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Modelling approaches in sedimentology: Introduction to the thematic issue

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ABSTRACT

As an introduction to this thematic issue on "Modelling approaches in sedimentology", this paper gives an overview of the workshop held in Paris on 7 November 2013 during the 14th Congress of the French Association of Sedimentologists. A synthesis of the workshop in terms of concepts, spatial and temporal scales, constraining data, and scientific challenges is first presented, then a discussion on the possibility of coupling different models, the industrial needs, and the new potential domains of research is exposed.

1. Introduction

Whether numerical or experimental, modelling is now widely used in sedimentology, but it covers a large range of domains both in time and space: experimental analogical models (notably used for geomorphological evolution of reliefs) enable us to characterize at a small scale erosion, transport, and deposition processes, to infer quantitative evolution laws, and to calibrate their relevant parameters. Hydro-sedimentary modelling is mainly used to understand the evolution of present environments using a detailed numerical modelling of these erosion–transport–deposition processes (solving the Navier–Stokes equations, for example). Process-based simplified approaches are applied to geological time scales: they are based either on solving deterministic laws describing main processes (genetic models, de Marsily et al., 2005), or with additional introduction of stochastic parameters into the laws (the so-called random-genetic methods). Reservoir architecture modelling is based on geostatistical approaches or mixed geometric/stochastic methods mentioned here as hybrid models: they enable us to quantify the uncertainty of the resulting geomodels, which are linked either to the data, or to the conceptual model (depositional environment, correlation scheme...). At the basin scale, stratigraphic modelling uses averaged transport and deposition laws (diffusion equation, for example) in order to reproduce large-scale depositional architectures and to test the impact of control parameters (accommodation, climate, clastic sedimentary input or carbonate production...).

Some of these approaches are coupled: process-based models are often calibrated on analogical experiments, and

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then applied to recent systems, before being used on outcrops or subsurface data. Process-based, random-genetic or hybrid models produce reservoir architectures that may be used as training images for geostatistical methods. At the basin scale, stratigraphic modelling may be coupled with thermo-mechanical models in order to get the timing of the deformation of the basin, through the evolution of the lithosphere, and analyze its impact on surface processes. Stratigraphic models may also be used as an input of large-scale fluid circulation models, which may be coupled with reactive transport simulation for environmental purposes (geothermal energy, CO_2 storage, wastes), or diagenesis-related problems.

During the 14th Congress of the French Association of Sedimentologists held in Paris from 5 to 7 November 2013, a workshop on "Modelling approaches in sedimentology" has been organized between researchers of these different communities in order to:

- exchange on the different concepts and approaches developed to model and solve problems in sedimentology;
- discuss the methodologies adopted to honour data, through parameter calibration, and in relation with uncertainty quantification;
- identify the limits and key issues of these approaches;
- evaluate the possibility and needs for coupling between models, in order to initiate new collaborations and research domains in relation with industrial needs.

2. Organization of the workshop

The workshop was organized in three stages.

First, a poster session, with 27 contributions, gathered the participants and illustrated their different modelling approaches and their latest results. The electronic version of some of these posters is available on the website of the French Association of Sedimentologists (ASF) at the address: http://www.sedimentologie.fr/.

Following the poster session, two discussions were held in parallel between modellers divided according to the scale of their models:

- **theme 1:** large-scale modelling of the history and sedimentary architecture of basins: geodynamical control, data synthesis, fluid palaeo-circulations (coordinators: P. Joseph, G. Caumon, D. Rouby);
- **theme 2:** modelling of sedimentary and diagenetic heterogeneities: processes, reservoir architecture and properties, fluid-flow behaviour (coordinators: V. Teles, R. Labourdette, P. Le Hir, S. Lopez, P. Weill).

These discussions were structured around three key-points and are summarized in the next section:

- presentation of the spatial and temporal scales, and main concepts of each model;
- use and availability of constraining data;
- identified scientific challenges in modelling approaches and coupling between models.

Finally, a round table with all the participants enabled to share and summarize the conclusions of the two thematic previous discussions and initiated a debate on academic and industrial needs and potential new research domains.

3. Synthesis of the workshop

3.1. Theme 1

This first theme gathered researchers working at a large geological scale with different approaches such as stratigraphic, thermo-mechanical, geological and/or fluid-flow modelling at the basin scale. Consequently, the considered space and time scales are quite homogeneous between these models. Spatial dimensions span from a few to thousands of kilometres, simulated time span from 100 ka to several (tens to even hundreds) million years. The modelling concepts presented during this workshop covered different aspects of basin-scale processes:

- *stratigraphic* and *geomorphological* models represent large-scale sedimentary processes either with diffusion-like or hydrodynamic equations;
- *geological* models can borrow different techniques from machine learning (e.g., neural networks), geostatistical methods or deterministic maps;
- *thermo-mechanical* models use rheological laws of solid behaviour;
- *basin-scale flow* models may couple fluid-flow laws in porous media, geochemical reactive laws and geomechanical laws.

