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Linking Measurable Phosphorus Pools With Simulations of Soil P Dynamics: Results for the Long-Term Experiment 'Rostock'

Michael Herbst[1] | Gihan Mohammed[1] | Bettina Eichler-Löbermann[2] | Wulf Amelung[1,3] | Jan Vanderborght[1] | Nina Siebers[1]

[1]Agrosphere Institute, IBG-3, Forschungszentrum Jülich GmbH, Jülich, Germany | [2]Agronomy and Crop Science, University of Rostock, Rostock, Germany | [3]Institute of Crop Science and Resource Conservation, Soil Science and Soil Ecology, University of Bonn, Bonn, Germany

Correspondence: Michael Herbst (m.herbst@fz-juelich.de)

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ABSTRACT

Phosphorus (P) is removed from agroecosystems through harvesting, and sustainable management must include P fertilization as P availability affects crop performance. However, accurate assessment of plant-available P is challenging. In this study, two promising approaches are combined to assess the plant-available P of a 22-year long-term experiment (LTE) near Rostock, Germany. We hypothesize agreement between a modern P test method and process-based model estimates of plant-available P. The diffusive gradients in thin films (DGT) technique offers an accurate P test method because it mimics the diffusion and desorption of soil P in the presence of root uptake. This was applied in a synergetic combination with a state-of-the-art agroecosystem model that was extended with a P cycling module. The simulations and yearly DGT-P analyses comprise 4 treatments: no P fertilization, mineral P fertilization with triple-superphosphate, organic P fertilization with compost, and mineral plus organic P fertilization. Soils at 0–30 cm depth were sampled in four replicates on a yearly basis between 1999 and 2021. In addition, a P fractionation was applied for 2015 using the Hedley approach, which made it possible to link non-plant-available, steady P fractions with the respective model pools. The comparison between DGT-P determined plant-available P up to a depth of 30 cm and that estimated from the pools of the agroecosystem model AgroC showed agreement with respect to the differences between the treatments and with respect to the temporal evolution (R^2 between 0.65 and 0.7). Less agreement was detected for DGT-P and the respective model pools in deeper soil. A closer match over soil depth was found between grouped Hedley P fractions and AgroC model pools. Both, model and DGT-P analyses indicate that a new plant-available P equilibrium will be established under the new P management after about 12 years for the Rostock site, which points to the resilience of P cycling in agroecosystems. We conclude that the combined application of DGT-P analysis and agroecosystem modeling offers a robust and accurate quantification of plant-available P in the plough layer and can be used to create an agricultural digital twin with respect to soil P availability and its impact on crop yield.

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Summary

- Combination of P-test data with process-based agroecosystem model AgroC.
- Diffusive thin gradient determined labile P at 0–30 cm depth agrees with model pools over time.
- Diffusive thin gradients P variations of fertilization treatments correspond to model estimates.
- New plant-available phosphorus equilibrium established after about 12 years.

1 | Introduction

The accurate assessment of plant-available phosphorus (P) is difficult, because its concentration depends not only on the amount of total P in soil, but also on its bioavailability, bioaccessibility, mobilization kinetics, diffusion gradients, distances, and pathways to the root surface (Weihrauch and Opp 2018). All of these processes additionally change over time, as does the P demand of the plant and its climate-controlled uptake rates (Khan et al. 2023). Furthermore, the bioavailability of P in soil is affected by the crops cultivated (Pearse et al. 2006; Eichler-Löbermann et al. 2021). The P removed from the soil via harvest must be replaced. The amount of fertilizer required to maintain a nutrient level can be calculated with fixed crop-specific P removal values or soil-specific tabulated estimates. A modern alternative for optimized P fertilization could rely on agricultural digital twins.

