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Macroscopic cellular automata for groundwater modelling: A first approach

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ABSTRACT

A groundwater model representing two-dimensional flow in unconfined aquifers is presented. The model is based on the paradigm of macroscopic cellular automata, that represents dynamical systems which are discrete in space and time, operate on a uniform regular lattice and are characterised by local interactions. Physically based equations are implemented to simulate the flow of water between adjacent cells. The model was validated against solutions of simple problems in both steady state and transient state conditions including analytical solutions and simulations performed with the MODFLOW-2000 model. The developed code is simple enough to facilitate its integration into other models such as land-surface models. The good performance without detriment to accuracy makes the model adequate to perform long simulation time analysis.

Software availability

Name of the software: MACCA-GW
Developer and contact address: Giovanni Ravazzani, Faculty of Civil and Environmental Engineering, Politecnico di Milano, Piazza Leonardo da Vinci, 32, I-20133, Milan, Italy. Tel.: +39 02 2399 6231, Fax: +39 02 2399 6207, E-mail: giovanni.ravazzani@polimi.it
Year first available: 2008
Required software: Fortran 90 compiler
Program language: Fortran 90
Availability and cost: Software and source code available free of charge upon request to the authors.

1. Introduction

Groundwater models historically have been applied to aquifer management problems (Besbes and deMarsily, 1984; Ponzini et al., 1989). To this purpose, many sophisticated numerical models have been developed to simulate water fluxes in complex heterogeneous multi layered aquifers (Rathod and Rushton, 1991; Oosterbaan, 1995; Owen et al., 1996; Diersch, 2002; Jackson and Spink, 2004; Zyvoloski, 2007; Hughes and Liu, 2008), while surface water processes are often oversimplified ignoring runoff, actual evapotranspiration, and snow dynamics (Carrera and Medina, 1999; Giudici et al., 2000). On the other hand, traditional Land-Surface Models (LSM) are designed with emphasis on surface water movement whereas the subsurface is commonly simulated by means of simple conceptual approaches or assumed as zero flux boundary (Niu et al., 2007). However, the interaction between surface water and groundwater plays a crucial role in many cases, so that integrated modelling approaches become fundamental to water resources planning and management (Facchi et al., 2004; Krause et al., 2007), also in light of the demands of the European Water Framework Directive (WFD; 2000/60/EU). In that respect, a few models try to consider the soil-vegetation-atmosphere-transfer phenomena (Maxwell et al., 2007) and the complexity of the vadose zone (Biondini, 2001) in a detailed and comprehensive way. In these situations, despite complexity of the aquifer system, the modelling of the superficial unconfined layer, is often sufficient to simulate water exchange between surface water and the underlying water table (Werner et al., 2006; Krause and Bronstert, 2007; Rodriguez et al., 2008; Wondzell et al., 2009). Moreover, in order to run long time simulations at fine resolution, the model is required to be as simple as possible to provide reliability, efficiency and flexibility. Fortunately, the common belief that very complex phenomena require necessarily sophisticated models has been shown to be erroneous: complexity can arise in a model even if governed by very simple rules (cf. e.g. Wolfram, 2002). Among these approaches Cellular Automata (CA) represents a simple, attractive and alternative modelling technique respect to traditional numerical models that solve differential equations to describe complex phenomena (Toffoli, 1984). Cellular Automata are dynamical systems which are discrete in space and time, operate on

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a uniform, regular lattice and are characterised by local interactions. They were introduced by Von Neumann (1966) to study self-reproducing systems and have been later used for modelling disparate complex physical phenomena (Di Gregorio, et al., 1999; Jiménez-Hornero et al., 2003; Parsons and Fonstad, 2007; Marshall and Randhir, 2008). Models based on CA are directly compatible with parallel programming and so they allow to easily exploit the power of modern computers.

Many CA applications in the field of fluid dynamics exist. Lattice Gas Automata (LGA) models were introduced to describe the motion and collision of particles on a grid (Frisch et al., 1987). They have been applied to simulate fluid dynamical properties (Di Pietro et al., 1994; Pot et al., 1996). A different approach is the Lattice Boltzmann Method (LBM), where the state variables can take continuous values, as they are supposed to represent the density of fluid particles endowed with certain properties located in each cell (McNamara and Zanetti, 1988; Succi et al., 1991; Chopard and Luthi, 1999). In the LBM, as in LGA, space and time are discrete and they have the advantage that microscopic components are intuitive. A drawback of both LGA and LBM is that fluid velocity and other properties such as density and momentum, cannot be calculated explicitly and one would average over a larger region in order to obtain reasonable results. Many complex macroscopic fluid dynamical phenomena seem difficult to be modelled in these CA frames, because they take place on a large space scale and require a macroscopic level of description. Empirical CA methods were developed on the macroscopic scale in order to overcome this problem, dealing directly with the macroscopic variables (Di Gregorio and Serra, 1999; D'Ambrosio et al., 2001). These CA make use of local laws that are ruled by empirical parameters. As these latter can have no direct link with classical physical parameters, an accurate calibration phase is generally required (Iovine et al., 2005). At the contrary, physically based macroscopic cellular automata (MCA), in which local rules derive directly by physical laws and depend on physical parameters, do not require a similar calibration (Bates and De Roo, 2000; Horritt and Bates, 2001; Mendicino et al., 2006).

In this work, physically based MCA are the reference computational paradigm of a new two-dimensional model developed to simulate water flux in saturated aquifers that is equivalent to an explicit scheme. The model is developed for its inclusion in a distributed hydrological model (Ravazzani et al., 2007; Rabuffetti et al., 2008), with the aim of simulating water exchange between surface soil, river network and the underlying aquifer. A specific focus of the model development is the assessment of stability and convergence. Explicit models are subject to a strict stability criterion, which must be satisfied if the model is to simulate natural conditions in a realistic way (Douglas, 1956). To maintain accuracy, the model must also satisfy a convergence criterion. We show that correct choice of computational time step guarantees both stability and accuracy. The model is validated against typical problems in the study of alluvial aquifers: solution of steady flow between two streams in response to uniform recharge, transient drawdown due to a constant pumping rate from a well, and aquifer response to stream-stage variation. Benchmarks include analytical solutions and numerical simulations performed with the MODFLOW-2000 model.

