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Processes affecting transfer of sediment and colloids, with associated phosphorus, from intensively farmed grasslands: a critical note on modelling of phosphorus transfers

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In this commentary we are concerned with mathematical models of phosphorus transfers from agricultural land, particularly intensive grassland, to receiving waters (Haygarth *et al*., 2006). We believe that the complexity of this problem requires an initially wide discussion of possible modelling concepts and the associated benefits or problems with these approaches. Hence we are reluctant to break the phosphorus-modelling problem down to smaller scales or detailed levels of complexity, e.g. sediments/colloids, which is the main concern of previous papers in this series of commentaries. However, many aspects of the following discussion could be applied equally to sub-elements of the phosphorus-modelling problem as well as wider environmental modelling applications.

Two objectives justify the building of mathematical phosphorus transfer models: (1) they formalize our knowledge about the system under study and in this way they act as vehicles for testing our understanding of phosphorus transfers; and (2) they may allow quantitative predictions under changing and complex environmental conditions. In the light of international legislation such as the EU Water Framework Directive (2000/60/EC), it is increasingly important to predict the impacts of land management practises and measures for mitigating diffuse pollution. This, however, requires a confidence in the process formulation (be it empirically or physically-based) and a predictive capability of models, which may not be justified in many cases, especially where there are limited observational data available to develop, test and drive model assumptions.

In the previous papers of this series of commentaries, we learned that our perceptual understanding of phosphorus, sediment and colloid transfers from intensive grasslands is far from perfect (Bilotta *et al*., 2007; Gimbert *et al*., 2007; Granger *et al*., 2007; Haygarth *et al*., 2006). However, this perceptual understanding is (and will always be) better than our translation of these perceptions into conceptual and, finally, procedural models.[1] Two main approaches to modelling the phosphorus transfer problem can be identified from the literature: (1) empirical phosphorus export models to calculate annual or seasonal loads (this includes empirical risk assessment techniques); and (2) process-orientated phosphorus models to simulate storm dynamics. This includes conceptual and physically-based models[2] (Table I). In the following sections, we highlight a few critical points regarding these approaches and, finally,

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[1] Here we refer to the three classic steps of model development: the 'perceptual model' is our qualitative understanding of system behaviour, the 'conceptual model' comprises the mathematical equations to describe this behaviour, and the 'procedural model' is the computer code to run the actual simulations. Note the term 'conceptual model' is also used with a different notion later in this paper, referring to a mathematical model class of intermediate complexity.

[2] The classification of models by the degree of complexity of their process descriptions as being empirical, conceptual or physically-based is widely used in hydrology (Rosbjerg and Madsen, 2005) even though none of these terms is unequivocal. We see the transition between these classes as continuous rather than discrete.

Table I. Example references of phosphorus (P) transfer models. Conc. = (mean[a]) concentration, DIP = dissolved inorganic P, DP = dissolved P, DRP = dissolved reactive P, IP = inorganic P, MRP = molybdate reactive P, OP = organic P, PP = particulate P, SS = suspended sediment, TP = total P

Model class		Modelling target	Scale of application[b]	References[c]
Empirical P export models	**Statistical models**	**Event DP load**	**0·57–1·46 ha**	**Edwards *et al.* (1996)**
		Event DRP conc.	**0·9–0·45 ha**	**Ekholm *et al.* (1999)**
		5 year mean DRP, SS, TP conc.	**9–139 km^2**	**Ekholm *et al.* (2000)**
		Annual TP load	**4–34 ha**	**Ulen *et al.* (2001)**
		Annual/seasonal MRP conc.	**Catchments**	**Daly *et al.* (2002)**
		Annual TP load	**<100 km^2**	**Kronvang *et al.* (2003)**
		Event DRP conc.	**0·72–0·79 ha**	**Schroeder *et al.* (2004)**
		Annual DRP, PP, TP conc./load	**3·7–57·8 km^2**	**Andersen *et al.* (2005)**
		Daily TP conc.	**5·1/15·6 km^2**	**Nour *et al.* (2006)**
		Annual TP (>0·45 μm), TP (<0·45 μm) load	**1·2–27·8 km^2**	**Schaerer *et al.* (In press)**
	Export coefficient models	**Annual TP load**	**46/363 km^2**	**Johnes (1996)**
		Ditto	**4·9–18·31 km^2**	**Johnes *et al.* (1996)**
		Ditto	**0·9–23·6 km^2**	**Johnes and Heathwaite (1997)**
		Seasonal TP load	**17·6 km^2**	**May *et al.* (2001)**
		Ditto	**41·4 km^2**	**Hanrahan *et al.* (2001)**
		Annual TP load	**10 km^2**	**Murdoch *et al.* (2005)**
		Ditto	**95 km^2**	**Khadam and Kaluarachchi (2006)**
	P indicators tool	**Annual TP load**	**218/366 km^2**	**Heathwaite *et al.* (2003)**
		Ditto	**0·93–23·62 km^2**	**Brazier *et al.* (2005)**
	P index	**Rating of vulnerability to P loss**	**1·1–125 ha (single[d])**	**Gburek *et al.* (1996)**
		Ditto	**26 ha (mixed[d])**	**Gburek *et al.* (1996)**
		Ditto	**39·5 ha (mixed[d])**	**Weld *et al.* (2001)**
		Ditto	**Regions**	**Birr and Mulla (2001)**
Process-orientated P models	**Physically-based models**	**3 min DP, PP conc.**	**100 m^2**	**Storm *et al.* (1988)**
		Daily DP, PP, SS conc.	**73 km^2**	**Cooper and Bottcher (1993)**
		Monthly TP conc.	**51/155 km^2**	**Wagner *et al.* (1996)**
		Daily TP conc.	**3·8 ha**	**Yoon *et al.* (1997)**
		Event SS, TP conc.	**77·15 km^2**	**Lenzi and DiLuzio (1997)**
		Monthly TP load	**0·46 ha**	**Knisel and Turtola (2000)**
		Daily DRP conc.	**0·72–0·79 ha**	**Pierson *et al.* (2001)**
		Hourly PP, SS conc.	**128·9 km^2**	**Rode and Lindenschmidt (2001)**
		1 min DP, PP, SS conc.	**30·6/98·6 ha**	**Hutchins *et al.* (2002)**
		1 min - 1 h DIP, SS, TP conc.	**0·5 m^2**	**Grant *et al.* (2004)**
		Hourly DP conc.	**1·44/128·9 km^2**	**Lindenschmidt *et al.* (2004)**
		Daily IP conc.	**750 ha**	**McGechan *et al.* (2005)**
		Daily DP conc.	**164 ha**	**Hively *et al.* (2006)**
	Conceptual models	**SS, TP conc.**	**>100 km^2**	**Jakeman *et al.* (1999)**
		Monthly TP load	**51–293 km^2**	**Lee *et al.* (2000)**
		Weekly TP conc.	**558 km^2**	**Smith and Wheater (2004)**
		Daily TP conc.	**150 km^2**	**Smith *et al.* (2005)**