With a perspective toward digitization in agriculture, agricultural digital twins have the potential to push the limits with respect to decision-making, support, and automation over a wide range of agricultural activities (Pylianidis et al. 2021). Digital twins are defined as synchronized virtual replicas of physical systems. The idea behind linking soil P test data with model estimates is to develop a blueprint for agricultural digital twins with respect to soil phosphorus dynamics and its impact on crop yield. An important step in the design of digital twins is the information flow from the physical to the virtual domain (Purcell and Neubauer 2023). At this point, it is not clear how classical or more modern experimental information on soil P availability to crops could automatically flow into a digital twin.

Over the years, a suite of P-tests with various advantages was developed (Nawara et al. 2017). For an accurate estimation of the available soil P, modern methods like the diffusive gradient in thin films technique (DGT) have evolved (Degryse et al. 2009; Kruse et al. 2015). In comparison to the batch techniques, such as double lactate or calcium acetate lactate methods and sequential extraction schemes of P pools in soil (Hedley et al. 1982; Cross and Schlesinger 1995), the DGT technique has advantages in assessing plant-available P by simulating the behavior of plant roots at the soil-solution interface. DGT-P has proven to be a valid indicator of plant-available P to crop growth in a range of studies (Mason et al. 2010; Nawara et al. 2017; Siebers et al. 2021).

In addition to the directly plant-available P, the amount and depth-specific distribution of the more stable P in the soil profile plays a role in the long-term perspective of P availability (Koch et al. 2018). Under fertilization, vertically stratified accumulation of P in the topsoil and depletion of P in deeper soil layers may occur. In case of reduced liquid-phase P concentrations, a desorption of P from stable pools may also be relevant in subsoils (Siebers et al. 2021). Bauke et al. (2018) applied Hedley fractionation and found for two LTEs that subsoil P stocks are used efficiently only when topsoil plant nutrient status is sufficient. Even though the Hedley fractionation is a commonly applied experimental procedure, it has been criticized for unreliable separation of organic and inorganic P and for not differentiating sorbed from “solid” pools (Klotzbücher et al. 2019; Barrow et al. 2021).

The accurate digital simulation of plant-available P is sensitive to the choice of the mineral P sorption concept. Physicochemical sorption approaches using Temkin, Freundlich, or Langmuir isotherms assume instantaneous equilibrium. Operating with P pools of different availability facilitates the inclusion of rate-limited steps for desorption and diffusion (McGechan and Lewis 2002). This helped in conceptualizing mineral sorption of P by fast sorption kinetics and slower desorption terms as suggested by Jones, Cole, et al. (1984), who further suggested differentiating between a labile, an active and a stable mineral P pool. This concept has finally become the basis for a substantial number of models, like EPIC (Williams et al. 2015) as a precursor of GLEAMS (Knisel et al. 1993) or RZWQM2-P (Sadukhan et al. 2019).

In general, P-test information can be used to initialize, calibrate, and validate (Lychuck et al. 2021) P pools in models. Jones, Sharpley, and Williams (1984) used the empirical functions established by Sharpley et al. (1984) to positively validate the model-based estimation of labile P over time with Bray P, Olsen P, and double acid extractable P for various LTEs in the United States. Similar approaches that rely on the assimilation of DGT-P measurements or Hedley fractionation data (Hedley et al. 1982) into digital models, however, are still lacking.

The extended AgroC model applied in this study enables the simulation of the entire P cycle of agroecosystems, including P sorption/desorption, uptake by crops, and mineralization of organic P (Mohammed et al. 2024). In combination with the application of the convection–dispersion equation for variably saturated solute transport in soil, this allows for a precise estimation of the liquid-phase P concentrations within a 1-dimensional soil column. This combination with the implemented pool concept for sorption/desorption is rarely found (Vogel et al. 2024), but it represents the most suitable model to combine with DGT-P measurements. A model with comparable features that we are aware of is the Agricultural Nitrogen Model (ANIMO) developed by Groenendijk and Kroes (1999).

A limitation of P uptake will affect the overall biomass increase and potentially reduce yield (Mason et al. 2010). For a new development, such as the AgroC P module, it is relevant to test the simulated response of biomass and crop yield to a potential P uptake limitation for a range of P fertilization levels and types.

