Towards an Effective Complexity for Modelling Nutrient Generation from Small Catchments

Adams, G.A. [1]

[1] Integrated Catchment Assessment and Management Centre, Fenner School of Environment and Society, and the Department of Mathematics, The Australian National University, Canberra, Australian Capital Territory.
Email: geoffrey.adams@anu.edu.au

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EXTENDED ABSTRACT

Models for predicting the water quality of runoff from rural catchments generally fall into one of two types. They can be either too simple to allow reliable prediction of changes to nutrient concentrations or loads arising from land use change. Or they can be too complex, with model and parameter uncertainty limiting the extrapolative ability of the models, often accompanied by extensive data requirements that restrict their practical applicability.

The problematic characteristics of such overly parsimonious and overly complex model types are reviewed, and a number of models that encompass the range of complexities of nutrient generation models briefly are described or identified.

Finally, the approach in developing a model structure of appropriate complexity for predicting the effects of changes in catchment conditions on nutrient generation is broadly described and success criteria indicated. The paper points out that the adopted complexity needs to take into account the specific model purpose, in particular the output of interest (concentration or load) and its form (average, time series, frequency distribution or extreme events).

1. INTRODUCTION

This paper describes the difficulties in selecting the most effective model complexity for representing nutrient exports from rural catchments. Existing rural-catchment water quality models are generally either:

-too simple to allow reliable prediction of changes to nutrient outputs arising from land use change on rural catchments with a range of soil types, geographical conditions and hydrological conditions; or
-too complex, with model and parameter uncertainty limiting the extrapolative ability of the models, and/or extensive data requirements restricting the practical applicability of the models.

Most nutrient generation models include both hydrological and nutrient components. Hence the complexity of modelling in two different physical sciences needs to be considered.

The objectives of this research are similar to those described in Jakeman *et al.* (1999), primarily: "Inferring the on-site" (~0.01-10km^2) "effects of variations in climate, landscape attribute and land use/management …" on discharge water quality outputs. The difficulties experienced in this research are therefore similar to those identified by Jakeman *et al.*, being the complexity of the natural system, and lack of detailed, accurate measurements of the system and its fluxes. These difficulties result in limitations to the detail in model responses that can reasonably be produced.

This paper briefly reviews issues of complexity in the context of catchment nutrient discharge models. It highlights the challenge of developing an appropriately complex model for predicting changes to nutrient exports resulting from changes to catchment conditions.

2. APPLICATION ENVIRONMENT

The problems that excessive nutrient runoff from catchments causes in streams, water storages, estuaries and water supply systems are well known both in Australia and overseas. The detrimental effects of nutrient pollution the natural and human environments has led to extensive research in quantifying and predicting nutrient outputs in catchment runoff over the years (e.g., Baginska *et al.*, 1998; Davis and Koop, 2006; Sharpley *et al.*, 2003). Nevertheless, it remains difficult to quantify one-to-one relationships between catchment land use and catchment nutrient export (Vanni *et al*., 2001).

Yet the significant detrimental effects of excessive nutrient outputs mean that it is important that nutrient outputs from both existing and potential future catchment conditions (whether land use or climatic) be able to be modelled – i.e., explained and quantified as far as possible. Without the ability to model nutrient exports it is not possible to reliably understand or to effectively manage catchment behaviour where nutrient generation is, or could be, a problem.

3. REVIEW

3.1. Model Complexity

Catchment water quality models range in complexity from parsimonious, few-parameter empirical models, through more detailed lumped, then distributed, multi-parameter conceptual models, to complex multi parameter physically based distributed models.

The inability of simple lumped models to reflect the effects of temporal variability of catchment processes and spatial heterogeneity of catchment properties has been recognised for many decades (e.g., Murray, 1970). It has been argued that the development and use of complex, physically based distributed models is needed because the less sophisticated conceptual models do not allow physical interpretation of the empirically fitted (or calibrated) parameters. And hence direct, physically-based analysis of changes to catchment properties (for example land use change) cannot otherwise be undertaken (Abbott *et al*., 1986). On the other hand, Beven (1989) argues that the equations of physically based models, typically derived from small scale analysis, do not necessarily represent physical reality at the larger catchment or hillslope scales at which the models are applied. He gives the example of the calculation of the vertical unsaturated water flux over a large scale using a physically based equation in the SHE model. This is determined by reference to capillary pressure. While spot measurements of capillary potential might readily be made across a catchment, it would be impractical to conduct enough measurements to obtain a realistic catchment or sub-catchment wide representative capillary potential given the spatial heterogeneity of typical catchments. Consequently, in practice, the capillary potential parameter may require calibrating. Grayson *et al.* (1995) provide the example that equations for both saturated and unsaturated subsurface flow developed from consideration of blocks of (effectively homogeneous) soil of size in the order of 1dm^3, are applied to soil mass on the catchment's surface some orders of magnitude larger, which include highly pervious macropores which are not even considered in the formulation. Drewry *et al.* (2006) discuss the influence of scale on nutrient mobilisation and transport.