[a] **We expect a mean concentration for large time steps even though this is not explicitly stated in most references.**

[b] **This does not necessarily mean that the application was successful at this scale.**

[c] **This list gives examples and is by no means complete.**

[d] **Land use.**

give our perspective of the properties that an alternative phosphorus-modelling strategy should possess.

Are there Limitations in Modelling Annual/Seasonal Phosphorus Loads?

Empirical phosphorus transfer models relate site characteristics, which are formalised as index parameters to phosphorus losses from these sites (spatially lumped or semi-distributed) on an annual or sub-annual basis. The simplest models within this class can be called *Statistical Models* since they are inferred from the data directly by statistical analysis (e.g. Daly *et al.* (2002); Andersen *et al.* (2005)). By their very statistical nature, these models are only valid for the data sets (e.g. catchments and years) they were applied to and their level of robustness will reflect the information content within these data sets. More assumptions about the meaning of model parameters are made in *Export Coefficient Models* (e.g. Omernik (1976); Johnes (1996)), which are usually calibrated against estimated in-stream phosphorus loads. The variability in export coefficient values reported in the literature from laboratory or plot scale experiments should lend itself intuitively to a treatment of these models within an uncertainty estimation framework (e.g. Murdoch *et al.* (2005); Khadam and Kaluarachchi (2006)). A more complex, multi-layered approach such as the *Phosphorus Indicators Tool* (Heathwaite *et al.*, 2003) further increases model parameter uncertainty. With currently available data sets, not all components of this type of model could be evaluated (Heathwaite *et al.*, 2003). Whereas the aforementioned models have at least the potential to be directly evaluated against observed data, this is less likely for qualitative risk assessment techniques such as the *Phosphorus Index* (e.g. Lemunyon and Gilbert (1993); Gburek *et al.* (2000)). Here, the boundaries of our conceptual formality that may be assessed with field observations are blurred into a more subjective ranking/weighting approach that lacks scientific scrutiny. Although this may sound critical, in fact, it may be the limit at which we can evaluate models and a level of subjectivity may be necessary as long as the assumptions made are explicitly identified.

On top of the model structural and parameter uncertainties mentioned above, we have to consider input and evaluation data uncertainties as well. The input data (e.g. land use and livestock density) are usually available in resolutions (grids or communes) that are different from the site dimensions (e.g. catchments) where they are applied. The evaluation data (in-stream phosphorus loads) are usually called ‘measured’ even though they are estimated from instantaneous phosphorus concentration and discharge measurements from coarse time resolutions.

Is there a Modelling Paradox in Representing the Process Descriptions of Phosphorus Transfers?