Within this study the following hypotheses were investigated: (i) the transient behavior of DGT-P measurements is consistent with that of the plant-available model pool for various P fertilization

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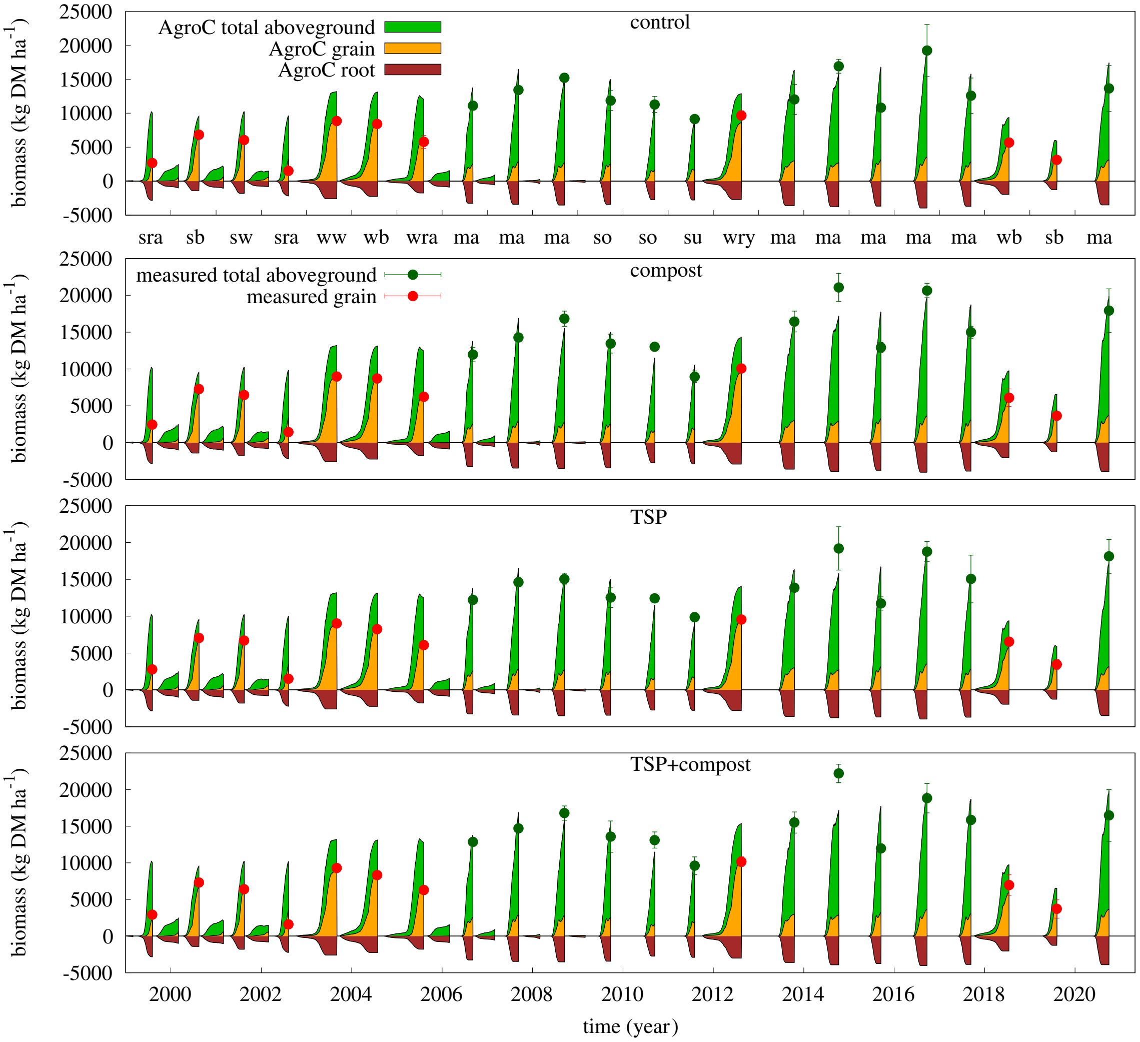