2. Model formulation

Models based on CA paradigm consist of four primary components: a lattice of cells, the definition of a local neighbourhood area, transition rules determining the changes in cell properties, and boundary conditions (Parsons and Fonstad, 2007). To simulate water flux in unconfined aquifer, a two-dimensional lattice of cells is created. A value of saturated hydraulic conductivity, K_s [LT^{-1}], a value of specific yield, S_y [−], elevation of the bottom of the aquifer [L], and initial head [L] are assigned to each cell. The cell size must be small enough so that physical properties can be considered homogeneous in the cell space, but large enough to achieve macroscopic description of the physical processes. The cell size is set as $\Delta s = \Delta x = \Delta y$.

The neighbourhood in CA models defines the area of process influence. Among those proposed in literature for two-dimensional CA with square tessellation, as that here presented, the von Neumann and Moore ones are the most adopted: the Von Neumann neighbourhood considers the group of four cells in the four cardinal directions from the central one, while the Moore neighbourhood also includes the adjacent cells along diagonals (Fig. 1). The Von Neumann neighbourhood has been chosen as the basis of the CA model developed in this work.

To give physical meaning to the rule defining water interaction between two adjacent cells, the Darcy's law is assumed. According to this, the water flux between central cell and, for example, northern cell, Q_{NC} [$L^3\,T^{-1}$], is calculated as:

$$Q_{NC} = \frac{2T_N T_C}{T_N + T_C}\left(h_N^t - h_C^t\right) \quad (1)$$

where T_N and T_C represent, respectively, the transmissivity [$L^2\,T^{-1}$] of northern cell and central cell, h_N^t and h_C^t represent, respectively, hydraulic head [L] of northern cell and central cell at previous time step, t. The term $2T_N T_C/(T_N + T_C)$ is the harmonic mean of transmissivity. It has been chosen because of its property to remove the impacts of large outliers by limiting the flux to the lower value of transmissivity. The flux is positive if entering the central cell.

The total flux entering the central cell is (Fig. 2):

$$Q_C = Q_{NC} + Q_{EC} + Q_{SC} + Q_{WC} + W_C \quad (2)$$

where W_C [$L^3\,T^{-1}$] is the volumetric flux representing sources (+) or sinks (−).

Hydraulic head at central cell is updated for the subsequent time, $t + 1$, applying the discrete mass balance equation:

$$h_C^{t+1} = h_C^t + \frac{1}{S_y}\frac{Q_C}{\Delta s^2}\Delta t \quad (3)$$

where Δt [T] is the time step.

The final component of a CA model is the boundary condition that describes what happens at the outer cells of the lattice. The boundary conditions can be of Dirichlet or Neumann type (Kilzenbach, 1986). Dirichlet conditions specify the head h; Neumann conditions specify the flux, i.e., the head gradient $\partial h/\partial x$ orthogonal to the boundary. Neumann conditions are type A (permeable) or type B (impermeable). A Neumann type A condition specifies a finite gradient, i.e., $\partial h/\partial x \neq 0$; conversely, a Neumann type B condition specifies a zero gradient, i.e., $\partial h/\partial x = 0$.

3. Model implementation

The CA for modelling water flow in unconfined aquifers, MACCA-GW (MACroscopic Cellular Automata for GroundWater modelling), was developed in the Fortran 90 programming language. Fortran 90 was selected as the development language due to its high portability and efficiency. In fact, Fortran 90 compilers exist for almost every operating system and, due to long experience accumulated during years, they have been optimized to provide faster performance. The code is composed of different modules that can be reused and integrated in other developed models.

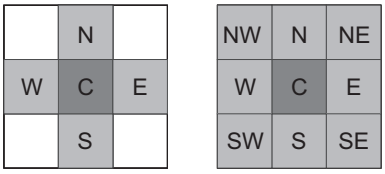

Fig. 1. Von Neumann neighbourhood definition (left) that considers the group of four cells in the four cardinal directions from the central one, and (right) the Moore method that includes the adjacent cells along diagonals.

Input data are raster layers in the Esri ASCII or Binary grid format. This format conforms to the description of lattice of cells and permits interoperability with many geographical information systems. A module was specifically developed for basic manipulation of grid. Two new types were defined to store lattice data and information necessary for the spatial positioning of the grid, one for floating point grid and one for integer grid (Fig. 3). The use of dynamic allocation makes the program suited for the analysis of problems of any dimension.

The groundwater module contains all variables and routines to initialise and update hydraulic head. A new type was defined to describe all necessary characteristics of a layer of an aquifer (Fig. 4). This new type is a container of several integer or floating point grids defining geometry (*top* and *bottom*), hydrogeologic parameters such as saturated hydraulic conductivity (*KsLayer*) and storativity (*porosity*), extent of the domain of analysis and boundary condition type (*domain*), values of boundary condition (*bc*), and saturated hydraulic conductivity of the eventually present underlying aquitard (*KsAquitard*). This latter feature was introduced to add the possibility to simulate aquifer composed of more than one layer, not investigated in the present work. The flow-chart of the program is shown in Fig. 5 and described in Table 1. When launched, MACCA-GW reads layer properties and initial condition. Then a time loop starts to simulate the transient flow. In each time step the model reads properties that may vary with time, well pumping rates, and boundary conditions; the model also updates for each time step the phreatic head with Eqs. (1)–(3) and writes results on file.

4. MODFLOW-2000

In order to test MACCA-GW model, a comparison with MODFLOW-2000, as the version incorporated into Visual MODFLOW 4.2 (Waterloo Hydrogeologic), was performed. MODFLOW-2000 (MacDonald and Harbaugh, 1988; Harbaugh et al., 2000), is a code developed by the USGS that is capable of simulating groundwater flow in transient, three-dimensional, anisotropic and heterogeneous systems. MODFLOW's governing three-dimensional flow equation for unconfined aquifer combines Darcy's Law and the principle of conservation of mass via

$$\frac{\partial}{\partial x}\left(k_{xx}h\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_{yy}h\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(k_{zz}h\frac{\partial h}{\partial z}\right) - W = S_y\frac{\partial h}{\partial t} \qquad (4)$$

where x, y, and z are Cartesian coordinates [L], K_{xx}, K_{yy} and K_{zz} are the principal components of saturated hydraulic conductivity along the x, y, and z axes, respectively (L/T), h is phreatic surface elevation (L), W is a volumetric source/sink term (L/T), and t is time (T).