In terms of input data, a wide range of data has been listed by stratigraphic and geological modellers: seismic data, fault geometry, climate data, dating, outcrop sedimentological sections, well logs and core data and their geological interpretation in terms of facies and depositional environments, hydrodynamic data (pressure and flow rates). Palaeogeographic, palaeo-bathymetry/palaeo-relief constructed by the geological modellers, as well as palaeoclimatic maps are interpreted data used by stratigraphic and basin-scale groundwater modellers. Thermo-mechanical models need information on the lithosphere structure and thermicity, and on mantle convective processes.

Simulation results of these models are calibrated mostly through a trial-and-error process, although some inversion techniques are also developed. Validation is done by comparison against well and seismic data, or interpreted palaeogeographic maps in the case of thermo-mechanical models.

It has been highlighted that the coupling of these different models would be a very interesting step forward. For example, stratigraphic models need a better estimate of subsidence and uplift rates through time that could be modelled by lithosphere thermo-mechanical models acting as providers of "boundary conditions". Basin-scale fluid-flow models are dependent on the timing and duration of the diagenetic events and on the geochemical composition of the fluids. Thermo-mechanical models would benefit from a better description of continental evolution and dismantlement. It was also noted that coupling with climate models would allow better estimates of water fluxes and temperature fluctuations through time.

3.2. Theme 2

This second theme gathered different modelling communities working at a smaller scale from hydro-sedimentary or experimental models on modern environments, to petroleum reservoir-scale models with either stochastic, geometric, hybrid or process-based approaches.

Time and space scales of these models are more variable than the ones of the previous theme. *Hydro-sedimentary* numerical or experimental models focus usually on one or several processes from the grain or ripple scale to the sedimentary body. Thus time scales taken into account span from seconds to several years. *Process-based* models simulate the sedimentary processes at a geological scale and they consider simplified or averaged laws often based on empirical observations. Simulated durations can as well be that of a specific sedimentary event as of several thousand years, because the objective is to reproduce the architecture and heterogeneity of the reservoir by stacking several sedimentary bodies. Stochastic and hybrid models also have this same objective and are mostly use at reservoir scale. *Stochastic models* first characterize mathematically the geometry and heterogeneity of the sediments from available data, and then they can reproduce them into several equiprobable simulations. Several algorithms are available depending on the object of interest. *Hybrid methods* were developed for specific cases whose structure and heterogeneity are difficult to model with stochastic methods: fluvial or turbiditic meandering channels (Lopez et al., 2008; Labourdette, 2007), deltaic mouth bars (Hu et al., 1994)... These models embed sedimentary concepts to produce geometries. They usually focus on significant heterogeneities or relation between geobodies. Hybrid models are close to stochastic models due to the fact that they usually can simulate several equiprobable realizations through stochastic concepts. The usual trade-off to be found between both alternatives is that stochastic models may explore unrealistic phase spaces, whereas over-simplified physical models may generate biased results and will not explore all possibilities. But both modelling approaches can easily lead to uncertainty assessment.

In terms of data, *hydro-sedimentary* models are based on field measurements of hydrodynamics and bottom morphology, and they also use mechanical, rheological characteristics. The results give the spatial and temporal (4D) distribution of sediments both inside the flow and over the floor surface, information such as bathymetry variation, state and composition of the floor down to the millimetre-scale. Inputs to *process-based* models are an initial topography, sediments description (grain size, density), and transport processes history (flow regime, successions of events). Calibration of the input parameters relies on trial-and-error testing. Eventually, they give architecture and facies distribution of deposits over the initial topography. They are also able to give information on the chronology and thus on genetic relationships between sedimentary structures. Finally, both *geostatistics* and *hybrid* models use well data (facies, porosity, permeability), production data, as well as geological concepts along with outcrop and seismic data (seismic attributes and horizons). Whether the variable of interest is continuous (petrophysical, mechanical, thermal, elastic parameters) or discrete (facies, diagenetic phase), both methods are able to produce spatially distributed data fields honouring the actual observed data.

During the discussion, it appeared that these modelling approaches face similar issues linked to their dimensions/scales and upscaling possibilities. Laboratory experiments need an appropriate scaling to adequately represent real-world processes. One of the issues of hydro-sedimentary numerical models as well as for process-based approaches is the upscaling of their equations both in time and space for the simulation of successive events. The link between processes or events and deposits and their preservation through time is an open question to know what is significant to consider at the simulation scale. Stochastic and hybrid models are confronted with the issue of upscaling when the modelling results must be transferred to the dynamic reservoir model.

