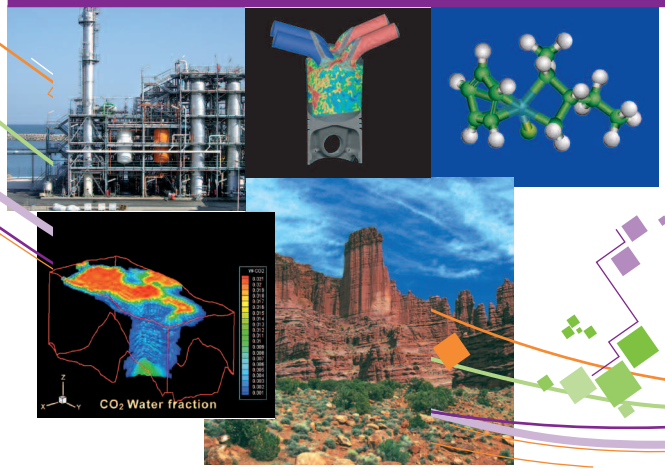


Science@ifp
No 5 - May 2009

Improving solvent selection for CO_2 capture

IFP has recently created an R&D network of expertise to make the most of its researchers' technical and scientific excellence and effectively promote it with its industrial, institutional and academic partners.
This community of IFP experts currently boasts 6 Expert Directors and 21 Experts.

This fifth issue of "Science@ifp" deals at length with work initiated and led by some of our experts.
In the future, we will often find the members of this community among our authors, and also future experts, since the very purpose of this newsletter is to report on the most significant scientific results to emerge from our R&D programs, while shedding light on their technological importance.

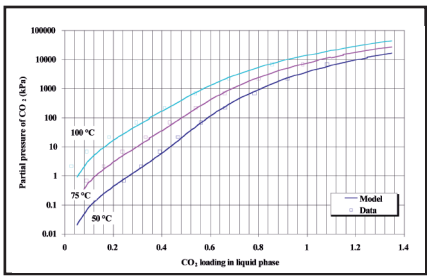
Hervé Toulhoat
Associate scientific director

Capture of the CO_2 contained in industrial flue gases (from conventional power stations, steel mills, cement works, etc.) is the key to controlling greenhouse gas emissions. The capture processes currently being considered absorb the CO_2 by using a basic amine solvent that makes it possible to purify the flue gases while the solvent is regenerated at high temperature and recycled.

A large share of the capture cost corresponds to the energy needed to regenerate the solvent, and considerable work is being done worldwide to identify an economical capture solvent. In addition to the problems of the chemical kinetics and the stability of the solvent, its thermodynamic behaviour in the presence of CO_2 is one of the main criteria in the technical-economic evaluation of a process.

The experimental characterization of a new solvent consists in measuring the quantities absorbed and the heats of absorption of the CO_2 in the solvent at different pressures.

These different kinds of thermodynamic data are then integrated in a model coupling chemical reactions and phase equilibrium. This approach serves to ensure the consistency of the various data and to enhance the predictive capabilities of the model. It is therefore possible to determine the profile of the species in the liquid phase during the charging of the solution (cf. diagram), which helps in understanding the capture mechanisms. This approach, successfully applied to various alkanolamines (MEA, DEA, MDEA), is being applied to new solvents under development.



Quantity of CO_2 absorbed by the solvent versus the partial pressure and temperature - Comparison of model and experiment.

