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AQUIVAL: A GUI for groundwater modelling incorporated into the simulation of complex water resources systems

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Abstract

The difficulty to integrate a groundwater model into the simulation of complex water resources systems is due to the complexity of sophisticated numerical models that have to be coupled with the simulation of surface water, and to the necessity to use a wide set of computer tools needed for preprocessing data and visualizing results. For this purpose AQUIVAL has been developed. AQUIVAL is a Graphic User Interface (GUI) integrated in a Computer Aided Support System for water resources planning and management including conjunctive use, called AQUATOOL (Andreu et. alt.[3]). It has been developed at the Universidad Politécnica de Valencia, Spain. It allows the integration of previously calibrated aquifer models based on the finite differences or finite elements methods in the simulation of a complex system of water resources. The aquifer modelling is performed through the approach due to Andreu and Sahuquillo[1], based on the eigenvalues method. AQUIVAL aids the user to graphically input the data that have to be process and to obtain a reduced set of vectors and matrices needed for the simulation of the aquifer. Its capabilities include also facilities to obtain written reports, zooming on screen, graphical edition of every datum, input through a digitizer, definition of typified stresses and control parameters representative of the aquifer state, etc. Thus, the described GUI makes accessible the means to simulate the surface and ground water systems avoiding the use of multiple computer tools and puts at the user's fingertips an efficient methodology.

1 Introduction

The possibility of using sophisticated methodologies or numerical techniques for the simulation of complex water resources systems use to be strongly limited by a very common requirement. This is the previous knowledge and instruction on the usage of several computer tools: operating systems, editors, spreadsheets and even basics about programming. This was a common situation found when different consulting firms and basin authorities started to apply the optimization and simulation models developed at the Universidad Politécnica de Valencia and it lead to develop the AQUATOOL system, a Computer Aided Support System for Water Resources planning and management including conjunctive use (Andreu et alt.[3,4]). AQUATOOL makes accessible to everybody who is familiar with the basic concepts on water resources, the use of powerful tools for planning and management of complex systems and allows to incorporate the simulation of the groundwater system in the decision-making processes. The latter is achieved by means of AQUIVAL, a Graphic Users Interface that helps the modeler to preprocess data from previously calibrated aquifer models in order to be incorporated as distributed parameters submodels in a more general simulation model of surface and groundwater. The technology underneath is due to Sahuquillo[10] and Andreu and Sahuquillo[1], who proved it to be more efficient than other existing methodologies, at least for common situations.

Following there is a brief description on how the groundwater submodels are incorporated in the conjunctive use simulation, and how the AQUIVAL GUI has been implemented to make this technology available to non-expert users. Due to obvious reasons, only a small subset of the interface windows, displayed by the GUI, have been included in the figures below.

2 The eigenvalue method and its integration in a complex water resources simulation model

2.1 The groundwater submodel

The equation that describes the linear flow problem in a confined aquifer can be transformed into a vector differential equation like that in eqn 1.

$$\mathbf{T}\cdot\mathbf{H}+\mathbf{Q}=\mathbf{SF}\,\frac{d\mathbf{H}}{dt} \qquad (1)$$

where, **H** is the vector of piezometric heads, **T** is a sparse and banded symmetric matrix the elements of which depend on transmissivity, boundary conditions and spatial discretization, **SF** is a banded symmetric matrix, the elements depending on the aquifer storage coefficient and spatial discretization, and **Q** is the vector of external stresses that accounts also for flows through boundaries.

