From modelling soil columns to large scale aquifers: an illustration of the MARTHE code capabilities.

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Abstract

In the last 20 years, numerical modelling of Groundwater flow and transport has become the best tool for water resources management and decision making. Numerous codes deal with flow, transport, density, unsaturated zone, surface water- groundwater interaction, etc…but only a few codes integrate these aspect simultaneously. The MARTHE code presented here tackles all of them in a dynamic way. This presentation intends to illustrate through case studies, how this modelling software can be used to treat various problems.

The scale of applications of this computer program ranges from detailed investigations, such as water movement in soils (soil volumes of a few cm^3 with cells of a few mm), to simulation of large multilayered aquifer systems (150,000 km^2, 1,500 m thickness). The temporal scale of applications ranges from a few seconds to 15,000 years for long-term geochemical predictions.

MARTHE has been applied to over 300 aquifer systems since its first release in the late 1980's. Fields of application have included i) the management of groundwater resources (e.g. water balance assessments, evaluation of the potential impacts of abstractions); ii) civil engineering and mining works (e.g. impact of underground activities); and, iii) environmental assessments, both point and diffuse pollutions, (Thiéry et al, 2004).

1. Introduction

Advances in computer resources observed in recent years have favoured and enlarged the use of modelling softwares for the treatment of hydrogeological problems. Memory, computer speed and storage become less and less a limiting factor. Technological improvement tend to popularize the use of numerical models. However, modelling has increased in complexity, dealing not only with flow and transport but also with density, variably saturated medium, reactive transport, river water / groundwater interactions, multiphase flow and so on.

Hydrodynamic and hydrodispersive modelling became during 20 last years, the principal management tool of the water resources. The possibility of taking into account space and temporal heterogeneities, by discretizing within a grid study area and by cutting out time periods called "time steps", makes it possible to the hydrogeologists to bring a quantitative response to problems which would otherwise only get approximate solutions. Without giving to model results an exaggerated importance, knowing of course that the value of the model depends primarily on that of the input data and of their analysis, the tool which we describe allows:

- to compute water balance over aquifer systems as well as specific zones (such as sub-catchment areas) defined by the user, distinguishing the amount of water corresponding to recharge, boundary conditions, storage, leakage, connexions between aquifers, and so on)

- to take into account the impact on the water table of civil works or hydraulics engineering (underground car park, excavations, tunnels, gravel pits, dams, etc.)
- to consider the interference between wells, to manage the abstraction, to work out scenarios of exploitation.
- to simulate the propagation of a pollutant in a variably saturated medium, considering the characteristics of the pollutant such as degradation, sorption or density.
- to represent the ~~spanning~~ extension of a contamination in order to evaluate its impact, the protection measures and the remediation scenarios.
- to envisage the impact on the groundwater quality of specific installations such as waste disposal or industrial settlement.

For more than 20 years BRGM has worked in the field of groundwater modelling and has developed a code, MARTHE (Thiéry 1991, 1993a, 1993b, 1994) able to tackle these problems in an integrated and dynamic way. The following description of the MARTHE software will not detail the code and numerical implementations. Its purpose is to share a user experience and show the ability of the software to answer a wide range of hydrogeological problems.

2. Main features

The field to be modelled is discretized according to a rectangular grid of "Scottish" type: each line and each column of cells have a constant width but the user is free to adapt this width according to local heterogeneities, to the density of information and to the required precision. It is moreover possible to locally refine the grid using nested (multi-stage) grids (cf. Figure 1). These features bring to the MARTHE software a flexibility generally not accessible to other finite differences models.

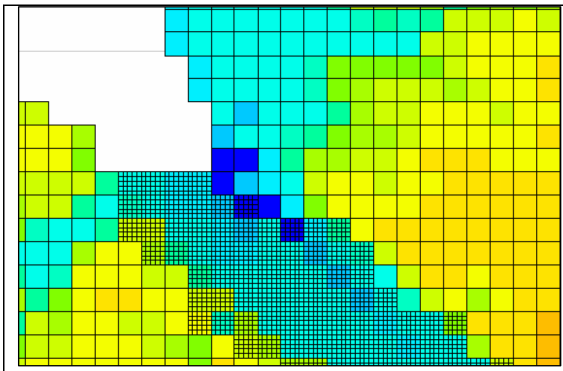


Figure 1: Example of a nested grid

The Somme river basin: The river bed is discretized by fine cells to better represent topography and better simulate the risks of flood event.

The cells can be associated to geographical co-ordinates, which makes it possible to interface them with a GIS software, or to work on cartographic background using the MARTHE interface. The volume of each cell is defined by its top and bottom elevation, which makes it possible to represent complex geometries. A set of tops and bottoms defines a model layer. It is possible to have discontinuous layers if in reality, the structure represented disappears locally (such as geological unconformities) which is quite common.

Input and output data files are text files which can be edited and manipulated with MARTHE interface, or with another tool (for example Excel to visualize simulated series)

Calculation of flows (hydrodynamic)

Hydrodynamic calculations are carried out according to a method with finite volumes. They make it possible to answer, for example, with the following situations:

- One-layered or multi-layered aquifers (stacking of aquifers separated by more or less continuous semi-pervious strata) or in full 3D.
- Free, confined or semi-confined water table in steady state or transient state. (cf. Figure 2)
- Taking into account of discontinuities such as free surface water (lakes, gravel pits), local dewatering, (and re-wetting), including in multi-layer aquifers, water table overflows (river, sources, drains), tight limits (sheeting piles…).
- Horizontal and vertical permeability anisotropies.

