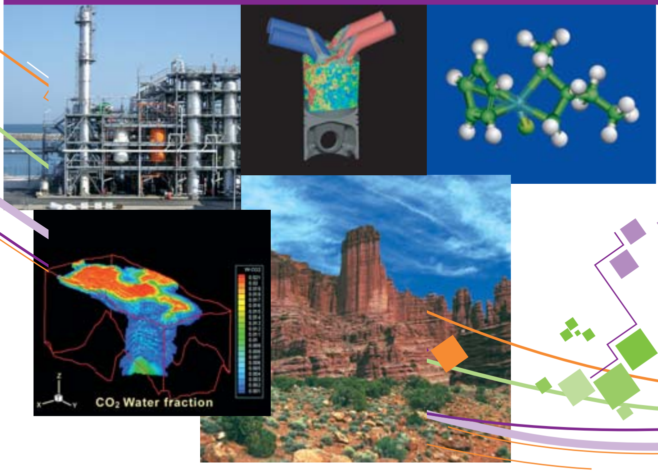

Science@ifp

No 2 - November 2007

The Grenelle Environment Forum has strengthened awareness of the need to cut emissions of greenhouse gases and atmospheric pollutants. This second issue of Science@ifp highlights scientific advances that will contribute to this. For example, low-temperature combustion in the new diesel engines reduces both the fuel consumption and the particulates emissions of automotive vehicles. Again, the molecular modelling tools developed by IFP and its academic partners are contributing to knowledge of the phase equilibriums relevant to the storage of CO_2 in underground reservoirs. As the other items show, in order to ensure a smooth energy transition, IFP also continues its work to improve oil technologies in exploration, production, and refining, which will remain essential to ensuring our energy supplies for a long time to come.

Philippe Ungerer
Scientific Director

Looking below diapirs

Seismic imaging is a basic tool for the characterization of reservoirs. Advances in the last few decades have made it possible to image complex structures in 3D, in particular diapirs (salt domes) as well as the structures below.

The difficulty lies in the contrast of wave velocities, of which the spatial distribution must be precisely estimated *(Fig. 1)*. In the context of the PSI and then the KIM consortiums, IFP has developed an original approach based on the inversion of the arrival times of certain seismic events. Correcting the pathologies inherent in this inverse problem made it possible, in particular through the use of prismatic reflections, to determine the overhanging geometry of the diapirs and so define the extent of some reservoirs *(Fig. 2)*. ■

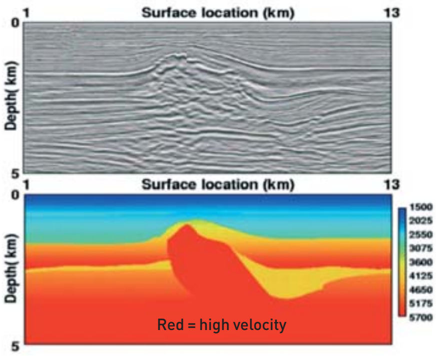

Fig. 1: 3D seismic image of a salt ridge and velocity model: the imprecise delineation of the overhanging part degrades the image

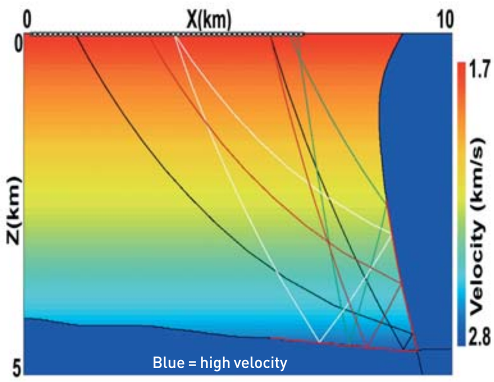

Fig. 2: The prismatic reflections provide precious information about the overhanging parts of the diapirs.

Delprat-Jannaud F. et Lailly P., *J. Geophys. Research, 98 , 6589-6605, 1993.*

Cavalca M. et Lailly P., *Inverse Problems, 23, 139-163, 2006.*

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IFP is a world-class public-sector research and training center, aimed at developing the technologies and materials of the future in the fields of energy, transport and the environment.

Innovation Energy Environment

NMR goes into the well

A molecular analysis and imaging tool well known in chemistry and medicine, Nuclear magnetic resonance (NMR) is now also used by petrophysicists to characterize porous media and petroleum fluids and thereby improve the production of oil and gas reservoirs.

