An overview of complex behaviour in the groundwater compartment of catchment systems and some implications for modelling and monitoring.

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Abstract
An understanding of non-causal relationships between processes in the air, soil and water compartments of the environment is fundamental to sustainable integrated management. This paper provides an overview of the groundwater sub-compartment and asserts that it exhibits many characteristics of a complex system, especially in relation to a wide range of non-linearities, although not all groundwater phenomena should be regarded as reflecting system complexity. Analysis of the groundwater compartment based on concepts such as emergence has been hindered by a long history of deterministic conceptualisation, while other aspects of complex systems such as self-organised criticality are difficult to investigate in the groundwater context due to problems of obtaining appropriate data. Despite this, conceptualising the groundwater compartment as a complex system would enable groundwater processes to be more fully integrated in a systems understanding of the environment. Some of the implications of complex behaviour for groundwater resource modelling and monitoring are briefly noted.

1. Introduction

The Natural Environment Research Council (NERC) have recognised, through their new strategy for the sustainable use of natural resources (NERC, 2007a), that there is a need to build an integrated understanding of interactions in the hydrosphere and biosphere. However, it is not yet known which, if any, of these interactions are non-causal, and so, by implication, we don't know if the patterns of interaction will repeat given the same starting conditions. An understanding of any non-causal relations is fundamental to the sustainable management of the environment, as we need to predict the effect of decisions, not least to mitigate and adapt to the impacts of environmental changes such as climate change.

With the increase in computing speed and memory, there has been a trend towards more integrated modelling of the water cycle facilitated by the linking of predominantly process-based models using software such as the MIKE suite of modelling tools (e.g. Li et al., 2007), HydroGeoSphere (e.g. Lemieux et al., 2008), and protocols such as OpenMI (Gregersen et al., 2007). But linking of process-based models may not always be appropriate if the phenomena arise from non-causal relationships or if critical dependencies or interactions are missed (Watkins and Freeman, 2008). Consequently, as described in the NERC strategy a 'new understanding using data derived using new network systems approaches and incorporating non-linearity and emergent behaviour and complexity science' (NERC, 2007b: section 3.3) needs to be developed in parallel with the existing environmental modelling approaches.

The concept of complexity has been used for to explain many aspects of the behaviour of systems in physics, biology, the social sciences and economics (Manson, 2001; Johnson, 2007) and it has been widely applied in some areas of the environmental sciences (Murray and Fonstad, 2007; Tetzlaff et al., 2008). Complexity concepts have been used by geologists in the context of understanding earthquake generation, fracture distributions, and the implications for hydrocarbon reservoir management (Heffer, 2005). Complexity concepts have only been used by the hydrogeological community in a limited way where work has been largely restricted to application to unsaturated zone flow and contaminant transport problems (Berkowitz and Balberg, 1993; Wood et al., 2001), and to date there has been no systematic overview of the application of complexity theory in the context of groundwater systems. This paper isn't intended to that systematic assessment or even a review of all work related to groundwater and complexity, instead the aim is to prompt discussion and investigation of the topic and to briefly note some implications for groundwater resource modelling and monitoring.

2. Characteristics of complex systems in the context of groundwater

It is difficult to point to a common set of concepts, terms or definitions for complexity, and there is no one, identifiable, ‘complexity theory’ (Manson, 2001; Frigg, 2003). Complex systems are perhaps best defined based on their characteristics. Table 1 lists and describes some commonly accepted features of complex systems and notes where the characteristic can be recognised in the groundwater compartment.

Table 1. A list of some commonly accepted features of complex systems and groundwater examples (Manson, 2001; Johnson, 2007; Brodu, 2008; Heylighen, 2008).

