



# Evaluation of different approaches to describe the sorption and desorption of phosphorus in soils on experimental data



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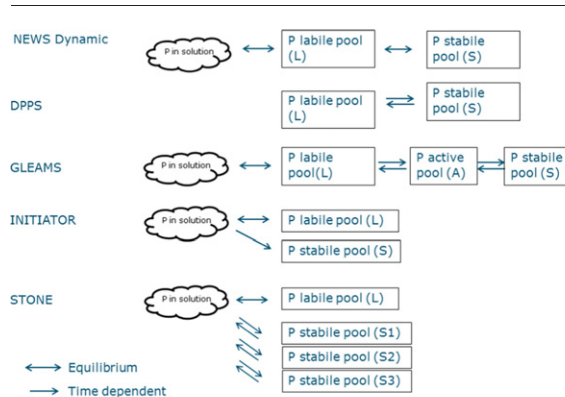
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## HIGHLIGHTS

- Five phosphate models with increasing complexity were compared with observations in P addition and P mining experiments.
- Model performance using site specific data compared well with observations for the included sand, clay and peat soils.
- Models with equilibrium and rate limited sorption performed better on P mining experiments than equilibrium only models.
- Model performance strongly reduced when using generic data, specifically for mining experiments and for peat soils.
- Models of intermediate complexity, with equilibrium and rate limited sorption, seem most suited for regional application.

## GRAPHICAL ABSTRACT



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## ABSTRACT

Phosphorus is an essential element to enhance the needed increase in crop production in the forthcoming century. On the other hand environmental losses of phosphorus cause eutrophication of surface waters. Both problems call for reliable models to predict the behaviour of phosphorus in agricultural soils. In this study the performances of five different sorption approaches were evaluated. The ultimate aim was to identify the most suitable concept for large scale predictions of P dynamics in soils, in terms of a high comparability between observations and predictions with a minimum amount of input data. The model results were compared with unique data from long term (10–15 years) experimental field studies of grassland including situations with P mining, equilibrium P fertilization and P surpluses and a pot experiment with P mining. The model performance was evaluated while using site specific constants and generic constants for adsorption and desorption. Three rate limited models (DPPS, INITIATOR and ANIMO) showed good performance when site specific constants were used but the performance of the equilibrium model (NEWS-Dynamic) was reasonably comparable. Model performance was better for experiments with a P surplus than for P mining and was also better for sandy soils as compared to clay and peat soils. However, long term desorption rates had to be calibrated for each application rate. The performance of all models declined when generic data were used. We conclude that none of the included models properly describe what happens when the soil changes its P status, considering that parameterization needs to

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be treatment-specific to obtain reliable predictions. Considering this flaw, models of intermediate complexity, including both equilibrium and rate limited sorption, and a limited data demand, like DPPS and INITIATOR, seem most suited for regional model application.

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## Annex on abbreviations

### Equilibrium constants and related parameters (not used in DPPS)

|                                     |   |
|-------------------------------------|---|
| $K_L$                               | Langmuir affinity constant ( $\text{m}^3 \text{mol}^{-1}$ )                               |
| $K_{F,i}$                           | Freundlich constant of a stable pool $i$ ( $\text{mmol kg}^{-1}(\text{mg l}^{-1})^{-n}$ ) |
| $\text{Al} + \text{Fe}_{\text{ox}}$ | Oxalate extractable Al and Fe contents ( $\text{mmol kg}^{-1}$ ).                         |
| $\beta$                             | Ratio of maximum labile P pool size to oxalate extractable Al and Fe contents             |

### Pool sizes

|       |  |
|-------|--|
| $L$   | size of the labile P pool ( $\text{mmol kg}^{-1}$ ).   |
| $L_m$ | maximum size of the labile P pool ( $\text{mmol kg}^{-1}$ ),                                     |
| $A$   | size of the active P pool ( $\text{mmol kg}^{-1}$ ); only in GLEAMS                              |
| $S$   | size of the stable P pool ( $\text{mmol kg}^{-1}$ ); ANIMO has three stable pools, S1, S2 and S3 |

### Sorption and desorption rate constants (not used in NEWS-dynamic)

#### DPPS

|            |  |
|------------|--|
| $\mu_{LS}$ | rate constant for the P transfer from the labile pool L to the stable pool S ( $\text{d}^{-1}$ ) |
| $\mu_{SL}$ | rate constant for the P transfer from the stable pool S to the labile pool A ( $\text{d}^{-1}$ ) |