FIGURE 1 | Simulated (filled curves) and measured (points ± standard deviation) harvest biomass for control, compost, TSP (triple superphosphate), and TSP + compost treatment. Crop rotation is indicated in the uppermost panel, where sra = spring rape, sb = spring barley, sw = spring wheat, ww = winter wheat, wb = winter barley, wra = winter rape, ma = maize, so = sorghum, su = sunflower, and wry = winter rye.

treatments; (ii) a link exists between P fractions and model pools over soil profile depth; (iii) the experimentally determined effect of P availability on crop growth is reflected similarly in P model pools and results.

2 | Materials and Methods

2.1 | Study Site “Stover Acker,” Rostock

The LTE site “Stover Acker” (54°3′41.47″ N, 12°5′59″ E) is located near Rostock, Germany (Eichler-Löbermann et al. 2021). According to the World Reference Base for Soil Resources, the soil is classified as a Stagnic Cambisol. Soil texture is loamy sand with clay, silt, and sand fractions of 9%, 26%, and 65%, respectively. Cation exchange capacity in the upper 30 cm is 6.7 ± 1.0 cmol+ kg^{-1}. The maritime climate is characterized by an average precipitation of 642 mm yr^{-1}, and an average 2-m air temperature of 9.31°C. Both averages were computed from on-site measurements over 22 years covering the experimental period 1999 to 2021.

In this study, we focus on four LTE treatments: fertilization with triple superphosphate only (TSP), biowaste compost only (compost), TSP plus compost (TSP + compost), and the control treatment without any P fertilization. Treatments were established as randomized split-plots with subplots of 120 m^2 each in four replications (Hu et al. 2022). All treatments were supplied with potassium, magnesium (Mg), calcium (Ca), and micronutrients. Mineral nitrogen (N) fertilizer doses varied between 30 and 120 kg ha^{-1} for a single application to avoid N limitation on crop growth (Koch et al. 2018; Requejo and Eichler-Löbermann 2014). TSP fertilization was applied on a yearly basis at 21.8 kg P ha^{-1} until 2013. Starting in 2014, the mineral P input was adjusted to 30 kg P ha^{-1}. Biowaste compost was applied every third year, with dry matter (DM) amounts varying between 12.7 and 38.4 t DM ha^{-1}. The crop rotation is given in Figure 1 and Table S1. The total P concentration in the compost was measured for each application and varied between 0.14% and 0.26% of fresh matter. This resulted in organic P amendments varying between 44 and 151 kg P ha^{-1} for a single application. Within the Rostock LTE, for spring rape and all cereals, only the grains were harvested.

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Subsequently, grain biomass and P content were determined. Leaves and stems were left on the field as harvest residue. In contrast, for maize, sunflower, and sorghum, the entire aboveground biomass was harvested, and only 10 cm of the stem remained on the field (Zicker et al. 2018). Biomass and P content of the entire harvested aboveground biomass was measured for maize, sunflower and sorghum.

The Rostock site is perfectly flat. Lateral P transport by surface runoff is negligible (Zicker et al. 2018). The measured soil P balance (P_{BAL}) at this site was computed as:

$$P_{BAL} = P_{fert} - P_{rem} - P_{leach} \tag{1}$$

where P_{fert} is the amount of fertilizer applied, P_{rem} is the P taken up by crops and removed as harvest product, and P_{leach} is the P leaching. Since leaching measurements were not available, the study site average of the AgroC simulated leaching at 120 cm depth of 0.22 kg ha^{-1} yr^{-1} was also assumed for the computation of the measured P balance.

2.2 | Soil P Fractions and DGT

Soil sampling of the 0–30 cm plough horizon for DGT analyses was performed on a yearly basis, usually during February/March. One exception was the sampling performed in August 2002. Three replicates were sampled for each treatment, and soil samples were air-dried for further analysis. Diffusive gradients in thin films were analysed with a standard procedure described in Supporting Information S1 and Siebers et al. (2021). The DGT-P concentrations measured in the eluent were determined at 100% water holding capacity, which prohibits a direct quantitative comparison to simulated liquid-phase concentrations of the unsaturated soil.