Feature	*Description*	*Groundwater example*
System is open	Complex systems exist in a thermodynamic gradient, dissipate energy and are typically far from an energetic equilibrium, but despite this they may show local dynamically stable patterns or phenomena	Groundwater systems are open, generally through continuous inputs of water via rainfall and outputs via evapotranspiration, discharge and abstraction
System boundaries	It is difficult to define or locate the boundaries of a complex system and it may require relatively arbitrary decisions by the observer. Complex systems are often nested and this may lead to difficulties in defining the boundaries Components of complex systems may themselves exhibit complex characteristics.	Many groundwater system boundaries are a matter of observer choice, and are often arbitrarily defined in terms of groundwater divides and flow direction, or in terms of the position of a zero-flux plane or other elements of the unsaturated zone. If any part of a groundwater system can be considered to be a complex system, then the presence of systems at different scales, for instance, local soil systems nested within shallow superficial aquifers that interact with deeper regional flow systems must inevitably demonstrate nested behaviour
Interactions between objects	Interactions between many linked objects or agents lead to a network that can share information. The rules of interaction are important and can lead to phenomena such as system memory and emergent behaviour	Commonly cited examples of agents in the complexity literature, such as traders in stock exchanges or termites, aren’t particularly useful analogies for many environmental systems. The components of the groundwater compartment include features of the soil, geology and hydrogeology that can be parameterised, for example: porosity, soil moisture and hydraulic conductivity, recharge, groundwater head, flux and quality, discharge, and abstraction
Feedback	Feedback happens when part of an output signal from a system is passed as an input to the system, affecting the dynamic behaviour of the system and modifying elements or components of the system.	The development of preferential flow paths in aquifers through dissolution is an example of a positive feedback, where increased flux increases permeability (Bloomfield et al., 2005), allowing further increases in flow. Equivalent negative feedbacks are associated with sediment clogging of pore spaces reducing flow and so reducing the potential for further clogging. Anthropogenic feedbacks may play an important role in groundwater systems, for instance where aquifers are actively managed to maintain a particular status
Memory and learning	Regularly occurring external relationships reinforce the growth of the same set of components and sub-systems in a complex system. This reinforcement can cause the system to appear to have a memory through the persistence of internal structures	Soil processes, groundwater levels, river stage in a groundwater dominated river and groundwater quality are all examples where a groundwater system can be thought of as having memory, in that the current state influences future response to external changes
Nonlinear behaviour and relationships	For a complex systems it is not possible to write a linear sum of independent components to solve for a nonlinear variable. Complex nonlinear systems are inherently unpredictable in that they have the characteristic that small perturbations in the system may cause large effects, a proportional effect or no effect at all (Phillips, 2006)	Groundwater systems demonstrate a wide range of nonlinear behaviours. These are discussed briefly later

Emergence Emergent phenomena arise out of nonlinear behaviour and simple interactions between numerous agents or objects Examples of emergent behaviour may include the spatio-temporal character of groundwater recharge, the development of secondary porosity systems, and the temporal variability of groundwater flow or quality delivered to a borehole, river, or spring

The system is dynamic Complex systems constantly change through the process of self-organisation, the property that allows systems to change their internal structure to more effectively interact with their environment. Some complex systems evolve towards a dynamically stable condition known as self-organised criticality (Bak, 1996; Frigg, 2003) with features that show spatial and or temporal scale invariance Although groundwater systems are undeniably dynamic over a wide range of time scales, self-organised criticality has yet to be demonstrated in the groundwater compartment.

3. Groundwater as a complex system

From Table 1 it is clear that the groundwater compartment exhibits many characteristics of a complex system. But how can conceptualising the groundwater compartment as a complex system add to our current understanding of phenomena such as groundwater flow? The origin of hydrogeology as a scientific discipline is often traced back to the work of Henry Darcy in the mid 1850s. Darcy showed empirically that specific discharge through a cylinder filled with sand is directly proportional to the head gradient across the cylinder and the hydraulic conductivity of the sand. Since then, hydrogeology as a quantitative science can be regarded as having been built to a large extent on empirical observation, the laws of fluid mechanics, and a strongly deterministic view of the groundwater compartment. Conceptual models and associated analytical approaches, such as those of Toth (1963), and widely used numerical codes, such as MODFLOW that solve the groundwater flow equations, have been used to satisfactorily understand, simulate, and predict many aspects of groundwater flow.