The introduction of in-well NMR tools, in the 1990s, allows remarkable *in situ* measurements, in particular using weak magnetic fields (0.05T). The information exploited is the relaxation of the nuclear magnetization carried by the molecules (superposition of exponential decays). More precisely, in a water saturated porous medium, the relaxation mechanism exploited is the interaction between the porous surface and the molecules of the fluid. By diffusion, these molecules in effect explore a small thickness at the surface (a few Å) and, in so doing, provide information about the pore sizes, in a range from 1nm to 1mm.

This makes it possible to characterize, *in situ,* the porous media relevant to the petroleum domain (clayey media, microporous carbonates, coal, catalysts).

But the interpretation of these measurements is difficult and requires an understanding of liquid-solid nuclear interactions, which depend on the fluid and on the surface. For this purpose, in collaboration with the École polytechnique, IFP has managed to estimate the residence times of molecules at the surface, and from them to deduce the surface diffusivities and their temperature dependency.

Godefroy S., Korb J.-P., **Fleury M.,** *Phys. Rev. E, 64, 2001.*

Godefroy S., Fleury M., Deflandre F., Korb J.-P., *J. Phys. Chem., 106, 2002.*

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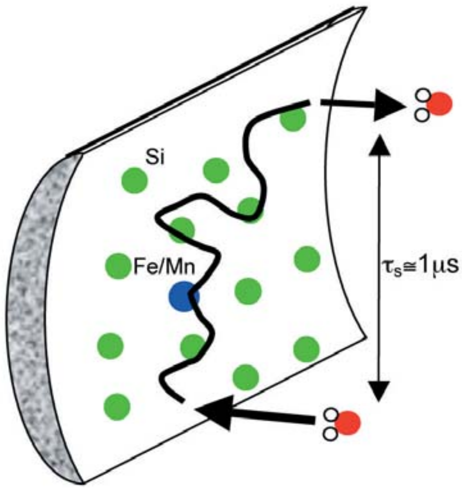

Schematic representation of the surface diffusion of the fluid (e.g. H_2O, red and white). The interactions with paramagnetic surface impurities (in blue, for example Fe or Mn, replacing Si, in green) are intense and cause a significant increment of relaxation. They provide information about the correlation time of the surface diffusion τ_m~1ps. This diffusion is limited by desorption, defined by the surface residence time τ_s~1µs.

Fluidized-bed reactors: optimizing the reaction zones

Fluidized-bed reactors, widely used in refining, are now being considered for new uses in the development of alternative sources of energy (biomass, gas, and coal) and the capture of CO_2 by Chemical Looping.

IFP has been working on these reactors for many years in order to achieve a better understanding of the flows and transfers, with a view in particular to optimizing the reaction zones of conversion processes. IFP has for example participated in many joint research projects, in particular with the University of Western Ontario (Canada), the INPT, the UTC, and PSRI (Particulate solid research inc.).

In fluidized reactors, the movement of the particles is beneficial but makes the hydrodynamics more complex. In spite of an abundant literature, predicting flows in this type of reactor is still tricky. For progress to be made, focused experiments and flow modelling must be combined. The experiments must be defined taking into account scale effects and inter-particle forces. Measurement methods must be adapted or developed and the phenomena that occur in reactors like catalytic cracking reactors must be described.

CFD (Computational fluid dynamics) has for ten years been used to calculate the flows in these reactors. Unfortunately, the physical models describing the gas-particle interactions are unsuited to fine particles. The closing laws will therefore have to be adapted and the simulations validated.

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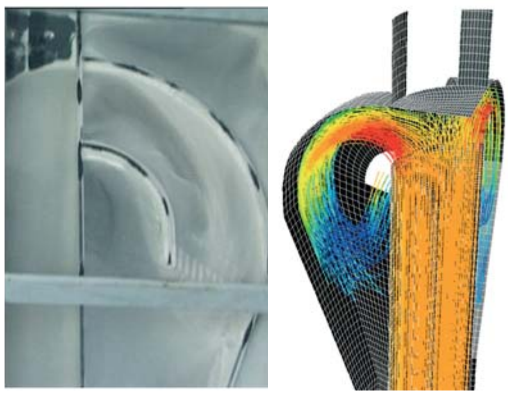


Experiments and 3D simulation of gas-particle separation in an FCC (Fluid catalytic cracking) reaction zone.