E. Blanchon Le Bouhelec , P. Mougin, A. Barreau, *R. Solimando, Rigorous modelling of the acid gas heat of absorption in alkanolamine solutions, Energy & Fuels, 2007, 21, 2044-2055 - DOI: 10.1021/ef0605706.*

A. Barreau, E. Blanchon Le Bouhelec, K. Habchi Tounsi, P. Mougin, F. Lecomte, *Absorption of H_2S and CO_2 in alkanolamine aqueous solution: Experimental data and modelling with the electrolyte-NRTL model, Oil & Gas Science and Technology - Rev. IFP, 2006, 61(3), 345-361- DOI: 10.2516/ogst:2006038a.*

scientific contact:
pascal.mougin@ifp.fr

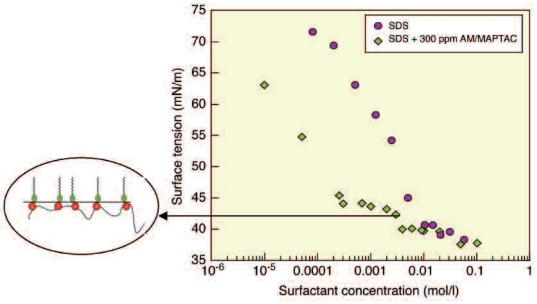
Stabilizing emulsions and aqueous foam

Polymers and surfactants are used in many fields, in particular to control the stability and rheology of colloidal systems such as emulsions and foams. However, it is essential to control the interactions between these two constituents so that their combination does not alter the macroscopic properties of the formulation. It is also possible to look for synergies between these two types of additives, in order to optimize the system in terms of performance and cost. In this context, combining polymers and surfactants having opposite charges is an innovating and promising approach.

Starting from an analysis of the interfacial properties of these systems conducted in partnership with the *Université d'Orsay*, it has been shown that the addition of a low concentration of a polyelectrolyte of opposite charge to an ionic surfactant could form and stabilize an emulsion or a foam with very low surfactant concentrations, typically less than the Critical Micellar Concentration. This stabilization is explained by the coadsorption of molecules of polymer and surfactant at the fluid/fluid interface and by the formation of a polymer /surfactant complex having a high interfacial activity.

In addition, it is possible to modulate the association and therefore the stability of the emulsion or of the aqueous foam by acting on the electrostatic attraction between the two charged species. Formulations based on polyampholytes or amphoteric surfactants can therefore be used as pH-sensitive systems to control the stability or breaking of emulsions or of aqueous foams. With a view to sustainable development, formulations based on biodegradable natural polymers might be developed in this way.

scientific contact:
j-francois.argillier@ifp.fr

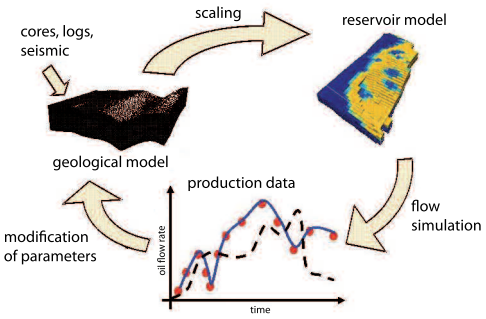


Interfacial tension of the anionic surfactant (SDS) alone and of the combined anionic surfactant and cationic polymer (AM/MAPTAC), with the formation (box) of a highly active polymer/surfactant complex at the interface.

*A. Asnacios, D. Langevin, **J.F. Argillier,** Complexation of cationic surfactant and anionic polymer at the air-water interface, Macromolecules, 29, 23, pp. 7412-7417, 1996. DOI 10.1021/ma960225n.*

***J.F. Argillier, S. Zeilinger, P. Roche,** Enhancement of aqueous emulsion and foam stability with oppositely charged surfactant/polyelectrolyte mixed systems, Oil & Gas Science and Technology - Rev IFP, to be published in Oct 2009.*

Reconciling reservoir models and production data



Fitting methodology.

In order to optimize oil & gas recovery, IFP is developing a reservoir modeling methodology based upon the fitting of dynamic data. The objective is to generate geological models satisfying all data collected: static data such as measurements on cores and dynamic data such as flowrates or time variations of seismic attributes (4D seismic).

The method comprises basically two phases: defining a sequence of activities and fitting the dynamic data. A sequence of activities is a sequence of operations that serves to go from the geological model to production responses. It includes, for example, a step in which the physical properties are modelled on the scale of the geological model, scaling to a coarser reservoir model, and flow simulation to obtain production responses.

