A Spatially-Distributed Conceptual Model For Reactive Transport Of Phosphorus From Diffuse Sources: An Object-Oriented Approach

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Abstract: This paper presents CAMEL, a spatially-distributed conceptual model for simulating reactive transport of phosphorus from diffuse sources at the catchment scale. A catchment is represented in the model using a network of grid cells and each grid cell is comprised of various conceptual storages of water, sediment and phosphorus. To allow for reactive transport processes of phosphorus between grid cells, two cascade routing schemes are used for groundwater and channel water flows, respectively. The model has a modular, object-oriented structure so that it can be easily modified or extended and, furthermore, it can even provide a library of hydrological and hydrochemical processes from which the user can select a sub-set of processes suitable for a particular application. A verification study of the model has been carried out for a hypothetical catchment with satisfactory results.

Keywords: Phosphorus; Diffuse source; Reactive transport; Spatially-distributed; Object-oriented; CAMEL

1. INTRODUCTION

Phosphorus (P) is an essential element for plant growth and its input to the soil has long been recognised as necessary to maintain profitable crop and livestock production. Excess inputs of P, however, may cause eutrophication of fresh waters. Many standing waters in the UK have undergone eutrophication and many UK rivers are heavily polluted with P [Withers and Lord, 2002]. This has focussed attention on the pollution of freshwaters by P loss from agricultural diffuse sources.

P is readily adsorbed to sediment particles and forms insoluble precipitates with cations such as iron, aluminum and calcium [Sample et al., 1980]. Because of this phenomenon, called P retention, P is strongly associated with sediment particles in the soil. Consequently, the majority of P from diffuse sources is transported by surface runoff in particulate forms. However, surface runoff or sub-surface drainage can also transport significant amounts of dissolved P particularly if the soil is overloaded with P and the soil/geology has a low adsorption capacity for P.

During the course of delivery from the soil to the river system, P undergoes numerous transformation processes. Important processes related to P transformation in the stream include: detachment and deposition of sediment particles; adsorption and desorption of soluble P to/from sediment particles [House et al., 1995]; co-precipitation of P with calcite in hardwaters [House and Donaldson, 1986; Jarvie et al, 2002]; formation of the ferrous phosphate mineral vivianite in anoxic sediments [Woodruff et al., 1999]; and P uptake by aquatic plants through either root or shoot. The combination of all of these processes, in tandem with variations in river flow and other environmental factors, makes the transport process of P very complicated.

The significance of each of the above processes varies greatly in space. A small portion of the catchment may contribute a large proportion of P load [Gburek and Sharpley, 1998]. These areas have been termed critical source areas and are characterised by having high potential to release P into surface or subsurface runoff in conjunction with hydrologic connectivity with streams or ditches. Targeting critical source areas would increase the efficiency and reduce the economic costs of control [Needelman et al., 2001]. Therefore, in the context of catchment management, it is important to identify critical source areas and major transport processes of P from those areas. A spatially-distributed P transport model can be a useful tool for these purposes.

This paper presents a spatially-distributed conceptual model, CAMEL (Catchment Analysis Model for Environmental Land-uses) v1.0, that has been developed for the assessment of long-term effects of agricultural land use changes on water quality in terms of sediment and P concentrations in the water.

2. A REVIEW OF EXISTING MODELS

There are a number of existing models that can simulate dynamics of P transport at a catchment scale in a distributed or semi-distributed manner. Examples of these models include AnnAGNPS [Cronshey and Theurer, 1998], ANSWERS-2000 [Bouraoui and Dillaha, 2000], SWAT-2000 [Neitsch et al., 2001], LASCAM [Viney et al., 2000] and INCA-P [Wade et al., 2002]. These models have been reviewed to identify critical requirements for the new model.

In some models that divide a catchment into small sub-catchments and regard them as homogeneous units, spatial parameters (e.g. ground surface slope) are aggregated for sub-catchments that are different in size. The aggregations are therefore carried out at different scale and this can cause significant errors in simulation results. For assessing effects of land use changes, the spatial consistency of simulation results of a model is of critical importance. In this respect, grid cell representation of a catchmant is the better option.