Following Sahuquillo[10], the solution of eqn 1 can be obtained by using eigenvalues and eigenvectors decompositions. Thus, vector **H** can be expressed as in eqn 2,

$$\boldsymbol{H}=\boldsymbol{A}\cdot\boldsymbol{E}\cdot\boldsymbol{A}^{T}\cdot\boldsymbol{SF}\cdot\boldsymbol{H}_0+\boldsymbol{A}\cdot(\boldsymbol{I}-\boldsymbol{E})\cdot\alpha^{-1}\cdot\boldsymbol{A}^{T}\cdot\boldsymbol{Q} \qquad (2)$$

where, α and **A** are the diagonal matrix of the eigenvalues and the eigenvectors

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matrix, respectively, obtained solving the eigenproblem $\mathbf{T}\cdot\mathbf{A} = \mathbf{SF}\cdot\mathbf{A}\cdot\alpha$. The set of eigenvectors, in matrix **A**, is orthonormal in the aquifer domain, with respect to the **SF** matrix, i. e., $\mathbf{A}^T\cdot\mathbf{SF}\cdot\mathbf{A} = \mathbf{I}$. **I** is the N × N identity matrix, N refers to the number of discretization nodes of the aquifer domain, **E** is a diagonal matrix, the elements of which are equal to $e^{-\alpha_i t}$, and α_i refers to the i th eigenvalue.

The solution for heads, **H**, can be expressed in the basis provided by the set of eigenvectors as shown in eqn 3,

$$\boldsymbol{H} = \boldsymbol{A}\cdot\boldsymbol{L} \tag{3}$$

where its components **L** are given by eqn 4,

$$\boldsymbol{L} = \boldsymbol{E}\cdot\boldsymbol{L}_0 + [\boldsymbol{I}-\boldsymbol{E}]\cdot\alpha^{-1}\cdot\boldsymbol{A}^T\cdot\boldsymbol{Q} \tag{4}$$

being $\mathbf{L}_0$ the initial conditions expressed in the eigenvector basis and obtained from $\mathbf{L}_0=\mathbf{A}^T\cdot\mathbf{SF}\cdot\mathbf{H}_0$.

It is assumed that the simulation of the system is divided into time periods of equal length τ, and that vector **Q** can vary from one period to the other. With these assumptions, and based on eqns 3 and 4, the state of the aquifer at the end of every time period **k**, can be computed through equations 5 and 6,

$$\boldsymbol{H}_k = \boldsymbol{A}\cdot\boldsymbol{L}_k \tag{5}$$

$$\boldsymbol{L}_k = \boldsymbol{E}(\tau)\cdot\boldsymbol{L}_{k-1} + \chi\cdot\boldsymbol{Q}_k \tag{6}$$

where, $\mathbf{E}(\tau)$ is a diagonal matrix the elements of which are equal to $e^{-\alpha_i \tau}$, and χ is a matrix obtained from $[\mathbf{I}-\mathbf{E}(\tau)]\cdot\alpha^{-1}\cdot\mathbf{A}^T$.

Eqns 5 and 6 provide the means to compute the state of the aquifer at the end of every time period, once the evolution of vector **Q** is known. In fact, matrices **A**, **E**(τ) and χ, need to be computed only once before starting the simulation. However, as it has been shown by Andreu and Sahuquillo[1], the information needed for the simulation can be simplified and condensed even more than in eqn 5 and 6. In order to do that, two concepts are introduced: "basic stresses" and "control variables".

The basic stresses are a set of unitary stresses (in the sense that the summation of their components is equal to one) that serves as a vector basis to express any stress configuration at any given time period k. Thus, if these basic vectors are arranged as columns of an $N \times N_b$ matrix, $\mathbf{Q}^b$, then $\mathbf{Q}_k$ can be expressed as $\mathbf{Q}_k=\mathbf{Q}^b\cdot\mathbf{B}_k$, where $\mathbf{B}_k$ is a vector the elements of which refer to the intensities at which the basic stresses are applied. It is realistic to think that the number of basic stresses, N_b, will use to be considerably less than N. Using the basic stress concept, it is defined the $N \times N_b$ matrix Ψ, as $\Psi= \chi\cdot\mathbf{Q}^b$ that has to be computed only once before starting the simulation and allows to obtain $\mathbf{L}_k$ using eqn 7,

$$\boldsymbol{L}_k = \boldsymbol{E}(\tau)\cdot\boldsymbol{L}_{k-1} + \Psi\cdot\boldsymbol{B}_k \tag{7}$$