The reservoir model produced in this way has predictive value if the simulated responses reproduce the dynamic data. The goal is therefore to minimize the function measuring the difference between the simulated results and the data. The integration of dynamic data of different types, such as 4D seismic in addition to the production data, poses difficulties that have not yet been completely overcome. This question is the purpose of the MC2 research consortium. The methodology set up has also led to the development of IFP's *CondorFlow* software, marketed by Beicip-Franlab.

***M. Le Ravalec, B. Noetinger, L.Y. Hu,** The FFT moving average (FFT-MA) generator: an efficient numerical method for generating and conditioning Gaussian simulations, Math. Geol., 32(6), 701-723, 2000.*

***F. Roggero, D.Y. Ding,** P. Berthet, **O. Lerat,** J. Cap, P.E. Schreiber, Matching of production history and 4D seismic data – Application to the Girassol field, offshore Angola, SPE ATCE, Anaheim, CA, USA, SPE 109929, 2007.*

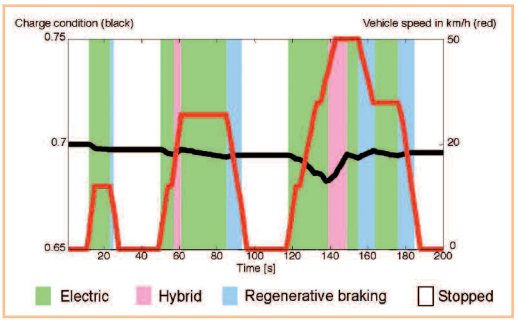
scientific contact:
mickaele.le-ravalec@ifp.fr

Optimizing energy management in hybrid vehicles

There have been hybrid vehicles for over a century, but it is only recently that their potential contributions to longer range and lower CO_2 emissions have been explored. One very important function among the keys to this success is the management of energy flows on board. This is a control problem that is complex, but is normally dealt with using heuristic management laws, calibrated case by case. A step forward towards energy managers that are general, but still powerful, can be taken thanks to mathematical optimization.

On the basis of judicious optimization criteria (fuel consumption, emissions, range, etc.) and constraints (battery life, drivability, etc.), IFP's researchers are developing original tools to calculate the optimal energy management laws for a specified driving profile. The tools apply to any hybrid vehicle architecture and are based on Pontryagin's Minimum Principle (PMP). Unlike most existing optimization techniques, such as Dynamic Programming, the kernel of the laws resulting from the PMP can be applied directly on board, even if the driving cycle is not known there in advance, thanks to the on-line estimation of an unknown parameter.

These innovative techniques are validated using the "HyHiL" system, a semi-virtual testing resource dedicated to hybrids, developed as part of a project financed by the *Fonds unique interministériel* ("French interministerial fund"). The tests have shown that on-line control allowed the best possible use of the available degrees of freedom. Current work is aimed at extending the optimization methods, for example to thermal management and to regenerative braking.



Optimal development of battery charge and operating mode versus vehicle speed.

*L. Guzzella, **A. Sciarretta,** Vehicle propulsion systems: Introduction to modeling and optimization, 2nd edition, Springer-Verlag, Berlin Heidelberg, 2007, ISBN 3540746919.*

***A. Sciarretta,** L. Guzzella, Control of hybrid electric vehicles: Optimal energy-management strategies, Control Systems Magazine, vol. 27, no. 2, April 2007, pp. 60-70. DOI: 10.1109/MCS.2007.338280.*

scientific contact:
antonio.sciarretta@ifp.fr

Visualizing unburnt hydrocarbons in low-NOx engines

The development of the new low-temperature diesel combustion modes, making it possible in particular to achieve very low levels of nitrogen oxides and particulate emissions, is hindered by the fact that this type of combustion can also generate significant emissions of unburnt hydrocarbons. It is for this reason that IFP has performed a study aimed at a better understanding of the phenomena concerned and propose ways for improvement.

