DEVELOPING AN INDEPENDENT, GENERIC, PHOSPHORUS MODELLING COMPONENT FOR USE WITH GRID-ORIENTED, PHYSICALLY-BASED DISTRIBUTED CATCHMENT MODELS

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ABSTRACT

Grid-oriented, physically based catchment models calculate fields of various hydrological variables relevant to phosphorous detachment and transport. These include (i) for surface transport: overland flow depth and flow in the coordinate directions, sediment load, and sediment concentration and (ii) for subsurface transport: soil moisture and hydraulic head at various depths in the soil. These variables can be considered as decoupled from any chemical phosphorous model since phosphorous concentrations, either as dissolved or particulate, do not influence the model calculations of the hydrological fields. Thus the phosphorous concentration calculations can be carried out independently from and after the hydrological calculations. This makes it possible to produce a separate phosphorous modelling component which takes as input the hydrological fields produced by the catchment model and which calculates, at each step the phosphorous concentrations in the flows. This paper summarise the equations and structure of Grid Oriented Phosphorous Component (GOPC) developed for simulating the phosphorus concentrations and loads using the outputs of a fully distributed physical based hydrological model. Also the GOPC performance is illustrated by am example of an experimental catchment (created by the author) subjected to some ideal conditions.

Keywords: Phosphorous modelling; Soil phosphorous, Phosphorus transport; Grid Oriented Phosphorous Component

INTRODUCTION

Modelling of phosphorous (P) loss from agriculture land and its transport consists of two distinct parts. The first part deals with simulating most of the chemical transformations and movements in the soil phosphorous cycle, whereas the second part focuses on the transport of phosphorous over and beneath the land surface. According to Stevenson and Cole, (1999) soil P compounds consist of soluble inorganic and organic P, weakly adsorbed (labile) inorganic P, sparingly soluble P, insoluble organic P, strongly adsorbed and/or occluded P by hydrous oxides of Fe and Al, and fixed P of silicate minerals. The detached and dissolved P compounds from the parent material can be transported by storm runoff in which they normally exist in dynamic equilibrium between the dissolved and sediment-bound or particulate forms (Lee et al., 1989).

Mathematical models of the soil P movement are generally in the form of storage accounting procedures, however in a very limited number of models this movement has been modelled by a set of partial differential equations derived from the actual physical and chemical laws which describe the process. Albeit the aim of the equations is to model the subsurface P movement they can also be considered as a method of representing the change in storage of the P soil solution or the labile pool in a partial differential equation formulation. An example of a P movement model is the one developed by Shah et al., (1975). In their work material balance equations for water in the soil pore spaces, P in the liquid phase, and adsorbed P on the soil were formulated. These equations are solved numerically to simulate the P concentration profiles in the soil solution as a function of depth for an operating waste disposal system. In another attempt to model P movement in the soil, Enfield and Shew, (1975) compared two nonequilibrium models for solving (in time and space) the concentration change of P in the liquid phase. The difference between the two models is the approach of describing the kinetics of the sorption process. Although the dynamics of the soil P cycle has been described adequately in the SWAT model (Arnold et al., 1998), the relations in the model have not been formulated in partial differential form. Nevertheless these relations can be utilised to build a more mathematically sound model to simulate the soil P dynamics.

In most of the nonpoint pollution models overland flow transport of the detached P is generally described by empirical or crude relations. However one of the few comprehensive models to include a detailed model of overland flow was developed by Lee et al., (1989). That model considers the effects of advection, infiltration, biological decay and uptake, the kinetics of chemical desorption from the soil surface to storm water, the adsorption kinetics of dissolved phosphorous to sediment in runoff, and the dynamic changes of sediment size fractions on chemical transport.

The work represented here aims to improve the spatial resolution and the level of physical description in phosphorous modelling by the development of a grid-based distributed phosphorous modelling component to allow the modelling of phosphorous using fully distributed catchment models. In comparison to other models, the soil P representation in the SWAT model offers a fair accounting for most of the variables in the soil P cycle and it can provide an adequate estimate of P loads transported with the overland flow in dissolved or particulate forms. The mathematical models describing the transformation and the chemical processes of the different soil P variables in SWAT were used along with models from other sources to develop a Grid Oriented phosphorous Component (GOPC). The hydrological variables required to drive

the GOPC can be calculated using any distributed physically based model (DPBM) capable of producing a reasonable simulation of the flow fields in the catchment. These include, (i) for surface transport: overland flow depth, flow in the coordinate directions, sediment load, and sediment concentration and (ii) for subsurface transport: soil moisture and hydraulic head at various depths in the soil. This paper presents the phosphorous mathematical models in the GOPC including processes of P in both soil and overland flow.