Otherwise, specific issues were mentioned for each approach and could be solved by coupling different methods:

- definition of initial and boundary conditions, conditioning to hard data through stochastic methods, uncertainty analysis and computing time are difficulties of hydro-sedimentary and process-based models;
- lack of realism in some cases, difficulty to take into account a priori connections or geological concepts for stochastic methods;
- extension to other sedimentary environments, inclusion of new sedimentary objects for hybrid models.

4. Main conclusions

4.1. Needs and possibility of coupling

The workshop set out the large diversity of scales and approaches that are used in the community of modellers, but it also appears that all models may be "customers" of the others. First, in terms of results that may give constraints to other approaches, but also, in terms of scientific concepts on which the models are built. Models working at different spatial and temporal scales could be nested: their coupling may therefore be made at their interfaces, where the results of some models may be used as boundary conditions or input for the initialization of other models (global sand-shale ratio from stratigraphic modelling as input for geostatistical reservoir modelling, for example). In other cases, models are complementary. The drawbacks or limits of some of them correspond to the intrinsic characteristics of others: for example, process-based models which give realistic results cannot be exactly fitted to conditioning data, which is the basis and one of the main benefits of geostatistical techniques. In that case, process-based results may be used as constraints for geostatistical methods (database of modelling parameters, training images...). Thus, coupling between these approaches has been naturally identified: the introduction of stochastic approaches in hydro-sedimentary process modelling, and the coupling of process-based approaches with methods of uncertainty quantification.

The focal point between the two themes could be found around the construction of a 3D static geological model, even though scales and resolutions are very different. This resulting object could be a federative, common objective where the different approaches could be coupled through a nested-scale 3D geological model.

4.2. Industrial needs and challenges

There are at least three main scales of models used in the industry.

The simulation of hydro-sedimentary processes is used for environmental purposes (continental erosion, littoral evolution, or transport and dispersion of pollutants, for example). There is a need now to introduce new forcings such as vegetation or biology. For ancient systems, their application may be limited by the difficulty of reconstructing past hydrodynamic parameters from sedimentary records (rainfall for example). A challenge is also the upscaling of erosion or transport laws in order to simulate geomorphological evolution over long geological time scales.

Reservoir modelling is mainly used for resource production or sequestration on human timescale (hydrocarbons, nuclear, water, CO_2). A significant number of techniques and methods have already been developed, but the key point remains the quantification of uncertainties through multi-realizations, and the calibration to well data. Geostatistical methods may be used in an inappropriate way because they are easy to apply. However, when available data are scarce, it is essential to integrate geological concepts as hybrid models do or by the use of trends or additional constraints in stochastic methods (constraints could derived from seismic images). Upscaling is also a key issue in order to correctly transfer information from geological static models to fluid-flow dynamic model (notably for complex environments such as carbonates, where diagenetic imprints are crucial).

Basin modelling is used during exploration to reconstruct the large-scale architecture of permeable and impermeable layers through the simulation of their evolution along geological times. One main difficulty is linked to data availability and integration, particularly in terms of quantity, spatial distribution, identification and elimination of aberrant data, assimilation of new data into existing models.

An essential step in basin modelling is the restoration phase of initial stages with decompaction of previous deposits, but it is time consuming. There is a clear need for coupling with geodynamical and deformation models to validate the basin's evolution. "Global" models integrating plate tectonics, palaeogeographical maps and climate evolution do exist now, but they must be used with caution, and the critical point remains the estimation of the palaeo-reliefs and of the palaeo-rainfalls.

For the modelling of large-scale fluid transfers, a key point is the characterization of the palaeothermicity and of the nature and geochemistry of the fluids, with a progressive transition towards full 3D thermo-hydro-mechanical models. Basin-scale fluid-flow simulation might benefit from the development made in reservoir production models (local grid refinement, inversion methods).

For all these models, the growing capacity of computers and the promises of High Performance Computing (HPC) open new areas for testing the coupling of complex phenomena. It has been noted, however, that dialog or interconnection between models is difficult if not often impossible, and therefore there is a clear need for shared access to different models (open source, interoperability) and to data (open data).

5. Examples of approaches

Several contributions from the workshop have been selected for this thematic issue to illustrate the high diversity of modelling approaches used in sedimentology, involving a wide range of space and time scales.

Poirier et al. (2016) show the application of a RUSLE soil erosion model to compute denudation rates and simulate sediment supply from the Charente River catchment since 1500. The forcing parameters of the model are the climate (through the rainfall intensity) and the nature of the land cover (crops, pastures, or forests). The model takes into account the sensitivity of the soil to erosion and the topography. It correctly predicts present-day Charente River sediment load and confirms that this contribution is minor comparatively to the input from the Gironde Estuary. The application to the 16th and 18th centuries shows that the sediment supply did not change significantly, because soil erosion resulting from the 18th century's deforestation was compensated by a drier climate reducing the average rainfall. The comparison of the simulated sediment load with the sediment record reveals the control of sedimentation (silt–sand alternations) by sub-decadal rainfall variability.

