Fluxes, numerical models and sustainability of groundwater resources

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Abstract Management of groundwater resources in a sustainable manner requires understanding of hydrological processes in space and time. Therefore the spatio-temporal complexity of subsurface fluxes is discussed with regard to their use in numerical models and their importance in judgement of sustainability. Sustainability of groundwater resources depends on two types of constraints: anthropogenic, resulting from human impact, and hydrogeological. Four hydrogeological constraints of sustainability: net recharge, aquifer storage, aquifer transmissivity and groundwater quality are important in groundwater management. The most important is the net recharge which represents the difference between recharge and groundwater evapotranspiration. In arid and semiarid areas, recharge and groundwater evapotranspiration are largely spatially and temporally dependent. In such conditions sustainability of groundwater resources can only be well evaluated by fully-transient models i.e. with spatio-temporally variable fluxes defined on the basis of long-term monitoring data. The standard management of aquifer storage can be undertaken successfully by using partially-transient models based on model calibration with excessive pumping abstraction and related drawdowns. Two, modelling studies from Spain (fully transient model of Sardon area) and Botswana (partially transient model of Serowe area) with different hydrogeological conditions and different degrees of socio-economic impact, are analysed with regard to sustainability of groundwater resources. In this analysis, the advantages but also the complexity of fully-transient models with spatio-temporally variable fluxes are emphasized and compared.

Key words fluxes; groundwater; numerical models; vulnerability

INTRODUCTION

Sustainability of groundwater resources refers to the development and use of groundwater in a manner that can be maintained for an indefinite time without causing unacceptable environmental, economic or social consequences (Alley *et al*., 1999). With changing climate, increasing population and adverse human impact upon the environment, the issue of sustainability of groundwater resources nowadays plays an important role in water resources management. This is particularly so because groundwater represents ~98.55% of the total freshwater resources of the Earth excluding ice caps and glacial ice (Hiscock, 2005) and because in many locations groundwater represents the only, or the main, source of water supply. Sustainability of groundwater resources depends not only upon hydrogeological (environmental) constraints (see below) but also upon the anthropogenic (human-related) constraints, often changing the environment in a hazardous way. One of the most important changes related to the state of groundwater resources and therefore their sustainability, is the change of groundwater flow systems resulting from excessive water abstraction. The multitude of factors influencing the flow system and their interaction, make the prediction of flow system responses a challenge that can be handled best by groundwater modelling. The critical issue in groundwater modelling is data availability, which often is a limiting factor in model design and its solution; for example a lack of temporal data does not allow calibration of models in transient mode. With insufficient amount of data or low quality of data, models suffer calibration non-uniqueness, a problem which occurs because of aquifer heterogeneity, scale effects, i.e. an increase of effective transmissivity with increasing scale of observation that is particularly distinct in fractured rocks (Sanchez-Vila *et al*., 1996), uncertainty in net recharge estimates and also difficulties in data extrapolation. Problems of non-uniqueness affect primarily steady-state models. Transient models are less affected because they are better constrained by the temporal data pattern and have less degrees of freedom in model calibration.

There are two types of transient models, partially-transient (quasi-transient) models and fully-transient (true-transient) models (Lubczynski & Gurwin, 2005). The standard, commonly used partially-transient models with spatio-temporally variable aquifer storage and temporally invariant fluxes are efficient in terms of calibration, but are dependent upon availability of substantial drawdown schemes, which unfortunately are rarely available in practice. The complex, fully-transient models with spatio-temporally variable aquifer storage and fluxes are at least as accurate as partially-transient models but, in contrast, they can be calibrated without need for heavy groundwater abstraction typically required to obtain large drawdowns. Instead, they require monitoring networks which are indispensable for temporal data acquisition.

GROUNDWATER FLUXES IN NUMERICAL MODELS

In contrast to spatially dependent parameters, fluxes are spatio-temporally dependent. The spatio-temporal variability of fluxes is largely dependent upon the climatic zone. In general, the more arid the climate, the larger is the spatial and especially temporal variability of fluxes. In arid, and often in semiarid climates, the yearly average recharge (*R*) is typically low. In the cases of aquifers overlain by a thick unsaturated zone it can be on order of 5 mm year^{-1} (de Vries *et al*., 2000). The temporal distribution of recharge is usually irregular, varying from no recharge in “dry” years to largely exceeding the yearly average in “wet” years. In the case of large temporal variability of recharge, models that are not designed to evaluate sustainability of groundwater resources may provide wrong solutions and consequently the wrong judgment of sustainability.

