International Conference on Multiscale Approaches for Process Innovation - MAPI 25-27 January 2012. Round Table Discussion.

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Oil & Gas Science and Technology – Rev. IFP Energies nouvelles, Vol. 68 (2013), No. 6, pp. 1109-1113

IFP Energies nouvelles International Conference
Rencontres Scientifiques d'IFP Energies nouvelles

MAPI 2012: Multiscale Approaches for Process Innovation
MAPI 2012 : Approches multi-échelles pour l'innovation des procédés

International Conference on Multiscale Approaches for Process Innovation – MAPI 25-27 January 2012 Round Table Discussion

Hervé Toulhoat*

IFP Energies nouvelles, 1-4 avenue de Bois-Préau, 92852 Rueil-Malmaison Cedex - France
e-mail: Herve.TOULHOAT@ifpen.fr

* Corresponding author

Résumé — Conférence internationale sur les approches multi-échelles pour l'innovation des procédés – MAPI – 25-27 janvier 2012. Comptes-rendus des discussions de la table-ronde — Cette table ronde avait été préparée avec l'objectif de recueillir les points de vue aussi bien des fournisseurs de nouvelles méthodes de simulation (chercheurs académiques) que d'industriels utilisateurs ou facilitateurs (distributeurs de codes et plateformes de calcul) sur quelques sujets clés :

– quel jalonnement vers la mise en pratique de la simulation multi-échelle pour innover dans les procédés ?
– pour quoi faire ? (conception de matériaux, de réacteurs, de schémas intégrés, prédiction de performances, pilotage en temps réel, etc.) ;
– quels verrous se présenteront sur ce chemin ? (représentation physique des phénomènes, capacité de calcul, constitution d'équipes pluridisciplinaires, validation expérimentale des prédictions, etc.).

Ce compte-rendu synthétique tente de faire ressortir l'essentiel des discussions et des réponses apportées.

Abstract* — *International Conference on Multiscale Approaches for Process Innovation – MAPI – 25-27 January 2012. Round Table Discussion — *The Round Table had been prepared with the aim to collect the views of both the suppliers of new simulation methods (academic researchers) than industrial users or facilitators (distributors codes and computing platforms) on a few key issues:*

– *what boundary mark to the implementation of the multi-scale simulation to innovate in processes?*
– *for what? (design of materials, reactors, integrated schemas, performance prediction, real-time control, etc.);*
– *what locks will be met on this path? (representation of physical phenomena, computing capacity, creation of multidisciplinary teams, experimental validation of the predictions, etc.).*

This report attempts to highlight synthetic most discussions and responses.

INTRODUCTION

This round table discussion was proposed as the last session of the MAPI conference. It was chaired by **Jean-Claude Charpentier**, and moderated by **Hervé Toulhoat**. The panel comprised **Richard J. Quann** (*ExxonMobil*), **Philippe Ungerer** (*Scientific Director Materials Design Inc.*), **Philippe Sautet** (*ENS Lyon, French Academy of Sciences*), **Hans Kuipers** (*TU Eindhoven*), and **Jan Verstraete** (*IFP Energies nouvelles*).

Our round table discussion had been prepared with the aim to obtain points of views of both industrialists (end users, enablers like software vendors) and academia (providers of innovative methods) for each issue addressed. In view of the limited time it also made sense to propose a focus on key topics:

- towards applicability of multiscale simulation for process innovation: roadmap and agenda? What for: design of materials? Of internals? Of flowsheets? Performance prediction *versus* for instance: changes in feedstock, operating conditions, ageing? Real time monitoring?
- where will be the bottlenecks along this roadmap? Physics? Team building involving cross expertise? Computational capability? Validation *versus* experiments? Precision?

