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Potential of ethanol-dedicated engines



Endorsing a sustainable development approach is one of IFP's major commitments.

This is further corroborated by its five strategic priorities: controlled CO₂, diversified fuels, fuel-efficient vehicles, clean refining and extended reserves. This fourth issue of Science@ifp presents a selection of recent publications that bear witness to IFP's action in this context. Simulating the complete dynamic of a sedimentary basin, mastering well fracture network geometry, reconstructing complex petroleum cuts by computer, proposing new engine control approaches for improved energy management aboard hybrid vehicles, or demonstrating another way of using ethanol potential as an alternative to conventional fuels are the contributions proposed here.

Hoping that you enjoy reading this issue...

Xavier Montagne
Associate scientific director

In a context that requires reducing greenhouse gas emissions and diversifying energy sources in the transport sector, ethanol has a great potential, especially when it is produced using the lignocellulosic approach (second-generation). In addition, ethanol properties, in particular its very high octane number, are extremely well suited to spark-ignition engines.

IFP has demonstrated the potential of such a fuel by developing and partially optimizing an ethanol-dedicated engine. A small-displacement SMART engine was modified in this way by optimizing its compression ratio and materials, but also the control laws (engine mapping). The result was a substantial increase of power and torque (expressed as Mean Effective Pressure, Fig. 1) and a clear

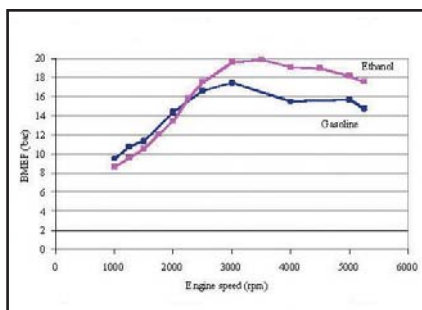


Fig. 1: Mean Effective Pressure (equivalent to engine torque) versus engine speed and fuel.

reduction in unburnt hydrocarbon emissions.

This optimization also allowed to reduce CO₂ emissions from the vehicle's exhaust by 9% (Fig. 2), which further strengthens the positive well-to-wheel balance of the ethanol approach.

This development demonstrates the potential of ethanol motor fuel and paves the way to further ethanol combustion optimization studies (studies now in progress at IFP) in particular on gasoline direct injection engines. ■

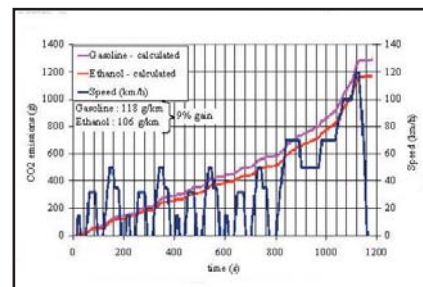


Fig. 2: Total CO₂ emissions on NEDC.

"Potentiality of ethanol as a fuel for dedicated engine", N. Jeuland, X. Montagne, X. Gautrot, *Oil & Gas Science and Technology - Rev. IFP*, Vol. 59 (2004), No. 6, pp. 559-570
DOI: 10.2516/ogst.2004040

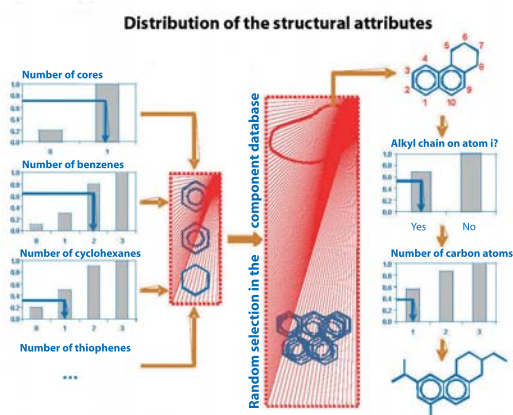
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IFP is a world-class public-sector research and training center, aimed at developing the technologies and materials of the future in the fields of energy, transport and the environment.