Let us consider the example of an arid area with a total yearly rainfall of 300 mm extending over a 5-day period, and also assume that this rainfall results in 35 mm of recharge acting in 7 days with a ~5 mm day^{-1} average recharge rate for that particular week. A groundwater model could be set up with a weekly time discretization (stress period), involving a 5 mm year^{-1} recharge rate for the week with recharge and no recharge for all other weeks of the year. Alternatively, it could be set up with a monthly time discretization involving average recharge of ~1 mm day^{-1} for the month with rain and no recharge for the remaining 11 dry months; or with a yearly time discretization (similar to steady-state solution) with average recharge of ~0.1 mm day^{-1}. Despite no difference in total recharge quantity, the implication of different time discretization for modelling calibration is substantial. The finer the temporal discretization, the larger is the recharge quantity in a given stress period. This implies larger calibrated transmissivities (as compared to the calibration for coarser stress periods) which are required to pass groundwater through the modelled aquifer system for a given head condition. Different calibrated transmissivities result in different model predictions and therefore also in different sustainability scenarios. This example emphasizes the advantage of fully-transient models, showing that only models with temporally variable recharge input can provide reliable solutions in circumstances of large temporal variability of rainfall and recharge (e.g. arid and semiarid areas).

Unfortunately it is common practice in groundwater modelling to use a recharge flux (R) as model input, without specifying whether the intention of the model setup is to assign recharge (R) or net recharge (R_n). The R_n is defined as $R_n = R - ET_g$ with ET_g being groundwater evapotranspiration flux (Lubczynski & Gurwin, 2005). In models where only R is specified and ET_g not, automatically the assumption is made that the assigned R represents R_n. For example, if in MODFLOW (McDonald & Harbaugh, 1996) only recharge package is active and the evapotranspiration package that specifies ET_g not, then the assigned R represents R_n. Use of R_n, instead of R and ET_g separately, is a simplification which works well but only if the true R_n (taking into account ET_g) is assigned in the model. Disregarding ET_g, particularly in models of semiarid and arid environments, which are characterized by large spatio-temporal variability and large contributions of ET_g (Lubczynski, 2000; Lubczynski & Gurwin, 2005), leads to inaccurate solutions and consequently to inaccurate or even wrong evaluation of sustainability of groundwater resources (see below).

ET_g is a sum of groundwater transpiration (T_g) and groundwater evaporation (E_g) as discussed by Lubczynski (2000) and Lubczynski & Gurwin (2005). In arid and semiarid locations, rainfall is not present for much of the year, so plants are typically adapted to dry soil conditions either capturing traces of surface and unsaturated water or taking up groundwater (with capillary fringe water). The roots of groundwater-dependent trees can tap groundwater at 60–70 m depth (Canadell *et al*., 1996; Le Maitre *et al*., 2000). Moreover, in arid and semiarid areas, the quantities of groundwater discharged by root systems can be substantial as compared with recharge, because normally T_g occurs for a much longer time per year than R, which in certain years may not even occur at all.

The second component of ET_g, called groundwater evaporation (E_g), represents direct evaporation from groundwater. It is particularly important in dry areas with a shallow groundwater table where capillary water, or in the case of coarse rocks groundwater, evaporates to the atmosphere. Recent research indicates that in dry areas with a deep groundwater table, water can also move upward (evaporate). Walwoorth (2002a,b) and Scanlon *et al*. (2003) showed evaporation from >20 m below the ground surface. Such movement occurs in a vapour and liquid form and is driven by the water potential and by the soil temperature gradient. The vapour movement is dominated by thermal gradient and it condenses in the shallow subsurface of a few metres below the ground surface depending on the soil type (Coudrain *et al*. 2003). The condensed water as well as the capillary-driven water then evaporate from the shallow subsurface to the atmosphere.