In his 10 mn introduction, Jean-Claude Charpentier sketched the essential driving forces for developing innovative chemical processes in today's global context: to "convert molecules into money" is still the job, and for that be "first on the market with the required end use properties of products". But now you cannot avoid doing it in a sustainable fashion. That is to say social and environmental constraints have to be taken into account, and this using less energy and raw materials. To manage such a complexity, the integrated multiscale approach appears as the third paradigm of chemical engineering, after the first: unit operations, and the second: transport phenomena and chemical reaction engineering. Integrating scales from molecular phenomena up to the industrial platform necessarily involves understanding. For instance in biotech, if you want to modify a microorganism towards the production of a desired metabolite, you need to identify metabolic networks, the key enzymes involved, and the connection between genome sequence and the expression or mutation of these enzymes as desired. In general, three breakthroughs are enabling: intrusive instrumentation gathering information in situ at various spatial and temporal scales (*e.g.* NMR, MRI), high throughput experimentation for screening materials or operating conditions, and powerful computational tools which opened the avenues to more and more realistic numerical simulations at all scales: molecular modeling, computational fluid dynamics, static and dynamic process simulation, etc.

Hervé Toulhoat invites the panel to express views related to the first key topic:

1 TOWARDS APPLICABILITY OF MULTISCALE SIMULATION FOR PROCESS INNOVATION: ROADMAP AND AGENDA?

Richard J. Quann provided a point of view from industry on the first issue: can we delineate a roadmap towards process innovation based on multiscale approaches? For him, the number one goal is not to build models, but to build processes, because it is the latter which make the money. Today, there has not been a universal approach, but many different types of models, for different applications. For instance, we are very good with engineering models based on Navier stokes equations. We have not been so good in physical chemistry, because there much more science is needed. Over 300 equations of state have been published but this means actually that we do not understand enough and much more science is needed in physical chemistry. Also notice that modeling tools are required to predict what happens in case of "irregular" operations. They should also take into account safety issues.

Philippe Ungerer underlines that a new generation of tools emerged recently, based on the resolution of the Schrödinger equation and on statistical mechanics, which is the appropriate model for the molecular scale, as typically needed to design microporous and nanoporous adsorbents, *e.g.* zeolites, and for instance organic templates used to direct their synthesis. At the macroscopic scale, flowsheeting tools such as delivered by *Aspen Technologies* are on the market, but processes rely on the blackbox properties of materials (*e.g.* catalysts and sorbents). Materials sciences have comprehensive tools, but we need ever more engineering to pass this science to engineers. Achieving good communication is essential. Currently, bankers forecast a 30%/year growth in software engineering for materials sciences.

From an academic perspective, Hans Kuiper finds the paradigm "Process innovation based on multiscale approaches" very attractive. It means fundamental research inspired by end uses in a very systematic way. It is a great opportunity for academy, and on the basis of a convergent analysis, *Eindhoven University of Technology* has established a multiscale multidisciplinary institute. In order to achieve their common goals, scientists in the different fields involved must ask each other the right questions. To give but one crucial example, the field of interfacial transport phenomena involved in dispersed flows should be much much more developed.

Nobody can predict coalescence and breakup even with Direct Numerical Simulation (DNS). The fracture of solid materials is also lagging behind: better collaborations are needed for people from solid mechanics and from process engineering.

Jan Verstraete states that modeling is used systematically at *IFP Energies nouvelles* on different levels. It allows to do a lot of sensitivity analysis. Facing the challenge of rationalizing complexity, modelers are always trying to simplify: they need therefore to validate the models at different levels, going from catalyst development to a complete process. Precision is crucial since discrepancies of 10% at a given level will cumulate at the end.

Answering to Hervé Toulhoat's question, Jan Verstraete finds difficult to prioritize the importance of applications among materials design, reactor and internals design, and flowsheet design: it is a chain, and all levels are needed. Hervé Toulhoat adds that he had been impressed by the demonstration of cost optimization by design in Ludovic Raynal's talk.

Philippe Sautet comes back to the view point of academics: their basic role is to generate new knowledge, and under this respect the multiscale approach is a fantastic opportunity. The *University of Lyon* has also set up its multiscale institute ("LABEX iMUST").

Hervé Toulhoat asks viewpoints from the audience on applicability:

Celine Chizallet (*IFP Energies nouvelles*) asks whether in order to be efficient one will have to train students and people to be expert at all scales?

Hervé Toulhoat rephrases this question in terms of teams building, and asks for Richard J. Quann's advice: "if I need brain surgery I will not apply to a foot doctor". Experts generally misunderstand the other disciplines. Therefore it is brainstorming at the interfaces which will produce the breakthrough concepts.

