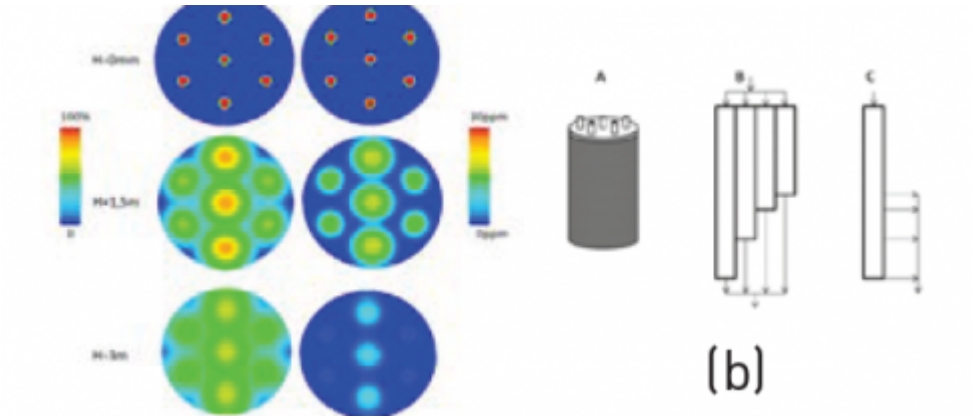
In addition, the results obtained from the employed computational workflow compare very favorably with experimental databases [2], particularly when molecular diffusion or superficial velocity vary. The same workflow could be used for other forms of catalyst without additional effort.

References:

[1] V. Petrazzuoli, Impact of packing and porosity filter use in G/S and G/L/S packed bed millireactors:experimental and numerical studies, Thèse de doctorat de l'université de Lyon, soutenue le 02/12/2020.
[2] V. Petrazzuoli, M. Rolland, V.Sassanis, V. Ngu, Y. Schuurman, L. Gamet, Numerical prediction of Péclet number in small-sized fixed bed reactors of spheres, Chemical Eng.ineering Science, 240, 2021.
[3] V. Petrazzuoli, M. Rolland, A. Mekki-Berrada, O Said-Aizpuru, Y. Schuurman, Choosing the right packing in millipacked bed reactors under single phase gas flow, Chemical Eng.ineering Science, 231, 2021.

Scientific contact : lionel.gamet@ifpen.fr

YOU MAY ALSO BE INTERESTED IN



In trickle bed reactor simulators, hydrodynamics count!

Improvements in chemical processes are regularly achieved as a result of the introduction of new internal geometries within reactors.

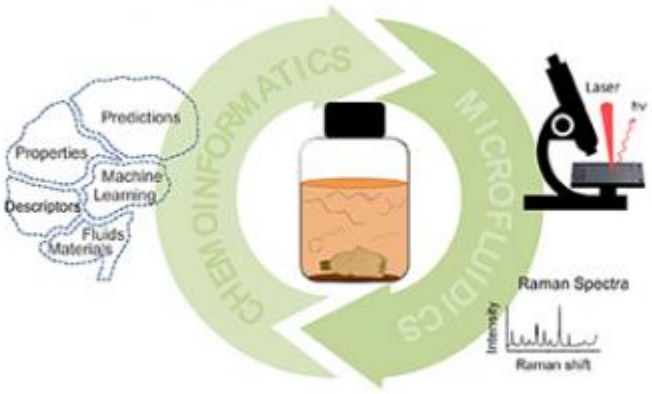
Chemical sciences | Catalysis and reaction kinetics | Engineering sciences | Fluid mechanics | Chemical engineering and process engineering | Systems modeling and simulation

HTE in a milli-fixed bed reactor boosts the development of slurry catalysts

THÈSE DE CHARLES BONNIN

Responsible oil and gas | Fuels | Petrochemicals

Chemical sciences | Catalysis and reaction kinetics | Analysis and characterization | High-throughput experimentation (HTE) | Engineering sciences | Chemical engineering and process engineering



Microfluidics and Chemoinformatics: a highly complementary approach to studying material/fluid compatibility

Pour de nombreuses applications industrielles, comme le recyclage chimique des plastiques, ou encore pour assurer la compatibilité entre polymères et nouveaux carburants, il est essentiel d’anticiper les interactions entre matériaux et fluides...

