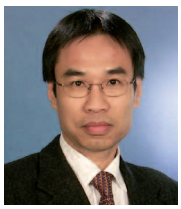
Science@ifpen
Issue 10 - October 2012



According to a recent bibliometric study, IFP Energies nouvelles (IFPEN) is now one of the world's top ten organizations in terms of scientific publications and quotations in the fields of engine and powertrain control. This result reflects our excellent position on the international stage and the broad influence of our research in these fields.

This special issue of Science@ifpen is dedicated to IFPEN's research in the field of digital sciences and technologies. In addition to questions directly linked to motor vehicle issues, readers will also find information concerning the numerical simulation of CO_2 storage, algorithmic geometry in geosciences, image processing for catalyst analysis, as well as real-time simulation in the design of complex physical systems. These few examples aim to demonstrate the full potential of numerical modeling and simulation in all the fields we operate in, including numerical chemistry, processes, engine combustion and geosciences.

We hope that you enjoy this issue.

Van Bui Tran,
Director, Technology, Computer Science and Applied Mathematics Division

Keeping a close watch on batteries

Subject to high dynamic stress, battery systems are the most critical components in electric vehicles. Controlling their state of charge (SOC) and state of health (SOH) is essential in terms of powertrain management and in order to reduce the performance deterioration and life span of the battery.

SOC and SOH cannot be measured directly onboard. So an accurate and reliable estimation on the basis of available measurements is necessary. This problem is difficult to deal with because, firstly, the cells composing the battery pack are the site of highly complex electrochemical phenomena and, secondly, the battery pack is equipped with few instruments.

State of charge estimators are conventionally based on integration of current over time. They are of limited predictive use since they are not capable of estimating the initial state, overvoltages and the available power. The solution proposed by IFPEN researchers consists in using an extended Kalman filter, able to estimate the internal state of the cell. This filter is based both on a dynamic model of the cell and voltage and current measurements at the battery terminals. The proposed approach is based on modeling of electrochemical phenomena by electrical analogy. Tested on IFPEN's HIL (Hardware in the Loop) bench on different battery technologies, this filter has demonstrated a good level of precision for estimating the charge, the energy and the available power. This level of precision will be further improved by using non-gaussian errors filtering methods, such as the particulate filter.

IFPEN's battery HIL bench is used to assess the behavior of a battery within an entirely virtual complex powertrain.

D. Di Domenico, *A. Stefanopoulou, G. Fiengo, Journal of Dynamic Systems, Measurement, and Control (JDSMC), 2010, 132 (6). DOI: 10.1115/1.4002475*

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CO_2 simulates its own storage

For effective and safe geological CO_2 storage, it is crucial to fully understand and control the chemical interactions that might occur between the gas, the water and the rock, during the injection operation, first of all, then throughout the long-term storage period.

Numerical modeling of these interactions can be used to assess the risks, as well as the potential for trapping the injected CO_2.

The numerical difficulties encountered in a reactive transport simulator are numerous. Hence, conventional solvers cannot be used to resolve non-linear systems comprising chemical equilibria equations and stiff kinetics. In addition, these methods usually require a large number of iterations and the successive failures generally lead to significant reductions of the time step. Since these difficulties are localized within a small area of the simulation domain, one possible solution is to isolate this reactive zone. Working in partnership with the *Laboratoire Analyse, Géométrie et Applications* (LAGA – Analysis, Geometry and Applications Laboratory) at the University of Paris 13, IFPEN researchers studied a time-space domain decomposition method, extended to the partial differential equation systems used for reactive transport. This research led to the development of a general coupling methodology, i.e. one applicable irrespective of the domain geometry, and with or without overlapping.

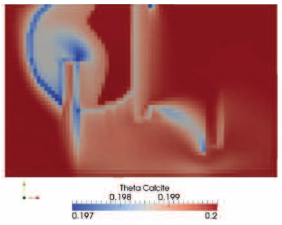
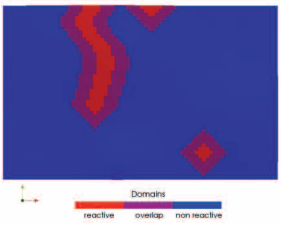


Image of the calcite dissolution front (blue) bordering the CO_2 storage zone.



Reactive sub-domain (red), non-reactive domain (blue) and overlapping (magenta).

This strategy has been applied in a prototype code as part of the ANR $SHPCO_2$ project and will be tested soon on real cases to assess its full potential.

F. Haeberlein, A. Michel, F. Caetano, Time space domain decomposition for reactive transport, *Procedia Computer Science, 2010, 1 (1), 753-760.*

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Simulation and Co.

HIL simulation platform used for real-time testing of engine control systems.

A common obstacle encountered when assessing new integrated systems is the physical absence of certain components or prototypes. Real-time simulation is the ideal solution to overcome this problem, making real elements interact with missing, but simulated, ones.