Molecular reconstruction of petroleum cuts

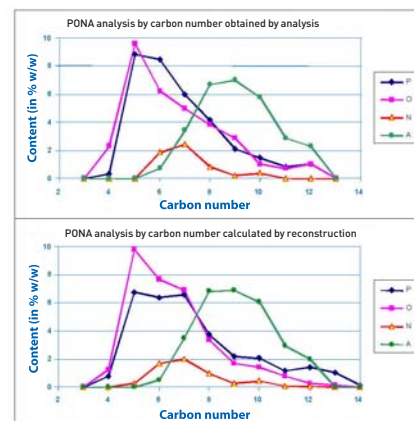
Optimizing refining processes calls for the development of ever more precise kinetic models. It is therefore important to rely on a detailed molecular representation of petroleum cuts. Current analytical techniques can characterize on a molecular level only fractions containing up to nine carbon atoms, because of the large number of isomers having similar properties.

Various methods have therefore been developed to numerically "reconstruct" mixtures of molecules from the available analytical data. These molecular reconstruction techniques, based on stochastic or statistical principles, or using information entropy maximization, have been successfully applied to gasoline, gas oil, vacuum distillate and residue fractions. They have made it possible to propose synthetic mixtures containing a large number of molecules and mimicking the properties of these petroleum cuts.



Stochastic reconstruction method.

The reconstructed mixtures subsequently serve as basis for the development of models. For example, in the case of residues, they provide a detailed representation that allows developing molecule-based kinetic models. The strength of this approach lies in the data reconciliation of the various analytical techniques and in the polydisperse representation of the mixture. ■



Comparison of PONA analyses (paraffins, olefins, naphthenes, aromatics) by carbon number obtained by analysis and predicted by information entropy maximization.

Molecular reconstruction of LCO gasoils from overall petroleum analyses, D. Hudebine, J. Verstraete, *Chem. Eng. Sci.*, 59, 4755-4763, 2004 - DOI: 10.1016/j.ces.2004.09.019

Molecular reconstruction of naphtha steam cracking feedstocks based on commercial indices, K.M. Van Geem, D. Hudebine, M-F. Reyniers, F. Wahl, J. Verstraete, G.B. Marin, *Comp. Chem. Eng.*, 31, 9, 1020-1034, 2007 DOI: 10.1016/j.compchemeng.2006.09.001

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Microkinetic models for complex petroleum cuts

Kinetic modeling of petrochemical processes, performed to optimize them, is especially difficult because of the very large number of reactants present in the charges. One solution is to lump the components. For this purpose, various strategies are proposed according to the type of petroleum cut.

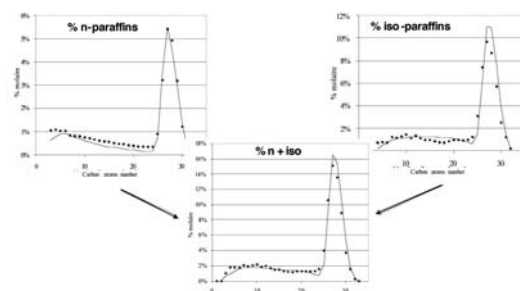
For distillates and bifunctional heterogeneous catalysis, the construction of a "single-events" model includes:

- the computerized generation of the complete network of elementary reaction steps between all the carbocations present at the surface of the acid phase,
- a strategy of reducing the number of kinetic constants,
- a rigorous *a posteriori* grouping procedure.

A second late lumping method, not requiring the generation of the reaction network but based on a computerized inventory of the complexes activated, has been developed. It opens up the possibility of extrapolating the model to heavy petroleum cuts, which has been demonstrated by simulation of the hydroisomerization of Fischer-Tropsch waxes. More recently, in co-operation with the University of Ghent (Belgium), it has been successfully extended to the description of metallic catalysis reactions. ■

A single events kinetic model: *n*-butane isomerisation. K. Surla, H. Vleeming, D. Guillaume, P. Galtier, *Chemical Eng. Sci.*, vol.59(22-23), 2004, pp. 4773-4779. DOI: 10.1016/j.ces.2004.07.036

A single events kinetic model for the hydrocracking of paraffins in a three-phase reactor, J.M. Schweitzer, P. Galtier, D. Schweich, *Chem. Eng. Sci.*, vol.54, 1999, pp. 2441-2452 - DOI: 10.1016/S0009-2509(99)00006-8



Measurements / Model comparison by carbon number (up to C35 on abscissa) in a process effluent.