Chemical analysis **Microfluidics** **High-throughput experimentation (HTE)**
Signal processing/Data science

An hydrodynamic study for more efficient catalytic millireactors

De nombreux procédés catalytiques utilisent les réacteurs à lits fixes arrosés car ils présentent de nombreux avantages. Simples d'utilisation, ils ont de bonnes performances en termes de mise en contact des gaz, liquides et solides. Néanmoins des phénomènes complexes y sont à l'œuvre et pour les comprendre il est nécessaire de recourir à la mécanique des fluides numérique. Un travail de thèse a permis d'obtenir des résultats en accord avec les observations.

An apparently simply design that hides considerable complexity

Due to **their relatively practical design and their ease of use**, fixed trickle bed reactors are considered to be **the best gas-liquid-solid contact technology** for a broad range of catalytic processes. Although simple to use, these reactors combine several complex phenomena.
In order to gain a better understanding of these phenomena, several literature reviews have focused on the characterization of reactors of this type, but few of them have tackled matter transfer at the interfaces. Moreover, **significant disparities have been observed in the estimation of parameters of interest**: feed loss, liquid saturation, wetting rate as well as gas-liquid and liquid-solid matter transfers.

Realistic estimation of parameters of interest

With a view to gaining a better understanding of local phenomena, a PhD thesis [1] using computational fluid dynamics (CFD) studied **the complex coupling between hydrodynamics and matter transfer** in realistic industrial operating conditions. To do so, predictive gas-liquid-solid transfer simulations were conducted. Hydrodynamic predictions concerning feed loss and liquid saturation were validated with respect to reliable models in the literature (Ergun's equation, [2]). Similarly, the grain wetting rate was compared to a previously established correlation [3], also taking into account the effects of gas flow and grain shape.

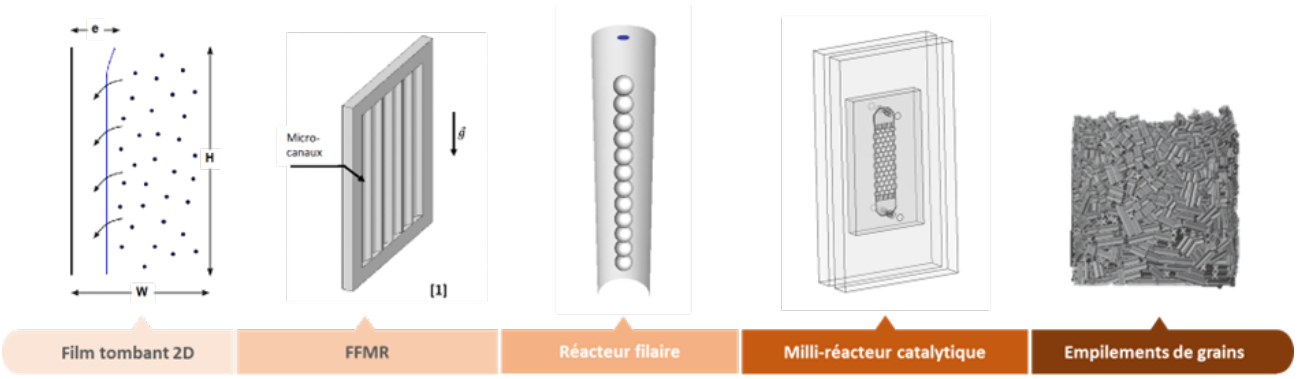


Figure 1: Research strategy followed to achieve thesis objectives.

A broad range of case studies, catalyst geometries and grain shapes

For CFD modeling, a strategy involving the gradual complexification of case studies was adopted (Figure 1), from the case of a two-dimensional, semi-infinite falling film to that of a three-phase reactive medium, with very good agreement concerning hydrodynamics and matter transfer flows.

The CFD model was evaluated to study the effect of the geometry of the solid catalyst in three configurations: (i) **a string reactor**, (ii) **a structured millireactor**, (iii) **three stacks of fixed trickle beds** comprising spheres, trilobes and quadrilobes. In these case studies, an acceleration of external transfers was revealed and quantified for tortuous flows, due to the convective contribution of the solute limiting the reaction. The study of transfer in fixed trickle bed reactors, for various grain shapes, demonstrated **an improvement in transfer coefficients for particles with a high surface/volume ratio**.