Koch et al. (2018) used soil sampled on April 29, 2015, for a modified sequential fractionation method according to Hedley et al. (1982). In short, consecutive extractions were carried out using: (1) resin, (2) 0.5 M $NaHCO_3$, (3) 0.1 M NaOH, and (4) 1 M H_2SO_4. The interpreted P fractions adhered to the recommendations of Hedley et al. (1982). $NaHCO_3$-P_i and $NaHCO_3$-P_o represent labile inorganic and organic bicarbonate P. NaOH-P_i and NaOH-P_o represent moderately labile inorganic and organic P sorbed and/or fixed by aluminum- and iron-(hydr)oxide, as well as P in humic and fulvic acids being potentially bioavailable. The H_2SO_4-P fraction represented insoluble (stable) P associated with Ca and Mg minerals in occluded or non-occluded forms.

2.3 | AgroC

AgroC is a one-dimensional agroecosystem model (Herbst et al. 2008; Klosterhalfen et al. 2017), based on three main modules for the simulation of soil water, heat, solute, and CO_2 flux (SoilCO$_2$; Simunek and Suarez 1993), crop growth (SUCROS; Spitters et al. 1989), and soil C turnover (RothC; Coleman and Jenkinson 2008). It was extended with a P module, which accounts for fertilization, convective–dispersive transport in the soil, sorption to an active and a stable P pool (Jones, Cole, et al. 1984), root uptake, the effect of P limitation on crop growth (Williams and Izaurralde 2008) as well as mineralization and immobilization of organic P (see Figure S1). The latter is closely linked to the turnover of organic carbon (C) and N following the approach suggested by Vereecken et al. (1991). We assumed that 20% of the organic P amendment was mineral and directly fed the liquid-phase pool (Mohammed et al. 2024).

The numerical mass error related to the total amount of P in the system at the last time step was −0.441%, 0.029%, −0.442%, and 0.029% for the TSP + compost, TSP, compost, and control treatment, respectively. We consider this range as acceptable for reactive solute transport simulations in unsaturated porous media.

The phosphorus available for plant uptake is assumed to be mobile in the soil. The concentration of P in the pore water P_{lab} [M P L^{-3} water] is simulated with the Convection–Dispersion equation. Fertilizer application, plant uptake, and leaching are computed with the solute transport module available in the HYDRUS-1D Version 4.17 (Simunek et al. 2013). One major process of P cycling in soils is sorption. AgroC simulates the sorption of labile P into mineral P pools, active P_{ACT} [M P L^{-3} soil] and stable P_{STAB} [M P L^{-3} soil], as suggested in the mineral P cycling approach of Jones, Cole, et al. (1984). This approach is based on instantaneous equilibrium and sorption/desorption rates between the labile P pool and the active P pool, and between the active P pool and the stable P pool. The equilibrium between P_{lab} and P_{ACT} is given as:

$$P_{lab} \times \theta = P_{ACT} \times \frac{PSP}{1 - PSP} \tag{2}$$

where θ is the soil water content, required to convert from the liquid-phase concentration to the soil volume related concentration of P_{ACT}, and PSP [—] is the non-sorption coefficient, defined as the fraction of P that remains labile. In case of mass transfer to P_{ACT}, the mass is added to the P_{ACT} pool and removed from P_{lab}, which is performed as a source/sink term. The direction of mass transfer reverses when $P_{lab} \times \theta$ is smaller than $P_{ACT} \times PSP/(1 - PSP)$. In that case, the reverse exchange is assumed to be much smaller, and mass transfer is scaled down with the reverse rate modifier R_{rev} (default value = 0.1, Williams and Izaurralde 2008). At equilibrium, P_{STAB} is assumed to be larger than P_{ACT}, and the corresponding exchange rate between the active and the stable P pool $R_{ACTSTAB}$ [M P L^{-3} T^{-1}] is given as:

