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Catchment water quality: the inconvenient but necessary truth of fractal functioning

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This commentary concerns catchment water quality functioning in relation to environmental impact assessment, with a view to proposing that much more emphasis be placed on issues of within-catchment complexity and its manifestation within stream water chemistry: fractal dynamics. The commentary is based, with closure, on my long-term research. Encouragement is given for new avenues to be pursued, including dealing with the complexities of within-stream biological functioning, and their integration into environmental legislation.

Understanding of catchment water quality functioning has grown immensely in the Earth Sciences and hydrogeochemical research arenas in relation to process understanding (weathering, ion exchange, hydrogeochemical typology, etc.: Drever, 1997) and thermodynamic modelling (Appello and Postma, 2006). Indeed, since the early 1980s the application of hydrogeochemical process understanding has led to the development of modelling approaches critical for describing and assessing the impacts of pollution and the potential means of remediation (Christophersen et al., 1982; Cosby et al., 1985; Whitehead et al., 2002). Paralleling this has been the growth of long-term monitoring programmes that describe the changes in water quality with environmental and pollution change (Stoddard et al., 1999) while picking up features that conventional view for their time missed (e.g. dissolved organic carbon and iron increases with acidification reversal: Evans et al., 2005; Neal et al., 2008).

Viewing catchments conceptually within simple accepted frameworks provides a key foundation for understanding how such “systems work” and in communicating science to students and non-specialist communities alike. It provides a valuable means of discourse within and across the spectrum of scientific, environmental and social communities. For example, within the “acid rain” debate, hydrochemical stirred-tank box models have commendably been widely used and generally adopted. They describe long-term changes in chemistry and short-term dynamics of the mixing of soil- and ground-water, with relatively simple hydrology, ion-exchange, solubility and weathering processes taking place that can be represented mathematically based on theory and laboratory measurements. They also provide excellent “learning tools” for describing relatively easily how systems might respond to change. In general, the field and modelling programmes have gone hand-in-hand, with great respect and admiration across and between the research communities, even if in detail there are strong differences. Nonetheless, there are problems over the extent to which conventional understanding of catchment water quality functioning based on generalised and accumulated theory compares with actual field measurement. For example, even just by looking at the panorama of many a catchment, there is much variability in topography and it is unreasonable to expect that water drains uniformly from rainfall via the soil and the bedrock to the stream (Figure 1, 2). Correspondingly, field measurements reveal a complex hydrological and chemical picture (Mulder et al, 1991; Taugbol and Neal, 1994; Neal et al., 1997a): both soil- and ground-water flow pathways can interact and there is really no simple “end-member composition” to define each typology (Hill and Neal, 1997; Neal et al., 1997b). However, issues of complexity have a low profile in relation to environmental management modelling. This is fully understandable as just stating issues of complexity have limited value without alternative solutions and guidelines for handling complexity. Generally, there are insufficient measurements taken to show the true degree of variability and the value of “more data” beyond the level of “pure research” is not clear for the high outlay required. In terms of modelling there are companion difficulties. For example, increasing the complexity will almost inevitably increase the number of parameters used to mathematically describe and model the system and there remain issues of independent validation and what constitutes negation.

There is proactive debate over how water and chemicals move through catchments and dealing with issues of complexity (McDonnell et al., 2007; Tetzlaff et al., 2008). Environmental tracers have clearly been critically important across a spectrum of catchment typologies. Their key value continues for instance in assessing sewage and agricultural sources of nutrients (Neal et al., 2010a) and indicating long-term storage along river reaches (Neal et al., 2010b). However, a fundamental development with regards to catchment water quality research has been the recognition that stream-water signals have a fractal structure which applies to both chemically conservative tracers of atmospheric inputs and, chemically reactive species within-catchments (Kirchner et al., 2000; Heathwaite and Harris, 2005; Godsey et al., 2010; Kirchner and Neal, 2013). By this, the issue of complex and erratic within-catchment variability transposes into a physically based mathematical framework that can be tested (Kirchner et al., 2001; Kirchner and Neal, 2013).

So, what is the inconvenient but necessary truth concerning the fractal functioning of catchments that the new drivers in hydrology and the new measurements in water quality dynamics are revealing?