MATHEMATICAL FORMULATION OF P PROCESSES IN THE GOPC

Quantifying the amount of P transported by the nonpoint sources pollution mechanism requires a calculation procedure that takes into account the soil P dynamics as well as the P transported by overland flow. Bearing this in mind, the GOPC is developed in such a way that can incorporate an accounting procedure for simulating the mass changes of P in the soil and the overland flow.

The basic concept in the GOPC is the mass balance which was employed to formulate mathematical equations for each of the state variables in the P estimation. As classified in the SWAT model (Arnold et al., 1998), the state variables of the soil P are: the soil soluble P (SSP), the fresh organic P (FROP), the fixed organic P (FXOP), the easily soluble inorganic P (ESIP), and the fixed or insoluble inorganic P (FIP). The FROP represents the organic matter that can be easily mineralised (e.g. manures, decayed plants, and microbial biomass) while the FXOP constitutes materials with slower rate of mineralisation. The inorganic phosphorous is divided into two types, the ESIP and the FIP (an assumption similar to that in SWAT model). The P in overland flow is carried in two forms, the dissolved P (DP) and the particulate P (PP) (Lee et al., 1989). Therefore in total there are seven P state variables of which two represent the P forms that exist in the overland flow. The interconnections between the soil P state variables and the overland P state variables as well as the external inputs of P material to the state variables are shown inside ellipses. Moreover the fluxes of P into and out of the storages are represented by arrows indicating the flux direction. Fluxes are denoted by the letter P with a subscript showing the origin and destination storages. The fluxes between the soil P state variables and those in the overland flow as well as external inputs of P are indicated by thick lines.

The general form of the mass balance equation (for each P state variables) is: the input fluxes minus the output fluxes for a particular storage. In mathematical form this can be demonstrated by the following general equation.

$$\frac{dP}{dt} = \text{Input } Pf\text{lux} - \text{output } Pf\text{lux}$$
(1)

When writing the mass balance equation for some of the P state variables, the fluxes between brackets represent processes of which one is the reverse of the other. Therefore one equation is used to simulate the net effect rather than the individual fluxes contributing to this net effect. Following are the equations of the seven state variables.

Soil Soluble Phosphorous(SSP)

$$\frac{\partial SSP}{\partial t} = P_{FP \to 1} + P_{DP \to 1} + (P_{21 \to 1} - P_{1 \to 21}) - (P_{1 \to 31} - P_{31 \to 1}) - P_{1 \to RU} - P_{1 \to LP} - P_{1 \to AD} - P_{1 \to DP}$$
(2)

$$\frac{1}{dt} = P_{MP \to 21} + P_{RD \to 21} - (P_{21 \to 1} - P_{1 \to 21}) - (P_{21 \to 22} - P_{22 \to 21}) - P_{21 \to PP}$$
(3)

Fixed Organic Phosphorous (FXOP)

$$\frac{dFOXP}{dt} = (P_{21 \rightarrow 22} - P_{22 \rightarrow 21}) - P_{22 \rightarrow PP}$$
(4)

Easily Soluble Inorganic Phosphorous (ESIP)

$$\frac{dESIP}{dt} = P_{PP \to 31} + (P_{1 \to 31} - P_{31 \to 1}) - (P_{31 \to 32} - P_{32 \to 31}) - P_{31 \to PP} - P_{31 \to DP}$$
(5)

Fixed Inorganic Phosphorous (FIP)

$$\frac{d\mathsf{F}\mathsf{IP}}{d\mathsf{t}} = \left(\mathsf{P}_{31\to32} - \mathsf{P}_{32\to31}\right) - \mathsf{P}_{32\to\mathsf{PP}} \tag{6}$$

Overland Flow Dissolved Phosphorous (DP)

$$\frac{\partial(y.DP)}{\partial t} = P_{1 \to DP} + P_{31 \to DP} + P_{RP \to DP} - P_{DP \to PP} - P_{DP \to BU} - P_{DP \to AD}$$
(7)

$$\frac{\partial(y.g.PP)}{\partial t} = P_{TSP \to PP} + P_{RP \to PP} + P_{DP \to PP} - P_{PP \to 31} - P_{PP \to AD}$$
(8)



Figure (1) Interactions between the soil P and the P transported in the overland flow

Most of the possible chemical and physical processes occurring to P in both the soil and the overland flow have been accounted for in the GOPC. Table (1) summarises the description of the P fluxes used in the mass balance equations along with their sources. The units of P state variables for all soil storages are mass per area while fluxes in and out of the same storages are in units of mass per area per time. For overland flow state variables units of mass per water volume are used for the DP storage whereas mass of P per mass of sediment particle are used for the PP storage. The fluxes in and out from the two overland storages are in the units of mass per area per time. To present equations (7) and (8) in units of mass of P per area per time, the rate of change of storage of DP is multiplied by the runoff water depth (y) while the PP rate of change of storage is multiplied by the concentration of the sediment (g) and runoff water depth (y).