Separate definition of recharge (R) and groundwater evapotranspiration (ET_g) is possible in steady-state, partially-transient and fully-transient models. In the former two types of models, due to the temporal flux invariance, the separate definition of R and ET_g is numerically equal to specifying only an R_n matrix but it provides a clearer definition of fluxes. In fully-transient models, the separate use of R and ET_g is significant.

Let us consider a simple example of a model consisting of two cells: one where recharge prevails (the "recharge cell") and the other where discharge, consisting of groundwater evapotranspiration (ET_g) and lateral groundwater outflow (Q_g), prevails (the "discharge cell"). Under natural conditions, R and ET_g fluxes change in time in such a way that the relative difference between the two as well as the flow between the two cells vary in time. These differences can change in time from being extremely high, when the "recharge cell" is recharged maximally and discharged minimally and the "discharge cell" is not recharged at all but discharged at the maximal rate, to being very low, when almost equal fluxes are applied on the two cells. Temporal averaging of fluxes, inherent in the steady-state and partially-transient models, masks the real flux and flow variability. The substantial recharge events, when simulated in fully-transient mode, result in short and large flows, larger than those simulated by steady-state and partially-transient models. As a result they require different (usually higher) model transmissivities to permit transfer of water from one area ("recharge cell") to another area ("discharge cell"). Therefore transmissivities confirmed in the fully-transient model calibration are more reliable than those obtained with steady-state and partially-transient model calibrations.

HYDROGEOLOGICAL CONSTRAINTS OF AQUIFER SUSTAINABILITY—MANAGEMENT IMPLICATIONS

Two types of sustainability constraints can be analysed, namely anthropogenic constraints (e.g. rate and distribution of water abstraction, expected increase of water demand, etc.) and hydrogeological constrains. There are four important hydrogeological constraints: (a) net recharge; (b) aquifer storage; (c) aquifer transmissivity; and (d) groundwater quality.

Net recharge represents the temporally variable balance between recharge and groundwater evapotranspiration. It depends upon climatic conditions, land cover (e.g. deep-rooting trees) and the nature of the subsurface medium (lithology, groundwater table depth, etc.). The balance between the net recharge and groundwater abstraction is the most important hydrogeological constraint on sustainability of groundwater resources. This constraint can be alleviated either by increasing recharge, e.g. by artificial recharge or by decreasing discharge, e.g. by reducing well abstraction, by decreasing lateral outflow through aquifer grouting or by reducing groundwater transpiration through replacing trees, such as e.g. eucalyptus (up to 500 L day^{-1} of water consumption per tree) that consumes the largest amount of groundwater.

Aquifer storage depends upon the rock type described by the storage coefficient, the aquifer volume and the degree of aquifer confinement. Long droughts (R = 0) and/or excessive pumping with active ET_g and lateral groundwater outflow (Q_g), can dramatically lower the groundwater table (and groundwater resources) in a way that disturbs the ecosystems so that total replenishment of aquifer storage may require many years. Exactly how many years may be uncertain because prediction of rainfall is very difficult, if not impossible. However, numerical models may be able to provide information necessary to process model scenarios, so that aquifer storage can be managed in sustainable manner.

Aquifer transmissivity depends upon the hydraulic conductivity of the medium and the aquifer thickness. Because aquifer transmissivity cannot be improved, the strategy of sustainable management relies mainly on adjusting rates and spatial patterns of pumping in relation to the particular transmissivity distribution, focusing on large transmissivity fields.

Groundwater quality in its natural state is dependent upon rock type, physical conditions (particularly temperature) and residence time. In natural conditions without human impact, quality is quite stable, especially when long time scales are analysed. Typical human impacts take place either by lowering or raising the groundwater table, which may, for example, increase groundwater salinity, or by aquifer contamination (directly or indirectly via the recharge area). The best strategy of sustainable groundwater quality management is simply to reduce human impact as much as possible, and in the case of aquifer contamination, to remediate it as quickly as possible, although protective policies may require a more sophisticated approach.