It is also reasonable to assume that in order to monitor the state of the aquifer, only a reduced number, N_c, of state variables need to be computed. Thus, if $\mathbf{C}_k$ is a vector containing the values of those state variables, here after referred to as control variables, at a given time period k, it can be obtained using eqn 8,

$$C_k = A^R \cdot L_k \qquad (8)$$

where $\mathbf{A}^R$ is an $N_c \times N$ matrix the rows of which are obtained as linear combinations of rows of matrix $\mathbf{A}$ and allows to compute any state variable of interest: average heads and/or volume of stored water in a given zone, flows through boundaries, gradients, etc.

Eqns 7 and 8 provide the means to compute all the control variables for every time period, having previously obtained the initial state vector, $\mathbf{L}_0$, and matrices α, Ψ and $\mathbf{A}^R$. These arrays condense all the information about the aquifer that could be needed: spatial discretization, hydrodynamic parameters, boundary conditions, spatial distribution of basic stresses, initial conditions and procedure to compute control parameters. If a series of intensity vectors, $\mathbf{B}_k$ (k=1,...), is given, eqns 7 and 8 will easily yield the successive control parameters vectors, $\mathbf{C}_k$ (k=1,...), that the modeler can need for any decision making process. It is even possible to reduce the computational cost just cutting down the eigenvectors basis. A subset of these vectors, corresponding to the smallest eigenvalues, can yield a good enough approximation for the simulation of the groundwater flow.

2.2 Integration in the simulation of a complex water resources system

The model constituted by eqns 7 and 8 have been proved, by Andreu and Sahuquillo[1], to be a very efficient flow simulator for cases in which the numbers of basic stresses, N_b, and control parameters, N_c, are small enough compared with the number of dicretization nodes, N. These authors have compared the eigenvalues technique with the Influence Functions method (see Maddock[6] and Morel–Seitoux and Daly[8]) and with the most common approach of solving the flow equation with a sequential time steps solver, concluding that the methodol–ogy they propose, is more efficient in speed and storage requirements.

These were the reasons why the eigenvalues approach was chosen as the methodology to include distributed aquifer models in model SIMGES (see Andreu and Capilla[2]). SIMGES is a general purpose model for the simulation of basin or complex water resources systems management, with conjunctive use of surface and ground water. It works on a monthly basis and includes several possibilities to decide about pumping from aquifers that rely on the aquifer state variables, on user–defined stored water indexes and on the availability of surface water for consumption units with different priorities. At the same time, the model simulates hydraulic connections of rivers reaches, artificial recharge to aquifers, seepage of reservoirs and streambeds, pumpings and recharges from irrigated zones. These capabilities lay on the fact that the simulation of the surface and ground water systems is fully coupled allowing to design, simulate and test any management alternative of interest for the basin authority.

This kind of valuable computer tools are often rejected by decision-makers due to the necessity of knowing and using a wide set of computer tools needed for preprocessing data and visualizing results. This is specially true as the complexity of preprocessing procedures increases. And computations needed to obtain the arrays $\mathbf{L_0}$, α, Ψ and $\mathbf{A^R}$ for a groundwater submodel are not a simple task.

In order to avoid this kind of inconvenience it was developed AQUATOOL, a Computer Aided Support System for Water Resources planning and management including conjunctive use. The core of this computer tool is basically made up by an optimization model and a simulation model, the latter being SIMGES. Around these models, and in a windows environment, several Graphic User Interfaces (GUI) have been implemented that can be invoked in order to access both models, manage hydrological series or make other kinds of preprocessing like preparing data for the aquifer distributed models simulation. The GUI designed for the latter purpose is called AQUIVAL. Further details on AQUATOOL can be found in Andreu et alt.[3,4].