Lastly, the effects of gas flow and grain shape on partial wetting of the solid surfaces were simulated in real process conditions, making it possible to broaden the scope of application of the correlation already stated [3].

A better understanding of local phenomena

Using computational fluid dynamics, this research has made it possible to study **hydrodynamics and gas-liquid-solid matter transfer on a local scale**, and improve both the understanding and determination of the parameters of interest. As a result, correlations are proposed to (i) estimate the wetting rate in grain stacks and (ii) correct the series resistance model, widely used in industry to estimate the global transfer coefficient.

References:

[1] Bouras, Hanane (2021) Etude expérimentale et numérique des transferts de matière externes dans différents réacteurs catalytiques triphasiques en régime ruisselant. En ligne : www.theses.fr/2021LYSE1021
[2] Boyer, C.; Volpi, C.; Ferschneider, G. (2007) Hydrodynamics of trickle bed reactors at high pressure: Two-phase flow model for pressure drop and liquid holdup, formulation and experimental validation. In : Chemical Engineering Science, vol. 62, n° 24, p. 7026–7032. DOI: https://doi.org/10.1016/j.ces.2007.08.036.
[3] Julcour-Lebigue, Carine; Augier, Frédéric; Maffre, Harold; Wilhelm, Anne-Marie; Delmas, Henri (2009) Measurements and Modeling of Wetting Efficiency in Trickle-Bed Reactors: Liquid Viscosity and Bed Packing Effects. In : Industrial & Engineering Chemistry Research, vol. 48, n° 14, p. 6811–6819. DOI: https://doi.org/10.1021/ie9002443.

Scientific contact : hanane.bouras@ifpen.fr

YOU MAY ALSO BE INTERESTED IN

HTE in a milli-fixed bed reactor boosts the development of slurry catalysts

THÈSE DE CHARLES BONNIN

Responsible oil and gas | Fuels | Petrochemicals

Chemical sciences | Catalysis and reaction kinetics | Analysis and characterization | High-throughput experimentation (HTE) | Engineering sciences | Chemical engineering and process engineering

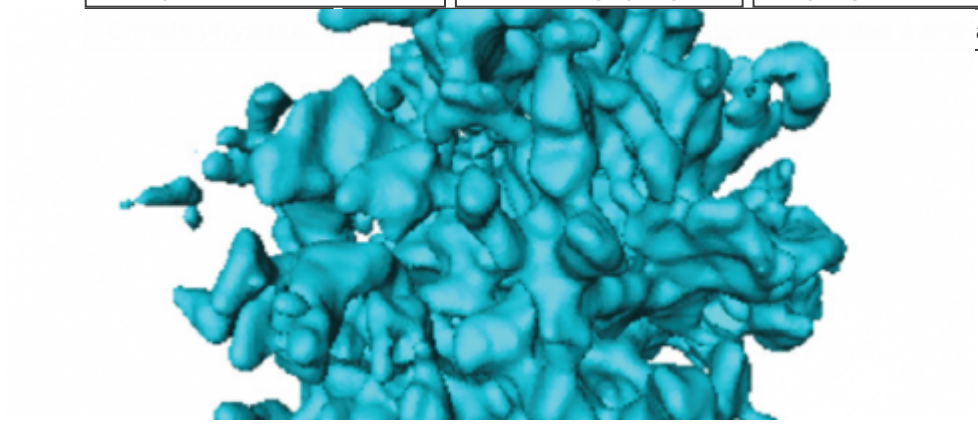
Recherche fondamentale

Actualités January 2018

Mieux comprendre les phénomènes de diffusion au cœur des catalyseurs

Hydrocarbures responsables | Carburants | Pétrochimie

Analyse et caractérisation | Sciences physiques | Physique du transfert et du transport aux



Characterizing catalysts for Fischer-Tropsch: a question of SWING

Fischer-Tropsch synthesis is a catalytic process to produce hydrocarbons from a syngas, which could come from biomass.

Responsible oil and gas | Fuels

Chemical sciences | Catalysis and reaction kinetics | Analysis and characterization | Chemical analysis | Structural analysis and Imaging

The gas-liquid-solid matter transfer in fixed trickle bed reactors

Porous media challenge scientists
17 October 2023

Link to the web page :