However, simulated component models may present complexities preventing their real-time execution. In routine practice, these models are reduced in these situations, but this leads to a reduction in their predictive capacities and their representativity. Additional validation work is required as a result.

To address this problem, IFPEN has adopted an original approach: application of a cosimulation method, facilitating parallelization of 0D model resolution and enabling modular and multi-rhythm integration. To achieve this, specific real-time execution models have been proposed. These provide a compromise between quality of results and performance of distributed execution on multi-core PCs. The new real-time scheduling methods that have become possible as a result have been described, studied theoretically and validated experimentally.

Among other things, this research has led to improvements in rapid engine control law prototyping methods and made it possible to extend the capacities of a high-dynamic test bench to validation of hybrid powertrain concepts.

The research is being continued today, the aim being to enable automatic parallelization of complex system 0D models.

P. Marti, A. Camacho, M. Velasco, ***M. Ben Gaid,*** *IEEE Transactions on Industrial Informatics, 2010, 6 (4), 503-520.*

M. Ben Gaid, *A. Cela, Y. Hamam, IEEE Transactions on Control Systems Technology, 2009, 17 (2), 309-326.*

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When grids become gridlocked

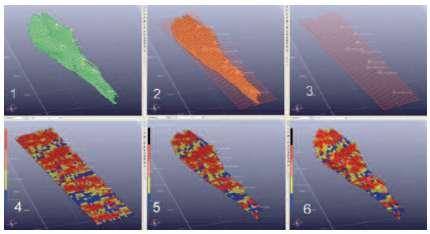
Reservoir models are essential if we are to have a clearer understanding of fossil resources and hence make better use of them. Feeding these models with physical properties on the basis of well data is a key step in their construction.

In current methods used to populate the properties of a CPG (Corner Point Geometry) stratigraphic grid, a Cartesian grid of equivalent size (in each direction), obtained by averaging the edge lengths, is first of all completed. The properties calculated in this way are then transferred as they are into the initial CPG grid, because there is cell-for-cell correspondence. This leads to distortion of the Cartesian grid, making it fit the shape of the CPG grid. However, this has the effect of altering calculations of correlation distances between well markers in geostatistical population simulations and, consequently, this primarily induces distortions on the simulated bodies.

To resolve this problem, IFPEN has developed innovative methods for a "smooth" conversion from a CPG grid of the structural space to a Cartesian grid of the geostatistical population space.

The basic principle is to calculate the correlation distances between wells on the basis of "quasi-isometric" flattening of the stratigraphic unit CPG grid in the filling space. This same flattening technique is then used for inverse transfer of the properties from the filling space to the structural space, as illustrated in the right hand figure. This is valid as long as these volumes are slim, something that is always the case in practice.

This research has led to a prototype, that is currently being tested and that will be industrialized in 2013.



The various steps in the methodology:
1: initial CPG grid
2: flattened CPG grid
3: Cartesian filling grid with transfer of wells on the basis of flattening
4: Cartesian grid populated by geostatistics
5: flattened CPG grid populated by upscaling from the Cartesian grid
6: initial CPG grid populated from the flattened CPG grid.

M. Poudret, C. Bennis, *H. Bourouchaki,* ***J.-F. Rainaud,*** New flattening-based methodology for more accurate geostatistical reservoir populating, *to be published in Engineering with Computers Journal.*

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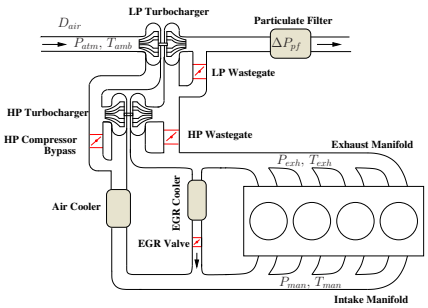
Turbo under control

Engine turbocharging systems are key components in new air loop architectures. They improve gasoline engine efficiency using the downsizing technique and reduce the pollutant emissions of diesel engines by allowing the intake of high levels of burned gases. There is an increasing diversity of turbocharging technologies available (variable-geometry turbine, double turbocharging, electric compressor), leading to modifications of their control systems.

The objective of turbocharging control is to satisfy pressure requirements by minimizing the system's response time, taking into account multiple constraints and interactions.

IFPEN's approach is based on the use of reduced system models, from which simple control laws are developed, with properties (stability, convergence, compliance with constraints) that can be verified on these reduced models. Experimental tests are then performed to validate the hypotheses produced at the model reduction stage. The control laws proposed are generally based on trajectory planning and feedback linearization.

One of the advantages of the approach lies in the reduced model proposed. This is because it provides an open loop action, which can be easily integrated into industrial engine control, without affecting its structure. Today, the two stage turbocharger control strategies developed at IFPEN have been integrated into a mass-produced vehicle computer and control strategies for a variable-geometry turbocharger are ready to be produced on an industrial scale.



