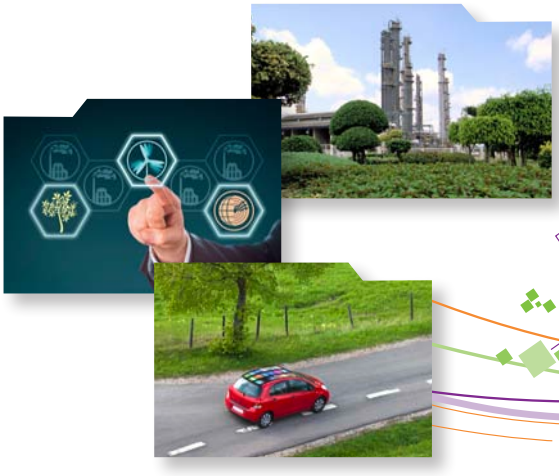

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SPECIAL ISSUE
Multiphysical and multiscale modeling

A number of until recently unsolvable complex problems are now within the reach of multiscale simulation following the rapid development of high-performance computation methods. We now have access to an extraordinarily effective combination of new ideas, advanced physical models, discretization and resolution methods, along with increasingly powerful computing tools.

This revolution, which has been made possible through the capacity of parallel computation, has resulted in, for example, calculations of one million CPU hours (i.e. a century) being obtained in the space of one month. This represents a huge step forward in the ability to deploy sophisticated modeling methods which are useful for designing complex technical systems as well as simulating the interaction of physical phenomena.

This issue gives us an insight into the development work being carried out at IFPEN on the modeling of coupled phenomena, with a view to scale change, and its implementation in various domains.

I hope you enjoy reading this issue,

Sébastien Candel,
Former Chairman of IFPEN's Scientific Board
Vice-President of the French Academy of Sciences

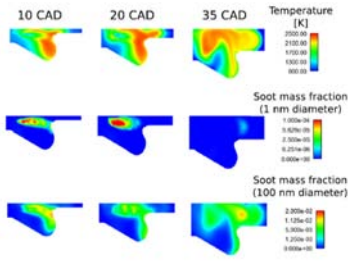
Soot "sectioned" for reduced air pollution

The capacity of researchers to understand and predict the formation of pollutants emitted by vehicles is a key challenge for sustainable mobility. This knowledge is essential, both to reduce emissions at source and optimize after-treatment systems.

In this context, the particles emitted by diesel engines represent a major modeling challenge since these emissions are regulated both quantitatively and qualitatively. Consequently, in order to be useful, models need to be able to predict — in addition to the overall mass — the number and size of soot particles emitted by engines, which also depend on the fuel composition and the vehicle's use profile. The development of such models is complex since they involve very advanced combustion chemistry and turbulent combustion modeling.

However, IFPEN has managed to overcome these difficulties. The model developed by its researchers has been implemented within a 3D engine simulation code. After grouping together soots on the basis of their size ("sectional" approach[a]) the model[1] describes the evolution of this distribution, taking into account collisions and exchanges with the gas mixture (including oxidation). Since these exchanges involve complex chemistry, their treatment is based on tabulated approaches[2] to simplify the calculations.

For diesel engines, it is therefore now possible to simulate combustion in the chamber, including fine representation of the particles formed at each location and time. The models developed are of interest to both the car industry and the aeronautics industry, where they will be integrated into an aeronautical combustion chamber simulation code.



Mapping of the temperature and of two soot sizes modeled in a diesel cylinder.

a - in which each soot size category is described *via* a specific transport equation

(1) ***D. Aubagnac-Karkar, J-B. Michel, O. Colin, P.E. Vervisch-Kljakic,*** *N. Darabiha, Combust. Flames, 2015, 162, 3081-3099.*
DOI: 10.1016/j.combustflame.2015.03.005

(2) ***J-B. Michel, O. Colin,*** *Int. J. Engine Res., 2013, 15, 346-369.*
DOI: 10.1177/1468087413488590

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For better irrigation of fixed beds

Eliminating impurities such as sulfur or nitrogen or increasing gasoline or diesel production yields are major challenges for the refining industry. Irrigated fixed-bed catalytic reactor technology is helping to address these challenges *via* processes such as the hydrotreatment of oil cuts or vegetable oils.