Eq. (4), when combined with boundary and initial conditions, describes transient three-dimensional groundwater flow in a heterogeneous and anisotropic medium, provided that the principal axes of hydraulic conductivity are aligned with the coordinate directions.

MODFLOW-2000 solves Eq. (4) using the finite-difference method in which the groundwater flow system is divided into a grid of cells (blocks). Development of the groundwater flow equation in finite-difference form follows from the application of the continuity equation: the sum of all flows into and out of the cell must be equal to the rate of change in storage within the cell. The continuity equation is written for each cell in backward-difference form leading to a system of equations that must be solved simultaneously for each time step.

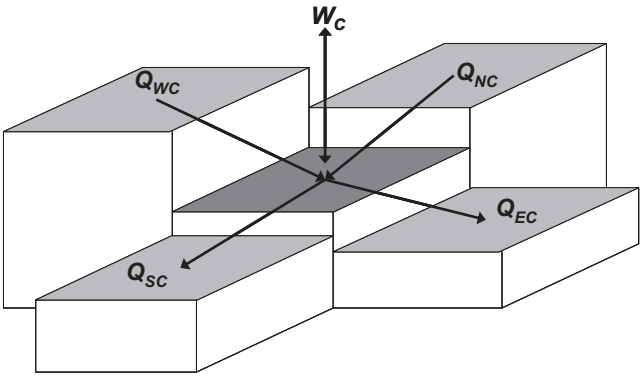

Fig. 2. Scheme for the calculation of water fluxes between the central cell and the four adjacent cells. W_C is the volumetric flux representing source (entering the cell) or sink (exiting the cell).

MODFLOW utilizes iterative methods to obtain the solution of the system of finite-difference equations for each time step. In these methods, the calculation of head values for the end of a given time step is started by arbitrarily assigning a trial value, or estimate, for the head at each node at the end of that step. A procedure of calculation is then initiated that alters these estimated values, producing a new set of head values that are in closer agreement with the system of equations. These new, or interim, head values then take the place of the initially assumed heads, and the procedure of calculation is repeated, producing a third set of head values. This procedure is repeated successively at each stage, producing a new set of interim heads that more nearly satisfies the system of equations. Each repetition of the calculation is termed an "iteration." Ultimately, as the interim heads approach values that would exactly satisfy the set of equations, the changes produced by succeeding stages of calculation become very small. This behavior is utilized in determining when to stop iteration (convergence criterion). MODFLOW-2000 comes with a choice of different solvers to use in solving the numerical equations for the flow simulation:

```
TYPE grid_integer
        INTEGER,POINTER :: mat (:,:)    !grid data
        INTEGER         :: jdim         !number of columns
        INTEGER         :: idim         !number of rows
        REAL            :: xllcorner    !lower left corner x coordinate
        REAL            :: yllcorner    !lowerleft corner y coordinate
        REAL            :: cellsize     !cell dimension
        INTEGER         :: nodata       !nodata value
END TYPE grid_integer

TYPE grid_real
        REAL,POINTER    :: mat (:,:)    !grid data
        INTEGER         :: jdim         !number of columns
        INTEGER         :: idim         !number of rows
        REAL            :: xllcorner    !lower left corner x coordinate
        REAL            :: yllcorner    !lowerleft corner y coordinate
        REAL            :: cellsize     !cell dimension
        REAL            :: nodata       !nodata value
END TYPE grid_real
```

Fig. 3. The two new user defined types to store floating point and integer grid. The individual components are defined to store georeferencing information (*idim*, *jdim*, *xllcorner*, *yllcorner*, *cellsize*) and data (*mat*, *nodata*).

```
TYPE layer
    TYPE (grid_real)        :: top          !top elevation
    TYPE (grid_real)        :: bottom       !bottom elevation
    TYPE (grid_real)        :: KsLayer      !layer hydraulic conductivity
    TYPE (grid_real)        :: porosity     !effective porosity
    TYPE (grid_real)        :: KsAquitard   !aquitard hydraulic conductivity
    TYPE (grid_integer)     :: domain       !domain of analysis and
                                            !boundary condition type
    TYPE (grid_real)        :: bc           !boundary condition values
END TYPE layer
```

Fig. 4. Definition of the new "*layer*" type to store all necessary characteristics of a layer of an aquifer.

strongly implicit procedure (SIP), preconditioned conjugate-gradient (PCG) and direct solver (DE4). Other solvers are made available in Visual MODFLOW such as WHS solver, a proprietary solver developed by Waterloo Hydrogeologic that is faster and more stable than other standard MODFLOW solver packages. The WHS solver implements a conjugate-gradient algorithm, called the bi-conjugate gradient stabilized (Bi-STAB) acceleration routine, using Stone Incomplete Decomposition as the pre-conditioning method (Obrecht, 1994). Discussions of the mathematical basis of various iterative methods can be found in many standard references, including Remson et al. (1971), Peaceman (1977), and Crichlow (1977).

MODFLOW-2000 supports several averaging schemes for computing interblock transmissivity: harmonic mean, logarithmic mean, and arithmetic mean thickness and logarithmic-mean hydraulic conductivity that reduces to arithmetic mean method when the aquifer is homogeneous (Goode and Appel, 1992).

5. Model testing

In order to test MACCA-GW numerical properties, a prototype artificial domain was considered, a 1-km^2 square aquifer (1 km $\times$ 1 km) with saturated hydraulic conductivity $K_s = 1.25 \times 10^{-5}$ m/s, and specific yield $S_y = 0.1$. The space interval was set as $\Delta s = 10$ m, i.e., a total of $100 \times 100 = 10{,}000$ grid nodes. The model was subjected to four tests: the first to verify model's convergence, that is its ability to return to the steady equilibrium condition starting from a depleted water table as initial condition, the second with the purpose to verify the numerical model with respect to steady state solution under Dupuit–Forcheimer conditions, the third to test model's ability to reproduce unsteady water table depletion due to pumping from a well, and the fourth to test the model in an important problem in the study of alluvial aquifers that is the simulation of aquifer response to stream-stage variation. The results of MACCA-GW simulations were compared to analytical solutions, where available, and MODFLOW-2000 numerical results.