A number of models estimate soil erosion using certain variants of the Universal Soil Loss Equation [USLE; Wischmeier and Smith, 1978] – namely, Modified USLE [Williams, 1975] and Revised USLE [Renard et al., 1997]. However, these MUSLE/RUSLE-based models are not only mathematically unsound [Kinnel, 2004] but also the USLE fails to deal with soils where organic matter contents are greater than 4 % [Lilly et al., 2002]. CAMEL is being developed for application in Scotland where soils with high organic matter content are common, which means that this is likely to be a significant issue.

Some models do not take into account in-stream P transformation processes. Without P in-stream processes, however, the dynamics of reactive transport of P cannot be properly simulated. Thus it would be impossible to identify where channel reaches are acting as sources or sinks at particular times. Furthermore, in some cases, simulation of conservative (non-reactive) transport of P may result in misleading results. For a comprehensive catchment management, therefore, it is essential to simulate reactive transport of P through channel routing across the catchment.

All the models listed above have a procedure-oriented top-down structure leaving little autonomy to the user. The resulting lack of flexibility and extensibility may constitute a barrier for potential users.

3. MODEL OVERVIEW

CAMEL is a dynamic, mass balance model that employs conceptual storages and spatially-distributed parameters. CAMEL contains a mixture of conceptual and physics-based components. Below is a list of the conceptual storages defined in each of the cells:

- Four water storages – canopy, soil, aquifer and channel;
- Two sediment storages – overland and channel-bed;
- Five P storages in the soil – active organic, stable organic, labile, active inorganic and stable inorganic;
- Three P storages in the aquifer and channel, respectively – labile, active inorganic and stable inorganic.

Unlike most existing models, CAMEL has a modular, object-oriented structure so that it allows the user to select from a library of hydrological and hydrochemical processes a sub-set of processes suitable for a particular application. In this way, the model provides a flexibility to 'build your own' model. The user is also allowed to determine appropriate spatial and temporal resolutions of the model.

CAMEL represents a catchment using a network of square grid cells. A cell can have a maximum of 8 neighbouring cells among which it can have up to 7 upstream cells and one downstream cell. Every cell represents the corresponding soil-aquifer column of the catchment and has a rectangular stream channel in the middle.

Input data requirements for CAMEL are in four main categories of parameters – topography, soil and aquifer, land cover and weather:

- Topography – ground surface elevation, slope, flow direction, flow accumulation, channel dimensions, channel roughness;
- Soil and aquifer – soil depth; soil water contents at saturation, field capacity and wilting point; median particle size, detachability and cohesion of the top soil;

saturated hydraulic conductivity of soil; aquifer water contents at saturation and field capacity; saturated hydraulic conductivity of aquifer for fast and slow layers;

- Land cover – canopy storage, overland roughness, soil cohesion increase by root reinforcement; crop height, crop coefficient, leaf area index at each of 5 crop stage dates; livestock excretion rates for cattle and sheep, incorporation rate of plant residue and application rates of fertiliser and manure;
- Weather – rainfall, air temperature, dew-point temperature, cloud cover, wind speed and mean sea level pressure at every time-step.

The current version of CAMEL provides the following outputs:

- Time-series outputs for a number of selected cells at every time-step;
- Snapshot outputs for the entire catchment at specific time-steps and cumulative snapshot outputs for the whole simulation period;
- Mass balance outputs of water, sediment and P for the entire catchment at every time-step.

4. INTRA-CELL PROCESSES

In CAMEL, hydrological and hydrochemical processes are calculated in two steps – intra-cell processes and inter-cell processes. Intra-cell processes include water flows, soil erosion and P transformations and are calculated for each of the cells.

4.1 Water Flows

CAMEL uses four conceptual storages – canopy, soil, aquifer and channel – for calculating water balance and water flows between them (Figure 1).