Hervé Toulhoat asks his opinion also to Jean-Claude Charpentier, as the former director of two major french schools of chemical engineering, *ENSIC* (*Ecole Nationale Supérieure des Industries Chimiques*) in Nancy and *CPE* in Lyon: 20 years ago, industry said to ENSIC "make good chemical engineers, the other parts they can learn along their carrier". CPE is Chemistry, Physics and Electronics, so multidisciplinary with majors, at the other end of the spectrum. Jean-Claude Charpentier raises a persistent problem for academics in France: breakthroughs are emerging indeed at the interfaces, but there you cannot make an academic career.

Hans Kuiper confirms that especially for multiscale we need topnotch specialists in their discipline, but also create interfaces through multidisciplinary projects.

Philippe Sautet argues that one key approach is to promote a rather wide initial training (*e.g.* double master) and then on this broad training you need to build specialization, but not too early.

Hervé Toulhoat quotes the Nobel prize 2005 in chemistry and former *IFP Energies nouvelles* colleague Yves Chauvin's favorite advice "Curiosity is essential", and concludes that one should include curiosity in the formal training (laughters in the audience).

Pascal Raybaud (*IFP Energies nouvelles*) from the audience points out that in MAPI the last initial is for Innovation. Thinking in this direction he would like more clarification on where the breakthrough will come from when trying to connect levels. For instance, in which way catalysts screening could be optimized from a multiscale approach?

Philippe Ungerer replies that if at the atomic level, DFT is increasingly successfully applied, it is not only a matter of managing reactions: in a process, separation steps are also important for energy budget, purity, poisons etc. For that the relevant scale is meso-scale, *i.e.* between 10 nm to microns, poorly addressed so far. Therefore, for this scale dedicated method are needed.

Richard J. Quann adds: Invention is by definition going into a new territory. The value of the tools should be to help us identifying what we do not know. They should both improve our knowledge and show us in which direction to go.

Jan Verstraete notices that a lot of work tends to be concentrated on the very small level. But a lot is missing at the interfaces between intermediate levels (ex bubble breaking, droplets interactions). We should look at these scales from different perspectives. It promises a lot of room for innovation

Philippe Sautet points out to missing links: they are numerous, for instance multidynamic issues of the fluid, of the reaction, but also of the catalyst itself. The latter is too often seen as a static solid, while it is dynamic (structure, surface speciation) in many cases, so this is another complexity to take into account.

Hervé Toulhoat then proposes to address the second key topic:

2 WHERE WILL BE THE BOTTLENECKS ALONG THIS ROADMAP?

Philippe Sautet elaborates on physics: one big challenge stands in the multiphysics, *i.e.* to build bridges between fluid dynamics, heat transfer, physics of chemical reactions. Also important challenges rest in the type of coupling. Today one sees more often weak coupling: one

parameter is extracted from the lower scale, and plugged into the upper scale. It needs to be much more self-consistent, not only bottom-up, but also top-down then -up and -down etc. insight will come not only from numbers but from a correct appraisal of feedbacks and feed forward between scales.

Philippe Ungerer raises the point that predicting the computing time is important in the practice of simulation. We all need increased parallelisation of codes since Moore's law will find its path through massive parallelisation rather than CPU speed for physical limitations (heat release, etc.). A petaflops machine might be found in an engineer's office in a few years. Finally user-friendliness of interfaces to big codes produced by academic laboratories is an important issue. Simulations will deliver increasingly huge amounts of information to organize. Automated convergence will be also required.

Hervé Toulhoat asks whether techniques like grid computing or GPU/CPU hybridization will really offer new opportunities.

Philippe Ungerer confirms that such techniques are already largely in use by simulations platforms for materials sciences.

Hans Kuiper recalls that validation is also critical for multiscale modeling. In this spirit, challenge problems awards have much value. They consist in inviting modelers to reproduce sets of complete, well defined, experimental data. This should be done for every scale and area.

From the room: for moving from scale to scale, one need concepts, a textbook, but bottlenecks will be found rather between disciplines.

Richard J. Quann insisted on the fact that often a breakthrough comes from adding value from another field. For instance, analytical chemistry brought many breakthroughs to process design.

Jan Verstraete comes back to the need for well documented experimental works when validation is attempted. One needs to know how the experiment was made, not just a number, for instance isothermal versus not. Serious misfits can come from what is behind the data.