For example, based on continuum assumptions, Toth (1963) demonstrated how steady-state groundwater flow fields develop in response to an assumed relationship between topography and the groundwater surface. His conceptualisation of regional groundwater flow has proved particularly robust and has been regularly used since. It has recently been used in the context of studies of groundwater-surface water interaction (Dahl et al., 2007; Jolly et al., 2008). Throughout their detailed review of the role of groundwater in supporting arid zone ecosystems, Jolly et al. (2008) repeatedly emphasise the dynamic nature of groundwater systems, the interaction between groundwater and water in the hyporheic zone, and the diversity of potential flow paths between groundwater and surface water. However, they still used a schematic illustration of Toth's steady-state model to characterise groundwater flow in relation to the hyporheic zone. Why was this? Probably because there is currently no suitable alternative conceptual framework that adequately captures the dynamic, heterogeneous, highly-non-linear nature of groundwater flow in and near the hyporheic zone.

Both Darcy's Law and Toth's conceptualisation of groundwater flow are based on continuum assumptions regarding porosity and hydraulic conductivity fields and assume macroscopic flow at or above a representative elementary volume (REV). This works well for a wide range of typical groundwater problems such as modelling groundwater levels or flow at the regional or catchment scale, averaged over relatively coarse time steps (months or weeks). However, for some groundwater phenomena, such as movement of contaminants, the concept of an REV is not so useful, since processes at the sub-REV scale may affect the macroscopic variable of interest. For instance, dispersion is caused by the sub-REV variations in water velocity, and the magnitude of the dispersion coefficient varies with the size of the REV (Gelhar et al, 1992). The underlying, often un-stated, assumption of an REV can cause difficulties when deterministic groundwater models are developed at one 'scale' and then used at a finer scale, when the model outputs may be an average over a larger volume than the measurement to which it is compared.

Modern monitoring techniques can now provide much more detailed information about temporal variability and potential non-linearities in river flow and stage and in groundwater levels. For example, Figure 1 shows groundwater level data for a borehole in the Chalk aquifer near the River Lambourn, in the Chilterns. It shows that weekly observations adequately describe the variation in groundwater levels at the site at the order of 10s of centimetres over the observation period. However, hourly observations show a much more complicated (although not necessarily complex) structure in the groundwater level time series.