The resolution algorithms use methods of conjugated gradients with possibility to select the more adapted solver to the problem (Choleski, Einsenstat, Orthomin)

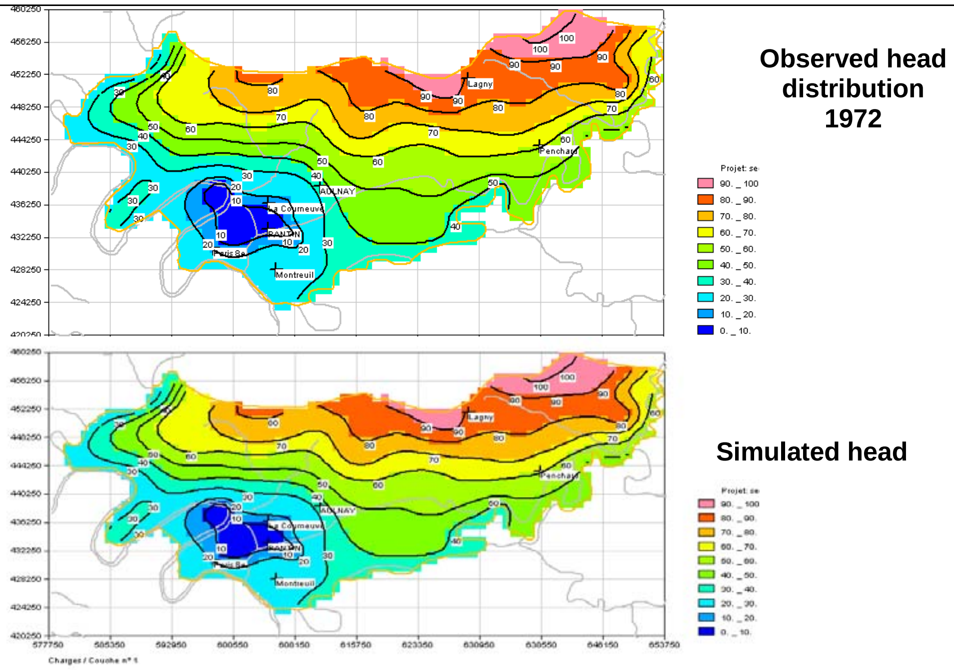


Figure 2: Observed and simulated head distribution in a monolayer steady state modelling. Modelling of the lower Eocene water table between the Marne river and the Oise river around Paris, using a one-layered model. It is a simple example where the permeability of the aquifer is homogeneous and where a fine knowledge of local geology (top and bottom of the aquifer layer) allows a good restitution of the heads by the model.

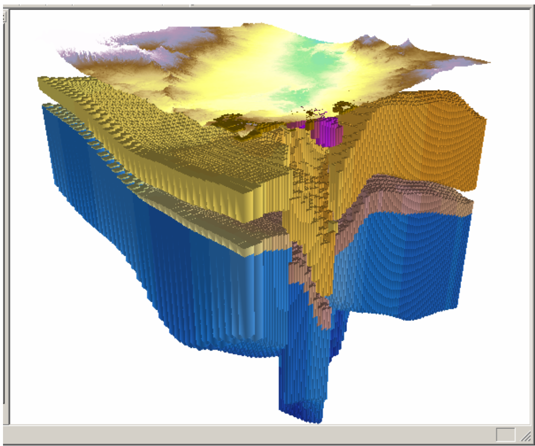
The model can represent a 2D map, a cross section, a portion in cylindrical coordinates or a 3D system. The case study #1 presents the modelling of a huge aquifer system using a 3D grid. The layers can be conformable or unconformable the ones over the others, creating short-circuits between aquiferous levels. This representation allows a perfect analogy between the layers of the model and the geological layers.

Case study # 1 : Transient modelling of the SAQ and overlaying aquifer systems (Saudi Arabia)

The Saq aquifer is a huge sandstone reservoir, over 375 000 sq Km (2/3 of France total area), in the North of Saudi Arabia. This area counts about 16 000 wells out of which only 600 are used for drinking water supply, the rest being used for irrigation in the desert.

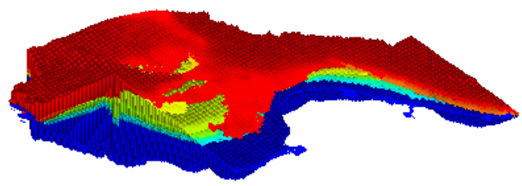
A model has been developed in 2005-2006 with the following objectives:

- To understand the functioning of the multilayer system
- To simulate abstraction scenarios and predict future difficulties
- To help defining a better management



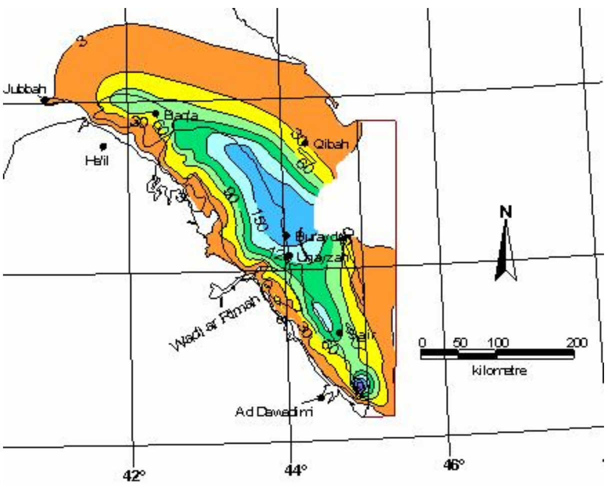
Prior to mathematical GW modelling a geological model had to be built. The shape of 26 layers, some of them not continuous (many unconformities are present) was reconstituted thanks to the numerous deep wells in the area and BRGM long experience in the country.