The need to calibrate parameters of models which were formulated as physically based, and possibly measurable at small scales, exposes physically based models to the risk of over-parameterisation, and its resulting disadvantages. Beven (1989) argues that "The calibrated parameters of such models may be expected to show a degree of interdependence, so that equally good results may be obtained with different sets of parameter values". More recently Beven (2001) has described equifinality, where "there may be many different model structures and parameter sets that will be acceptable in simulating the available data". In such a situation a model may not be capable of adequately, or uniquely, explaining the effects of physical changes within the catchment – such as land use change.

There is a corresponding danger of over-parameterisation with simple conceptual models which are configured in a distributed manner. Such an arrangement effectively creates many more parameters than inferred by the original conceptualisation. Blöschl and Sivapalan (1995) point out the dangers of using a distributed model to predict catchment outflow - incorrect sub-catchment responses could aggregate to give an acceptable total catchment outflow, with model errors in different sub-catchments compensating each other. Although this comment was made in the context of more complex physically based models, the same argument applies to distributed conceptual models. Murray (1970) identified the risk of "compensatory changes in parameters leading to unacceptable values but providing a good fit" when explaining that temporal and spatial lumping in (conceptual) models limited the ability of a model to accurately simulate runoff. Blöschl and Sivapalan did however suggest that subcatchment outflows could be used to ensure appropriate parameter calibration, although recognised problems with the additional data requirements to achieve this. Blöschl and Sivapalan (1995), in the context of physically based models, point out that state variables have been used to check model performance and parameter values, but that the measurements would typically be point values, and so would not necessarily be indicative of overall model performance.

Viewing the complexity/parameter estimation problem from a different perspective, Leavesley (1994) recognised the need for both more parameters and data if more complex responses are to be predicted. Wagener *et al.* (2001) point out that when simplifying model complexity (number of parameters) to reduce uncertainty in parameter values, care needs to be taken to ensure that important processes are not omitted. Such omission could result in the model being unsuitable for predicting response to the variation of interest.

Beven (1989) suggests that fitting three to five parameters should be sufficient for a model to adequately define the hydrological response of a catchment. Having more parameters than this would result in over-parameterisation of the model. Such comments are consistent with the findings of Perrin *et al.* (2003), Edijatno *et al.* (1999), Wagener *et al.* (2001) and (Boughton, 1984).

In a paper on model uncertainty, Beck (1987) describes the consequences of poor model identifiability as being “uncertain and ambiguous interpretation of past observed behaviour and … the possibility of ambiguous (and even contradictory) predictions…” (where identifiability is the ability to uniquely define model structure or parameters within the optimisation framework). In exploring parameter identifiability using both real, and ideal (i.e., controlled error) simulated data, Jakeman and Hornberger (1993) found that information on internal states is required to identify more than two components in catchment discharge.

The data set available for describing and predicting the hydrological response of a typical catchment generally consists of catchment surface discharge, point rainfall and some indication of evaporation. Yet the typical conceptual and physically based models will have representations of catchment processes occurring for which there are no, or insufficient, data. Such ‘hidden’ processes could include infiltration, exfiltration, overland flow, rill flow, channel flow, interception, and groundwater flow. Hidden states could include surface storage, groundwater storage, interception storage. (Some catchments may have other data available, such as soil moisture content, phreatic level, transmissivity or capillary potential. As each of these are point measurements representing a larger area the additional data do not help inform a catchment scale model to the extent that might be expected.) Beck (1987) explains this situation thus: "The crux of the problem is that what one would like to know about the internal description of the system ... is of substantially higher order than what can be observed about the external description of the system..." Beck (1987) also succinctly explains the consequences: "… the absence of a uniquely 'best' combination of parameter values that fit the data (many combinations are 'equally good') and in parameter estimates with high error variances and covariances."