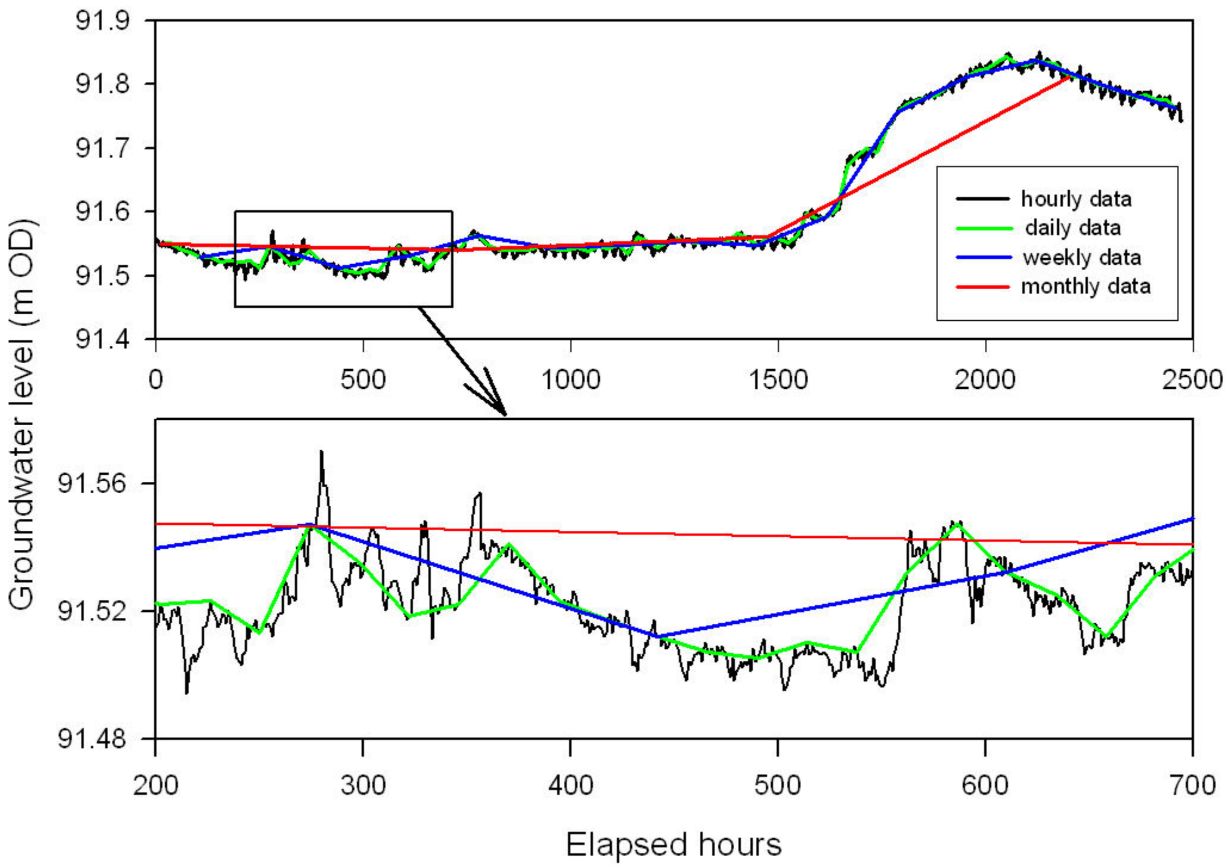

Figure 1. Illustration of the variation in the degree of information in groundwater level data as a function of measurement resolution. The lower graph is an enlarged section of the upper graph.

It is very difficult to adequately represent these more complicated groundwater level signals by models such as those of Toth with their assumptions of infinite uniform structure. Smaller scale, process-based models that account for natural heterogeneity can be used to explain some variation in groundwater levels. For example, the weak diurnal fluctuations in groundwater levels seen in Figure 1 might be explained in terms of a simple causal relationship between phreatophytic consumption and daily lowering of the water table near a river, but this still doesn't account for all the observed variability. In any case, it can never be certain that the postulated mechanism (in this case transpiration) is the sole cause of the effect being described. Complexity techniques can provide insights into groundwater-surface water interactions that process based models cannot provide when the phenomena examined are not described by simple causal relationships.

As noted in Table 1, a number of non-linear phenomena can be identified in the groundwater compartment. Non-linearity gives rise to the possibility of complex behaviour, though not all non-linear systems are complex. Non-linearity in a system has three major implications: the system may exhibit sensitivity to initial conditions, it may exhibit emergent properties, and the overall large-scale, long-term behaviour of the system may not be predictable from small-scale, short-term processes (Phillips, 2006). Sources of non-linearity in the groundwater compartment include spatial heterogeneity (land-use, soil and rock properties), critical thresholds (saturation state, zero flux plane, river or spring flow or absence of flow, and hydrogeochemical thresholds such as the redox boundary), and external forcing factors (climate factors, anthropogenic impacts, river and sea base levels and tectonics).

It is perhaps inevitable, given the range of non-linearities in the groundwater compartment that groundwater systems should demonstrate emergent behaviour and potentially self-ordered criticality. However, there are few documented studies in the peer-reviewed literature where groundwater phenomena are explicitly presented as being emergent phenomena, e.g. the spatio-temporal distribution of groundwater recharge (Bracken and Croke, 2007; Saco et al, 2007; Kollet and Maxwell, 2008), or the development of secondary porosity systems (Bloomfield et al., 2005). In addition, self-organised criticality has yet to be demonstrated in the groundwater compartment.