Included in the canopy storage processes are rainfall interception, throughfall and evaporation. For the estimation of potential evaporation and reference crop evapotranspiration, CAMEL uses two Penman equation derivatives suggested by Shuttleworth [1993].
The soil storage processes include saturation-excess surface runoff, groundwater recharge, interflow, transpiration and soil evaporation. For estimation of groundwater recharge and interflow, a simple storage routing technique is applied to each of the 100 vertical sections of the soil column based on the relationship between soil water content and hydraulic conductivity.
The aquifer storage processes are discharge to the channel, discharge to the downstream cell and groundwater rise to the soil. Each aquifer is
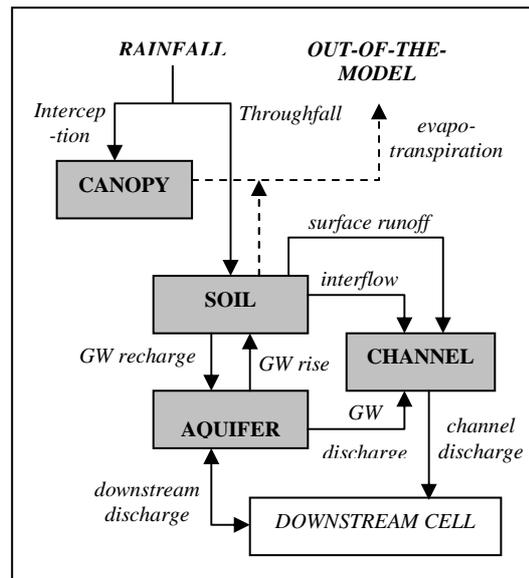

Figure 1. Conceptual water storages and hydrological processes in CAMEL.

assumed to have two layers – namely, fast and slow layers – with different hydraulic conductivities to accommodate fast flows through fissure openings of weathered layers near the ground surface. Groundwater flows are assumed to be Darcian and are estimated based on differences in hydraulic heads. Thus groundwater flows in the model can be bi-directional, allowing for an estimation of channel-aquifer interactions.

For channel water storage processes, channel evaporation is assumed to occur at the rate of potential evaporation.

4.2 Soil Erosion

For simulating the effect of sediment supply on sediment transport, two conceptual sediment storages – overland storage and channel storage – are assumed in CAMEL (Figure 2).

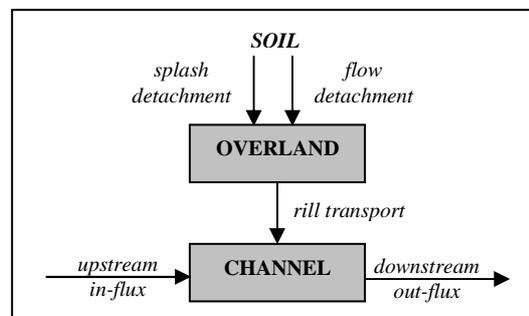Sediment particles detached by raindrops (splash concentrations in the rill flow. If the sediment

Figure 2. Conceptual sediment storages and sediment transport processes in CAMEL.

transport capacity of the rill flow is greater than the initial sediment concentrations, more sediment particles are detached (flow detachment) and transported to the channel. Otherwise, a part or all of the detached sediment is deposited and added to the overland sediment storage. Sediment transported to the channel is added to the channel sediment storage and is transported downstream by channel flows. The equations for splash detachment and flow detachment have been taken from EUROSEM [Smith et al., 1995], a physics-based soil erosion model.

4.3 P Transformations and Transport

The structure of the soil P transformation component of the model has been widely taken from the EPIC model [Jones et al., 1984] and the SWAT model [Neitsch et al., 2001] and then further simplifications have been made.