Kuczera has written extensively on parameter uncertainty (e.g., Kuczera, 1983; Kuczera and Mroczkowski, 1998) and also developed the program suite NLFIT (Kuczera, 1994), which assists modellers identify highly cross-correlated, or redundant parameters, within a model. NLFIT also identifies poorly determined parameters by calculating the posterior distribution of each parameter, and can use data from other responses to better identify parameter values. A case study is presented in Kuczera and Mroczkowski (1998), in which poorly identified and redundant parameters are identified in a nine parameter model, and in which estimates of parameter values were substantially improved by joint fitting to a water quality parameter (chloride).

Leavesley (1994), when commenting on the need to calibrate parameters because of uncertainty of the relationships between “measurable basin and climate characteristics” and associated parameters argues that the result is “a large degree of uncertainty” in the ability of the model to be used in different climatic and geographical situations. Boughton reported on the difficulty of relating particular parameter values to definable catchment characteristics in complex conceptual models (including a version of the pre-SFB Boughton model) - and that in the case of the Boughton model it would be difficult to quantify changes to parameter values as a result of land use change (Boughton, 1984). Kokkonen *et al.* (2003) illustrated how difficult it is to predict parameter values from catchment characteristics for the relatively parsimonious IHACRES model.

From the above discussion it can be seen that the appropriate level of complexity, and number of (in principle adjustable) model parameters in a catchment model should take into account:

- the number of parameters and their structural configuration requiring calibration should be kept to a minimum, having regard to the purpose of the model
- parameters should be selected to have minimal cross correlation
- the number and types of responses to be described, and forcing mechanisms to be

considered, will influence the number of parameters that will need to be modelled

- the number of independent, representative, data types (including state variables) observable or with some *a priori* knowledge will affect identifiability of parameters and model performance
- a physically based model with measured parameter values does not help solve the identifiability problem if the scales of model formulation and application are so different as to affect the validity of the representation of the modelled processes.

Kuczera and Mroczkowski (1998) succinctly summarize the difficulty in choosing the appropriate level of complexity of a model thus: "A simple model cannot be relied upon to make meaningful extrapolative predictions, whereas a complex model may have the potential but because of information constraints may be unable to realise it."

3.2. Nutrient Generation Models

This section provides examples of nutrient mobilisation models covering the spectrum of complexity.

Hydrologic response of a catchment is fundamental to both the mobilisation and transport of sediments and pollutants, including nutrients (Grayson *et al.*, 1992). Hence even simplistic nutrient runoff models generally include a hydrologic representation. A notable exception is the CMSS (Catchment Management Support System). CMSS uses nutrient generation rates (ie, kg/Ha/Yr), specified according to land use. The program was designed to enable prediction of changes to nutrient runoff rates caused by changes to land use. CMSS' principal method of dealing with variation in nutrient generation rates due to factors such as variation in soil type or slope is by the specification of uncertainty bounds around the adopted nutrient generation rates (Davis and Farley, 1997; Marston *et al.*, 1995). The slightly more complex L-THIA takes into account catchment discharge. Aggregate nutrient generation rates are determined from the product of a predefined event mean concentration (EMC) for the nutrient, and runoff volume - determined using the United States Department of Agriculture – Soil Conservation Service Curve Number method (SCS-CN) (Baginska *et al.*, 2005).

CMSS and L-THIA represent the less complex, empirical end of the model spectrum, and would typically be used for indicative analysis of excess nutrient load problems. A range of models represent some of the processes in more detail. In conceptual models the representation of the processes is by analogy, rather than an explicit physics based formulation. The relative sophistication of the hydrology versus the water quality components in conceptual models varies. Some conceptual models have greater sophistication for the hydrology component, some have greater sophistication for the quality component, and others use a comparable degree of complexity for both. Conceptual models need to be empirically fitted to each catchment, as the parameters generally have no direct physical relationship with catchment properties.

CREAMS (a field scale model for Chemicals, Runoff and Erosion from Agricultural Management Systems) uses a range of empirical and physics based algorithms for simulating both surface and sub-surface water flows. Smith and Williams (1980) describe the representation of hydrology within the model. Frere (1980) describes the many nutrient mobilisation and transport processes represented within CREAMS.

AGNPS models hydrology simplistically using the SCS-CN, with much more complexity used for nutrient modelling (Baginska *et al.*, 2003).