$$R_{ACTSTAB} = b_0 \times \left(Q_{STAB/ACT} \times P_{ACT} - P_{STAB}\right) \tag{3}$$

where b_0 [T^{-1}] is an exchange rate coefficient and $Q_{STAB/ACT}$ is the stable to active pool ratio (default value = 4). The mass of P transferred via $R_{ACTSTAB}$ is added to the P_{STAB} pool and removed from P_{ACT}. Again, a reverse exchange, given when $P_{STAB} > Q_{STAB/ACT} \times P_{ACT}$, is assumed to be slower and is scaled down with R_{rev}. Parameters PSP, $Q_{STAB/ACT}$, R_{rev}, and b_0 are material-specific model inputs. PSP (between 0.05 and 0.75) can be calculated from the pedotransfer functions suggested by Jones, Cole, et al. (1984). Parameter b_0 is 0.0076 for calcareous soils or $= \exp^{(-1.77 \times PSP\ -7.05)}$ for all other soils.

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2.4 | Model Inputs

Potential grass reference evapotranspiration was computed with the Penman–Monteith approach as proposed by Allen et al. (1998). The required meteorological information was provided by an on-site station maintained by the University of Rostock. Gaps in the meteorological data, occurring mainly for the 1999 to 2004 period, were filled by establishing regressions to the measurements performed by the German Weather Service (DWD) at Warnemünde station, located about 12 km apart.

Spatial discretization in the vertical is generally 1 cm and decreases to 0.1 cm near the soil surface. Depth-specific soil hydraulic properties (Table 1) were estimated from soil texture, bulk density, and organic C content as reported by Koch et al. (2018), applying the Pedotransfer functions of Weynants et al. (2009) and Weihermüller et al. (2017). The measured depth-specific organic C stocks were used to infer the initial organic C pools. Assuming an equilibrium state, the Pedotransfer functions of Weihermüller et al. (2013) were used to estimate the reactive initial organic C pools. The corresponding initial organic N pools were estimated from the respective initial organic C pool using the measured C/N ratio varying between 9.1 and 11.4 over depth (Koch et al. 2018). Analogously, the initial organic P pools were determined, assuming medium nutrient-rich organic matter with a C/P ratio of 150, which is in the lower range of soil organic C/P ratios between 62 and 919 reported by Tipping et al. (2016). This procedure was required to provide a consistent C:N:P stoichiometry for each initial organic pool. Total initial organic C, N, and P stocks at the beginning of the simulation period in January 1999 are summarized in Table 1. The initial mineral P pools, as defined by Jones, Cole, et al. (1984) were first derived from spin-up runs, where the simulation-period crop rotation, fertilization, and meteorological data was looped 10 times, covering a period of 220 years. This provided equilibrium states for the soil mineral P pools over soil depth. However, the initial labile pool estimated for the 0–30 cm layer was low and thus manually adjusted to match the measured DGT-P concentrations for the TSP-compost treatment over the first years of the experiment. Initial mineral P pools are summarized in Table 2. Please note, all treatment models were initialized with identical values regarding organic C, N, and P pools, as well as with respect to the mineral P pools and soil hydraulics.

The default SUCROS parameter sets for most crops (all cereals and maize) were available as compiled by Vanclooster et al. (1994). For rape, sorghum, and sunflower, parameter sets did not exist. In that case, available parameter sets were modified with literature values (Brogi et al. 2020).

2.5 | Model Calibration/Inversion

All calibrations and inversions were exclusively performed with the TSP + compost treatment model. This allowed for a calibration/inversion where processes related to both fertilization types were involved. After calibrating/inverting photosynthesis, crop P demand, and P sorption parameters for the TSP + compost model, the parameter sets were used in a forward manner to the other three treatments. The model inputs only differ in terms of the organic or mineral fertilization inputs specific to that treatment.