For simulating P transformation and transport processes in the soil, aquifer and channel, CAMEL assumes conceptual storages for organic and inorganic P (Figure 3). Organic P in the soil is divided into two storages: the active organic P storage (P_{AO}) and the stable organic P storage (P_{SO}). P_{AO} consists of P in undecomposed plant residues, livestock excretion, manure and microbes, whereas P_{SO} is composed of P in stable organic matter i.e. humus. Soil inorganic P is divided into labile P (P_{LB}), active inorganic P (P_{AI}) and stable inorganic P (P_{SI}) storages. P_{LB} is in rapid equilibrium (several days or weeks) with P_{AI} which in return is in slow equilibrium with P_{SI}. When inorganic fertiliser P is added to P_{AI}, it rapidly equilibrates between P_{LB} and P_{AI}. The slow reaction between P_{AI} and P_{SI} then follows. It is assumed P_{SI} is four times larger than P_{AI}. In the aquifer and the channel, only inorganic P storages (P_{LB}, P_{AI} and P_{SI}) are assumed and, therefore, P sorption is the only process simulated in the model.

All P transformation rates are calculated using first-order kinetic equations taking into account the effect of soil water content and temperature. The soil water content effect on organic matter decomposition, mineralisation and immobilisation is estimated using a segmented linear function. Soil temperature is calculated using the approach of Kang et al. [2000] and its effect on transformation rates is estimated using the Q10 function [Van Clooster et al., 1994]. Plant uptake of P is assumed to be proportional to transpiration rate and labile P concentrations in the soil water.

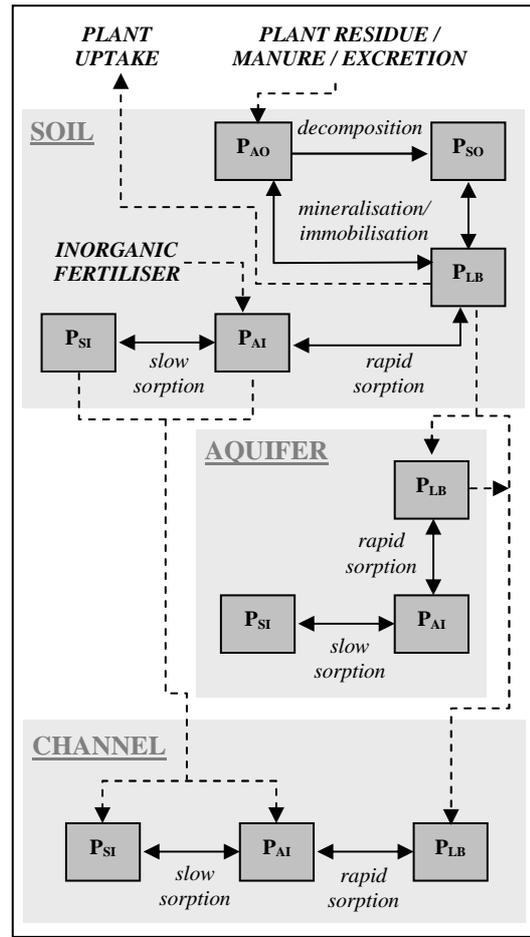Intra-cell P transport processes in the model include transport of sediment-bound P (P_{AI} and

Figure 3. Intra-cell P transformation and transport processes between conceptual P storages in CAMEL (P_{AO} = active organic P; P_{SO} = stable organic P; P_{LB} = labile P; P_{AI} = active inorganic P; P_{SI} = stable inorganic P).

P_{SI}) by surface runoff and transport of dissolved P (P_{LB}) by surface runoff, groundwater recharge and groundwater discharge. Transport of sediment-bound P is estimated using an enrichment ratio that exponentially decreases with the sediment flux. Dissolved P transport is estimated using an extraction ratio that is an exponential function of water flows.

5. INTER-CELL PROCESSES

Inter-cell processes are calculated after the intra-cell processes are evaluated for the entire catchment. To allow for reactive transport processes of P between cells, two cascade routing schemes are used for groundwater (dissolved P) and channel water (particulate and dissolved P) flows, respectively.

5.1 Channel Water Routing

For routing of the channel water, the spatially distributed unit hydrograph approach proposed by Maidment [1993] is adopted in CAMEL with modifications. The flow travel time from a cell to a given downstream cell is estimated by assuming constant flow velocities. The constant flow velocities for individual cells are estimated using Manning's equation on an assumption that channel water depth is 1/10 of the channel width. The volume of channel water leaving each of the cells is then routed to the given downstream cell in a certain time-step according to the isochrone of flow travel time to the cell.