HSPF (Hydrological Simulation Program – Fortran) (Bicknell *et al.*, 1997), while a semi-distributed conceptual model, represents both hydrological and nutrient processes with a high degree of complexity – utilising a large number of parameters for both the hydrology and nutrient components.

E2 (Argent *et al.*, 2006) can model catchment runoff with a range of complexities, while nutrient generation can be modelled using the less complex methods of the CMSS or L-THIA. E2 also offers filters for influencing transport of nutrients.

The models at the more complex end of the model spectrum are the physically based, distributed models. These models have explicit physics based mathematical formulations for the different hydrological and nutrient mobilisation processes which occur in the catchment, which are applied at a fine scale Examples of these include SHETRAN (Ewen *et al.*, 2002) and MIKE-SHE (Refsgaard and Storm, 1995). Despite the physical basis of such models, calibration is still required (Refsgaard and Storm, 1995).

4. DISCUSSION

The challenge of the current research is to develop models with sufficient complexity for their purpose to incorporate more causality than models such as CMSS or L-THIA, while avoiding the equifinality or extensive data requirements of more complex models. The approach is to partition discharge into surface and sub-surface runoff, thus enabling representation of the different mobilisation and transport capacities inherent to each flow path. Partitioning algorithms will be based on analysis of constituent properties of runoff (Clark and Fritz, 1997; Dewalle *et al.*, 1988; Lepisto *et al.*, 1994), rather than quick flow and slow flow as used in some methods (Argent *et al.*, 2006; Pilgrim, 1987), as it has been shown that quick flow is in fact often associated with sub-surface flow paths (Clark and Fritz, 1997; Dewalle *et al.*, 1988; Lepisto *et al.*, 1994). Where predictions of the impacts of localised catchment change are required, catchments will be subdivided according to land use and condition, soil type and slope. Consideration will be given to whether concentration or load outputs are considered the most important. Likewise, whether detailed time series outputs, long term average outputs, extreme event outputs, or some other characterisation of outputs such as frequency distribution is required, will affect the appropriate complexity of the model, data requirements, and mode of operation of the production version of the model.

Constituent concentration and runoff response data from the rural study catchments in S.E. Australia indicate that nutrient mobilisation and transport has a complex response (Figure 1).

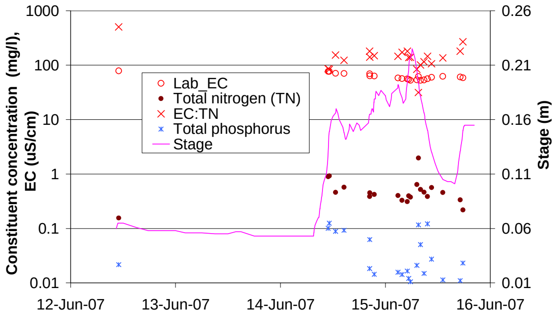

Figure 1. Runoff and constituent concentration response for a 2 Ha. catchment.

The task is further complicated by the low data resolution (spatially and temporally for quality data, and spatially for quantity data), and measurement errors. Clearly, a few-parameter, parsimonious model will be incapable of reproducing the complex time varying concentration changes of such responses. Fortunately the objective of typical nutrient generation models is not necessarily to reproduce the detailed time-series of chemical concentration signatures in the runoff. Rather the typical objective of the models is to quantify the aggregated nutrient exports to receiving reservoirs, or to characterise the nutrient concentrations in receiving streams.

If it is considered that the success of a model is not dependent on modelling the exact time of release of a nutrient discharge within an event, or even over which particular event a nutrient discharge occurs, then it is likely a more parsimonious model can be used to quantify catchment nutrient discharge for different catchment conditions. In other words, being explicit about purpose can allow simplification of model complexity.

Success will be achieved if nutrient discharge from the small catchments can be predicted on the basis of land use, cover, slope, and soil type, and catchment runoff.

5. CONCLUSION

Catchment water quality models are generally too simple to allow reliable prediction of changes to nutrient generation resulting from change to catchment or climatic conditions, or too complex, resulting in poorly identified parameters, probably exhibiting equifinality, and/or having extensive data requirements. The detrimental effects of excessive nutrient runoff from catchments however requires that we be able to predict the effects of changes to catchment conditions on nutrient levels. The current research is aimed at developing a reasonably parsimonious model with the ability to make sufficiently accurate predictions of the output of interest in an appropriate form.

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