1. Fractal functioning of water quality is not an oddity but “a fact of life” that is widely applicable but rarely recognised due to (a) lack of data, (b) the difficulties of tackling complexity within environmental models and (c) communicating issues of fractal processing in a generalised proactive and useful way.
2. Fractal processing of water quality should really be expected within catchments due to the “longitudinal” shape of catchments and the heterogeneity of the landscape, soils and groundwater, with the huge significance of hydrology linked to complex within-catchment transfer of water and chemicals to the stream.

3. The scatter in water quality data largely represents true observations when high quality sampling and chemical analysis is undertaken. Issues of data scatter and degree of fit then lies with the model conceived and the underlying assumptions that generate the statistical test.
4. Within the detailed dynamics of stream water time series and with comparison for rainfall inputs, there are important but cryptic clues to hydrogeochemical and hydrological controls within catchments. However, in order to recognise the inferences from the signals, a huge number of measurements need to be taken and this is costly in terms of longevity, intensity and all manner of resources. Nonetheless, “If we want to understand the full symphony of catchment hydrochemical behaviour, then we need to be able to hear every note, but under different hydrometeorological or pollution climates the notes may follow a different score” (Kirchner et al., 2004; Neal et al., 2012).
5. Commonly used equations depicting the major hydrogeochemical controls may not be useable employing “lumped” modelling procedures as the formulae do not strictly apply when “lumped” averages are considered as neither the equilibrium constant nor the power term need fit the thermodynamic relationship for any curvilinear relationship as, for example, average values plot to the convex side of any theoretical curve (Neal, 1996). Further, recognition is required of the extent to which the “thermodynamics” within the models actually translate to fitting terms given factors such as latitude in solubility between crystalline and amorphous forms of the same mineral or group of minerals and the need to match field data such as exchangeable cations with computed average soilwater chemistry. Nonetheless, in trying to obtain a more exact relationship, more elaborate heterogeneous models are needed. In turn, however, unproven assumptions are still required while there are an increased number of fitting parameters that cannot be independently assessed.
6. With fractal processing, abnormally long recovery time from pollution incidences may occur (Kirchner et al., 2000). This is relevant to how quickly systems react to change and is of major relevance to water quality management and issues such as socioeconomics, legislation frameworks and the law. It is also critical in terms of the funding of science as driven by policy where science management guidelines may not be achievable in terms of reliable outcomes, irrespective of the pressures from political and legislative drivers.

For me, several needs stand out.

1. The need to make fuller use of long-standing catchment studies covering decades of monitoring coupled with high-resolution data (Neal et al., 2012, 2013) so as to allow spectral and other analysis across a wide range of frequencies (Halliday et al., 2012; Kirchner and Neal, 2013). Within this, there is the need for full disclosure of data on water-quality with hydrology in relation to rainfall, runoff and internal catchment functioning. Further, there is the need for processed data that are rigorously quality control checked coupled with raw data and metadata that explain the reasons for exclusion of data in order to provide transparency and a level playing field for modelling (Neal et al., 2012, 2013).
2. There remains a lack of sustained high resolution water quality data that pick up the complex dynamics that occur within the stream and truly challenge views on how catchment systems function (Neal et al., 2012).
3. There is a need to model elements of contrasting hydrogeochemical character and source. This will provide a rigour of testing that will tax many environmental impact models and provide an independent means of validation. For example, it is extremely difficult to simultaneously describe inert atmospherically derived components and within-catchment hydrochemically active

components without introducing too many untested fitting parameters (Christophersen and Neal, 1990).

4. There is a need to directly measure water storage and to assess critical water pathways in order to compare modelling results with independent physical measurements. In this context, the relative importance of “passive water stores” needs to be established. For water quality, there are important questions as to how chemicals transfer between active and passive water within catchments. Indeed, transpiration may result in water movement towards the plant root, resulting in “Donnan membrane processes” that attenuate both cations and anions even if there is no ion exchanger within the system. Such a process will impact on issues such as passive and other storage volumes as assessed using tracers.
5. The use of terms such as “soilwater” and “groundwater” is notional in catchment studies and a more refined approach is ultimately required. Indeed, the endmembers may well be characterised by compositions within fine pores that are rarely measured. The catchment may then be defined in terms of “matrix soilwater” and “matrix groundwater” endmembers plus a “macropore network” that spans within and across the soil- and ground-water zones.
6. There is a need to view modelled prediction of change in terms of simulations for a wide variety of models that are constrained to fitting present-day conditions. This moves away from the norm of individual modelling approaches where uncertainty of prediction is expressed in terms of varying the parameter space, to one more akin to climate change modelling and the use of assemblages of models.
7. A critical advance may be to use “virtual catchment” simulations (Weiler and McDonnell, 2004) that link observation, field experience and theory to test model structures, isolate key pathways over a range of environmental conditions and provide a much needed learning tool.
8. There is a need for more refined and consistent approaches to issues of structural and other forms of uncertainty with clear conveyance to decision makers. Nonetheless, the tensions concerning negation and validation of concepts and model outcomes within contexts such as necessity, convention and structural change, need continued and proactive debate.
9. I hope that the extensive long-term and high-resolution water quality data for the Afon Hafren catchment in mid-Wales provides a good starting point for examining many of the water quality issues highlighted here. The data are freely available (Neal et al., 2013), as is a wealth of relevant soils, geomorphological and hydrological information, at the GEH Information Gateway (http://www.ceh.ac.uk/sci_programmes/plynlimondatasets.html)!