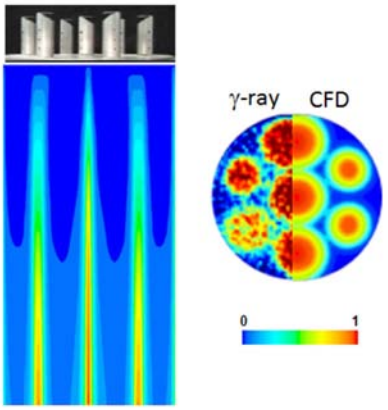
Today, the development of CFD[a] models and the increase in calculation potentials using HPC[b] are making it possible to simulate increasingly complex multiphase industrial reactors. By coupling hydrodynamics with reaction kinetics, these simulations make it possible to predict the performance of reactors, incorporating the impact of fluid distribution at the bed head.

The 3D hydrodynamic model recently developed at IFPEN is based on a space-averaged description of the interactions between phases (Eulerian model with two fluids in porous media). The physical laws involved in movement quantity assessment are derived from internal developments (frictions between phases, capillary pressure) and the literature (mechanical dispersion).

This model was successfully validated on several experimental cases, including one conducted on a model fitted with a γ-tomography analysis system, mobile depending on the height and giving access to the distributions of fluids on the basis of different sections (see figure). It was then coupled to a kinetic catalytic cracking model to determine the impact of distribution on the overall performance and thereby propose quantitative targets for distributors' future technologies.

In addition, in order to limit the calculation time and ensure the model can be incorporated — if necessary — into simulators employing detailed kinetic diagrams, the model was reduced to a "1D-multi-output" equivalent, parametrized on the basis of preliminary CFD simulations.

Future studies conducted on this model will consist in incorporating the hydrodynamic and diffusional limitations, due, primarily, to partial wetting of the catalysts.



Liquid saturation in a catalytic bed: simulations and experimental data.

a - Computational Fluid Dynamics
b - High Performance Computing

(1) ***Augier and al.,*** *CJCE,2016.*
DOI: 10.1002/cjce.22618

(2) ***Solomenko and al.,*** *CES, 2014.*
DOI: 10.1016/j.ces.2015.01.013

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Basin modeling: crude oil on the menu for microorganisms

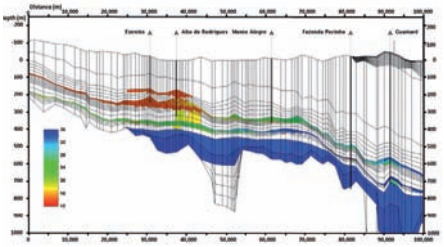
Sedimentary basin modeling is used to locate and determine the quality of future oil fields, during an exploration phase, thereby helping to reduce the risks and costs before drilling. The quality of hydrocarbons present in these fields also depends on another factor, only recently taken into account: its modification by microorganisms. The latter, which are present in shallow oil reserves, preferentially consume light components.

This reduces the economic value of the field and makes production technically more difficult since the oil in these reserves is consequently denser, more viscous and often sourer. Predicting the microbial modification of hydrocarbons is therefore crucial before launching the exploration phase.

Recent research, bringing together geologists, geochemists and microbiologists at IFPEN, led to this biodegradation being taken into account in basin models. In particular, the results obtained using this multiphysical approach and integrated into TemisFlow™ basin modeling software were applied to the Potiguar field (Brazil), where they were used to more clearly describe filling and oil modification phenomena in the fields[1].

This enhanced basin modeling method also provides new tools to help improve our understanding; they help explain, for example, the origin of large gas fields discovered in the Mediterranean. Supported by the data acquired as part of the Pamela[a], the new microbiological component of the model will be able to back up the hypothesis that microorganisms may have degraded the buried solid organic matter before it was transformed into oil.

a - Passive Margins Exploration Laboratories: consortium, a project led by Ifremer, with the assistance of Total, IFPEN and the universities of Brest, Rennes and Paris VI



Cross-section of the Potiguar basin: prediction of the density of the hydrocarbons trapped in the geological formation.

(1) ***M. Ducros, B. Carpentier, S. Wolf*** *and* ***M.C. Cacas,*** *Journal of Petroleum Geology, Vol. 39(1), January 2016, pp 61–78.*
DOI: 10.1111/jpg.12628

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Multiphysical all down the line

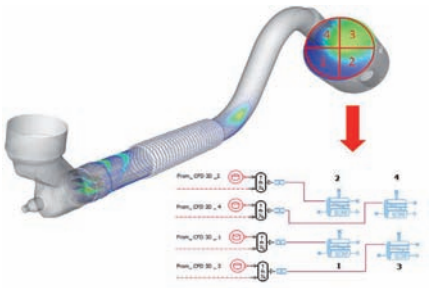
The development of more effective systems to reduce pollution in vehicle exhaust gases is a lever for the improvement of air quality in urban environments. The design of increasingly sophisticated systems draws on simulations coupling multiphase fluid dynamics and chemical reactivity models.