3 AQUIVAL: A GUI to apply the eigenvalues method

The AQUIVAL Graphic Interface, a modular component of AQUATOOL, is made up by a main kernel written in the Visual Basic programming language, for the Microsoft Windows environment, and four external procedures written in Fortran 77. These are fully controlled by the above kernel and are dedicated to solve the posed eigenproblem and to compute the arrays $\mathbf{L_0}$, Ψ y $\mathbf{A^R}$.

The primary function of AQUIVAL is to ease the preprocess of aquifer data, advising the process from the data input itself to the obtention of the arrays that condense the aquifer information for the simulation model SIMGES. All these tasks are performed without requiring the user to have a especial background in the usage of specific computer software.

Previously to start AQUIVAL a complete study of the aquifer including a calibrated model and the definition of basic stresses and control parameters, is needed. The model can be based on the finite difference method (following one of the schemes due to Prickett and Lonnquist[9] or to McDonald and Harbaugh[7]), or based on the finite elements method with linear triangles (as in the model by Carrera and Neumann[5]). The user can input the discretization data directly through the application windows, through a digitizer or from ASCII (plain text) files. AQUIVAL also allows to input basic stresses and control variables definitions through interactive windows, graphically clicking on the aquifer discretization chart shown in the main window, or even from ASCII files. Figure 1 shows the main window of AQUIVAL where it can be seen a finite elements discretization and the main printing options available through the application menus. The upper bar shows the entrance titles of the main menu: 'FILE', 'GEOMETRY', 'BASIC STRESSES', 'CONTROL VARIABLES', 'CALCULATION', 'SIMULATION' and 'HELP', all of them clearly referencing

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their purpose. Figures 2 and 3 show some of the interactive windows asking for discretization data in turn for the Finite Elements and for the Finite Differences I (Prickett et alt.[9]) methods.

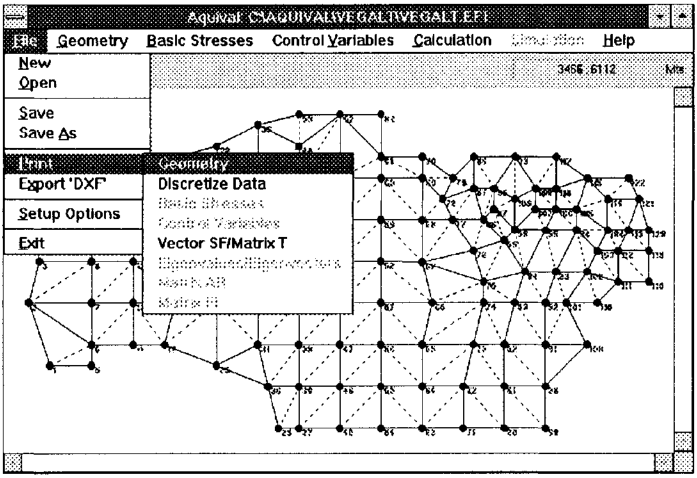

Figure 1: Main window showing an example of aquifer discretization an the main printing options.

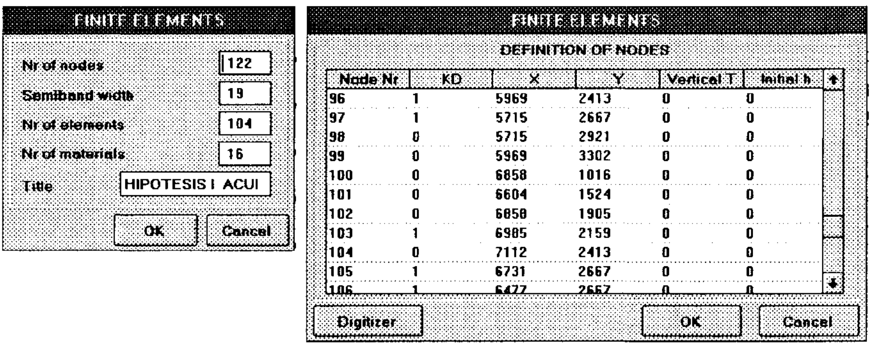

Figure 2: Two of the windows to interactively input the aquifer discretization data for the finite elements method.