TWO MODELLING CASE STUDIES

Two contrasting case studies based on MODFLOW models are presented: an investigation of the Serowe (Botswana) using a partially-transient model, and one of the Sardon (Spain) employing a fully-transient model. The Serowe study area is characterized by: (a) a deep, sandstone aquifer with substantial aquifer storage; (b) a low R, mainly due to the large retention capacity of the unsaturated zone and; (c) a significant ET_g as compared to R, dominated by T_g due to very deep, groundwater tapping root systems of certain trees such as *Boscia albitrunca* and *Acacia erioloba*, as proven by lithium tracers (O. Obakeng 2004, personal communication); because of the ~60–70 m deep groundwater table, the E_g is assumed as not relevant. In contrast, the Sardon study area is characterized by: (a) a shallow, granite aquifer with low aquifer storage; (b) a substantial R, due to the low retention capacity of the unsaturated zone composed of coarse, weathered rocks and/or densely fractured rocks; (c) an ET_g dominated by E_g but also with a significant T_g component.

The Serowe sandstone case study (Botswana)

The Serowe study area of ~2500 km^2 is located on the eastern fringe of the Kalahari in Botswana and is marked by a distinct escarpment running approximately north to south

(Fig. 1). The escarpment feature cuts the study area into two parts, the western "sandveld" and the eastern "hardveld". In the sandveld part, the main aquifer, which comprises the Ntane sandstone at depths of >60 m below the ground surface, is overlain by a 60–90 m thick Kalahari sand cover. In the hardveld part, the Ntane sandstone layer is generally outcropping (overlain only by a thin 0–5 m cover of Kalahari sand or by basalt) and the groundwater table is shallower, at ~10–30 m below the ground surface. In the eastern part of the hardveld, the Ntane wedges out to the east. Across the entire study area, the Ntane aquifer is mainly unconfined, except when overlain by scattered, non-fractured basalt. The main recharge area is located along the groundwater divide and it runs parallel to the escarpment on its western side. From the groundwater divide line, groundwater flows generally to the west and to the east. The westward groundwater flow is towards the central Kalahari, whereas the eastward flow, due to the wedging out of the Ntane aquifer, has no physical outlet and therefore discharges through evapotranspiration in the hardveld area.

In order to evaluate groundwater resources and to provide prediction scenarios for the response of the Ntane aquifer to the increased water consumption in the study area, a numerical 1-layer groundwater MODFLOW model of the Ntane aquifer was made, first in steady-state mode and later in partially-transient mode. The head (*H*) matrix was krigged from the geodetically surveyed borehole measurements. Because of the log-normal distribution of transmissivity (*T*), its spatial distribution was derived by krigging of the logarithms of the pumping test transmissivities and finally by formulating the transmissivity matrix from the antilogarithms of the interpolated grid values. The groundwater recharge (*R*) of the MODFLOW Recharge Package was distributed by a GIS overlay method (Lubczynski & Gurwin, 2005) according to the point measurements using chloride mass balance and ^{14}C half-life degradation methods. The groundwater evapotranspiration (ET_g) matrix of the MODFLOW Evapotranspiration Package was defined by scaling (Lubczynski, 2000) the energy