Simulations with MODFLOW-2000 were performed using harmonic mean scheme for the computation of interblock transmissivity and the WHS solver with residual tolerance for the convergence criterion = 0.0001 m.

The tests were performed on a computer with a Intel Pentium D dual core 2.80 GHz CPU and 1 GB RAM.

Table 1
Description of the main modules of MACCA-GW.

Module	Description
Allocate and read	Allocate grids and read layer properties and initial conditions
Advance time	Read external sources and sinks and update boundary conditions
Water budget	For each cell calculate local lateral fluxes and update hydraulic head
Output	Write head at specific cells and maps in Esri ascii grid format
Deallocate memory	Deallocate memory, close files and terminate the program

5.1. Convergence test

The scheme implemented in MACCA-GW is equivalent to an explicit finite-difference model and thus subjected to stability criterion that imposes the use of sufficiently small time step, Δt. Moreover, explicit as well as implicit models, are subject to a convergence criterion that places an upper limit on the time step (Ponce et al., 1978, 1979). The aim of this analysis is to verify the method proposed by Ponce et al. (2001) to find the minimum value of time step that satisfies stability and convergence.

Defining the hydraulic diffusivity of the aquifer (Freeze and Cherry, 1979) as

$$\upsilon = \frac{T}{S_y} \tag{5}$$

where T is the transmissivity, following Roache (1972), the cell Reynolds number, D, is defined as the ratio of physical and numerical diffusivities, leading to:

$$D = \frac{\upsilon}{(\Delta s/2)^2/\Delta t} = 4\upsilon\frac{\Delta t}{(\Delta s)^2} \tag{6}$$

Stability requires that $D \leq 1$. Therefore, $D = 1$ is the maximum cell Reynolds number that can be used in practice. For $D = 1$, the time step results:

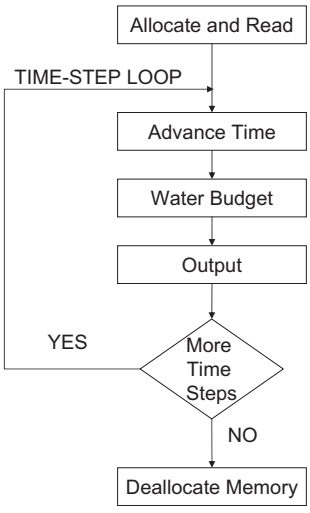

Fig. 5. Flow-chart of MACCA-GW.

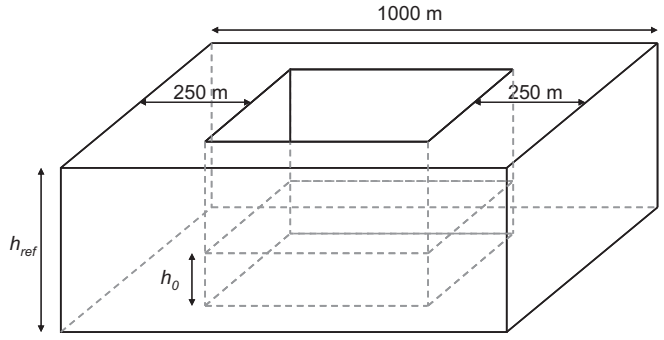

Fig. 6. Scheme of the artificial domain to test model convergence.

Table 2
Time interval in seconds, Δt, adopted in runs to test model convergence, for different combination of cell Reynolds number, D, and reference head, h_{ref}, located on external area of the test case.

D	$h_{ref} = 50$ m	$h_{ref} = 100$ m	$h_{ref} = 200$ m	$h_{ref} = 400$ m
1	4000	2000	1000	500
0.5	2000	1000	500	250
0.25	1000	500	250	125
0.125	500	250	125	60

$$\Delta t = \frac{(\Delta s)^2}{4\upsilon} \tag{7}$$

Sixteen test cases combining time step sizes, Δt, and reference heads values h_{ref} were perfomed to evaluate the convergence of the MACCA-GW model. The initial condition was specified as $h_0 = 25$ m in a square area of 500 m × 500 m centered in the computational domain, while the reference head, located on the external area of the computational domain, was set equal to $h_{ref} = 50$, 100, 200, and 400 m (Fig. 6). Moreover, the time interval was changed so that four cell Reynolds numbers ($D = 1.0$, 0.5, 0.25, and 0.125) were considered (see Table 2). Fig. 7 shows head recovery at centerfield node, while in Fig. 8, head recovery deficits, are reported. We observe that deficit increases nonlinearly with decrease in cell Reynolds number, denoting increase in model's inability to return to steady equilibrium, i.e., lack of convergence. The condition $D = 1$ guarantees the most accurate results and is also the most economical in term of model iterations as the time step is larger.

5.2. Steady flow between two streams in response to uniform recharge

The second stage of MACCA-GW testing has the purpose to verify the numerical model with respect to steady state solution. Under the hypothesis that Dupuit–Forcheimer conditions are assumed valid, for the problem of steady flow between two streams in response to uniform recharge (Fig. 9), the following analytical solution predicts the height of the water table (h), at any distance x from the origin (Harr, 1962):

$$h^2 = h_0^2 - \frac{\left(h_0^2 - h_L^2\right)x}{L} + \frac{W}{K_S}(L - x)x \tag{8}$$

where W is the recharge rate [LT^{-1}], h_0 and h_L [L] are the water elevations of the two rivers at, respectively, $x = 0$ and $x = L$.