#### GLEAMS

|            |   |
|------------|---|
| $\mu_{LA}$ | rate constant for the P transfer from the labile pool L to the active pool A ( $\text{d}^{-1}$ ). |
| $\mu_{AS}$ | rate constant for the P transfer from the active pool A to the stable pool S ( $\text{d}^{-1}$ ). |

#### INITIATOR/ANIMO

|                      |  |
|----------------------|--|
| $\mu_{\text{DisSi}}$ | rate constant for the P transfer from soil solution Dis to a stable pool $i$ , Si ( $\text{d}^{-1}$ )      |
| $\mu_{\text{SiDis}}$ | rate constant for the P transfer from a stable pool $i$ , Si, to the soil solution Dis ( $\text{d}^{-1}$ ) |

## 1. Introduction

A strong increase in food production is needed to feed the projected world population in 2050 (FAO, 2009) and to cope with the increasing demand for biofuels. Phosphorus (P) is an essential element to sustain and/or increase plant growth (Von Liebig, 1841). The world amount of phosphate ore is limited and studies indicate that the availability of P may limit the growth of the agricultural production in the forthcoming decades (Cordell et al., 2009) or centuries (Syers et al., 2011; van Vuuren et al., 2010; Scholz and Wellmer, 2013) although others found that past depletion concerns were refuted by means of new resource appraisals (Ulrich and Frossard, 2014). On the other hand the use of P in intensive

agriculture has led to accumulation of P in soils (Csatho and Radimsky, 2009) and losses to surface waters causing eutrophication of the aquatic environment (Rabalais et al., 2002; Selman et al., 2008). An improvement of the resource use efficiency of P is thus essential for a sustainable world food production (Sutton et al., 2013). Simulation models are needed to predict the availability of P in agricultural soils and P losses to the environment in the forthcoming decades and to obtain insight in options for improving the resource efficiency of P in the food chain. The P availability in soil is strongly determined by the binding and resulting accumulation of P in the soil. The binding of P to the soil is due to various processes, including fast and reversible adsorption on soil particles and various slower rate limited (time dependent) processes, described as solid state or slow diffusion, diffusion-precipitation or fixation (see e.g. Schoumans, 1995, 2013, 2014). A wide range in models exists to describe this complex range of processes (McGechan and Lewis, 2002).

Most models have been developed to make predictions for limited areas like a field, a catchment or a region (Lewis and McGechan, 2002). These models generally include a fairly complex description of the sorption of P in the soil to describe the accumulation or depletion of P in the soil due to either over- or under fertilization and losses by erosion and leaching (McGechan and Lewis, 2002). Models that are used on a larger regional to global scale generally use a less complex process description for the dynamics of P accumulation. Examples of such models are ANIMO (Groenendijk and Kroes, 1997), INITIATOR (De Vries et al., 2005) and GLEAMS (Tattari et al., 2001; Larsson et al., 2007) for use on a regional to national scale and DPPS (Wolf et al., 1987; Sattari et al., 2012) and an adapted version of Global NEWS (Mayorga et al., 2010) including P dynamics (Strokal and de Vries, 2012) for use on a global scale. The main differences between the models is the complexity of the description of the adsorption and desorption processes, in terms of the use of equilibrium (NEWS-Dynamic) or time-dependent descriptions of the sorption reactions (all other models) and the number of P-pools in the soil (two in DPPS and INITIATOR, three in GLEAMS and four in ANIMO). At present little information is available on the needed model complexity to simulate the behaviour of P in the soil under field conditions both in case of net P addition and P mining.

In this paper we evaluate the performance of different sorption models in the above mentioned five large scale models (NEWS-Dynamic, DPPS, INITIATOR, GLEAMS, ANIMO). This was done by comparing the simulated P behaviour with observations in long term experimental field studies and in a pot experiment. In performing the comparison, use was made of site specific (Langmuir) adsorption constants and calibrated rates for rate limited desorption. Site specific sorption constants are, however, generally not available when studying the fate of phosphorus on a regional scale. We therefore also evaluated the model performance using generic sorption constants, neglecting the available information for site specific parameterisation. The ultimate aim was to identify the most suitable concept for a large scale prediction, defined as an acceptable description with a minimum amount of input data, of P dynamics in soils. The novelty of this study is that we compared the performances of the five different sorption approaches with unique data from long term (10–15 years) experimental field studies including situations with P mining, equilibrium P fertilization and P surpluses.

## 2. Material and methods

### 2.1. Data sets

To test the selected models, two datasets of long-term experiments on grassland were used. The first dataset was from a long term field

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