5.2 Groundwater and P Routing

A Darcian groundwater flow from an upstream cell is transported to the downstream cell completing the process in two time-steps. The downstream out-flow from a cell in the current time-step contributes to the upstream in-flow of the downstream cell in the next time-step. Due to this separation of upstream in-flows and downstream out-flows in time, groundwater is routed downstream in a fully cascading way, which allows for P sorption processes in the aquifer of indi vidual cells. It should be noted, however, that this routing scheme is valid only when the groundwater flow velocity does not exceed the cell length per time-step.

5.3 Channel Sediment and P Routing

For reactive transport of sediment and P in the channel, a comprehensive cascade routing scheme has been developed. For calculating the channel sediment budget of a given cell, primary cells that have no upstream cells are first identified. Then the amount of sediment and P leaving the primary cells are estimated and routed downstream cell-by-cell to the given cell taking into account the isochrones. Sediment transport processes in the channel (i.e. detachment and deposition), P sorption and transport (in both dissolved and particulate forms) processes are evaluated using the same equations applied to rill flows within a cell.

6. MODEL VERIFICATION

A verification study of the model has been carried out for a small hypothetical catchment (0.8 km^2) with 200 m grid cells for one year period at daily time-steps. For this study, a set of daily weather data from a UK meteorological station was used and the catchment was assumed to have a homogeneous land cover (winter wheat) and a soil/geology layer (sandy silt loam underlain by

well-fissured granite). To avoid unnecessary confusion, it should be noted that no comparison with field data has been carried out in this verification study.

Parameter values were initially taken from various sources and adjusted during verification simulations to obtain reasonable results. Table 1 lists some of the parameter values used for the final verification simulation.

The hydrological simulation results including evapotranspiration, soil water content, discharge and groundwater table elevation show strong seasonal variations as expected. The overland sediment is delivered to the channel mostly by the first few storms in autumn when the soil is fully saturated. The comprehensive cascade routing scheme for channel sediment and P works well with very little mass balance errors.

Simulation results of P transformation processes in the soil, demonstrated in Figure 4, show strong temporal variations reflecting the effect of agricultural practices such as harvest and applications of fertiliser and manure. For example, when mineral P fertiliser is applied in spring, P is rapidly adsorbed to the soil and then, as plant uptake increases in the growing season, P adsorption rate gradually decreases leading to P desorption in summer.

The model also reasonably represents P transport processes. In the model, P is transported to the channel in both particulate and dissolved forms. However, simulation results show that most of P is transported in particulate forms (Figure 5), which

Table 1. Selected parameter values used for the final simulation

| Parameter	Unit	Value
Saturated hydraulic conductivity for soil	m/day	0.56
Saturated hydraulic conductivity for aquifer:		
- fast-flowing layer	m/day	2.50
- slow-flowing layer	m/day	0.25
Organic matter decomposition rate	1/day	0.10
Humus decomposition rate	1/day	0.03
Rapid adsorption rate	1/day	0.50
Slow adsorption rate	1/day	0.01
Fertiliser application rate	KgP/ha/y	35.0
Manure application rate	KgP/ha/y	5.0
Plant residue incorporation rate	KgP/ha/y	5.0
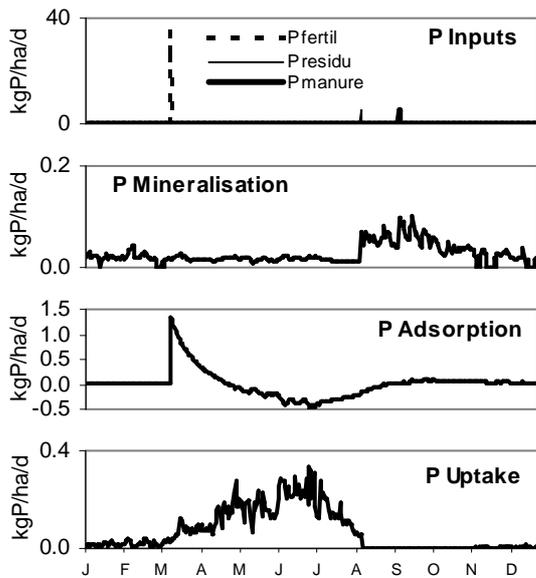
Figure 4. Simulation results of P transformation processes in the soil.