Physically-based phosphorus transfer models conceptualise the processes governing phosphorus input, mobilisation and transport (physically and chemically) in a potentially very detailed and spatially distributed way. Many of the models are founded on similar equations (Viney *et al.*, 2000), so we restrict ourselves here to citing two of the first codes: ANSWERS (Beasley *et al.*, 1980) and CREAMS (Knisel, 1980). However, physically-based phosphorus transfer models do vary in their degree of process incorporation (driven by the scale of application for which the models are developed), their underlying hydrological model structure and their numerical design. Nevertheless, if processes are understood as the actual mechanisms going on in reality, they can in no way be completely represented in any of the models. Although a model may have been ‘validated’ at one scale this may not be the same as the scale at which it is applied. These validation difficulties are conditioned by two facts: (1) measuring model parameters and input/output variables at the required resolution is impossible given our current observational techniques (Kavetski *et al.*, 2003); and (2) many parameters and variables are non-measurable as they reflect effective processes for the scale of application (Beven, 1989).

As a pragmatic response to these drawbacks, conceptual phosphorus transfer models, i.e. hybrids consisting of empirical and physically-based components with mostly semi-distributed spatial organisation (e.g. Haith and Shoemaker (1987); Jakeman *et al.* (1999); Smith and Wheater (2004)), are being developed to acknowledge explicitly the effective nature of any model process representation. However, for all model variants the uncertainty problem in modelling remains: not only do we have insufficient data to support many of our perceptions in the field, we are also data-limited in identifying and evaluating model structures and parameters. Moreover, what limited data we have are uncertain in themselves because of measurement and interpolation errors as well as the mismatch between variables in the model and those that we can measure in the field. Experience suggests that many model structures and parameter combinations can describe the available observations equally ‘well’ (the ‘Equifinality’ problem described by Beven (1993)) and this should have a bearing on the type of evaluation framework we use to assess these models.

Can an Alternative Uncertainty Learning Framework for Phosphorus Models be Defined?

We have briefly outlined the difficulties of understanding phosphorus transfer across scales (see also the field perspective in the previous papers of this series of commentaries), especially the limits of available data to identify processes in a model evaluation exercise. We believe conceptualising these processes requires a 'top-down' strategy of model development, i.e. keeping the model as simple (parametrically parsimonious) as possible but as complex as necessary to describe the available data well while ensuring physical and chemical relevance. Such a model would describe the dominant modes of behaviour of phosphorus transfer, where these can be supported by field observations. In a perceptual sense, this would include critical phosphorus source areas (defined by Heathwaite *et al.* (2005), for example), linked by dominant phosphorus transport pathways, and complemented by the relevant mechanisms of phosphorus mobilisation and redeposition. The number of possible model structures and parameterisations for any given modelling application is potentially large. Hence the assessment of these competing hypotheses within a model-learning framework (i.e. with the aim of rejecting specific models where possible) seems appropriate. This framework should essentially incorporate uncertainties in model structure, parameters and data. Uncertainty estimation techniques are well known in hydrology (e.g. Beven and Binley (1992); Gupta *et al.* (1998); Kavetski *et al.* (2003)). They mainly differ in the assumptions they make in characterising the model error sources, the discussion of which is beyond the scope of this commentary.

We want to emphasise again that we may face a dilemma in relying on uncertain data to identify models of phosphorus transfers, which are themselves only weakly supported by experimental evidence (see previous papers of this series of commentaries). It is here that the necessary dialogue between modellers and field experimentalists (Seibert and McDonnell, 2002) comes into play. The field scientists, on one hand, have to communicate the basis of their perceptual understanding of phosphorus transfers to identify possible models. The modellers, on the other hand, have to identify points where any translation from perceptual to conceptual models is not sufficiently supported by data and can, therefore, help to understand (and guide new) field observations. This would enable the field experimentalists and modellers to learn more about the spatial and temporal dynamics of the controlling processes of their system under study through an iterative scheme of observation and model testing. A close collaboration would also be beneficial for the quantification of data uncertainties and limitations.

So, do we think we can meet the two modelling objectives outlined at the beginning of this paper? Adopting the proposed modelling approach and utilising data from research sites would meet the first objective of identifying phosphorus transfer processes. However, we doubt that ensembles of dominant processes derived for specific sites (of different scales) will be universally applicable (see discussion by Beven (2000), for example). We believe that any model is generally confined to the temporal and spatial scale for which it has been developed. Consequently, we have to be honest and explicit about the capabilities of any model to meet the second objective of predicting future scenarios. Qualitatively, we are confident that the dominant modes of behaviour derived for specific sites and periods will hold for similar sites and for future behaviour as long as there is no severe shift in the dominant processes (of the kind reported by Lazzarotto *et al.* (2005), for example).

We shall now summarize what we believe are the main requirements of an efficient strategy for future modelling of phosphorus transfers:

1. With phosphorus transfer we have an ill-posed process problem. This can only be confronted with a top-down strategy of model development aiming for the dominant modes of system behaviour.
2. The approach above has to be embedded in a model evaluation scheme that accounts for model structural and parameter uncertainties and that aims for rejecting competing model hypotheses. In this way, modelling is learning about the system studied.
3. We have to understand the limitations in our observations, both for identifying and for driving model components. This includes the quantification of data uncertainties and their incorporation into the model evaluation scheme.
4. Understanding phosphorus transfer from diffuse agricultural sources is very complex. Only by adopting an iterative learning framework that includes experimentalists and model developers working together are we likely to resolve some of the complexities and build better predictive models.

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