The bringing together of process understanding with within-catchment complexity represents a major challenge for both pure and applied aspects of the aquatic, Earth and environmental sciences. Never has there been a greater need to bring together the “measurers” and the “modellers” in an open research climate, with developments in community research in hydrology providing an important marker. Education is required to insert issues of complexity within the curricula of these sciences. The word “fractal” needs to enter the vocabulary much more within the scientific discourse and it must be linked to wider environmental usage when dealing with the physics and chemistry of catchments. A critical challenge will be in the constraining of environmental policy to what is actually achievable, with the associated caveats over the overall uncertainty, rather than what one would wish to happen.

Finally, the aim of dealing with pollution issues and remediation strategies must lie in goals connected with biological improvement for the environment. This means that water quality issues must translate-into and be subservient-to ecosystem functioning and biodiversity, with major issues of feedback mechanisms and complex interactions, where highly dynamic and uncertain outcomes are to be expected (Brown et al., 2002; Marques et al., 2003; Harris and Heathwaite, 2012; Page et al., 2012). Introducing biology raises the bar for reliable predictions of biological response to physical and chemical change, as the issues of scale, boundary conditions and breadth of measurement are magnified. Predicting biological change to physical and chemical drivers also raises the bar with respect to environmental management: portraying overall uncertainty in a meaningful and consistent way at a level understandable by environmental managers and legislators and for setting clearly achievable goals within the context of risk. This critically impinges on the key goal of environmental legislation with appropriate rather than well-meaning but misdirected socioeconomic cost. There is a long and scientifically exciting but challenging way to go.

Figures

Figure 1. The upper Hafren catchment. The top-left plate illustrates a variable topography: it is inconceivable that rain falling onto the catchment will pass uniformly to the stream. The top-right plate shows a dense network of conifers: the vegetation critically affects the soil profile with a wide and shallow distribution of roots. Indeed, part of the water and chemical flux is upwards through the soil profile due to a combination of transpiration via the root and wind-blow that leads to a “rocking motion” of the flat root structure and a pumping mechanism that transfers water upwards. At times when the trees reach maturity, the upward movement can result in small intermittent water fountains at the soil surface and the upward transfer to the soil surface of small pebbles. The lower-left plate illustrates that soils are thin (typically 1 m and less) and that there are fracture zones below the soil profile where shallow groundwater is transported. A major point with these plates is that with catchments of kilometre or more scales but with soil and groundwater of a few metres depth, the main transport of water is horizontal relative to the soil and groundwater profile. The bottom-right plate illustrates riparian zone inputs of water at periods of baseflow. This chemistry can be very distinct from normal soil- and ground-water. In this case, the seepage waters are reducing and enriched in ferrous iron that is oxidised by the air to generate ferric ions and precipitation of amorphous $Fe(OH)_3$: both the riparian and hyporheic areas may be hydrochemically important under baseflow conditions.

Figure 2. The heterogeneous transfer of water at Plynlimon through the soils (left hand plate: photograph kindly provided by Brian Reynolds) and groundwater (right hand plate). In the case of the soils, macropore flow is widespread and manifest as natural soil pipes. The groundwater issue is illustrated by a gushing artesian borehole located next to the Nant Tanllwyth stream. The introduction of the borehole permanently changed the groundwater level in a borehole at the other side of the stream. Artesian boreholes occur at just two locations within our network and groundwater levels vary substantially and erratically across the catchment. This illustrates the dominance of groundwater routing via complex fracture pathways.

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