Once the discretization data input is complete, AQUIVAL automatically performs the calculations to obtain matrices **A** and **SF**, allowing them to be browsed or even modified through windows like the one shown in figure 4. In fact, there is an option to input these matrices directly from an ASCII file. The process to define basic stresses and control parameters or to input them from files can be started at this point through windows like in figures 5 and 6. After all these data are ready it is possible to complete the calculations, through the 'CALCULATION' menu option, to obtain the arrays required by SIMGES. Then, AQUIVAL allows the possibility, see figure 7, to run a flow simulator for a

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given series of intensity vectors $\mathbf{Q}_k$, defined by the user.

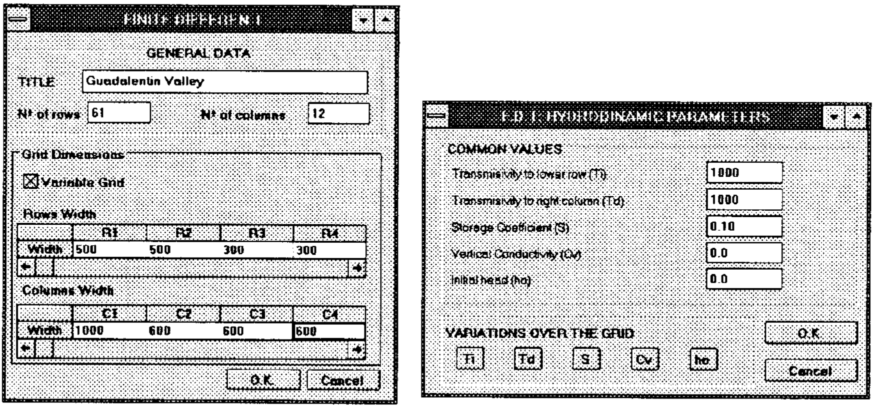

Figure 3: Two of the windows to interactively input the aquifer discretization data for the finite differences method I (as in Prickett et alt.[9]).

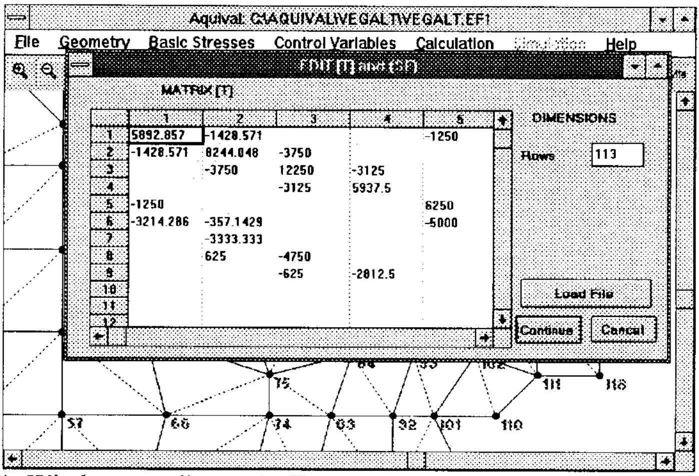

Figure 4: Window to edit matrix **T**.

The multiple functions and capabilities implemented in AQUIVAL, reachable through its menus, can be summarized as follows:

+ Input/Edit/View of discretization geometric data, hydrodynamic parameters, boundary and initial conditions, basic stresses and control parameters, through interactive windows, digitizer, on screen selection or ASCII files edition. The user can choose any of the given optional ways. At any moment there is the possibility to view/edit any element or block datum required, just clicking with the pointing device (mouse) on it (on its representation on screen). There are menu entrances to print, to a file or to a printer/plotter, any subset of data, or even a hard copy of the aquifer chart shown on