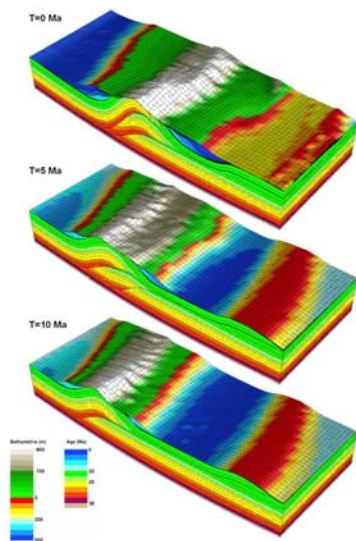
Kinetic methods in petroleum process engineering. P. Galtier, *Advances in chemical engineering*, 2007, vol.32, pp.264-307.

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Complex stratigraphic and tectonic modeling

To improve the success rate in exploratory drilling, IFP has since the beginning of the 1990s been developing a numerical stratigraphic model, *Dionisos*, that simulates the evolution of sedimentary basins over geological time. The early work investigated the evolution of deltas and carbonate-containing platforms. During the last four years, much work has been done in sedimentology and in applied mathematics, in order to optimize the numerical diagrams and enrich the list of physical processes taken into account by the *Dionisos* model (erosion of mountainsides, avulsion of rivers, growth of coral reefs, formation of diapirs, etc.).

Dionisos can now simulate the interaction between tectonic and sedimentary processes, from the growth of a mountain chain to the transport and deposit of sediments in deep basins. It is currently



Modeling of the filling of sedimentary basins in active tectonic zones.

used in oil exploration, during the evaluation of frontier zones or the delineation of prospects.

Work is underway to better describe the transport of fine sediments and the production of evaporites. This will make it possible in the longer term to associate *Dionisos* with climatic models and to simulate the complete dynamics of a sedimentary basin.

This project has been led by a research consortium supported by eight partners for ten years and has already produced industrial software, marketed by Beicip-Franlab. ■

H. Alzaga-Ruiza, D. Granjeon et al., 2008, *Gravitational collapse and neogene sediment transfer across the western margin of the Gulf of Mexico: Insights from numerical models, in tectonophysics* DOI:10.1016/j.tecto.2008.06.017

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Automation and signal processing for engine control

Automation and signal processing henceforth play a pivotal and growing part in vehicle operations. To meet requirements in terms of consumption and pollution, energy production and its distribution to the wheels must be optimized.

From the technical standpoint, the best combination of actuators must be achieved based on measured or estimated information about the system's condition. Estimating parameters that are not measured (temperature in the combustion chamber, battery charge condition, etc.), designing multivariable and nonlinear controllers, and implementing them in on-board real-time software are the main obstacles to be overcome. In addition, on-board systems and variable frequency are obstacles for algorithmic design. From the scientific standpoint, original approaches are

sought. For example, the cyclo-stationary nature of the engine was used to increase the convergence of a torque estimator.

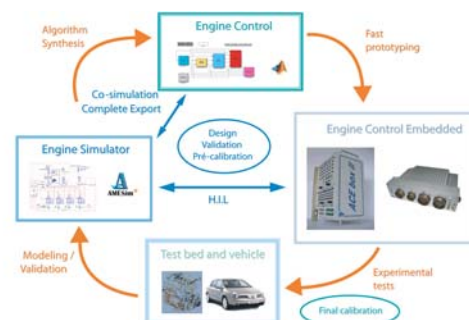
Vehicle hybridization strengthens the role of control, with energy management becoming the key to cutting consumption. The new generation of energy managers relies on automation techniques, which will ultimately replace the heuristics which were used initially. ■

J. Chauvin, G. Corde, N. Petit, P. Rouchon, *Automatica*, vol. 43, pp. 971-980, 2007.
DOI : 10.1016/j.automatica.2006.12.012
L. Guzzella, A. Sciarretta, *Vehicle Propulsion Systems - Introduction to Modeling and Optimization*, Springer 2005.
ISBN 3540251952, 9783540251958

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Hybrid natural gas vehicle in which IFP developed the whole ICE-hybrid control system. Partners in the project: ADEME, GDF SUEZ, Inrets, Valeo



Powertrain control system design and development chain.

