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Are groundwater nitrate concentrations reaching a turning point in some chalk aquifers?

J.T. Smith [a,*], R.T. Clarke [b], M.J. Bowes [c]

[a] School of Earth and Environmental Sciences, Burnaby Building, University of Portsmouth, Portsmouth, PO1 3QL, UK
[b] School of Conservation Sciences, Bournemouth University,Talbot Campus, Poole, Dorset, BH12 5BB, UK
[c] Centre for Ecology and Hydrology, Maclean Building, Crowmarsh Gifford, Wallingford, Oxfordshire, OX10 8BB, UK

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ABSTRACT

In past decades, there has been much scientific effort dedicated to the development of models for simulation and prediction of nitrate concentrations in groundwaters, but producing truly predictive models remains a major challenge. A time-series model, based on long-term variations in nitrate fertiliser applications and average rainfall, was calibrated against measured concentrations from five boreholes in the River Frome catchment of Southern England for the period spanning from the mid-1970s to 2003. The model was then used to "blind" predict nitrate concentrations for the period 2003–2008. To our knowledge, this represents the first "blind" test of a model for predicting nitrate concentrations in aquifers. It was found that relatively simple time-series models could explain and predict a significant proportion of the variation in nitrate concentrations in these groundwater abstraction points ($R^2 = 0.6–0.9$ and mean absolute prediction errors 4.2–8.0%). The study highlighted some important limitations and uncertainties in this, and other modelling approaches, in particular regarding long-term nitrate fertiliser application data. In three of the five groundwater abstraction points (Hooke, Empool and Eagle Lodge), once seasonal variations were accounted for, there was a recent change in the generally upward historical trend in nitrate concentrations. This may be an early indication of a response to levelling-off (and declining) fertiliser application rates since the 1980s. There was no clear indication of trend change at the Forston and Winterbourne Abbas sites nor in the trend of nitrate concentration in the River Frome itself from 1965 to 2008.

1. Introduction

Historically rising nitrate concentrations in rivers and groundwaters in the south of England, as a result of increasing fertiliser applications, are well documented (for example, Heathwaite et al., 1996; Stuart et al., 2007). In many cases, groundwater nitrate concentrations are currently approaching, or exceeding, the 11.3-mg $NO_3–N\ l^{-1}$ Drinking Water Standard as discussed by, for example, Jackson et al. (2008). Understandably, therefore, in past decades there has been much scientific effort dedicated to the development of models for simulation and prediction of nitrate concentrations in groundwaters. Owing to the large number of hydrological, soil, land use and aquifer processes involved in the transfer of nitrate from fertiliser applications to extracted groundwater, the development of truly predictive models remains a major challenge.

In an evaluation of nitrate transport in chalk catchments, Jackson et al. (2008) provide a very useful summary of types of model applied to this problem based on earlier work by Wheater et al. (1993). They distinguish – with increasing levels of representation of physical processes – between "metric", "conceptual" and "physics-based" models. As defined by Jackson et al. (2008), metric models are "essentially statistical relationships between existing input and output data sets with rudimentary, if any, physical basis"; conceptual models "involve specifying a model structure *a priori*, normally on the basis of a system of conceptual stores"; and physics-based models "seek to capture a system's response by incorporating significant processes through fundamental physical equations". The full range of models, from "metric" statistical analyses of data (for example, Roy et al. (2007)) to "physics-based" models such as the INCA model (Mathias et al., 2007; Wade et al., 2002; Whitehead et al., 1998) are currently being used for nitrate research and management.

Although very useful, such categorisation of models is – in one sense – meaningless, since all models are neither more nor less than mathematical constructs designed to quantify the logical consequences of scientific hypotheses. Models cannot be evaluated by (necessarily) ad hoc categorisation, only by the comparative testing of their predictions against empirical data (Popper, 1963). It is, however, clear that different modelling "philosophies" lead to different levels of model complexity. Increasing complexity (the "reductionist" or "mechanistic" approach: detailed modelling of processes; greater

* Corresponding author. Tel.: +44 2392 842416.
E-mail address: jim.smith@port.ac.uk (J.T. Smith).

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spatial and/or temporal resolution) has both advantages and disadvantages. The advantage is that more physically based models – *if* they can accurately simulate the real physical processes in an environmental system – may be better able to predict (extrapolate) real-world events which are temporally, spatially or environmentally outside the scope of the model calibration. Less physically based models may also achieve this, but because the process representation is less detailed, the basis for extrapolation is likely to be cruder (though it cannot be concluded, on this basis alone, that it will be any less successful).

Whilst having obvious advantages, physically based models can suffer from two well-known problems. Firstly, they tend to be data intensive, often requiring detailed site-specific information on the physical processes they incorporate: this may not always be available, particularly for large-scale applications. In an evaluation of models applied to the radioactive contamination of catchments after the Chernobyl accident, Monte et al. (2004)) concluded that, in the context of post-accident prediction, "the inclusion of more processes in a complex model does not guarantee greater accuracy of model performance. Indeed the overall uncertainty of the model is strongly influenced by the uncertainty of large numbers of model parameters whose values cannot be known with a sufficient accuracy at site-specific level". This can make extrapolation to other sites very difficult.