The geological model was later simplified to 13 significant formations (7 aquifers and 6 aquitards). The spatial discretisation consists in a regular grid of square cells (2x2 km). The grid covers approximately 1000 x 1000 km. It is composed of 3 millions of cells, out of which 1.5 million are active cells.



The use of satellite image of various dates allowed the reconstitution of irrigated areas and associated abstraction in the last 20 years.

The transient state was calibrated with time series from about 50 observation wells. It is run with a yearly time step over 45 years.



The model spots the areas affected by abstraction between 1960 and 2005, where huge drawdown take place. As aquifer recharge is very weak (0 to 5 mm/a), any significant groundwater abstraction is clearly a mining operation.

Reference: BARTHÉLEMY Y., BÉON O., LE NINDRE YM., MUNAF S., POITRINAL D., GUTIERREZ A., VANDENBEUSCH M., AL SHOAIBI A., WIJNEN M.. 2006. Modelling of the Saq aquifer system (Saudi Arabia): an essential tool in water management. Proceedings of the AIH international workshop – Dijon – France – 30 April – 2 May 2006. (in press)

Mass transport calculation

MARTHE is frequently used to simulate the dispersive migration of an effluent in the aquifer.

According to the type of problem arising (predominance of the convection or dispersion), the user can choose between four techniques of calculation to optimize the transport scheme implemented:
- Finite volumes;
- Method of characteristics (MOC) using particles;
- TVD method (Total Variation Diminishing) in transient state;
- Method of Random Walk, known also as particle dispersion method;

All these methods perfectly respect the mass conservation.

Transport in aquifer is simulated under its advective, diffusive and dispersive components. Four options are proposed for reactive transport:
- Exponential decay of the effluent with time;
- Filiation of sub products (metabolites);
- Retardation factor using the partition coefficient kd (phenomena of adsorption-desorption).
- Freundlich and Langmuir isotherms

In the case study #2, a 3D model is used to simulate the propagation of chlorides in the alluvial aquifer of the Alsace Valley in the East of France. This modelling combines transport and density effects.

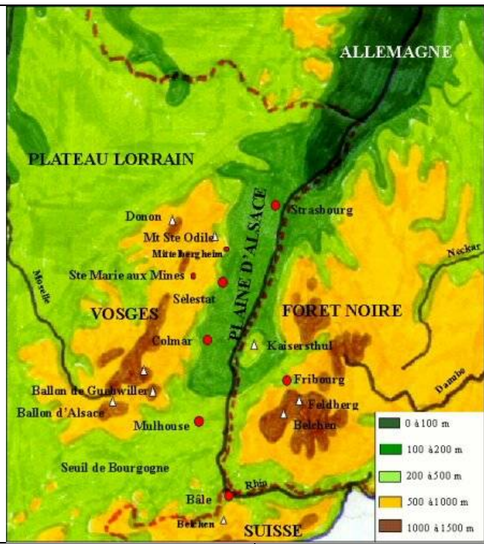
River – aquifer coupling

An hydrographic network can be integrated into the model. In this case, the bed of the river is cut out in sections of river having particular characteristics such as the permeability and the thickness of the banks, the dimension of the bottom, the width and the length of the section. The sections are superimposed on the grid. They receive water from upstream and convey it downstream. They can drain or feed the water table according to the height of the water calculated in the river and the head of the water table. Sections can be dried up temporarily. Withdrawals or direct injections in the river can be taken into account. The coupling between the height of water in the river and the discharge of river is carried out in a dynamic way by a Manning-Strickler relation. The coupling between the river and the water table is also dynamic and can be coupled with a hydro climatic water balance assessment over a specific zone (such as a catchment area), using rainfall and potential evapotranspiration records.

Case study #3 illustrates a simulation with river – aquifer interactions. For this modelling, the river valley is defined using a nested grid with fine cells (as in **Figure 1**). The calibration was performed in transient state from 1989 to 2003 and validated later using updated observations. This type of model is useful for predicting the location of flood events and helps the authorities in taking proper decisions.

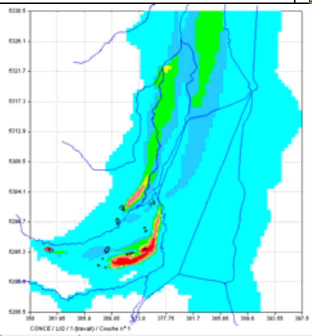
Case study # 2: Mass transport computation. Example of the Alsace Valley (France)

Exploitation of potash (potassium hydroxide) near the city of Mulhouse since 1913 is responsible for an important chloride contamination of surface water and groundwater.