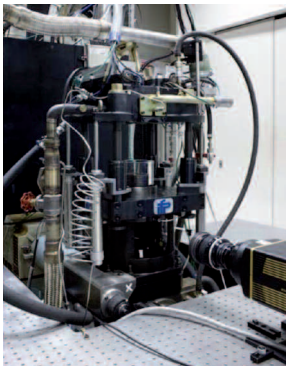
For this purpose, measurements have been made on a "transparent" engine, using various specially developed laser-induced fluorescence techniques in order to visualize not only the zones of formation of unburnt hydrocarbons, but also the liquid film deposits on the piston wall. These measurements have been coupled to the results of parametric variations performed on a standard, all-metal engine, including changes of engine configuration. Two preponderant mechanisms have been identified in this way: bulk quenching (deficit in combustion temperature or local equivalence ratio, leading to incomplete reactions) and the formation of liquid film on the piston wall with some injection strategies.

The application of fluorescence measurement techniques also made it possible to understand how the liquid film deposited on the surface of the piston separates from it during the expansion stroke, by a film flash-boiling phenomenon, thereby emitting unburnt hydrocarbons in the engine exhaust.

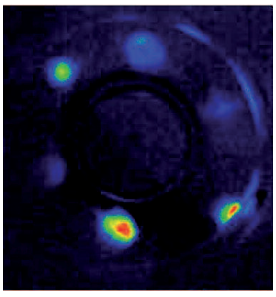
***J. Kashdan, G. Bruneaux,** Mixture preparation and combustion in a optically-accessible HCCI diesel engine, Oil & Gas Science and Technology – Rev IFP, vol. 61, n° 1, pp. 25-42, 2006.*

***J. Kashdan, G. Bruneaux,** An investigation of unburned hydrocarbon emissions in wall-guided, low temperature diesel combustion, Oil & Gas Science and Technology – Rev IFP, vol. 63 n° 4, pp.433-459, 2008.*

scientific contact:
gilles.bruneaux@ifp.fr



Optical engine used for the tests.



Visualization of the liquid films formed on the piston surface, by laser-induced fluorescence through the transparent piston.

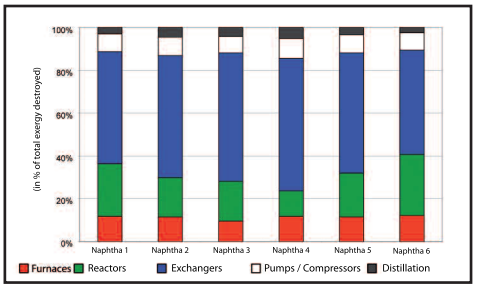
Exergetic analysis and sustainable development of processes

In order to propose materials transformation processes that are effective and environmentally-friendly, it is essential to incorporate the limitations and requirements in terms of greenhouse gas emissions and resource depletion as early as possible in their development. The environmental impact of a process can be determined by a Life Cycle Analysis, but this requires a level of detail not available at the conceptual design stage of a process. For a qualitative estimate, a simplified life cycle analysis is used, which delivers a mean value of greenhouse gas emissions for various types of utility (water, steam, electricity, etc.).

The exergy, a thermodynamic function that relates the enthalpy, the entropy, and a reference to a standard environment, represents the "useful" part of the energy of a fluid. In consequence, the more exergy is destroyed, the more useful energy is lost. The features of a process requiring improvement can in this way be highlighted by determining the destruction of exergy in each individual operation.

Coupling the exergetic analysis and the simplified life cycle analysis reveals that greenhouse gas emissions increase as more exergy is destroyed. In this way, elements of the process contributing most to its environmental impact may be identified.

Current developments aim at incorporating, in this analysis, the notion of value of the flows produced by the process, in order to obtain an index that will steer development to a process that is both economically viable and environmentally-friendly.



Exergy destroyed by type of unit operation in a catalytic reforming process.