AN EXAMPLE OF THE GOPC APPLICATION

The GOPC has been tested using an experimental catchment created (by the author) for the purpose of demonstrating the results. This example can also be considered as a verification to the conceptual representation of the GOPC. The fully distributed physically-based hydrological SHETRAN model (Ewen et al., 2000) has been used in the example to obtain the flow and sediment variables required by the GOPC. As illustrated in fig. (2) the catchment was assumed to be comprised of five grid elements (shown in the boxes numbered from 1 to 5) and five river links (shown as arrows).

In order to test the performance of the GOPC in simulating the soil P variables, when fertiliser over the catchment has been applied during a rainfall event, two hydrological extreme situations can be considered. The first situation occurs if the element is very dry and any rainfall water reaching the soil is lost by infiltration and accordingly no overland flow depth results. Conversely in the second situation the soil is wet enough to allow significant overland flow depth to be produced.

1E: Water Resources Management

To achieve both situations in the catchment, the hydrological properties (elevations, hydraulic conductivity, etc.) and the initial conditions (soil moisture content, overland flow depth, etc.) of the grid elements have been defined in such a way that either of the two situations occurs in any element. The reason for this set up is to explore the effects of the continuous and the pulse applications of fertiliser on some of the soil P variables. The rainfall input to the catchment was assumed to be a constant value of 0.8mm/hr for a period of 14hrs whereas two cases of fertiliser inputs were investigated. In case (1) constant fertiliser application of 10gP/n² for a period of 14hrs was assumed while in case (2) a pulse input of 10gP/n² was applied at the first hour only. Furthermore the initial values for the soil P variables are all set to zero.

Flux	Description of the flux			
	Input of fertiliser to the SSP storage (1)			
$P_{DP \rightarrow 1}$	Infiltration of DP from the overland flow into the soil (2)			
$(P_{21\rightarrow1} - P_{1\rightarrow21})$	Mineralisation /Immobilization processes (3)			
P _{1→RU}	Root Uptake of P from the SSP (4)			
P _{1→LP}	Loss of SSP by the leaching process (5)			
P _{1→DP}	Dissolution of SSP in the surface overland water (3)			
$P_{1 \rightarrow AD}$	Advection transport of SSP (1)			
$\left(P_{1\to31}-P_{31\to1}\right)$	Adsorption/desorption processes (3)			
$P_{MP \rightarrow 21}$	Input of Organic Manure P to the FROP (1)			
$P_{RD \rightarrow 21}$	Input of P the decayed roots to the FROP (1)			
$P_{21\rightarrow 22}$	Decaying of the FROP that added to the FXOP (3)			
P _{22→21}	Decomposing of the FXOP that added to the FROP (3)			
P _{21→PP}	Input from the soil FROP detachment to the PP (1)			
$P_{22 \rightarrow PP}$	Input from the FIP detachment to the PP (1)			
$P_{PP\to31}$	Input of the PP deposition from overland flow water to the ESIP storage (2)			
$(P_{31\rightarrow32} - P_{32\rightarrow31})$	Precipitation/desorption processes between the ESIP and the FIP (3)			
P _{31→PP}	Input from the ESIP detachment to the PP (1)			
P _{31→DP}	Desorption of ESIP that enters the overland flow DP (2)			
$P_{32 \rightarrow PP}$	Input from the FXOP detachment to the PP (1)			
P _{RP→DP}	Input of P from the rainfall water to the overland flow DP (2)			
$P_{DP\toPP}$	Adsorption of the overland flow DP into the overland flow PP (2)			
P _{DP→BU}	Loss of the overland flow DP due to biological uptake (2)			
$P_{DP\toAD}$	Advection of the overland flow DP (2)			
$P_{TSP \to PP}$	Total input from the soil detached P to the overland flow PP (3)			
P _{RP→PP}	Input of P from the rainfall to the overland flow PP (2)			
$P_{PP \rightarrow AD}$	Advection of the overland flow PP (2)			

Table (1) Description of the phosphorous fluxes in GOPC

Sources of the flux equations used in the GOPC: (1): Proposed by the first Author, (2): GRAPH model (Lee et al., 1989)(3): SWAT model (Arnold et al., 1998), (4): HSPF model (Donigian et al., 1984), (5): Oddson, et al., (1970).