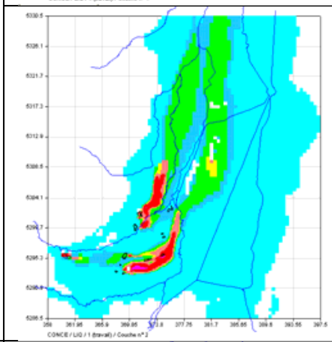


Initially, salts (NaCl) issued from exploitation, after extraction of potassium, where disposed in heaps ("terril"). Precipitation, which have leached these heaps, have contaminated the groundwater. By runoff on the banks or infiltration through the heap, meteoric water becomes brackish (350 mg/l) before reaching surface water (Rhine) or groundwater where it is diluted.

Contamination was maximum in 1972 when 170 km^2 of the water table had a chloride (Cl) concentration over 200 mg/l. Since 1976, direct input of Cl in river have stopped. Other measured include drilling of wells to fix and treat the pollution (70 depollution wells in 2000), accelerate the salt dissolution by aspersion (photo) and recuperation of water in trenches and wells, reduce infiltration on heaps with a tight cover.

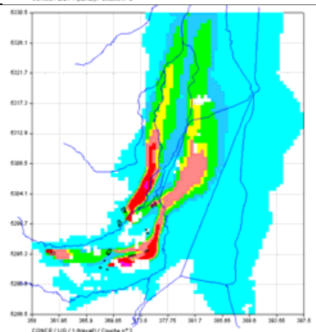


Layer 1



Layer 2

The model was used to simulate propagation of salts under given scenarios. The above simulation results show impact of density in the propagation of Chloride in the groundwater.



Layer 3

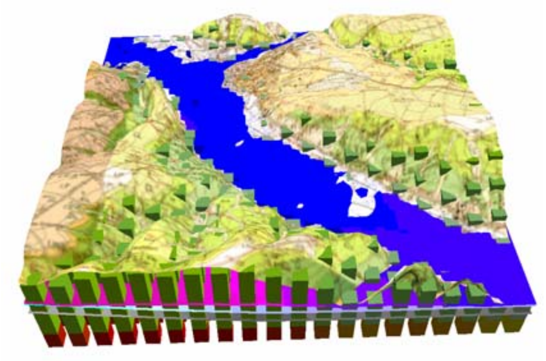
Chloride concentration (mg/l)

References:

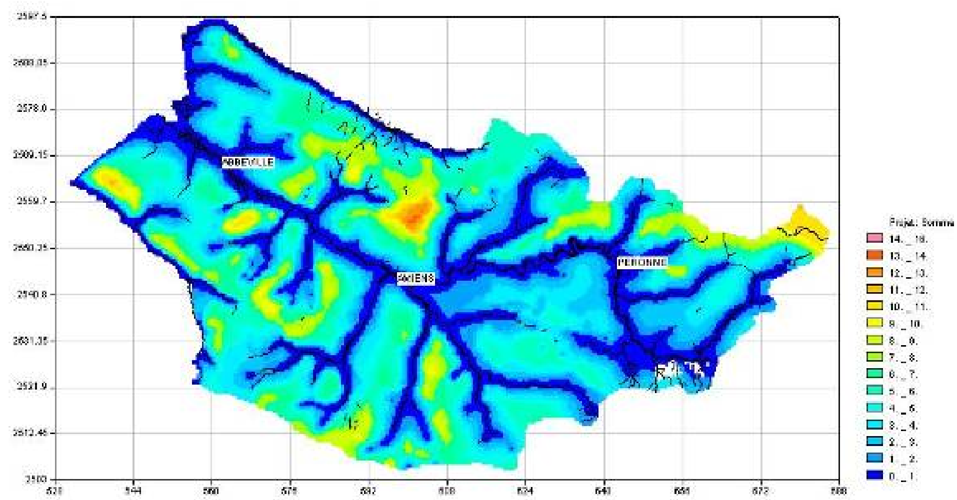
NOYER.M.L., ELSASS.P. (2006) Modelling aquifer salinity in the Potash Basin (Alsace), in Proceedings of the AIH international workshop “Gestion des grands aquifères” – Dijon – France – 30 April – 2 May 2006. (in press)

Case study #3 : River – Aquifer relationship : Flooding in the Somme river valley

The flood in the Somme river valley during the winter of 2000-2001 highlighted the possible contribution of groundwater to flooding and led to observations that can be extrapolated to other regions. A flood phenomenon is the combination of rainfall, runoff and groundwater flow. The proportion of each component in this combination depends on the basin's morphology, hydrogeology, surface conditions (including frozen soil in winter), land-use and rainfall records.



The Somme river valley (France): 3D representation of the 2001 flood in the south of Abbeville. The cells are represented by parallelepipeds The geological map is draped over. Fine overflowing cells are coloured in blue to represent flooded areas.



The model has shown that the contribution of compartments of the chalk aquifer to the Somme discharge increased proportionally upstream to downstream. While the groundwater contribution to stream flow during the summer months is nearly 100%, it was estimated to have accounted for around 80% during the 2001 flood.