*J.F. Portha, J.N. Jaubert, **S. Louret,** M.N. Pons, Definition of a thermodynamic parameter to calculate carbon dioxide emissions in a catalytic reforming process, Int. J. of Thermodynamics. Vol.11 (2), pp.81-89, June 2008.*

scientific contact:
sylvain.louret@ifp.fr

Photos : © IFP, X

Appointments

• **Christian Angelberger,** *IFP Expert, was appointed a member of section 10 (Fluid and reactive media: transport, transfer, transformation processes) of the CNRS by the Ministry of Higher Education and Research on 16 September 2008.*

• **François Roure,** *IFP Expert in Structural Geology, has been renewed in his positions with the Publications Committee of the AAPG (American Assoc. of Petroleum Geologists).*

Collaborations

• **IFP, the CNRS and ENS-Lyon** *are starting up a research project in molecular modeling for catalysis with King Abdullah University of Science and Technology (KAUST), a world-class university and research center under construction in Saudi Arabia.*

• **IFP and the BRGM** *have signed a research partnership agreement in the modeling of CO_2 storage facilities, organized around IFP's Coores™ simulation software and supported by their complementary skills and expertise.*

Chairs at the IFP School

• **Philippe Joseph,** *IFP Expert, holds the chair of "Sedimentology and reservoir characterization" supported by Total*

• **Antonio Sciarretta,** *IFP Expert, has been named to the chair of "Hybrid vehicles and energy management" (January 2009).*

Awards

• **Prix Yves Chauvin 2008 :** *IFP's thesis prize has been awarded to* **Antoine Fécant** *for his opus entitled "Synthesis of new zeolites having pore openings with 10 and 12 tetrahedral atoms".*

• **Marc Fleury,** *of the Reservoir Engineering Division, has been awarded the Darcy prize for 2008, the Society of Core Analysts' highest honor, for his work in petrophysics.*

• **Caroline Chaux** *has been awarded the 2008 Thesis Prize of the Electronics, Electrical Engineering, and Automation Teachers and Researchers Club for her thesis, "Analysis in M-band wavelets in dual tree; application to image restoration", supervised by J.-C. Pesquet (Université Paris-Est) and L. Duval (IFP).*

Accreditations to Supervise Research (HDR)

• **Gilles Bruneaux,** *IFP Expert, HDR, Université d'Orléans: "Experimental investigation of the structure of the diesel jet and its combustion" (25 June 2008).*

• **Gerhard Pirngruber,** *HDR, Université Claude Bernard Lyon 1: "Breakdown of N_2O and synthesis of biomimetic catalysts" (11 December 2008).*

Book

"La nouvelle donne du charbon" - ("The New Deal in Coal")
F. Kalaydjian, S. Cornot-Gandolphe
Éditions Technip - ISBN: 9782710809265.

Scientific conferences at IFP

• **IFAC Workshop on Engine and Powertrain Control, Simulation and Modeling**
30 November - 2 December 2009,
IFP, Rueil-Malmaison
Organizational contact: bettina.caruso@ifp.fr
Scientific contact: paolino.tona@ifp.fr

• **1st International Conference on Chemical Looping**
17-19 March 2010, IFP-Lyon, France
Organizational contact: frederique.leandri@ifp.fr
Scientific contact: thierry.gauthier@ifp.fr

• **The AAPG-European Region Conference** *will be hosted by IFP at Rueil-Malmaison on 23 and 24 November 2009.*

ANR (French National Research Agency)

• **L'IFP** *has been chosen by the ANR as support organization for the VTT (Vehicles for Terrestrial Transport) program, aimed at promoting energy efficiency in vehicles, lower emissions, and transport systems efficiency.*

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To get in touch with IFP or receive Science@ifp:
Communications Division: Tel.: +33 1 47 52 59 00 - Fax: +33 1 47 52 70 96 - Science@ifp.fr
1 et 4 avenue de Bois-Préau - 92852 Rueil-Malmaison Cedex - France
Press contact: A.-L. de Marignan - Tel.: +33 1 47 52 62 07
Institutional contact: K. Ragil - Tel.: +33 1 47 52 58 75

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