Philippe Sautet remarks that we deal with 10 orders of magnitude in space, and 20 in time so there is room for plenty of models. Therefore, it is important to discuss articulations, otherwise these models will remain "local" multiscale approaches.

Pierre Galtier (*IFP Energies nouvelles*) from the audience: he is surprised to hear so few emphasis about the need for kinetics/microkinetics studies. He views it as an important intermediate level which sets a bridge between chemistry and physics.

Hervé Toulhoat asks whether this is considered from an experimental standpoint or from a modeling standpoint?

Pierre Galtier proposes in return that we need to work on elementary steps in relation to the catalyst's structure.

Philippe Sautet remarks that this relation was hidden as an very important part in the topic "modeling the chemical reaction". Indeed, activation barriers have to be determined from first principles and translated into rates. Microkinetics and molecular modeling have to work together.

Hervé Toulhoat recalls that in connection to what Hans Kuiper and Jan Verstraete said about "well defined experimental data" experimental thermochemical properties provides crucial tests for the validation of new theoretical chemistry methods. He has been personally much concerned by looking for "chemical trends" in catalysis thanks to DFT theoretical descriptors: it works well as long as good experimental reactivity "patterns" are available for consistent sets of catalysts. It is quite difficult to find such sets of turnover frequencies at same operating conditions for instance. He would like to push for the fresh acquisition of such data.

Philippe Sautet observes that schools in kinetics are not developing anymore. It is not a popular discipline, in contrast with the current needs. It should develop.

Richard J. Quann confirms that so far we have not been good enough at relating kinetic data to materials structure.

Marianna Yiannourakou (*Materials Design*) from the room asks provocatively whether we should not also focus on multiple viewpoints on the same scale. For instance, should not there be a third axis for the result of different methods on the same scale? In adsorption for instance, Monte-Carlo simulations and experiments will provide isothermal loadings, but are not we also interested in mechanisms? Where adsorbates stand? Why? Which factors are important? You would like more or less to complete the picture so that in the next step you can design better.

Hans Kuiper confirms that from his experience it is essential that this third dimension is included.

Philippe Sautet warns that for each scale there is an opportunity for a ten years research program. So what do we do? We have to mix and keep developments so that each scale is pushed.

Philippe Ungerer states that there is no market for a tool dedicated to one problem only. Forcefields for instance were in the past designed by brilliant researchers, but two decades of improvements on transferability followed before applicability.

Hervé Toulhoat mentioned that as users, we expect flexibility from the tools, *e.g.* choice of different force-fields.

Hervé Toulhoat asks Philippe Sautet whether the *French Academy of Science* has a position with respect to the topic of this conference.

Philippe Sautet cannot speak in the name of this Academy since the point has not been discussed specifically yet, but he mentions that the Academy has a special section on the applications of science to industry. In general, the Academy will certainly support multidisciplinary efforts. Moreover, at *CNRS* physics and engineering institutes are very pushing towards multiscale approaches.

Hervé Toulhoat informs the audience that it is now also formally included into the scientific policy of *IFP Energies nouvelles*.

Bob Diawara (*Chimie Paristech*) from the audience: upon treating systems at the same scale, *e.g.*, using kinetic Monte-Carlo (kMC) for deriving stresses, mechanical properties, you have to relax, and for that it is convenient to use molecular dynamics. We need therefore algorithms and tools which couple techniques at the same scales. Each development in kMC is unfortunately specific currently (geometry, energy database, etc.) There is a need to develop general softwares for doing that. This is a particularly big challenge.

Philippe Ungerer notices that molecular modeling already covers several scales, but would be happy to see the emergence of exchanges between *e.g.* density functional theory, molecular dynamics, Monte-Carlo, dissipative particle dynamics.

Jean-Claude Charpentier proposes concluding statements: we shall succeed because engineering sciences are under the constraint of success. There are two sets of keywords:

– "Product Design and Engineering for end use" "*Un biscuit est craquant ou craquelant ou craquotant ...*" for the chemist it is the same material, but not for the customer;
– "Process intensification": here we are completely engaged with the multiscale approach to obtain an end-use property required by the customer.

He would be pleased if at the end of this meeting, participants bring back home the following messages:

– integrated multiscale approach, integrate to use at upper scale;
– make the models at each scale as simple as possible but not simpler.

Manuscript accepted in July 2013
Published online in October 2013