References:

Pointet.T., Amraoui.N., Mardhel.V., Negrel.P., Noyer.M.L., Pennequin.D., Thiery.D. – 2005 La contribution des eaux souterraines aux inondations. Modélisation des hautes eaux de la Somme., Géosciences - La revue du BRGM pour une terre durable, N°2 - pp. 80-85

Pointet.T., Amraoui.N., Golaz.C., Mardhel.V., Negrel.P., Pennequin.D., Pinault.J.L. – 2003. La contribution des eaux souterraines aux crues exceptionnelles de la Somme en 2001. Observations, hypothèses, modélisation, La Houille blanche, p. 112-122

N. Amraoui, C. Golaz, V. Mardhel, Ph. Negrel, V. Petit, J.L. Pinault, Th. Pointet 2002 - Simulation par modèle des hautes eaux de la Somme. BRGM report BRGM/RP-51827-FR.

Calculation in the unsaturated zone

Sometimes the modelling of a natural or experimental system requires to take into account the unsaturated zone between ground surface and the water table. This taking into account utilizes characteristic laws of the terrain (retention law and permeability law) which represent the variation of the capillary pressure and the permeability according to saturation of the medium. MARTHE proposes the choice between several usual schemes. For example, with regard to the retention law, the models of Van Genuchten, Brooks-and-Corey, homographic or logarithmic curves are implemented. For the law of relative permeability, the schemes of Van Genuchten, Brooks-and-Corey, a power or an exponential law are available. The treatment is continuous between the saturated zone and the unsaturated zone.

To meet needs related to modelling for the transfer of the pesticides, the taking into account of the vegetation was integrated (cf. Figure 3). The incidence of the development of the plants (leaf and root) on the water content of the terrain, and consequently on the propagation in depth of a contaminant can be thus simulated. Research are still on-going in this field (cf. case study #4). One of the most recent developments of the MARTHE model was the integration of the macroporosity in the ground.

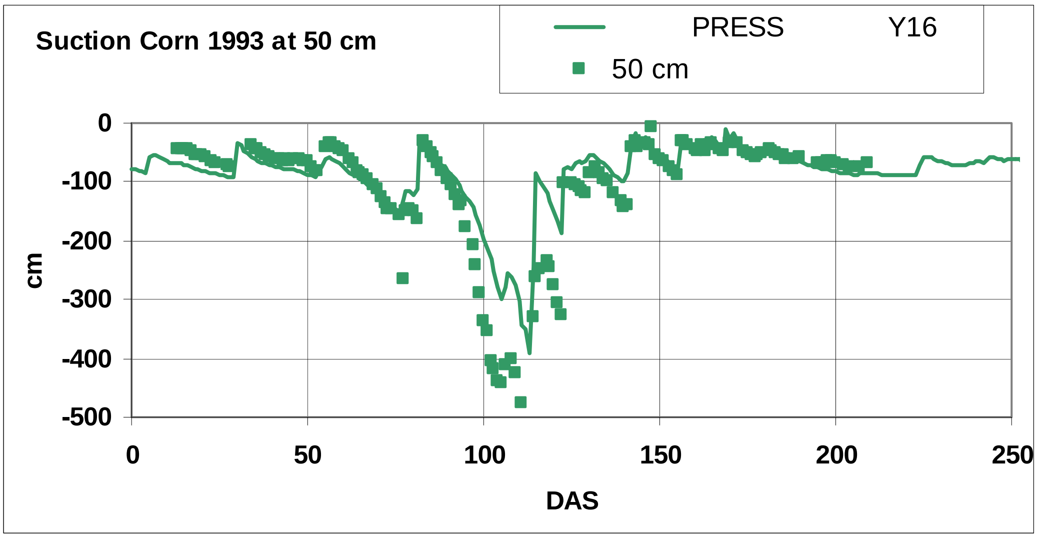


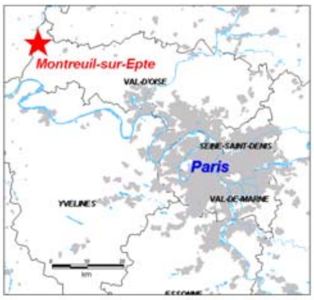
Figure 3 : Simulation of the capillary pressure in unsaturated zone under a corn field
The capillary pressure, which governs the flows in the unsaturated zone, is represented here according to time (in days) at 50 cm of depth in the ground of an experimental field. Strong suctions are created (and are simulated) when the growth of the plant is maximal and when precipitations are scarce.

Automatic calibration, optimization and sensitivity analysis

An option of MARTHE makes it possible to automatically obtain a field of permeability starting from a given piezometry, by inverse modelling. This functionality may be practical to rough a problem and to identify zones of permeability in the absence of data. The recommended methodology remains however to define zones of permeability according to geological and hydrogeologic criteria. The calibration can then be optimized by entrusting to the model the choice of the best parameters between intervals of values fixed by the user.