To run MACCA-GW, the model domain was set with two Dirichlet conditions on the west boundary ($h_0 = 20$ m) and the east boundary ($h_L = 17$ m) to represent the stage in the river. In addition, a Neumann type B condition on north and south boundaries was considered. Recharge was set to 5.78704×10^{-9} m/s equivalent to 0.5 mm/day. The time step was set to 8000 s. Initial head was set to 17 m on every cell. Simulation with MODFLOW-2000 was performed as steady state flow run type. In Fig. 10 the comparison between analytical and numerical solution by MACCA-GW and MODFLOW-2000 is reported after sufficient simulation time to permit that steady condition was reached. The root mean squared error, RMSE, is 0.003 m for MACCA-GW and 0.014 m for MODFLOW-2000.

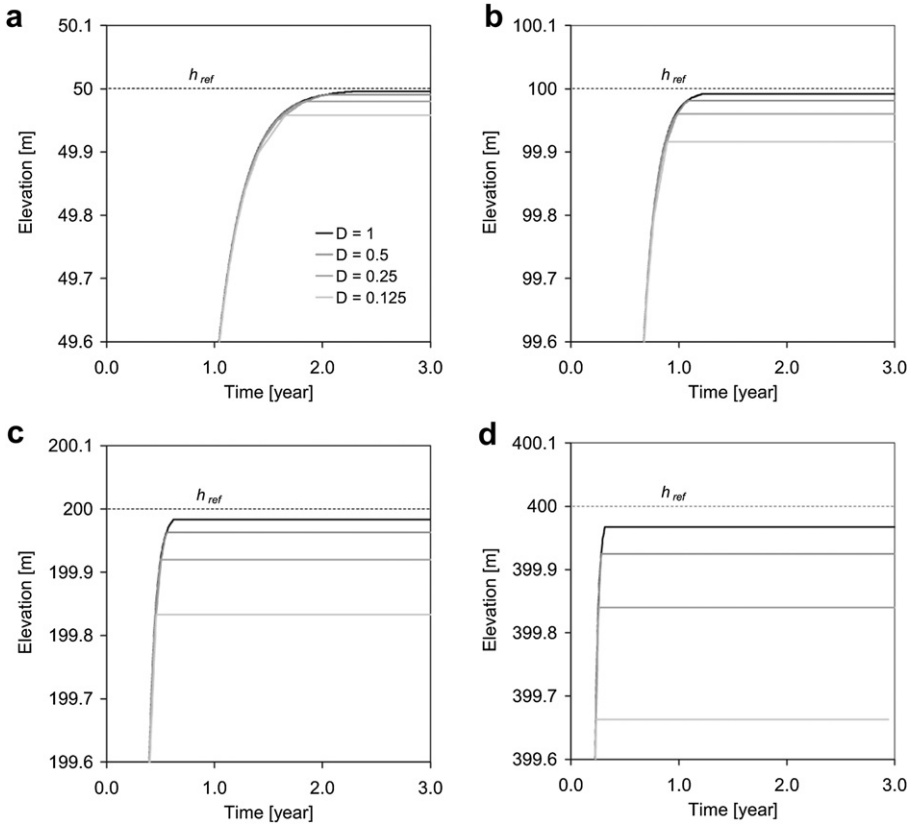

Fig. 7. Results of model convergence test: head recovery at centerfield node for $h_{ref} = 50$ m (a), $h_{ref} = 100$ m (b), $h_{ref} = 200$ m (c), and $h_{ref} = 400$ m (d).

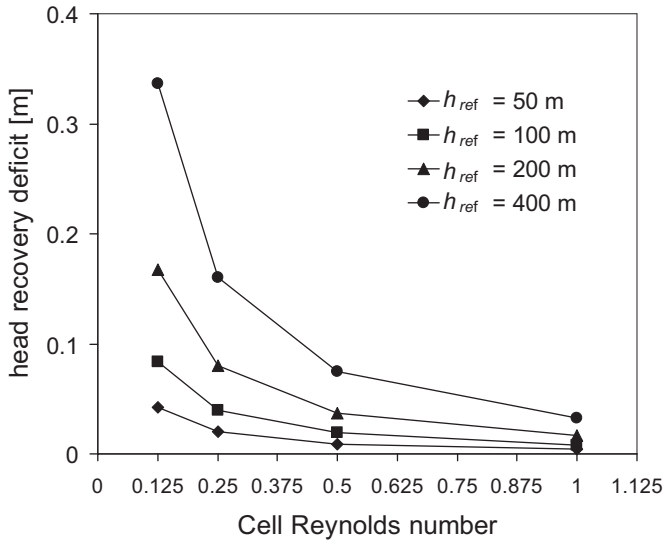

Fig. 8. Head recovery deficit for $h_{ref} = 50$, 100, 200 and 400 m as a function of cell Reynolds number.

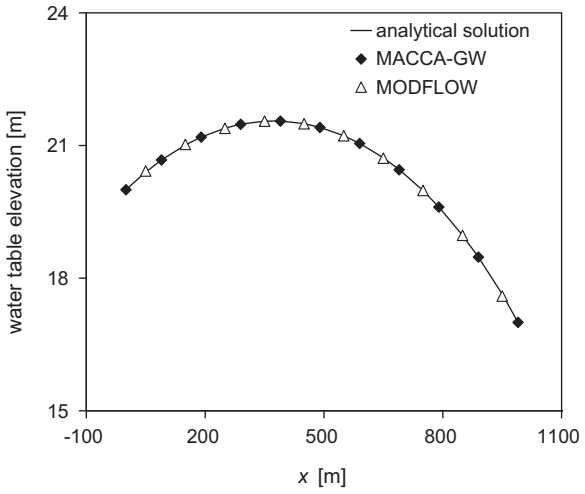

Fig. 10. Comparison between analytical and numerical solution (MACCA-GW and MODFLOW) for water table elevation between two streams in response to uniform recharge.

5.3. Drawdown due to a constant pumping rate from a well

The third stage of MACCA-GW testing has the purpose to verify the numerical model with respect to transient solution of head drawdown due to a constant pumping rate from a well. The first mathematical analysis was obtained by Theis (1935), under the assumptions that: (a) the aquifer is confined and compressible; (b) there is no source of recharge to aquifer; (c) water is released instantaneously from the aquifer as the head is lowered; (d) the well is fully penetrating.