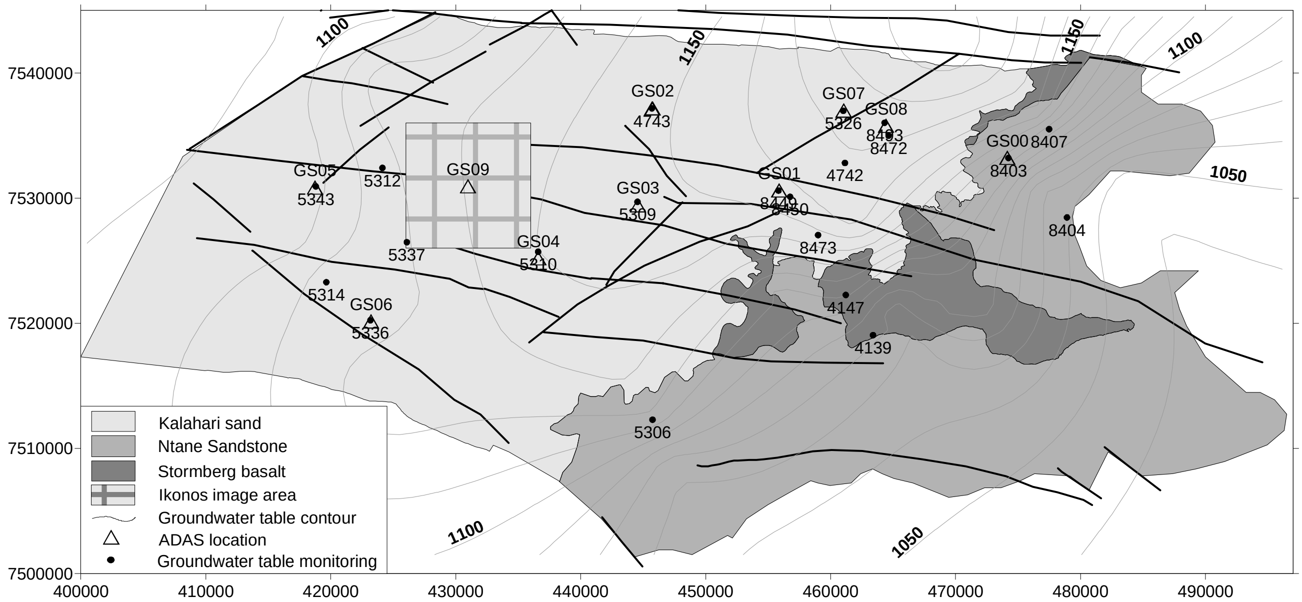

Fig. 1 The Serowe study area in Botswana (after Lubczynski & Obakeng 2004).

balance solution of surface evapotranspiration derived from remotely sensed data (Timmermans & Meijerink, 2000). The model was calibrated first in the steady-state mode, using historical data from before 1986, i.e. before the public groundwater supply was established. The result of the steady-state calibration was taken as an initial condition for the partially-transient model, and the known borehole abstractions were imposed on the model and calibrated against the known monitored drawdowns. In this calibration process the storage coefficient (S) was adjusted. The calibrated S was verified against two piezometric pumping test points, three core sample points and against well-described borehole log data points for which the ranges of the most likely S values were deduced from descriptions of borehole lithology. The final S matrix was by far less spatially variable than the T matrix and was well fitted in the S range of 0.02–0.08, which was typical for the Ntane sandstone aquifer.

The Sardon granite case study (Spain)

The Sardon catchment of ~80 km^2 was selected as being representative of granite areas in western Spain (Fig. 2). The watershed boundaries of this catchment match well with the catchment groundwater divides. The granite rocks of the study area are weathered in the upper 0–5 m zone and fractured in the underlying zone. The depth of the massive, non-fractured basement, considered as the base of the flow system, varies from 0 m in areas of non-fractured rock outcrops (mainly along the watershed boundary locations) to several tens of metres in the centre of the catchment. The central part of the catchment is occupied by a north–south fault zone, approximately matching the course of the intermittent Sardon River. The hydrostratigraphy of the system, as well as its parameterization, was investigated in the study area by shallow percussion drilling, by magnetic resonance sounding (MRS), and by electromagnetic and resistivity methods. The investigations were undertaken as part of the hydrogeological fieldwork programme carried out by ITC students from The Netherlands. In order to provide transmissivity data in the form of a matrix for steady-state model calibration, the three cross-sectional FLOTRANS models were calibrated. The results of the three models, as well as additional point data from other locations, were integrated in an ILWIS GIS and finally calibrated in MODFLOW (Lubczynski & Gurwin 2005). In order to provide spatio-temporal distributions of heads and fluxes (R and ET_g), required as input of the fully-transient models, an electronic monitoring network was installed in the study area at the end of 1996 and has been operated continuously since then. The network consists of two multi-sensor automated data acquisition systems (ADAS towers) and 10 automated groundwater table recorders (AGTR). The ADAS towers were designed to monitor rainfall, the climatic components of potential evapotranspiration (PET), unsaturated zone moisture and suction pressure, groundwater table fluctuation and also tree transpiration (by measurements of temporal variability in sap velocity). At both ADAS sites, the sensors were managed by multi-channel loggers synchronized for operation at the temporal resolution of 1 h that was the same as the resolution of AGTRs. As the AGTRs were much cheaper than ADAS, they have been used in larger numbers to increase spatial data coverage of groundwater table fluctuations that were directly used in the transient model calibration. In addition, one AGTR was used for flow measurement at the outlet of the Sardon River.