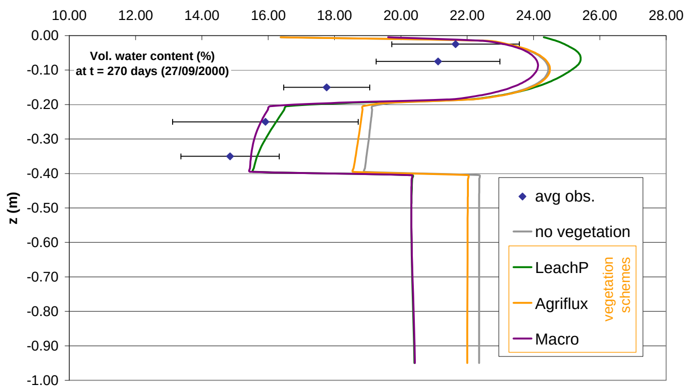
The results and forecasts given by the model correspond to a single response in reaction to a set of requests (inputs of the model). Various parameters of the model may come from estimates rather than measurements (for example storage coefficient or permeability which are generally only known at discrete locations). It is thus useful, even essential, to accompany any modelling by an a sensitivity analysis. MARTHE proposes an automatic method to carry out this sensitivity analysis and to possibly determine confidence intervals.

Case study #4 : Modelling the unsaturated zone. Work in the frame of AquaTerra project

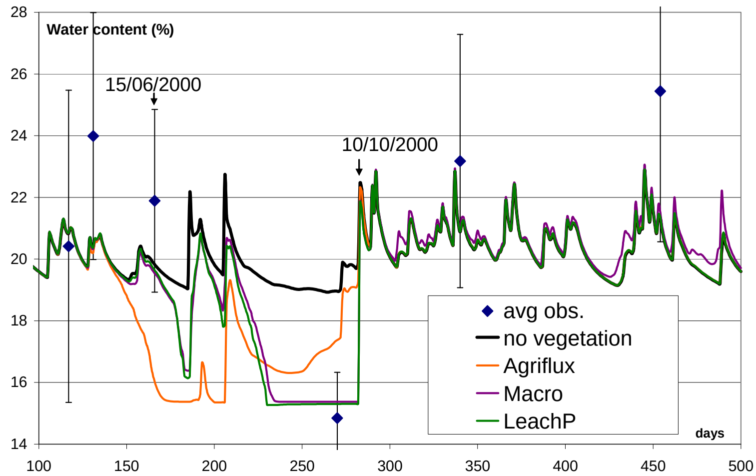


Within the Aquaterra project, BRGM together with Avignon University (France), DTU, Liège and Gembloux Universities (Belgium), is studying a small catchment located 70 km North west of Paris. At Montreuil sur Epte, a spring was used for drinking water until 2001 when the authorities prohibited this use because of its level in pesticides (Atrazine 0.2; DEA 0.7 µg/l) and nitrates (65 mg/l). The catchment is studied since 2000: farmers were convinced to replace Atrazine with Acetochlor. We are following Acetochlor in the soil and waiting for its appearance at 19 piezometers and at the spring.

Works regarding modelling have been done in a progressive manner: starting from 1D column with the ambitious objective to finish with 3D model. The soil zone (1st meter) is known by numerous measurements (16 cores/plot at 5 depth and 6 different dates during year 2000) regarding water content, Bromide and Acetochlor, which were both spread simultaneously in April 2000. We consider a column constituted of 2 horizons of soils (H1 and H2) overlaying the Lutetian limestone (over 30 m of unsaturated zone). Soil properties (retention curves and permeability laws) comes from a fitting of Van Genuchten law to observed soil characteristics (using the RETC program).

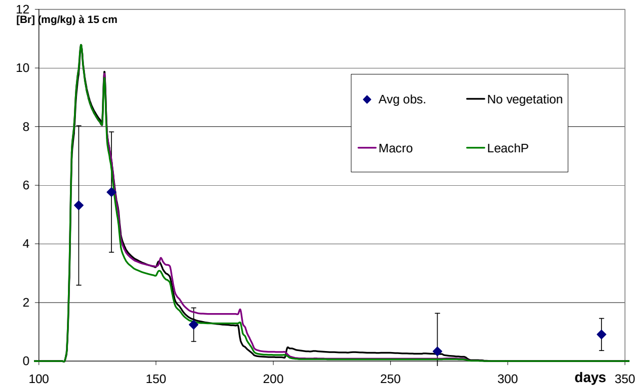


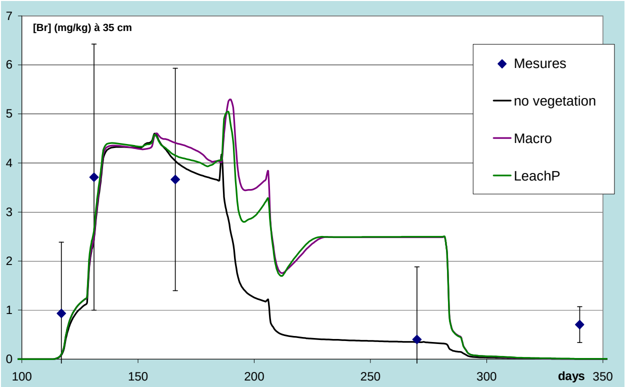
Simulation of water content with depth, under several hypothesis of vegetation effect are presented here. Dots represent average of water content (16 samples) with standard deviations. Date t=0 corresponds to 01/01/2000 and observed rainfall and PET are applied as surface condition with a daily timestep. MARTHE offers the possibility to use several methods which are used in well known soil models, to take into account the vegetation (i.e. to consider the development of roots and leafs of the plant: here maize). The MACRO scheme is the closest from observed values. If we do not consider vegetation, a discrepancy appears with depth (black line).