The solution of unsteady distribution of drawdown is expressed by:

$$s(r,t) = \frac{Q}{4\pi T}\cdot W(u) \tag{9}$$

with

$$u = \frac{r^2\cdot S_y}{4tT} \tag{10}$$

and

$$W(u) = \int_u^{\infty} \frac{e^{-z}}{z} \tag{11}$$

where s, is drawdown [L]; Q, is the constant pumping rate [$L^3\,T^{-1}$]; t, time since pumping began [T]; r, radial distance from the pumping well [L]. The integral expression in Eq. (11) is termed the well function. It is generally evaluated with analytical approximation. In this paper we adopted the solution proposed by Barry et al. (2000) valid for all values of the argument of exponential integral. The Theis equation can be extended to describe flow in unconfined aquifers if the drawdown is small relative to the saturated thickness of the aquifer (Jacob, 1950).

The domain was setup applying Dirichlet condition on the entire boundary with hydraulic head $h = 50$ m, as well as initial condition. A well with a constant pumping rate of 0.001 m^3/s was placed in the central cell. The time step was set to 4000 s. Monitoring wells were placed along cardinal directions at a distance of 150, 200, 300 m from the pumping well. Two monitoring wells were placed on the 45° direction at a distance of 127 and 170 m to investigate the eventuality that von Neumann neighbourhood could generate privileged directions. A further monitoring well was positioned at

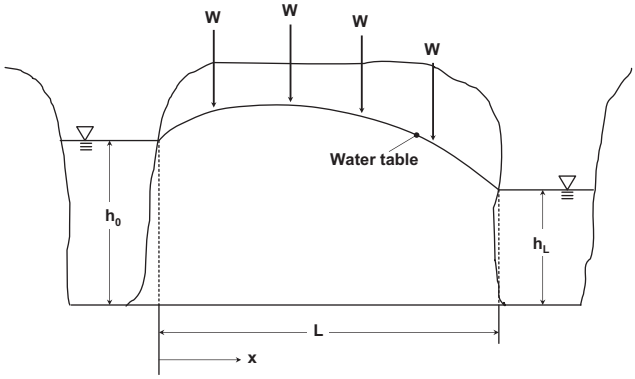

Fig. 9. Schematic diagram of flow between two streams in response to uniform recharge.

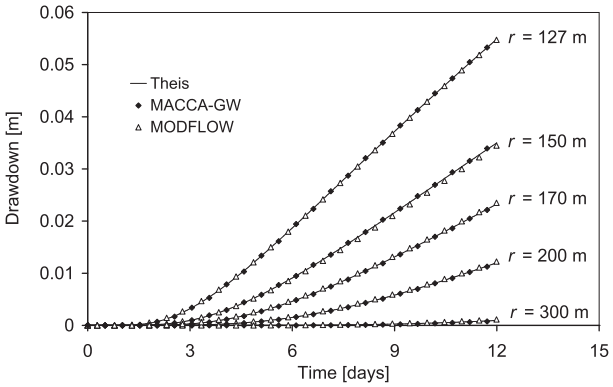

Fig. 11. Comparison between analytical (Theis) and numerical solution (MACCA-GW and MODFLOW) for head drawdown due to a constant pumping rate of 0.001 m^3/s at distance $r = 150$, 200 and 300 m from the well along cardinal direction, and $r = 127$ and 170 m on the 45° direction.

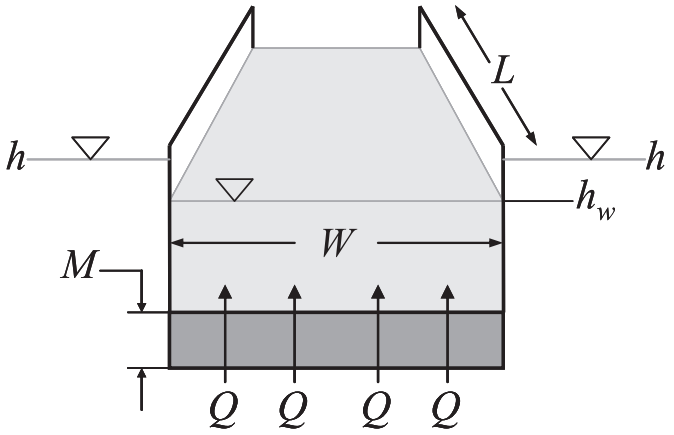

Fig. 12. Conceptual representation of river-aquifer interconnection: Q is the discharge, L is the stream length, W is the stream width, M is the streambed thickness, h_w is the hydraulic head in the stream, and h is the hydraulic head in the aquifer.

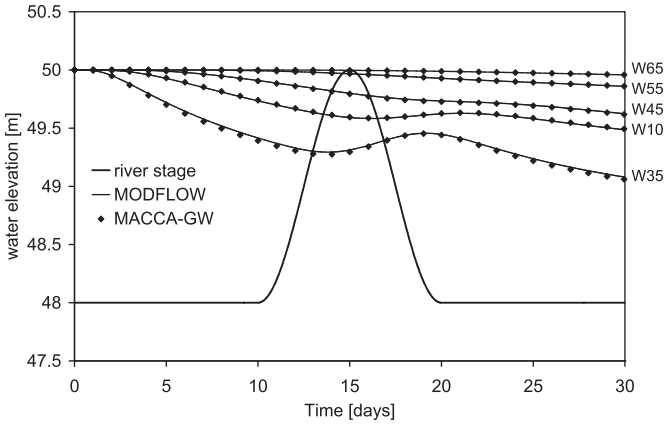

Fig. 14. River stage variation and response of the water table at the five monitoring wells simulated by MODFLOW-2000 and MACCA-GW.

the cell adjacent to the boundary to verify if boundary condition could have influence on the cone of depression.

Fig. 11 illustrates the depletion computed by MACCA-GW and MODFLOW-2000 compared to analytical solution for a 12 days duration after the beginning of the pumping. A very good fit can be observed in both monitoring wells along cardinal and diagonal direction.

5.4. Aquifer response to stream-stage variation

Rivers contribute water to or drain water from the groundwater system, depending on the head gradient between the river and the groundwater regime. Quantification of stream/aquifer hydraulics is an important problem in the study of alluvial aquifers.