4. Some approaches to analysing complex systems

Once it is accepted that the groundwater compartment of the hydrosphere represents a complex system it becomes apparent that the traditional (deterministic) approach used in conventional hydrogeology is unlikely to provide usable ‘simple’ solutions. In this context, ‘simple’ is used to describe an approach which is readily transferable from one groundwater body to another, or from an expert hydrogeologist to a generalist manager or policy maker. Deterministic modelling, by its very nature, requires that the relationships between the agents are well understood, can be quantified and that the relevant parameter values are known in sufficient detail (both spatially and temporally). Whilst many of the processes can be described by well known (partial differential) equations it is not always clear whether these equations are valid for the full range of parameters and conditions which occur in nature. For example, most work on the unsaturated zone is carried out by solving Richard’s equation. However, this equation takes no account of the air and water vapour that is present in the unsaturated zone. Under some conditions, for instance that of intense rainfall or rapid changes in atmospheric pressure, the presence of the gaseous phase can be have a significant impact on the recharge rate and the position of the water table. This introduces non-linearities into the system which are difficult to model deterministically.

From this it follows that a different approach may be required to quantify some of the more important inter-relationships within the groundwater compartment. Little work has been carried out to date using systems analysis techniques on groundwater problems, but several techniques show some promise. These include spectral analysis and cellular automata. Percolation theory examines the clustering of connections that form in lattice networks. Statistical relationships have been developed to describe these connections and there is an obvious parallel with the pore-scale detail of flow in porous media. Cellular automata are a class of mathematical model that seem to capture the complex behaviour found in many natural systems as a result of the interaction of a number agents which follow relatively simple rules. From their study it is possible to abstract general laws that encompass complex and self-organising systems.

Commonly in hydrological problems cellular automata ‘rules’ are solved using simulations based on discrete approximations of continuum behaviour. The rules applied to the individual cells in order to describe fluid behaviour preserve mass and momentum and regular grids can be shown to correspond to the standard Navier-Stokes equation for fluid flow. Goa and Sharma (1994) developed a lattice gas model that can be used to obtain a representative permeability for a heterogeneous porous medium with irregular boundaries. These models are not easy to develop, but their nature is such that the inherent complexities of the system are incorporated in the basic ‘rules’.

Spectral analysis of time-series data is an established method of investigation for surface water systems (Li and Zhang 2007, Zhang and Schilling, 2004, Feng et al., 2004, Zhang and Li, 2005, 2006). However, little work has been carried out in respect of groundwater data. Spectral analysis techniques, require long data sets, which either means a long time with infrequent data or a shorter time but with more frequent data. Feng et al. (2004) compare 3 year daily data and 17 year weekly data sets and conclude that more frequent data is needed to distinguish rapid dynamics. They also conclude that low frequency data combined with high frequency data during storm events can cause spectral artefacts which are difficult to remove. As an example of how important it is that the real, complex nature of groundwater flow is considered, Giudici and Vassena (2008) use spectral analysis to show that the information contained in groundwater hydrographs is not sufficient to determine the hydraulic conductivity field in the aquifer.

5. Some implications for modelling and monitoring

5.1 Modelling

Early analogue models were superseded by numerical equivalents, most notably with the development of MODFLOW by the USGS. At the heart of these models is a uniform aquifer block into and out of which water flows according to the heads in the adjoining blocks. Calibration and validation is by comparison with water level measurements at various locations and by flow output in the simply modelled rivers. The conceptual models that have been represented by these numerical models are developed by consideration of the geology and recharge patterns. The models can generally only be calibrated by comparison with measured groundwater heads. This is despite the fact that in most cases the groundwater flow in the aquifer is the property that is of real interest. An example of a groundwater hydrograph from a state-of-the-art groundwater model is shown in Figure 2. When this is compared with the real data in Figure 1 it can be seen that much of the complexity of the flow system represented by the hydrograph has been missed.