In a first step, the optimum photosynthesis parameter A_{max} was manually adjusted for each crop type to match the measured harvested biomass. During the manual calibration of the crop-specific P demand, it appeared impossible to simultaneously match the P removed by maize harvest for the 2006 to 2010 period and the second maize cropping period from 2013 to 2017. The maize variety changed from the first period to the second period. The measured average P content was 2.2 g P kg^{-1} DM and 1.3 g P kg^{-1} DM for the first and the second period, respectively. Thus, two P demand parameters, XPC_{tot} (see Equation S5), were inverted for maize from the measured P removal. We used the downhill simplex algorithm (Nelder and Mead 1965) to invert AgroC.

Thereafter, the stable to active pool ratio $Q_{STAB/ACT}$ (see Equation 3) was manually adjusted to achieve agreement between measured and estimated total soil P. In the last step, the inversion algorithm was also applied to estimate the P sorption parameter PSP (see Equation 2) for the 0–30 cm layer

TABLE 2 | Depth-specific initial mineral phosphorus pools labile P_{lab}, active P_{ACT}, stable P_{STAB}, and soil pH.

Depth	P_{lab}	P_{ACT}	P_{STAB}	$pHCaCl_2$
cm	kg ha^{-1}	kg ha^{-1}	kg ha^{-1}	—
0–30	138.8	688.7	2592.6	5.8 ± 0.1
30–60	8.9	304.1	1420.1	5.7 ± 0.1
60–90	1.2	200.2	825.3	5.8 ± 0.1

TABLE 1 | Initial organic carbon (C_{org}), nitrogen (N_{org}), and phosphorus (P_{org}) pools for simulation; soil hydraulic parameters water content at saturation θ_s, inverse air entry pressure α, shape parameter n, and saturated hydraulic conductivity K_s assigned to pedogenetic layers.

	Depth	C_{org}	N_{org}	P_{org}	θ_s	α	n	K_s
Horizon	cm	kg ha^{-1}	kg ha^{-1}	kg ha^{-1}	cm^3 cm^{-3}	cm^{-1}	—	cm day^{-1}
Ap	0–32	53,168.6	5842.7	354.5	0.4347	0.0304	1.240	23.6
Bv	32–54	16,145.4	1630.8	107.6	0.4223	0.0300	1.225	22.9
BvSw	54–75	12,359.7	1084.2	82.4	0.4193	0.2621	1.199	17.9
Sd	75–120	0.0	0.0	0.0	0.3984	0.2622	1.199	10.6

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using measured DGT-P concentrations of the TSP + compost treatment.

2.6 | Model Performance Criteria

For model agreement quantification in the calibration/validation procedure, mean absolute error (MAE) and root mean square error (RMSE) were applied. Both provide errors in the unit of the investigated variable. We further calculated the model efficiency (ME), also referred to as the Nash–Sutcliffe coefficient (Nash and Sutcliffe 1970), which varies between $-\infty$ and 1. The coefficient of determination R^2 varies between 0 and 1. Both are dimensionless criteria, but R^2 can exhibit values close to 1 even if the model just reproduces the pattern and not the overall magnitude. In contrast, ME is a stricter criterion as it is sensitive to deviations between simulated and observed mean values.

2.7 | Linking Experimental P Data With AgroC Model Pools

The measured DGT-P concentration is assumed to directly reflect the amount of plant-available P. For AgroC, the plant-available P was defined as the simulated liquid-phase mass plus the fraction of the mass of the active mineral P pool that could desorb over the time duration of the DGT-P experiment (=1 day):

$$P_{PA} = P_{lab} + P_{ACT} \times \frac{PSP}{1 - PSP} \times R_{REV} \hat{=} F_{DGTP} \tag{4}$$

where P_{PA} is the plant-available P, P_{lab} is the AgroC labile P pool, P_{ACT} is the AgroC active P pool (see Equations 2 and 3), PSP is the sorption parameter partitioning the P between the P_{lab} and the P_{ACT} pool, R_{REV} is the desorption rate modifier (=0.1 in this study), and F_{DGTP} is the measured DGT-P concentration. For comparison between simulated and observed P_{PA}, the simulated P_{PA} concentrations were averaged over a period starting 5 days prior and ending 5 days after the DGT-P sampling date. This compensated for any inaccuracies in the simulation of P_{PA} resulting from the short-term variations in water content.