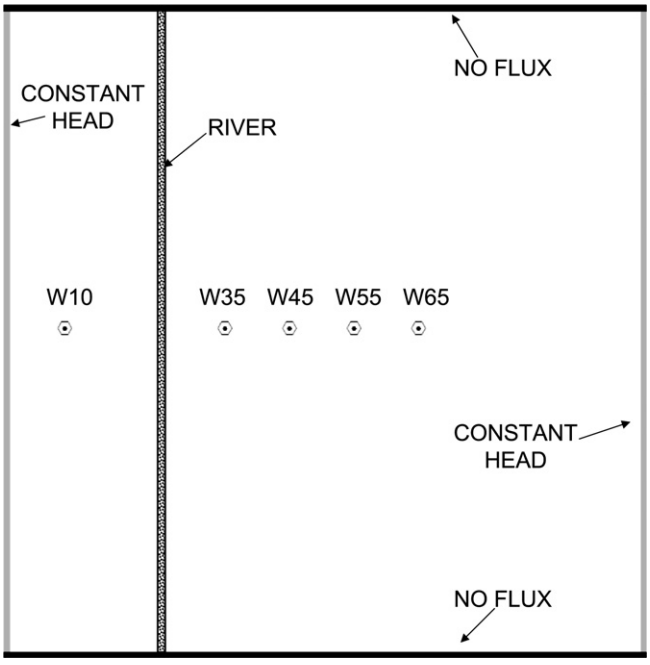

Fig. 13. Scheme of the domain setup to perform the simulation of the aquifer response to stream-stage variation: location of river, boundary conditions and monitoring wells (W10, W35, W45, W55, and W65) is shown.

This section has the purpose to test MACCA-GW's ability to simulate the aquifer response to stream-stage variation compared to the solution obtained by MODFLOW-2000.

The river interconnection was simulated using the RIVER package in MODFLOW-2000, which allows stream to gain or lose water. The stream stage is used to calculate the flux between the stream and the aquifer system, proportional to the head gradient between the river and the aquifer and a streambed conductance parameter. When the aquifer head is above the bottom of the streambed, MODFLOW-2000 assumes that the discharge through the streambed is proportional to the difference in hydraulic head between the stream and the aquifer (Fig. 12):

$$Q = \frac{K_{sb}LW}{M}(h_w - h) \tag{12}$$

where Q is the discharge [$L^3 T^{-1}$] with a downward flux assumed positive, K_{sb} is the streambed hydraulic conductivity [LT^{-1}], L is the stream length [L], W is the stream width [L], M is the streambed thickness [L], h_w is the hydraulic head in the stream [L], and h is the hydraulic head in the aquifer [L]. The term $K_{sb}W/M$ is defined hydraulic conductance of the streambed [LT^{-1}]. If the aquifer head drops below the bottom of the streambed, the model assumes that the seepage is no longer proportional to the aquifer head and becomes dependent on the water level in the stream and the streambed thickness:

$$Q = \frac{K_{sb}LW}{M}(H_w + M) \tag{13}$$

where H_w is the water level in the stream above the surface of the streambed [L]. At the beginning of each iteration, terms representing river seepage are added to the flow equation for each cell containing a river reach.

The same scheme was implemented in the MACCA-GW model. The domain was set up applying a constant head $h = 50$ m on the west and east boundaries, a Neumann type B condition on north and south boundaries, and an initial condition to perform the test. The time step was set to 4000 s. A river was placed with north-south direction at a distance of 250 m from the west boundary (Fig. 13). River bottom was set at 46.5 m. Riverbed conductivity and thickness were 1×10^{-5} m/s and 0.5 m, respectively, and the width of the river was equal to 5 m. Monitoring wells were placed at a distance of 100, 350, 450, 550, and 650 m from the west boundary as shown in Fig. 13.

Table 3
Summary of the results of the computational performance analysis using different specific yield values (S_y), saturated hydraulic conductivity (K_s), and cell Reynolds Number (D). Table shows calculating time, T_{calc}, in seconds, and root mean square error at monitoring well at 127 m distance in 45° direction (RMSE W = 127) and 200 m distance in cardinal direction (RMSE W = 200) from the pumping well.

Case	S_y (−)	K_s (m/s)	Δt (s)	D	Model	T_{calc} (s)	RMSE $W = 127$ (m)	RMSE $W = 200$ (m)
1	0.1	1.25E−05	4000	1	MACCA-GW	1.125	9.54E−05	2.72E−05
					MODFLOW	5.204	2.35E−04	1.39E−04
2	0.1	1.25E−05	16,000	4	MODFLOW	1.406	2.51E−04	1.64E−04
3	0.1	1.25E−05	32,400	8.1	MODFLOW	0.812	6.50E−04	2.66E−04
4	0.1	1.25E−05	64,800	16.2	MODFLOW	0.531	1.04E−03	4.66E−04
5	0.3	1.25E−05	12,000	1	MACCA-GW	0.375	1.95E−04	2.07E−05
					MODFLOW	2.703	7.86E−05	5.28E−05
6	0.3	1.25E−05	48,000	4	MODFLOW	0.562	2.44E−04	9.01E−05
7	0.3	1.25E−05	99,692	8.3	MODFLOW	0.375	5.33E−04	1.41E−04
8	0.3	1.25E−05	185,143	15.4	MODFLOW	0.235	1.00E−03	3.05E−04
9	0.1	1.25E−04	400	1	MACCA-GW	10.265	6.61E−4	6.65E−4
					MODFLOW	29.781	2.47E−3	2.32E−3
10	0.1	1.25E−04	1600	4	MODFLOW	8.125	1.00E−3	9.93E−4
11	0.1	1.25E−04	3240	8.1	MODFLOW	4.454	6.51E−4	6.74E−4
12	0.1	1.25E−04	6480	16.2	MODFLOW	2.719	5.18E−4	5.49E−4

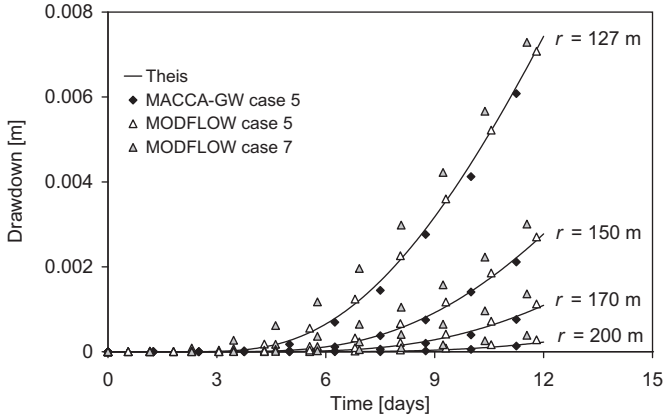

Fig. 15. Comparison between analytical (Theis) and numerical solution (MACCA-GW and MODFLOW) for cases 5 and 7.