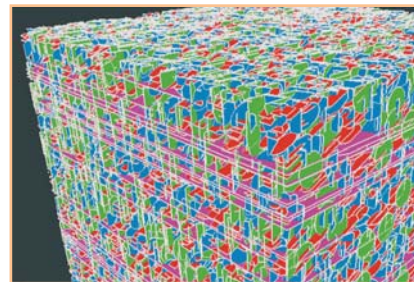
Homogenization of a fractured rocky medium

The numerical simulation of fluid flows in the rocks of a petroleum reservoir or a gas storage facility calls for information on various scales about their hydraulic properties, in particular their permeability. In the case of fractured reservoirs, this physical quantity is linked to characteristics of the network of fractures discernible on a scale much smaller than the mesh of a reservoir model.

Providing well data analysis tools to more effectively constrain the determination of the geometrical and hydraulic properties of the fracture network and from them deduce the macroscopic permeability of the volume through which this network passes is one of the FracFlow software's objectives, a software program developed by IFP.

Recent methods make it possible to estimate the permeability without resorting to stochastic representations. For example, effective media theory has in particular been used to account for the simultaneous presence of microfractures and closely spaced long fractures in an arbitrary anisotropic context. The method yields an estimate of the percolation threshold in the case of microfractures alone.

The method can also provide estimates of other properties: elastic (these can be linked to seismic attributes), thermal, or electrical. By fitting the model to several types of data, the uncertainty on fracture network characteristics can be minimized to improve reservoir development. ■



Stochastic generation of a realistic network of fractures.

Barthélemy J.-F., Effective permeability of media with a dense network of long and micro fractures, accepted for publication in *Transport in porous media*, 2008. DOI: 10.1007/s11242-008-9241-9

Barthélemy J.-F., 2007, Mechanical and hydraulic effective properties of an anisotropic fractured medium, in *Particle and continuum aspects of mesomechanics*, pp. 805-812. ISBN: 9781847040251.

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Awards

- **Alain-Yves Huc**, associate director of the Geology-Geochemistry-Geophysics division and IFP Professor, has received an "Honorable recognition award" for his work as "distinguished lecturer" as part of the EAGE's "Student lecture tours" program.
- **Denis Guillaume** has won the 2008 prize of the Catalysis division of the Société française de chimie for his research work conducted since 1999 in various heterogeneous catalysis fields.
- **Pierre Duret**, director of the Center for IC engines and hydrocarbon utilizations at IFP School, on 9 April last was awarded the medal of recognition of the Société des ingénieurs de l'automobile (SIA).
- **Ludovic Métivier, Florence Delprat-Jannaud and Patrick Lailly**, (IFP) and Laurence Halpern (University Paris XIII - Villetaneuse) won a prize at the CANUM conference (Congrès d'analyse numérique - May 2008), awarded by the Société de mathématiques appliquées et industrielles (SMAI) for their poster entitled "2D inversion of well seismic data".
- **Philippe Ungerer**, Scientific director of IFP, has been named Chevalier de l'Ordre national du mérite, by decree of the President of the French republic dated 30 January, on the proposal of the French Minister of higher education and research.

Other news

- On 13 February 2008 the **Gérard de Soete thesis prize** was created: it recognizes research work on the chemical kinetics of combustion. The prize will be awarded every two years in tribute to this former IFP researcher, co-founder of the Groupement français de combustion (GFC).
- **Pascal Barthélemy** joined IFP on 5 May as Executive vice-president. He holds a PhD in physical chemistry and was in charge of External relations, Industrial development and in particular Sustainable development for R&D with Rhodia. Pascal Barthélemy was also the founder and chairman of the Lyon and Rhône-Alpes Chemistry-Environment competitiveness cluster (Axelera).

Appointments to IFP's Scientific Board

As advisors:

- **Sébastien Candel**, École Centrale de Paris
- **Guy Marin**, University of Ghent (Belgium)

As expert members:

- **Paul Colonna**, INRA
- **Philippe Sautet**, ENS Lyon
- **J. M. Tarascon**, University of Picardie, French academy of sciences

IFP International Conferences

- **Advances in hybrid powertrains**
25-26 November 2008, IFP, Rueil-Malmaison
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Scientific contacts: francois.badin@ifp.fr and antonio.sciarretta@ifp.fr
- **Deep saline aquifers for CO₂ and energy storage**
27-29 May 2009, IFP, Rueil-Malmaison
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Scientific contact: etienne.brosse@ifp.fr

Book

A. Rojey - *Énergie et climat - Réussir la transition énergétique*, Éditions Technip
ISBN 978-2-7108-0908-1

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