Engine fitted with a double turbocharger.

P. Moulin, J. Chauvin, Modeling and control of the air system of a turbocharged gasoline engine, *Control Engineering Practice, 2011, 19 (3), 287-297. DOI: 10.1016/j.conengprac.2009.11.006*

J. Chauvin, O. Grondin, P. Moulin, Control Oriented Model of a Variable Geometry Turbocharger in an Engine with Two EGR Loops, *Oil & Gas Science and Technology – Revue d'IFP Energies nouvelles, 2011, 66 (4), 563-571. DOI: 10.2516/ogst/2011103*

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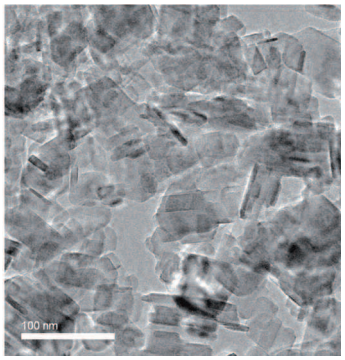
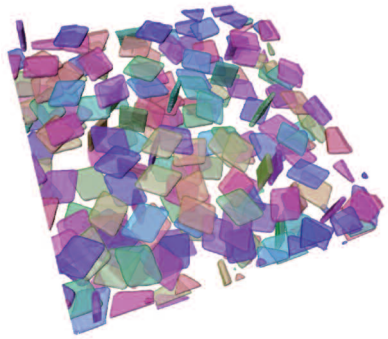
Getting inside catalysts

To make refining technologies more efficient and cleaner, improving the activity of catalysts is mandatory. This activity is partially linked to their microstructure, itself highly dependent on the morphology of the nanoparticles composing it. To address this key property, standard characterization methods presently used only provide information on the average size of these nanoparticles. While the microstructure is effectively visible by transmission electron microscopy (TEM), nanoparticles are semi-transparent and overlap. Their exact dimensions thus cannot be measured directly, as these nanoparticles are very difficult to disentangle.

The solution developed by IFPEN, in partnership with the *Centre de Morphologie Mathématique* (CMM – Mathematic Morphology Center) of Mines ParisTech, uses a numerical model of stochastic structure. It enables to access the size distribution of the nanoparticles observed, using statistical indicators estimated on the basis of experimental data. The approach has been employed to analyze boehmite nanoparticles used to create catalyst supports.



TEM observation of boehmite nanoparticles (0.41 nm.pixel^{-1}).



3D stochastic model simulated from statistical indicators based on observed experimental data.

The results obtained – unprecedented in terms of their precision – help us gain a greater understanding of the microstructure of these supports and the relationships between their properties (activity) and their structure. This paves the way for potential future innovations, the aim being to improve the performance of next-generation catalysts.

M. Moreaud, *D. Jeulin, V. Morard,* ***R. Revel,*** TEM image analysis and modelling: application to boehmite nanoparticles, *Journal of Microscopy, 2012, 245 (2), 186-199. DOI: 10.1111/j.1365-2818.2011.03560.x*

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Only one of these images is real... but which one?

Images of boehmite nanoparticles

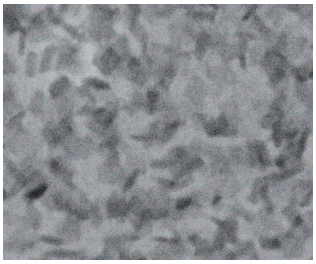

Image No. 1

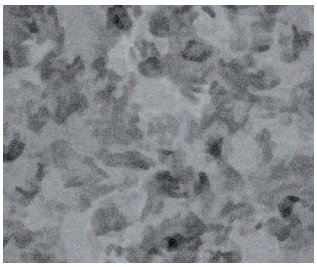

Image No. 2

The real one is the Image No. 2. *It is obtained by electron microscopy. The investigator is interested in the dimensions of the platelets (length, width, thickness), but these are difficult to measure from the image itself.* ***Image No. 1*** *is a simulation from a numerical model of this observation, obtained using mathematical methods from image processing. On this model, it is possible to measure the dimensions of the platelets and, consequently, to perform a precise analysis of characteristics that are not readily accessible using experimentally-obtained images.*

Upcoming scientific events

- *IFP Energies nouvelles' "Rencontres scientifiques" event* ***– IFAC Workshop on Engine and Powertrain Control, Simulation and Modeling, E-COSM'12 –*** *23-25 October 2012, IFPEN Rueil-Malmaison.*
- *IFP Energies nouvelles' "Rencontres scientifiques" event* ***– LES for Internal Combustion Engine Flows –*** *29-30 November 2012, IFPEN Rueil-Malmaison.*

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