An emblematic example is the selective catalytic reduction (SCR) process of nitrogen oxides (NOx), in which a urea/water mixture, injected upstream of the catalyst, is decomposed into a variety of products. Optimizing this decomposition is crucially important, ensuring the availability of reducing species in the catalyst, thus maximum NOx conversion. One of the consequences of poor decomposition is the formation of deposits, which clog up the exhaust pipe and further reduce the efficiency of the pollution control system.

For several years, IFPEN has been working on the development of a unique model[1] coupling the evaporation of urea solutions, the interaction of their spray with the wall, the decomposition of urea and the formation of deposits within realistic configurations (see figure). This model has been incorporated into the Converge™ 3D multiphase combustion code developed by our partner, Convergent Science. The quality of this modeling ensures the complementarity of the two models, thanks to precise specification of the conditions at the catalyst entrance, while minimizing the "computational cost" for the simulation of the catalytic section.

The model was then coupled with the IFPEN catalyst model[2] available on the LMS Imagine.Lab Amesim™ [a] system simulation platform.

This combination of two codes enables rapid, precise assessment of the potential for NOx reduction by a given after-treatment line, at the same time taking into account the development of any deposits or inhomogeneities in the composition of the exhaust gases.



Coupling between 3D and 0D multiphysical modeling for studying deposits and dimensioning an SCR system.

a - Integrated simulation platform for multi-domain mechatronic systems simulation

(1) ***V. Ebrahimian, A. Nicolle, C. Habchi,*** *AIChE Journal, 2012, 58(7), 1998-2009. DOI: 10.1002/aic.12736*

(2) ***S. Dosda, D. Berthout, G. Mauviot, A. Nogre,*** *SAE Technical Paper, 2016-01-2281. DOI: 10.4271/2016-01-2281*

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Very often, we need to scale things down

Geological porous media, even when homogeneous on a large scale, can present major heterogeneities on a microscopic scale (from the size of a pore to several thousand pores). And yet the behavior of fluids on a large scale is significantly dependent on this microscopic structure. That is why the modeling and simulation of flow and transport in porous media require fine structural characterization of the rock.

To achieve this, IFPEN relies on the observation of samples using high-resolution imaging techniques: X-ray imaging techniques (micro-tomography), implemented both at IFPEN and at the Grenoble synchrotron (ESRF), reveal the structure of the porous medium, with a resolution ranging from 0.3 to 3 µ.

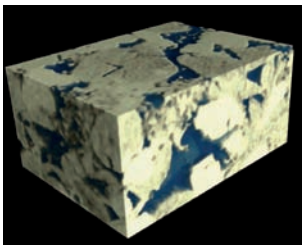
From these observations, two methods are used to simulate flow and transport in the porous medium:

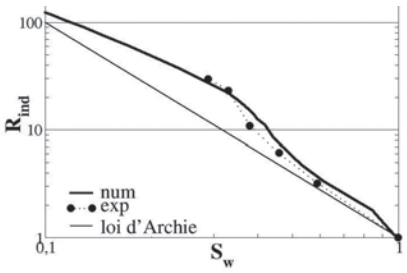
- the Lattice Boltzmann method, a direct method that uses a grid corresponding to discretization in space of the image obtained,
- Pore Network Modeling (PNM), based on the resolution of linear equations, which describe transport within a network, itself obtained from a skeletonization algorithm applied to the images.

The importance of taking into account the structure of the porous space when modeling properties on a large scale was demonstrated in the case of a parameter widely used to estimate the oil saturation of a petroleum reservoir: the resistivity index, determination of which is based on an empirical law, known as Archie's law, relating this property to saturation of the medium[a].

In fact, it has been observed experimentally[1] that this law is not respected for certain types of carbonate rocks, when water saturation is low. PNM simulation has been used to explain this divergence and proposes a predictive model for the resistivity index. Hence, it has been shown that the deviation from the empirical law increases when the water present in the medium is reduced to films covering the rock walls.

a - $R_{ind} = S_w^{-2}$ (R_{ind} being the resistivity index and S_w the fluid saturation)





Microtomographic image of a rock and comparison of resistivity index measurement versus simulation.