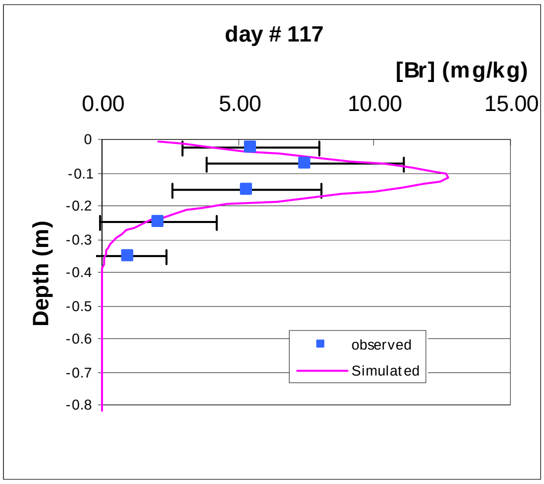


The modelling is in transient state. Vegetation effect becomes important during summer time. AGRIFLUX scheme was probably badly parameterised because the plant development is too fast. LeachP and MACRO schemes are giving similar results. If no vegetation is considered, the water content during summer time is over estimated.

Bromide was applied (as well as pesticides) on the soil at day 110 (20 of April 2000). At 15 cm depth, the "tracer test" is well simulated. LeachP and MACRO give similar results. However at 35 cm, the best simulation is oddly the "no vegetation" simulation. This shows the difficulty and sensitivity of such simulations.
After 300 days, Bromide observed in the soil could come from decomposition of roots and leafs from plants which absorbed part of the Bromide (measurements in plants showed that up to 50% of Br was absorbed this way). The MARTHE code takes into account this consumption by plants but does not consider the plant decomposition after harvesting. Moreover, the soil is reworked during winter and mixing occurs in the 40 first cm.

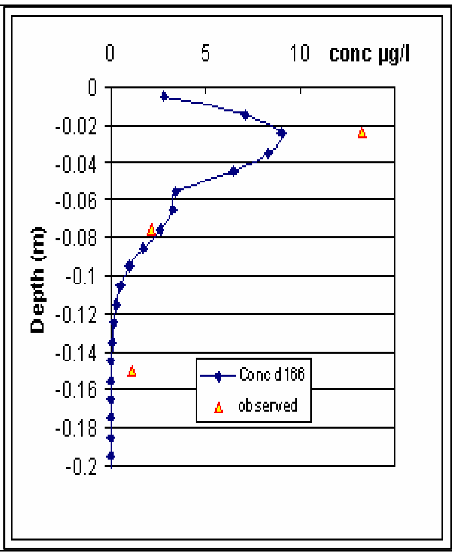






Bromide can be considered as perfect tracer and proper simulation of flow is the condition of success. Although extremely simplified, the 1D modelling globally respects the concentrations and delay of Bromide transfer, 7 days after application.

When it comes to pesticide transport, new parameters have to be introduced: mainly sorption which vary with depth (linked to Carbone organic content) and degradation which vary with temperature and water content. Sorption and degradation were estimated from soil samples in laboratory, giving the above results. It would be possible to get a better fit by playing with parameters, however the purpose was here to see whether pesticide transport might be simulated from parameters obtained by measurements (without calibration), considering the simplifications of the modelling .



References :

THIÉRY D., GOLAZ, C., GUTIERREZ A., FIALKIEWICZ W., DARSY C., MOUVET C. & DUBUS I.G. 2004 - Refinements to the MARTHE model to enable the simulation of the fate of agricultural contaminants from the soil surface to and in groundwater. Proceedings of the COST international workshop, Saturated and unsaturated zone: integration of process knowledge into effective models, Rome, Italy, 5-7 May 2004, Eds. Aagaard P., Bedbur E., Bidoglio G., Candela L., Nuetzmann, G., Trevisan M., Vanclooster M. & Viotti P., Publ. La Gollardica Pavese, ISBN 88-7830-387-9, pp. 315-320.

Other features

The correct resolution of calculations is checked by criteria of convergence. Convergence can be controlled following the variation of average (and maximum) head between two successive iterations, as well as the residual error of flow computation. For the latter, a total residual discharge is given for each iteration, but the cell recording the strongest residual flow is indicated. It is also possible to follow convergence in one or more particular cells of the model.

Numerous options, which are not described here, are available in MARTHE:
- Calculations of fresh Water/salt Water interfaces in monolayer or multi-layer systems.
- Density effects induced by heterogeneous salinities and/or temperatures.
- Calculation of the temperature field, for geothermic problems or energy storage.
- Taking into account of the viscosity variations with temperature.
- Coupling with a drain network (for example to simulate a gallery or a karstic system).
- Coupling with water balance modelling over hydro climatic zones.
- Taking into account of vertical fractures using equivalent transmissivity.
- Transport with interactions between water, chemical species and porous matrix.
- Multiphase flow: water and gaz ; water and oil.
- Gaz flow.

The MARTHE software consists of a computing core written in FORTRAN 95, and of an interface called WinMarthe (written in Visual C++) which plays at the same time the role of pre-processor for data preparation and of post-processor for results visualization. The WinMarthe interface allows in particular to work out the grids, to display and modify the values on a cell basis, on a selection of cells or on a whole layer, to visualize the data in a given layer and in cross sections, to visualize the model using a 3D viewer, to interpolate the results, to draw path lines, to represent velocity vectors… WinMarthe also offers numerous ways of importing and exporting data to other software (such as GIS software).