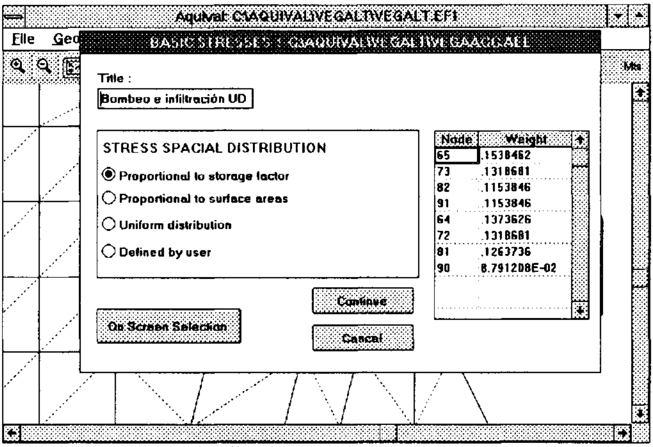

Figure 5: Window to create/edit/view basic stresses.

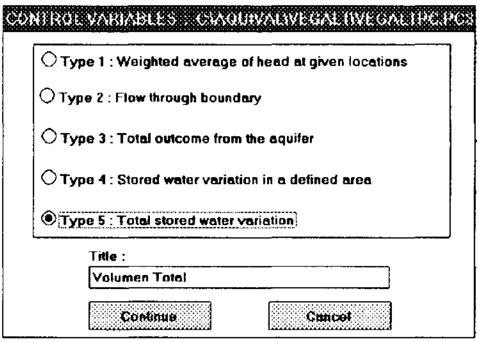

Figure 6: Main window to decide/browse the type of a control parameter.

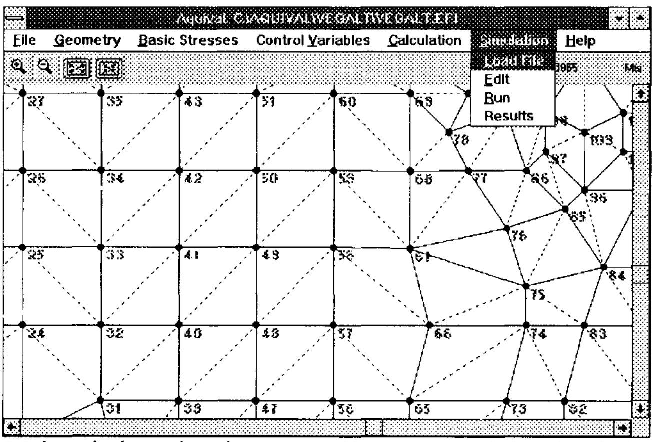

Figure 7: Main window showing an aquifer zoom and the simulation menu.

screen, very useful prepare a report. There are also 'zoom in/out', 'center' and'adjust to window' functions available on buttons under the main bar menu (see figure 7).

+ Guide and completion of the calculation process following the sequence: a) matrices **T** and **SF**, b) **A** y α, c) $\mathbf{L_0}$, Ψ y $\mathbf{A^R}$, d) simulation for a given series of intensity vectors $\mathbf{Q_k}$. The GUI controls the sequence of calculation stages to ensure that the data and results needed for every step are ready.

+ Management of files corresponding to different aquifer models.

+ Setup options to modify the presentation of aquifer charts and the system units.

+ Check of data to prevent input of anomalous or hydrologically inconsistent information.

+ Complete on-line help based on hypertext, accessible from any point in the program, the objective of which is to guide and provide supplementary information on any data, result or calculation process conducted by the GUI.

4 Conclusions

AQUIVAL is a GUI thought to preprocess aquifer data from aquifers for which there are previous calibrated models. Its purpose is to prepare distributed parameters submodels to be integrated in the simulation of complex water resources systems. It is part of AQUATOOL system, a Computer Aided Support System for Water Resources planning and management including conjunctive use.

The development of this Graphical Interface and the successful resulting product shows the possibility and utility of creating these kind of tools that make easily accessible, for decision-makers, powerful technologies for planning and management that, otherwise, are difficultly accessible and even avoided.

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