Herbert P.M., ***Gauthier T.A.,*** *Briens C.L. and Bergougnou M.A., Powder technology, 80 (3), 243-252 (1994).*

Gauthier T., Andreux R., Verstraete J., *Roux R., Ross J., International journal of chemical reactor engineering, vol.3, A47 (2005)*

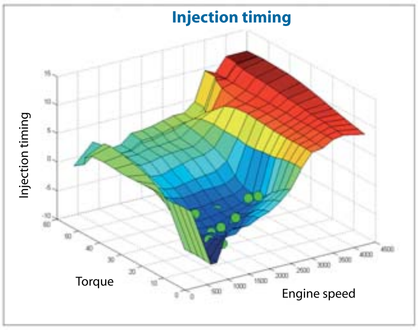
Optimizing complex systems

Optimization takes place in many IFP applications: estimating the parameters of numerical models from experimental data (earth sciences, combustion in engines), design optimization (networks of oil pipelines), optimizing the settings of experimental devices (calibration of engines, catalysis). These optimizations consist in minimizing a functional that is complex (nonlinearities, noise) and expensive to estimate (solution of a numerical model based on differential systems, experimental measurements), and for which derivatives are often not available, with nonlinear constraints, and sometimes with several objectives among which it is necessary to find the best compromise.

IFP has engaged an active research in this field for a number of years and develops its own optimization tools in order to meet the needs of its applications as well as possible.

SQPAL, for example, is a successive quadratic programming method suited to constrained nonlinear optimization problems, developed in partnership with the INRIA (for the TOMOinv[1] and CondorFlow industrial codes).

IFP is also developing optimization methods based on approximate models that are relatively inexpensive to evaluate: (i) reduced physical models as for the inversion of stratigraphic models (Lithopsi, Dionisos[2] codes), (ii) response surfaces constructed using a limited number of evaluations of the complex numerical model (historical matching of production data in oil reservoir engineering) or using experimental data (calibration of engines, *cf. Figure*).



Example of an optimized engine map: injection timing settings (in the engine operating domain described by the speed and torque) that minimize emissions of pollutants in a diesel engine. The reference operating points associated with the New european driving cycle (NEDC) are indicated in green.

[1]**Delbos F.,** *Gilbert J.C., Glowinski R.,* **Sinoquet D.,** *Geophys. J. Int., 164, pp. 670-684 (2006).*

[2]*Blum J.,* **Dobranszky G.,** *Eymard R.,* **Masson R.,** *Inverse problems, 22, pp. 1207-1225, (2006).*

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Cut pollution by controlling valves

With their combination of good thermal efficiency and low CO_2 emissions, diesel engines are currently very well placed to meet the energy and environmental requirements of tomorrow's transport sector. However, the expected evolution of standards calls for reducing their emissions of nitrogen oxides and of particulates.

This can be done using new low-temperature diesel combustion processes such as the NADI™ concept developed by IFP. However, these processes still have non-negligible drawbacks, such as a limited range of operation in which emissions of nitrogen oxides (NOx) are very low, a large demand for Exhaust gas recirculation (EGR) and, most particularly, high emissions of unburnt hydrocarbons (HC) and of carbon monoxide (CO) at low power.

To meet this challenge, IFP, in the context of the European Spacelight and Nice projects, has improved the potential of the new low-temperature combustion processes by using a Variable valve actuation system (modulation of the valve lift and timing, VVA) to create an internal recirculation of the burnt gases that keeps part of them in (or returns it to) the combustion chamber. The configuration with re-opening of the exhaust valve(s) during the intake phase yields the best compromise at the very low load points, which are the most problematical (low power, catalyst too cold, so not yet activated) and cuts emissions sharply (HC by 70%, CO by 40%, NOx to less than 0.1 g/kWh), while fuel consumption is controlled.

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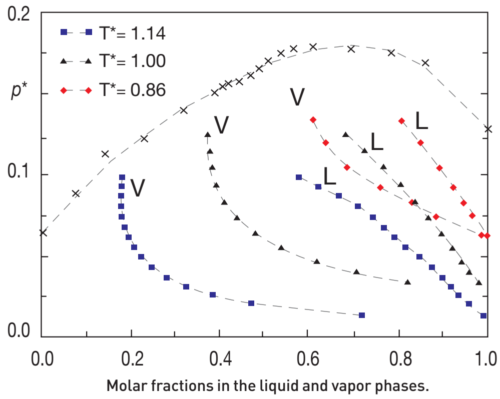
Schematic view of IFP's single-cylinder engine with Lotus VVA system

Walter B., Pacaud P., Gatellier B., *Journée SIA Variable valve actuation, November 2006.*