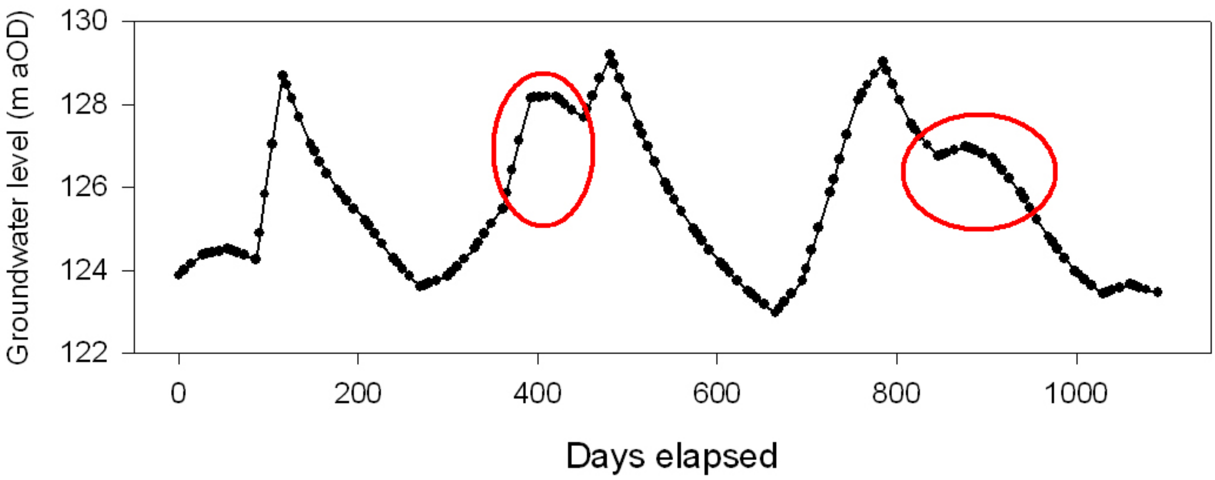

Figure 2. Modelled approximately weekly groundwater levels at an observation borehole in the Chalk aquifer of the Berkshire Downs, UK for a three year period. An annual cycle and the buffered effects of seasonal recharge anomalies (circled in red) are apparent, but finer scale complexity is missing.

An acceptance that the groundwater system is inherently complex (rather than just complicated) should mean that less is expected of deterministic groundwater models. At present regional groundwater models are usually developed for specific purpose, but the investment that is involved in developing a well calibrated model means that it will be used for other predictions. Systems analysis techniques which are applied to complex systems could be used to decide under which circumstances this is an appropriate use of a model and when a new model is required.

5.2 Monitoring

Groundwater monitoring is increasingly focused on addressing regulatory issues, monitoring water quality for compliance with statutes controlling potable water quality and environmental issues (Ward et al, 2004). Economic constraints can lead to a prioritization of monitoring onto individual sites which may demonstrate whether constraints are met, or not, but at the expense of loss of detail which may be key to understanding the detail of aquifer behaviour. Monitoring designed to gather information to show that groundwater systems act as complex systems may need a different focus.

A key implication of the concepts of complexity discussed above, when applied to groundwater monitoring, is a need for observations which simultaneously sample the different elements of the water cycle. Co-located measurements of meteorological inputs, soil moisture, runoff and groundwater level will be key to establishing the complex feedbacks and non-linear interactions between components (Kollet and Maxwell 2008).

Examination of groundwater systems for evidence of self-ordered criticality has been hampered by the relatively infrequent sampling interval of time series, such as piezometric level and spring discharge that has been considered adequate for aquifer management. Long time series with sampling intervals of less than 1 hour are relatively rare in groundwater datasets, with decisions on monitoring frequencies influenced by the relatively slow response of many aquifer systems and a desire to minimize the cost of data collection and the burden of subsequent data handling. Modern data gathering techniques open up the possibility of collecting data at very high spatial resolution over sufficiently long periods of time to provide the data frequency and sampling regularity required to apply frequency based spectral analysis, and explore for self-organized criticality. The benefit of such an approach has been demonstrated for karst springs, where multifractal analyses evidence scale dependent behaviour (Labat et al, 2002).

6. Summary

There is significant potential for the application of a range of systems analysis techniques to understand complex groundwater behaviours, and insights gained from this approach would complement findings from more commonly applied deterministic approaches. However, more high quality groundwater data, relatable to other environmental parameters will be needed.

Acknowledgements

Thanks to Chris Jackson for his review comments. This paper is published with the permission of the Executive Director of the British Geological Survey (NERC)

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