The simulation time was 30 days and the river stage was supposed to increase with a sinusoidal variation to a maximum of 50 m as reported in Fig. 14 where the comparison between MACCA-GW and MODFLOW-2000 results is performed. A good agreement can be observed.

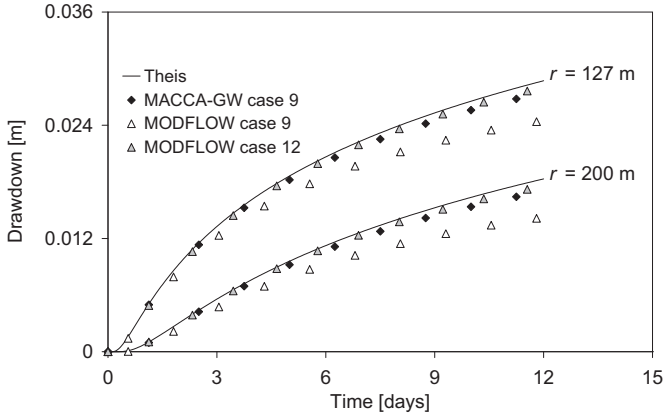

Fig. 16. Comparison between analytical (Theis) and numerical solution (MACCA-GW and MODFLOW) for cases 9 and 12.

6. Computational performance

To test the computational performance of the MCA approach, test case "Drawdown due to a constant pumping rate from a well" (Section 5.3) was employed to compare MACCA-GW to MODFLOW-2000. Simulations were performed with two different values of specific yield S_y, 0.1 and 0.3, and two different values of saturated hydraulic conductivity K_s, 1.25×10^{-5} m/s and 1.25×10^{-4} m/s. Time step of simulations performed with MACCA-GW was set so that cell Reynolds number was $D = 1$. Use of greater time step is not possible as it makes MACCA-GW to become unstable. Simulations with MODFLOW-2000 were performed using different time steps until condition $D \approx 16$ was reached. Simulation results are summarized in Table 3 where RMSE computed at the monitoring wells at distance 127 m on the 45° direction and 200 m distance along cardinal direction from the pumping well is reported. For $D = 1$, MACCA-GW shows lower RMSE than MODFLOW-2000, except for the 127 m distance monitoring well in case 5. MACCA-GW also shows better computational performance in the simulations performed with the same time step: it resulted from 2.8 to 7.2 times faster than MODFLOW-2000.

For $K_s = 1.25 \times 10^{-5}$ m/s, with the increase of time step, MODFLOW-2000 computational time decreases but RMSE increases of nearly two orders of magnitude. A comparison between case 5 and case 7 is shown in Fig. 15. For case 5, the two models are run with the same time step. Although accuracy of the two models is comparable, MODFLOW-2000 takes more than seven times longer to complete simulation. In case 7, in which time step is more than eight times greater than case 5, MODFLOW-2000 performs exactly as MACCA-GW in case 5 but exhibits loss of accuracy.

For $K_s = 1.25 \times 10^{-4}$ m/s, the behavior of MODFLOW-2000 is different. For $D = 1$ (case 9), MODFLOW-2000 shows significant underestimation of drawdown (Fig. 16). With the increase of time step, and consequently D, drawdown is better predicted giving a RMSE that is comparable to MACCA-GW in case 9, as if loss of accuracy can compensate underestimation when $K_s = 1.25 \times 10^{-4}$ m/s.

7. Conclusions

A cellular automata on a regular grid representing two-dimensional groundwater flow in unconfined aquifer was presented. Physically based equations are implemented to simulate the flow of

water between adjacent cells. This makes easier the setting of model parameters and their calibration. The model can account for sources or sinks and boundary conditions of Dirichlet or Neumann type. River-aquifer interaction can be simulated: the stream stage is used to calculate the flux between the stream and aquifer system, proportional to the head gradient between the river and aquifer and a streambed conductance parameter.

Test of the model under hypothetical conditions showed that the model is stable and convergent when the time step satisfies the condition that cell Reynolds number $D = 1$.

The accuracy of the model was evaluated considering three testing problems both in transient and steady state: the steady flow between two streams in response to uniform recharge, the drawdown due to a constant pumping rate from a well, and the aquifer response to stream-stage variation. Comparison with analytical solution and MODFLOW-2000 numerical results showed a good agreement.

The MACCA-GW model, thank to the explicit numerical scheme based on macroscopic cellular automata that does not perform inner iterations, proved to be fast in simulating the investigated transient phenomena. Simulations were performed investigating drawdown due to a constant pumping rate from a well with different values of specific yield and time step. For cell Reynolds number, $D = 1$, MACCA-GW generally exhibited more accuracy and resulted from 4.6 to 7.2 times faster than MODFLOW-2000. For $D > 1$, with the increase of time step, as expected from convergence test in Section 5.1, MACCA-GW showed instability and MODFLOW computational time decreased but RMSE increased of nearly two orders of magnitude.

The code of MACCA-GW model is simple enough to facilitate its integration into other models such as distributed models that simulate water and energy fluxes at the interface between soil and atmosphere. The good performance in terms of calculating time without detriment to model's accuracy, makes the MACCA-GW adequate to perform long simulation time analysis. However the motivation for the development of MACCA-GW was the simulation of unconfined aquifers and their interactions with surface water; it is not intended as alternative to MODFLOW for the simulation of 3-dimensional fluxes in complex and heterogeneous stratified confined aquifers.

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