Bression G., Soleri D., *Savy S., Dehoux S., Azoulay D., Ben-Hadj Hamouda H., Doradoux L., Bastardie B., Lawrence N., 6th Symposium towards clean diesel engine - Napoli, 2007.*

Thermodynamics: from nano to macro

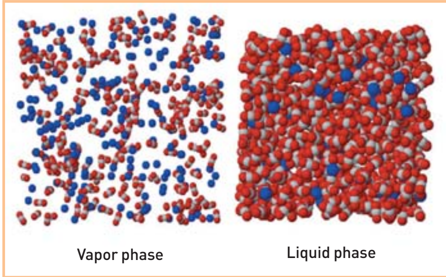
IFP has for many years been developing molecular simulation methods, applied in particular in the context of CO_2 storage. The thermodynamic models currently used for the design of processes (equations of state, group contributions) must generally be based on a large set of experimental data. Furthermore, they yield a poor representation of the vicinity of the critical point.



Binary mixture of two types of Lennard-Jones particles. Pressure and temperature are reduced with respect to the Lennard-Jones parameters. The crosses represent the locus of critical points of the mixture.

For more than ten years, IFP has been contributing to work on this problem by developing molecular simulation methods in collaboration with the University of Paris Sud and other laboratories. These methods, based on Monte Carlo algorithms, have a better physical basis. They make it possible to compute the properties of systems that have been little studied, or the critical points, with good scale behavior. Thanks to their implantation in the versatile GIBBS software program, these methods are being applied to systems of industrial interest; H_2S -hydrocarbon mixtures, for example- understanding them is useful in the production of certain gas fields, but their experimental characterization would be dangerous (collaboration with Total).

Several ANR projects are providing the data necessary for the underground storage of CO_2. ■



Simulation boxes illustrating the liquid-vapor equilibrium of a CO_2-Ar mixture (248 K, 5 MPa) (one center of force per atom; C=gray; O=red; Ar=blue)

Ungerer P., *Beauvais C., Delhommelle J., Boutin A., Rousseau B., Fuchs A.H., J. Chem. Phys. 2000, 112, 5499-5510.*

Ungerer P., Lachet V., Tavitian B. *Oil and gas science and technology 2006, 61, 387-403.*

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Visit from the NSF

The NSF (National Science Foundation, USA) sent a group of four experts to IFP in September 2007 for a look at the most advanced scientific techniques in the field of catalysis. This visit was part of a survey by the NSF of the world's leading laboratories in the synthesis of catalytic structures, the characterization of catalysts on the nanometric scale, modelling, and applications.

ANR projects in 2007

Of the 35 projects proposed in which IFP took part, 19 were accepted (6 in a complementary list) in the Predit, CO_2, PNRB, Blanc, Stock-E, RNTL, Intensive computation, and materials-processes programs.

Publications

Pierre Duret and Bertrand Gatellier wrote the chapters on 2T CAI and the NADI process for the book, "HCCI and CAI engines for the automotive industry" edited by Hua Zhao, from Whoodhead Publishing.

Honors

- **Nadège Bouchonneau** *won the 1st "A'Doc 2007" prize, awarded by the University of Franche-Comté, for her thesis, "Étude du comportement des systèmes d'isolation thermique pour les grandes profondeurs d'eau" ("Study of the behavior of thermal insulation systems for large depths of water"), defended on 14 March 2007.*

- **Jean Kittel** *was awarded the Cefracor's "Young corrosion researcher" certificate for 2007 for his work on corrosion mechanisms and the modes of protection of metallic surfaces.*

- **Véronique Smanio** *was awarded the Young researcher prize of the Eurocorr 2007 conference (9-13 September 07, Freiburg im Breisgau).*

Colloquia

- **Reducing CO_2 emissions**
(22-24 January 2008, IFP-Lyon).
Joint workshop of the European Castor, Encap, Cachet, and Dynamis projects.

- **ESCAPE 18** – European symposium on computer aided process engineering (1-4 June 2008, Lyon)

Accreditation as director of research (HDR)

- **Alain Méthivier**
HDR from the University Claude Bernard (Lyon 1): "Sélectivités d'adsorption dans les systèmes zéolithes / hydrocarbures" ("Adsorption selectivities in zeolite/hydrocarbon systems") (12 September 07).

- **Christophe Boyer**
HDR from the Institut national polytechnique of Toulouse: "Contribution à l'étude des phénomènes de transport dans les contacteurs gaz/liquide supportés" ("Contribution to the study of transport phenomena in supported gas/liquid contactors") (19 October 07).

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