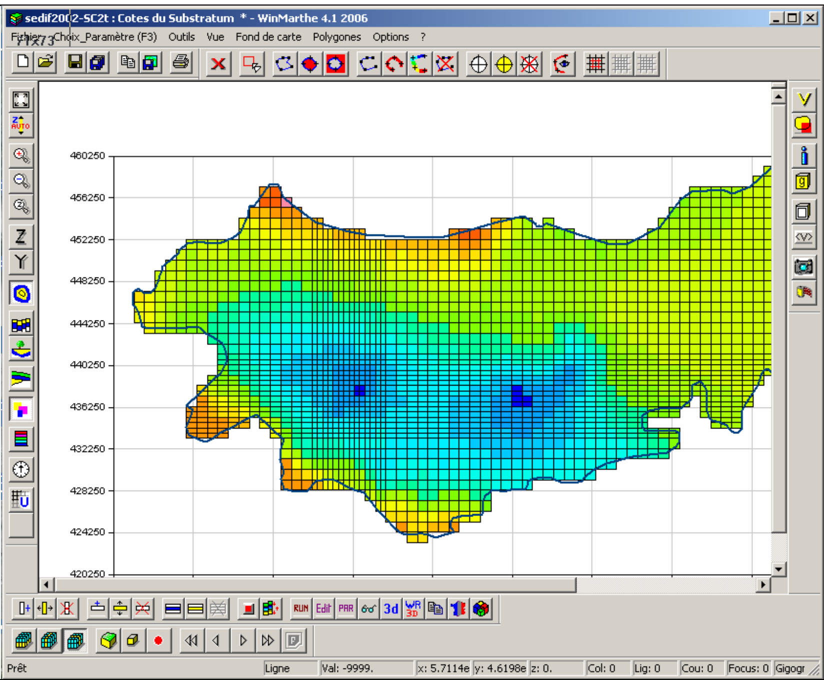


Figure 4 : The WinMarthe interface
Many tools are available for the modeller to work out the data or to display the results.

Conclusion

Illustrated by a series of examples, the use of the MARTHE software, developed at BRGM, has been described. It allows a large variety of simulations, from single multilayered columns to huge aquifer systems. From a user point of view, the software and its interface, benefiting from years of improvements, can be considered as one of the most powerful tool dedicated to groundwater modelling.

References

AMRAOUI ,N., GOLAZ, C., MARDHEL, V., NEGREL, P., PETIT, V., PINAULT, J.L., POINTET, T. 2002 - Simulation par modèle des hautes eaux de la Somme. BRGM report BRGM/RP-51827-FR.

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NOYER.M.L., ELSASS.P. 2006 - Modelling aquifer salinity in the Potash Basin (Alsace), in Proceedings of the AIH international workshop “Gestion des grands aquifères” – Dijon – France – 30 April – 2 May 2006. (in press)

POINTET.T., AMRAOUI.N., MARDHEL.V., NEGREL.P., NOYER.M.L., PENNEQUIN.D., THIERY.D. 2005 - La contribution des eaux souterraines aux inondations. Modélisation des hautes eaux de la Somme., Géosciences - La revue du BRGM pour une terre durable, N°2 - pp. 80-85

POINTET.T., AMRAOUI.N., GOLAZ.C., MARDHEL.V., NEGREL.P., PENNEQUIN.D., PINAULT.J.L. 2003. - La contribution des eaux souterraines aux crues exceptionnelles de la Somme en 2001. Observations, hypothèses, modélisation, La Houille blanche, p. 112-122

THIÉRY D., GOLAZ, C., GUTIERREZ A., FIALKIEWICZ W., DARSY C., MOUVET C. & DUBUS I.G. 2004 - Refinements to the MARTHE model to enable the simulation of the fate of agricultural contaminants from the soil surface to and in groundwater. Proceedings of the COST international workshop, Saturated and unsaturated zone: integration of process knowledge into effective models, Rome, Italy, 5-7 May 2004, Eds. Aagaard P., Bedbur E., Bidoglio G., Candela L., Nuetzmann, G., Trevisan M., Vanclooster M. & Viotti P., Publ. La Gollardica Pavese, ISBN 88-7830-387-9, pp. 315-320.

THIÉRY D., 1994 - Calibration of groundwater models by optimization of parameters in homogeneous geological zones in "Stochastic and Statistical methods in hydrology and environmental engineering". Kluwer Academic Publishers (The Netherlands) - Vol. 2, pp. 69-82 K.W. Hipel (ed.).

THIÉRY, D. 1993a. "Modélisation des aquifères complexes. Prise en compte de la zone non saturée et de la salinité. Calcul des intervalles de confiance". Hydrogéologie Volume: 4, pp. 325-336.

THIÉRY D. 1993b.- Tridimensional and multi-layer modelling of transfers in unsaturated porous medium. GEOCONFINE Symposium international Géologie et confinement des déchets toxiques. Montpellier, juin 1993. Geoconfine 93 - Balkema Rotterdam, pp. 467-472.

THIÉRY D., 1991.- Modelling contaminant transport through the unsaturated zone in transient state with a random walk particles scheme.
Congrès : Modeling in groundwater resources. Proceeding of the international conference on modeling groundwater flow and pollution. Nanjing, 1991.