0	0	0	0	0
0	8	5	0	0
0	2	3	4	0
0	8	1	8	0
0	0	0	0	0

Figure (2) Shape of the catchment which has been used to test the GOPC

On running the hydrological model (SHETRAN) on the catchment, a significant water depth (>0.005m) resulted in elements 2, 4, and 1 while the remaining two elements (3, and 5) recorded a practical zero water depth (<0.005m). It was assumed that the applied fertiliser contained mainly inorganic P added to the SSP and ESIP with an equal amount throughout the simulation period. This in turn would affect the inorganic related soil P variables (SSP, ESIP, and FIP) in each of the catchment elements. When applying the GOPC, the parameters have been chosen so that the dissolution of the SSP in the runoff water is the major P loss mechanism. As a demonstration the results of the GOPC application is presented for elements 5 and 2 only. Fig. (3) and (4) show the results of the SSP, ESIP, and FIP simulation in element 5

1E: Water Resources Management

for cases (1) and (2) of the fertiliser application respectively. Whereas fig. (5) and (6) show the results of three soil P variables in addition to the water depth in element 2 for cases (1) and (2) of the fertilis er application respectively. It is expected that there will be a constant increase in the storages of the SSP, ESIP, and FIP when there is continuous fertiliser application without experiencing any loss by any of the nonpoint mechanisms. Fig. (3) confirms this and as it has been shown that during the first period (up to 4hrs) the SSP and ESIP increase equally since they both received the same amount of fertiliser. The FIP has also increased but with slower rate since the only source of P to this form is the transformation of the ESIP. There were also transformations occurring between SSP to ESIP and vice versa (desorption/adsorption) and the rate of these transformations can be equal when both the P forms have same amount (this is another reason for getting typical values of SSP and ESIP at the beginning of the simulation). However the ESIP started in deviation from the SSP when the FIP amount increased significantly as more ESIP transforms into FIP. Fig. (4) shows the effect of the dissolution loss of P from the catchment on the three soil storages for the case of continuous application of fertiliser. The rate of increase of the water depth as obtained from the hydrological model was somehow exponential until it reaches the significant water depth for the dissolution to occur which was assumed to be 0.005m. Therefore the graphs of the three storages followed the same patterns as those in fig. (3) up to the point when the water depth became effective (approximately at about 12 hr). Before reaching this effective depth the increase of water depth influenced the SSP earlier at around 2hr when the SSP started to decrease. The drastic decrease in all the three variables was coincident with the point when the water depth has become effective (0.005m). At this point there was an abrupt decrease in the curves of the three variables as there are inter relationship between them. After the dissolution loss has commenced, any further addition of P to SSP was lost immediately and hence the values for three soil P variables were practically zero.





Figure (3) GOPC results of SSP, ESIP, and FIP for element 5 - case (1) of fertiliser application

Figure (4) GOPC results of D, SSP, ESIP, and FIP for element 2 - case (1) of fertiliser applicationr

The effect of the pulse fertiliser input on the three soil P variables was demonstrated in fig. (5) for element 5 and fig. (6) for element 2. As shown in fig. (5) when there was no enough water for the dissolution loss to occur, the SSP had a high value at the beginning due to the application of pulse input of fertiliser. Afterwards and as the addition of fertiliser stopped at the beginning this variable showed a small decrease in its values with time. The effect of the pulse fertiliser input on the ESIP at the beginning was similar to SSP, however since ESIP represents the source for FIP its values continued to decrease with similar rate of increase in the FIP. The shape of the graphs for the three soil P variables in fig. (6) for the case of pulse input of fertiliser on element 2 and with increasing water depth with time were typical to those in fig. (4) where there was continuous application of fertiliser. The reason for that is the dissolution loss in this case had same effect as in the case of continuous fertiliser application. The only difference is that there was no accumulation in the SSP and ESIP storages and therefore the initial sotrages created by the pulse input of fertiliser were diminished by the dissolution loss.

CONCLUSIONS

A component for modelling soil phosphorus dynamics, soil phosphorus loss, and overland transport of phosphorus has been developed. This component can be coupled with any fully distributed physically-based hydrological model which provides the required hydrological variables. The representation of the soil phosphorus state variables in SWAT model and the overland phosphorus state variables in GRAPH model were adopted to build the structure of the GOPC. The chemical processes occurring to the various phosphorus state variables were accounted for in the GOPC using equations from existing models.

Several outputs can be obtained from the GOPC making it an efficient tool in the phosphorus modelling. However in this paper the performance of the GOPC in simulating three of the soil phosphorus variables (SSP, ESIP, and FIP) for two elements of an experimental catchment of five elements (created for demonstration purposes) was presented. The catchment has been subjected to two cases of fertiliser inputs (continuous and pulse) and the results from the GOPC for both cases were in agreement with what can be logical. An application of the GPOC on an Irish catchment (Clarianna in

county North Tipperary) can be found in the paper (Modelling phosphorous loss from agriculture catchments: a comparison of the performance of SWAT, HSPF and SHETRAN for the Clarianna catchment by Nasr et al., (2003)).

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