Teles et al. (2016) present new developments on a process-based model for the simulation of submarine diluted turbidity currents. The CATS model is derived from Cellular Automata concepts, with a flow distribution ruled by a balance between potential energy and kinetic energy. Empirical laws are used for water entrainment, erosion, and deposition of several lithologies. A new approach is proposed, which takes into account the concentration profile of different grain sizes and the flow capacity to carry sediments in suspension. The model can simulate a sequence of several turbidity events in order to predict the resulting reservoir architecture and facies distribution. The application to a synthetic topography (sinuous channel and unconfined basin) and to a real case (Makran accretionary wedge in offshore Pakistan) gives realistic results, in agreement with observations.

In subsurface, the building of a geological reservoir model is very dependent on the correlation scheme between wells, because the correlation lines are generally used as limits of the modelling units. Lallier et al. (2016) address the quantification of uncertainties on the stratigraphic correlations, and thus on the conceptual geological model which is the basis for numerical modelling. They generate several possible correlations between stratigraphic logs by developing a stochastic and sequential application of the classic Dynamic Time Warping (DTW) algorithm. The correlations can be constrained by prior knowledge such as correlation lines extracted from seismic interpretation. This new technique enables us to quantify the cost of each correlation, using sedimentological knowledge, for example consistency with the slope palaeo-angle and with the palaeo-depositional profile in the case of a carbonate ramp in southeastern France. This case study shows the strong impact of the correlation uncertainty on the facies distribution in the resulting reservoir model.

Beucher and Renard (2016) describe new geostatistical methods that help to build geological reservoir models by distributing facies or lithotypes in space: this can be done in a nested manner (heterogeneities within sedimentary bodies for example), and categorical variables (facies) and continuous properties (grade, porosity, permeability...) can be jointly simulated. These simulation methods are based on a Gaussian framework. The Truncated Gaussian Simulation (TGS) has first been developed to reproduce ordered sedimentary depositional sequences: its flexibility enables to account for external constraints (trends) and to easily condition to numerous data. Pluri-Gaussian simulation (PGS) takes into account several Gaussian fields and enables one to reproduce very diverse textures, at the level of the rock sample, the outcrop or the subsurface field. New developments are in progress to better simulate oriented/anisotropic shapes or high-frequency layering.

Hamon et al. (2016) present an innovative workflow for the 3D joint modelling of facies and diagenesis at reservoir scale applied to a carbonate formation outcropping in Spain. The study is based on a detailed sedimentological characterization, which led to a depositional model and correlation of different modelling units through a sequence stratigraphy approach. Diagenetic phases were identified and quantified through thin sections analysis (point counting). These different phases are put in relation with the sedimentary facies and a bi-plurigaussian simulation (Bi-PGS) is used to model both facies distribution and diagenetic imprints in a consistent way. This application demonstrates the ability to model heterogeneities linked both to sedimentation variability and postdepositional diagenetic development, and the need to integrate the sedimentary and petrographic analysis in the modelling workflow.

In order to evaluate the impact of sedimentary heterogeneity on CO_2 storage efficiency, Issautier et al. (2016) lead a sensitivity analysis on a 3D model of a fluvial meandering reservoir, composed of stacked sandy point bars (first-order level of heterogeneity) embedded in a shaly floodplain. The CO_2 storage capacity after 50 years of injection can vary by more than 50% between different realizations of the model, because of the different connectivities between point bars. When a second level of heterogeneity is introduced (shaly plugs corresponding to the infilling of oxbow lakes inside the meandering belts), the final capacity can be reduced by 30% and dynamic simulations show a strong effect on the pressure field, on the shape of the CO_2 plume and on the CO_2 dissolution, which impacts the storage efficiency. A comparison with static estimates of the storage capacity highlights that, in such heterogeneous reservoirs, dynamic simulations on several geostatistical realizations are necessary to access the real storage potential.

Lastly, at basin scale and on geological time scale of several millions of years, Violette et al. (2016) test numerically the hypothesis of carbonate cementation due to meteoric recharge of Bathonian carbonate aquifers at the edge of the Paris Basin during the Lower Cretaceous. They use a 1D reactive transport model, coupling palaeo-fluid-flow simulation and fluid-mineral geochemical reactions. With a parameter sensitivity analysis, they show that this process alone does not suffice to reach the reduction by 10% of primary porosity observed in subsurface in the basin's centre, and that other processes such as infiltration of meteoric waters or upward migration of deeper fluids might probably be involved.

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