reflects the characteristics of P being adsorbed to sediment particles. The amount of dissolved P transported to the catchment outlet is negligible (0.02 kgP/ha/y) compared to that of particulate P (2.14 kgP/ha/y).

In calculating dissolved P concentrations in the channel water, CAMEL uses the size of labile P storage in the channel to estimate the amount of dissolved P in water. The assumption here is that water is fully interacting with the labile P storage. This is reasonable when enough water flows in the channel, but this becomes invalid when very little water flows in the channel. In reality, during low flow, water occupies a fraction of the channel bed and the interaction between water and the labile P storage is limited. In the model, the channel water evenly distributes across the channel bed and thus a full interaction is assumed even in very low flow conditions. This limitation can cause unrealistically high concentrations of dissolved P at very low flow conditions as shown in Figure 6.
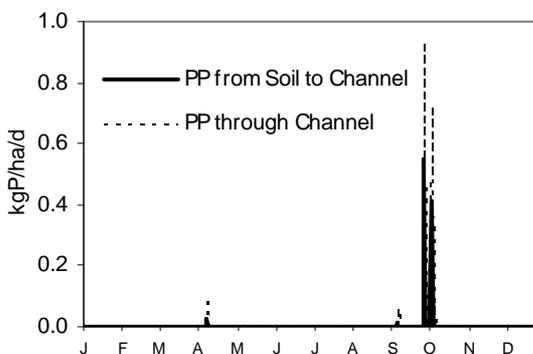

Figure 5. Catchment-mean transport rates of particulate P (PP)
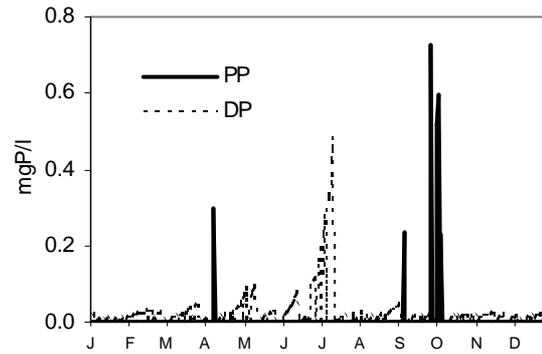

Figure 6. Simulated concentrations of P at the catchment outlet (PP = particulate P; DP = dissolved P)

It is anticipated that this problem will be resolved in the next version of CAMEL.

Despite some limitations, the model simulation results are generally reasonable and the mass balance errors of water (-4.34E-12 mm/y), sediment (9.23E-09 kg/ha/y) and P (3.26E-13 kgP/ha/y) are negligible. It is therefore considered that CAMEL has been correctly coded to represent the conceptual model.

7. CONCLUSIONS

A spatially-distributed conceptual model, CAMEL, has been developed for simulating reactive transport of P from diffuse sources at the catchment scale. Although based on conceptual storages, CAMEL evaluates the majority of processes using physics-based equations. The model has comprehensive cascade routing schemes that allow for reactive transport of P across the catchment. Because of its modular and object-oriented structure, CAMEL can be easily modified or extended. Furthermore, the model provides a library of hydrological and hydro-chemical processes from which the user can select a sub-set of processes suitable for a particular application. In this way, the model provides the user a flexibility to 'build your own' model. A verification study on a hypothetical catchment has shown that CAMEL has been correctly coded to represent the conceptual model.

With a network of self-contained cells and comprehensive routing schemes, CAMEL can identify the critical source areas in a catchment and the major transport processes of P from those areas. This information may then be used for improving the efficiency and/or effectiveness of catchment management practices.

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