A second problem, also related to information availability, is that physically based models may in practice be (unavoidably) over-parameterised with respect to the limited available test empirical data as discussed by, for example, McIntyre et al. (2005). This leads to difficulties in testing and determining parameter values for these models. Parameter estimates are often statistically highly correlated, leading to problems of equifinality of model outcomes: no single "optimal" model can be found (Beven, 2006). Insufficient appropriate data makes it difficult not only to calibrate model process parameters, but also to compare the predictive ability of different models for scenarios involving spatial and/or temporal extrapolation. It should be noted that the equifinality problem also applies to other model types, but is seen as less of a problem, since they do not aim for an accurate simulation of specific processes.

So, no modelling approach can be said, *a priori*, to be better than any other and (if the aim is prediction rather than "mechanistic" understanding) we must, where possible, rely on a subjective evaluation of utility (is the model "fit for purpose"?) coupled with Popper's (1963) critical test of scientific hypotheses (models): the falsification of predictions against empirical data. It is with this in mind that we here present a preliminary predictive test of time-series models for nitrate concentrations in groundwaters. The approach is analogous to unit hydrograph based models for river flow rate and hence could be said to be at the less "physically based" end of the nitrate modelling spectrum of Jackson et al. (2008). Our purposes are to test the extent to which such models can make useful predictions in this context and to assess the important limitations to this approach. We further hope that this exercise will provide a predictive benchmark against which to evaluate other – possibly better – models and modelling approaches. To our knowledge, this represents the first "blind" test of a model for predicting nitrate concentrations in aquifers.

1.1. Study area

The River Frome catchment, Dorset, UK, drains an area of 414 km^2, draining an area from the village of Evershot (ST 047576) on the Dorset–Somerset border, to Poole Harbour (Fig. 1). The dominant bedrock geology for the majority of the catchment is Cretaceous Chalk, with areas of Cretaceous Greensand in the River Hooke sub-catchment and fluvial sands and gravels in the lower reaches of the Frome. The land use within the catchment is primarily agricultural, mainly grassland and cereals. The town of Dorchester, with a population of ca. 27,000, is the only large town in the catchment. More detailed descriptions of the land use (Hanrahan et al., 2001), river chemistry (Bowes et al., 2009) and geology (Arnott et al., 2009) are given elsewhere.

2. Methods

2.1. Data for model calibration and testing

Groundwater nitrate concentrations were measured by Wessex Water Plc in public supply boreholes extracting groundwater from five sub-catchments within the catchment of the River Frome at various intervals during the period 1976–2008 (Table 1 and Fig. 1). Up to the mid-1990s, sampling was relatively infrequent (typically several samples per year), but from the mid-1990s onwards, samples

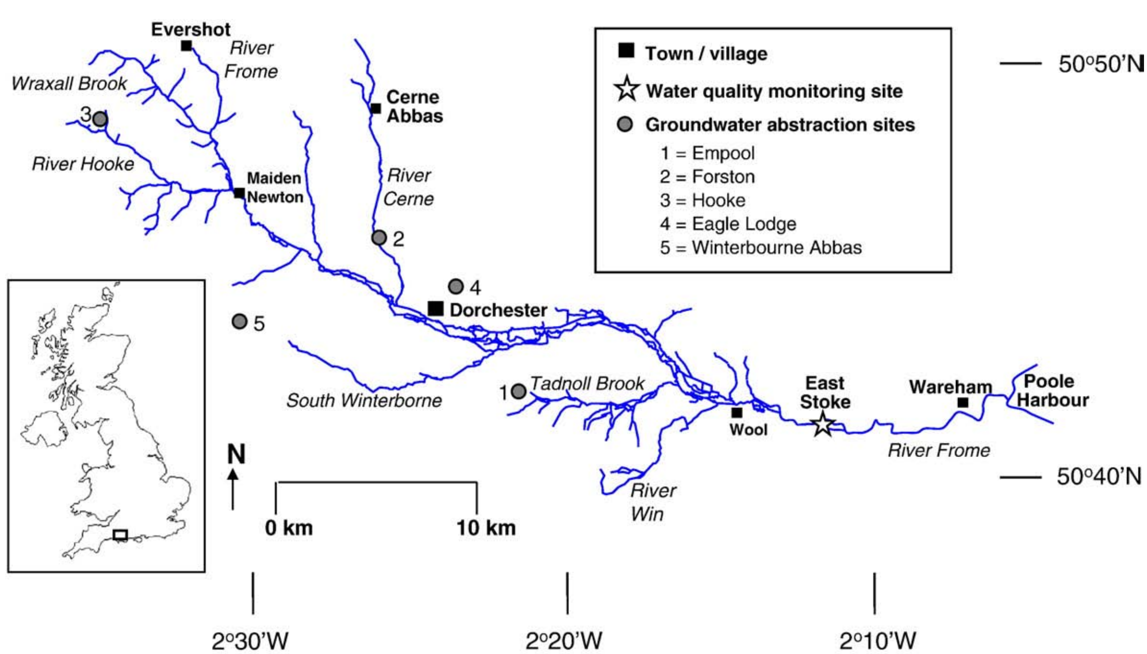

Fig. 1. Map of the Frome catchment showing the sites of groundwater abstraction and river water quality monitoring.