(1) ***D. Bauer, S. Youssef, M. Han, S. Bekri, E. Rosenberg, M. Fleury,*** and ***O. Vizika,*** *Physical Review, 2011. DOI: 10.1103/PhysRevE.84.011133*

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In search of bridges between multiple scales and multiscale

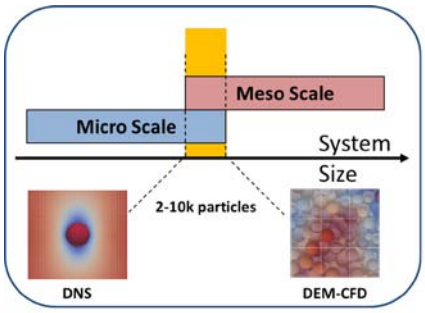
Be it for its design or the optimization of its operation, the numerical simulation of a complete chemical reactor, with fine, relevant resolution as regards the mechanisms involved, is probably an objective that it will be impossible to achieve over the next few decades, despite the anticipated evolution of computation powers. Indeed, a resolution around 1/30th of the equivalent diameter of the smallest particles involved[a] is thus necessary and, on this scale — what we call the "micro" scale — a numerical system may then require geometric discretization, involving up to 10^{15} cells.

This observation has promoted the use of meso and macro scales for simulation, with averaged approaches involving far fewer computational resources but requiring the development of "sub-grid" models, with more statistical and global consideration of the physical phenomena involved. The development of a coherent multiscale strategy — describing and quantifying the necessary and sufficient information to be transferred from one scale to another for a more realistic description of the physical mechanisms — is therefore an important challenge for these simulations.

Recently, IFPEN reached a new milestone[1]. Micro-scale simulations[b] were performed, with a reasonable computational cost, on an elementary representative sample of around 2,000 fluidized particles. The direct comparison between the micro and meso scales, made possible as a result, led to the validation and improvement of current models[2], as well as the methodologies for moving from one scale to another.

This promising work, for the time being applied to the description of fluid/particle flow hydrodynamics, is currently being continued *via* a collaborative research project[c], with a view to constructing a multiscale modeling method for reactive particle flows.

a - for example, catalyst granules
b - www.peligriff.fr
c - www.more4less.fr
d - DNS: Direct Numerical Simulation
DEM-CFD: Discrete Element Method - Computational Fluid Dynamics



Strategy adopted for direct comparison of the two scales: on the left, micro scale with a DNS[d] method and on the right, meso scale with a DEM-CFD[d] method.

(1) ***A. Wachs, A. Hammouti, G. Vinay, M. Rahmani,*** *Computers & Fluids, 2015, 154-172. DOI: 10.1016/j.compfluid.2015.04.006*

(2) ***A. Esteghamatian, M. Bernard, M. Lance, A. Hammouti, A. Wachs,*** *submitted to the International Journal of Multiphase Flow.*

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News

IFP Energies nouvelles' Oil & Gas Science and Technology journal (OGST) notched up 1,353 article quotations in 2015, giving it a two-year impact factor of 1.087, up from 2014.

Appointments

• ***Marie-Françoise Chabrelie,*** *Head of the Economics and Information Watch and Management Division at IFPEN, has been appointed director of the Ancre's (French National Alliance for Energy Research Coordination) theme-based Technology Transfer Consortium (CVT).*

• ***Jean-François Gruson,*** *Expert Director at IFPEN's Economics and Information Watch and Management Division, has been appointed onto the scientific and technical board for ADEME's (French Environment and Energy Management Agency) Graine* call for research proposals to provide expert advice and help select projects from among the 99 applications filed.*

** Managing, producing and converting biomass: a bioeconomy serving the ecological and energy transition*

Award

• ***Carmen Claver,*** *a member of IFPEN's Scientific Board, has just been awarded the Franco-Spanish prize by the Société chimique de France (SCF - French Chemistry Society). Professor of inorganic chemistry at the University of Rovira i Virgili in Tarragona (Spain), she brings to IFPEN her experience in the conduct of top-level scientific studies in the fields of organometallic chemistry and homogeneous catalysis.*

Publications

• *OGST – IFP Energies nouvelles journal – Issue 3, volume 71 (2016). Issue dedicated to process development methodologies at IFPEN.*

• *OGST – IFP Energies nouvelles journal – Issue 4, volume 71 (2016). Issue dedicated to characterization and modeling of low-permeability media and nanoporous materials.*

http://ogst.ifpenergiesnouvelles.fr

Upcoming scientific events

• *IFP Energies nouvelles' "Rencontres scientifiques" event –* ***LES4ICE 2016: Large-eddy simulation for flows in internal combustion engines –*** *30 November and 1 December 2016, IFPEN Rueil-Malmaison - www.rs-les4ice.com*

• *IFP Energies nouvelles' "Rencontres scientifiques" event –* ***Computational chemistry to reduce atmospheric pollution –*** *13 and 14 March 2017, IFPEN Rueil-Malmaison - www.rs-compchemistry.com*

• ***DEPOS27: deformation of solid polymers –*** *22 to 24 March 2017, Dourdan, France - www.depos27.fr*

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