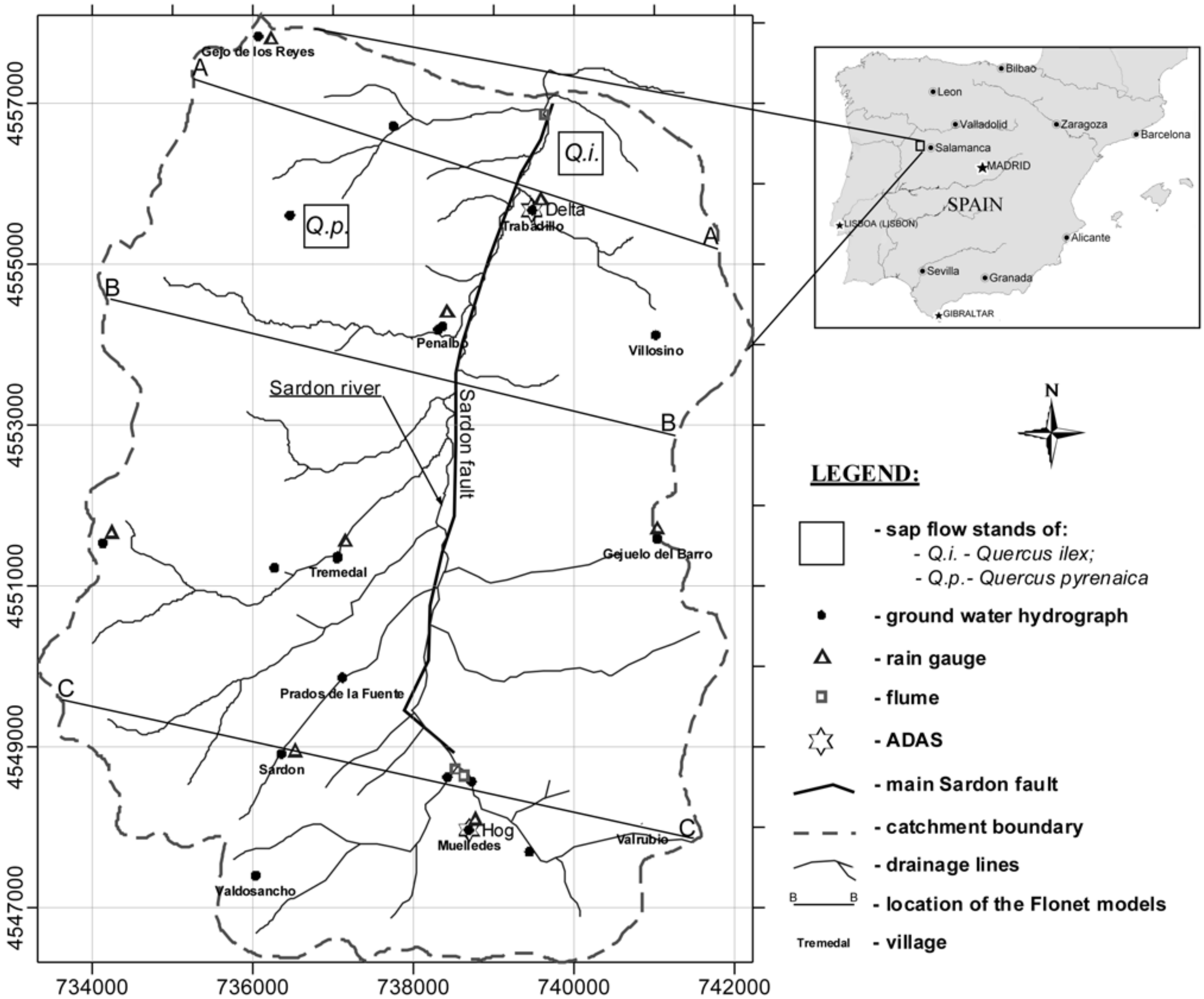

Fig. 2 The Sardon study area in Spain (after Lubczynski & Gurwin, 2005).

In the steady-state model calibration, the R and ET_g fluxes, estimated as long-term averages, were distributed spatially in a similar way to the procedure adopted in the Serowe case study and were optimized using the PEST code. In order to improve temporal flux data input (particularly recharge), and also to discretize the time scale of the transient MODFLOW simulations, the EARTH 1-D models (Van der Lee & Gehrels, 1990) were calibrated for each location with groundwater table monitoring data. In addition, sap velocity measurements (Granier, 1987) of tree transpiration were carried out for scaling of ET towards ET_g (Lubczynski & Gurwin, 2005). With such data, the spatio-temporal patterns of R and ET_g were adjusted and calibrated in fully-transient mode. In this procedure, the automated PEST calibration technique used in the steady-state mode was replaced by a manual trial and error method, which turned out to be more appropriate and more efficient. The result of the fully-transient model calibration is presented in Fig. 3.

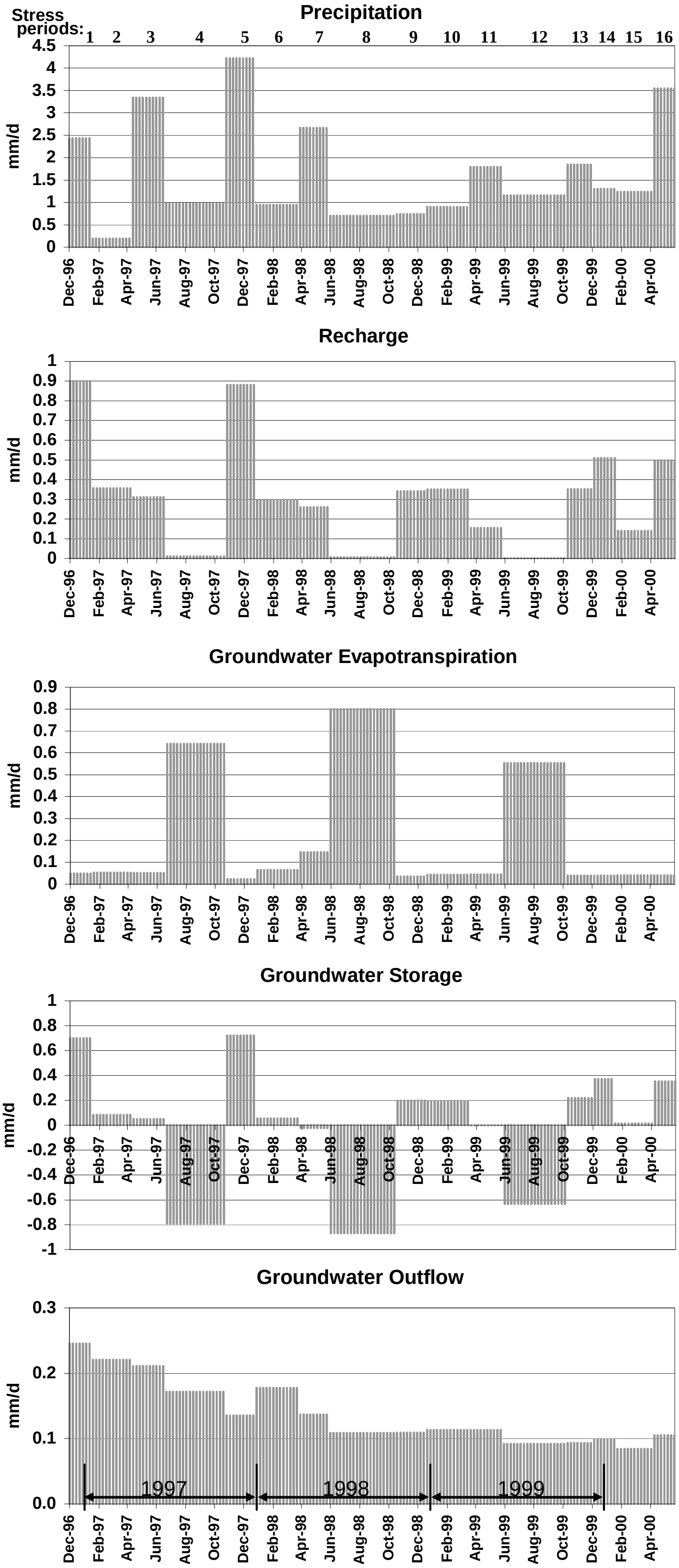

Fig. 3 Temporal variability of groundwater fluxes (after Lubczynski & Gurwin 2005).

DISCUSSION AND CONCLUSIONS

Sustainability of groundwater resources at a given location with given hydrogeological constraints is dependent upon anthropogenic constraints. An aquifer with low water demand compared with water availability, and without potential sources of contamination, can be considered as sustainable even if groundwater resources are low. This, for example, is the case in the Sardon area where water is supplied mainly from outside the Sardon watershed, population density is low and not increasing, and there is no industrial activity. In this area, the public groundwater use is so small (nearly natural conditions), that it was not even considered for model calibration. Moreover, the minor importance of groundwater as a drinking and irrigation water supply (other sources of water are available), has resulted in a lack of interest in groundwater resources and therefore also in a lack of a groundwater monitoring system. Such a system, however, was installed in this area (by ITC), although purely for research purpose, as a prerequisite for developing a fully-transient model. The main objective of that model was to study the spatio-temporal complexity of subsurface fluxes in natural, unbiased granite conditions and this objective was fulfilled (Fig. 3).

In contrast, the sustainability of groundwater resources of the Serowe area is a much more serious issue. In that area, recharge is very low and erratic, so the groundwater is the only source of drinking water supply and its use increases rapidly. The partially-transient model of the Serowe aquifer was set up and calibrated as a response to the increasing water demand and to the general Botswana policy of improving groundwater management by distributed numerical modelling. According to this policy, all strategic aquifers of the country are to be modelled. A number of the aquifers have already been modelled but unfortunately the majority were calibrated only in a less reliable steady-state mode, due to shortage of appropriate transient data. The Serowe partially-transient model was completed successfully because of the availability of the well-monitored drawdowns and corresponding well-documented well abstractions.

The dry, semiarid Serowe area with a deep groundwater table is characterized by erratic R and significant ET_g. Considering that in many locations in the Kalahari, the recharge event occurs once per several years and that ET_g is significant and relatively constant due to the presence of tree root water uptake, R_n is negative in most of the years considered as "dry". R_n is positive only in "wet" years with excessive rainfall, say once in 5 to 15 years, when recharge is in the order of several tens mm year^{-1}. The last such recharge event took place in 1999/2000 when large parts of Southern Africa were flooded. The "wet" recharge events are usually so "productive" that even with an erratic occurrence, they maintain positive long-term average R_n in the order of a few mm year^{-1}. With the large retention capacity of the buffering unsaturated zone, low lateral groundwater flow and significant tree root water uptake, a typical Kalahari groundwater table pattern is quite stable and comprises a gentle declining trend in dry years and distinct recoveries in "wet" years. These recoveries typically lag behind the corresponding rainfalls by a couple of months. With such unfavorable conditions of aquifer replenishment, the sustainability of groundwater resources is largely dependent upon the management of aquifer storage. Groundwater modelling is the best tool to perform such management because it is convenient and allows the design of optimal management solutions, provided the model is well calibrated in transient mode (partially or fully-transient). Transient models are more reliable in aquifer management than steady-state models because they are more constrained by temporal data and involve calibration of the storage coefficient, which is critical in storage prediction scenarios.

In the context of sustainability of groundwater resources (as in Botswana), the recharge-related renewability of the aquifers is the most important issue. In this regard, there has been an ongoing discussion in Botswana for many years as to whether the available groundwater resources are fossil or recharged from rainfall and, if so, at what rate. The solution of such problems requires long term monitoring of water fluxes and consequently the development and calibration of complex, fully-transient models (similar to the one presented for the Sardon study area). This requires a significant monitoring equipment investment in terms of finances and man-power, but is the only way to provide comprehensive answers. This challenging task has recently (in 2002) been undertaken by ITC and the Geological Survey of Botswana, by setting up the Kalahari Monitoring Project, in which the monitoring network appropriate for a fully transient model has been installed. In the next step, a fully-transient model of the Serowe study area will be developed and calibrated.

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