To relate the sequential P fractions determined by Koch et al. (2018) to AgroC model pools according to Jones, Cole, et al. (1984), the following assumptions were made:

$$P_{imed} = P_{ACT} + P_{DPM} + P_{RPM} \hat{=} F_{NAHCO3Po} + F_{NAHCO3Pi} \tag{5}$$

$$P_{stdy} = P_{STAB} + P_{HUM} \hat{=} F_{NAOHPo} + F_{NAOHPi} + F_{H2SO4P} \tag{6}$$

where the sum of the moderately labile fractions $F_{NAHCORPo}$ and $F_{NAHCORPi}$ is assumed to relate to the sum, further referred to as the intermediate P pool (P_{imed}), of the active P model pool (P_{ACT}) plus the labile organic P pool for decomposable plant material P_{DPM} and the labile organic P pool for resistant plant material P_{RPM}. Further, the sum of the stable P pool (P_{STAB}) and stable organic material (P_{HUM}), referred to as the steady P pool (P_{stdy}), was assumed to correspond to the sum of the F_{NAOHPo}, F_{NAOHPi}, and F_{H2SO4P} fractions.

3 | Results

3.1 | Harvest Biomass and P Exports

Figure 1 shows the comparison of simulated biomass and measurements. Please note that for maize, sorghum, and sunflower (green dots), almost the entire aboveground biomass was harvested. For all other crops (red dots), only the yield biomass was determined. The harvested biomass simulated by AgroC corresponds well with the measurements as ME varies between 0.75 and 0.89 over all treatments.

With respect to the amount of P removed by harvest products, agreement between AgroC and the observations can be stated (Figure 2) with coefficients of determination between 0.63 and 0.75. Average maize annual P exports by harvest were observed to be 22.6, 25.1, 25.7, and 26.3 kg ha^{-1} for the control, TSP, compost, and TSP + compost treatment, respectively. Respective simulated values were 24.2, 24.6, 25.8, and 26.2 kg ha^{-1}. The simulations of the calibrated TSP + compost treatment marginally overestimated the total sum of P removed as a harvest product over the 22 years by 5 kg ha^{-1} (Table 4). For the other three treatments, the respective errors between observed and simulated exported P were just slightly larger, varying between −7 kg ha^{-1} for the TSP treatment and 18 kg ha^{-1} for the control treatment. Nevertheless, the order of P removed by harvest was identical between the model and observations in the different treatments.

3.2 | P Pools Over Depth

The pools and respective fractions were related according to Equations (5) and (6). The distinguishment of the labile, intermediate, and steady pool in the AgroC model showed agreement with the corresponding extracts of the sequential P-fraction across different soil depths (Figure 3). ME varied between 0.91 and 0.98 (Table 3). Also, differences between the treatments were usually reproduced correctly, except for the measured steady fraction of the compost treatment at 0–30 cm depth, which was unexpectedly large but also characterized by a high standard deviation.

Total P stocks (P_{tot}), defined as the sum of all P pools/fractions up to a depth of 90 cm, show agreement for the 2015 sampling. The bulk density data used to convert P concentrations to P stocks were identical for the model and measurements. According to the sequential P-fractionation, P_{tot} amounts to 6307 ± 841, 5491 ± 1021, 6301 ± 1803, and 4992 ± 1055 kg ha^{-1} for the TSP + compost, TSP, compost, and control treatment, respectively (Koch et al. 2018). The stocks simulated by AgroC for P_{tot} were 6116, 5838, 5805, and 5582 kg ha^{-1}, respectively. Basically, the ranking of P_{tot} stocks between treatments was also reproduced by the model, except for the compost treatment. The larger P_{tot} stock of the compost treatment corresponds to large amounts of P in the H_2SO_4-P extract of the 0–30 cm layer.

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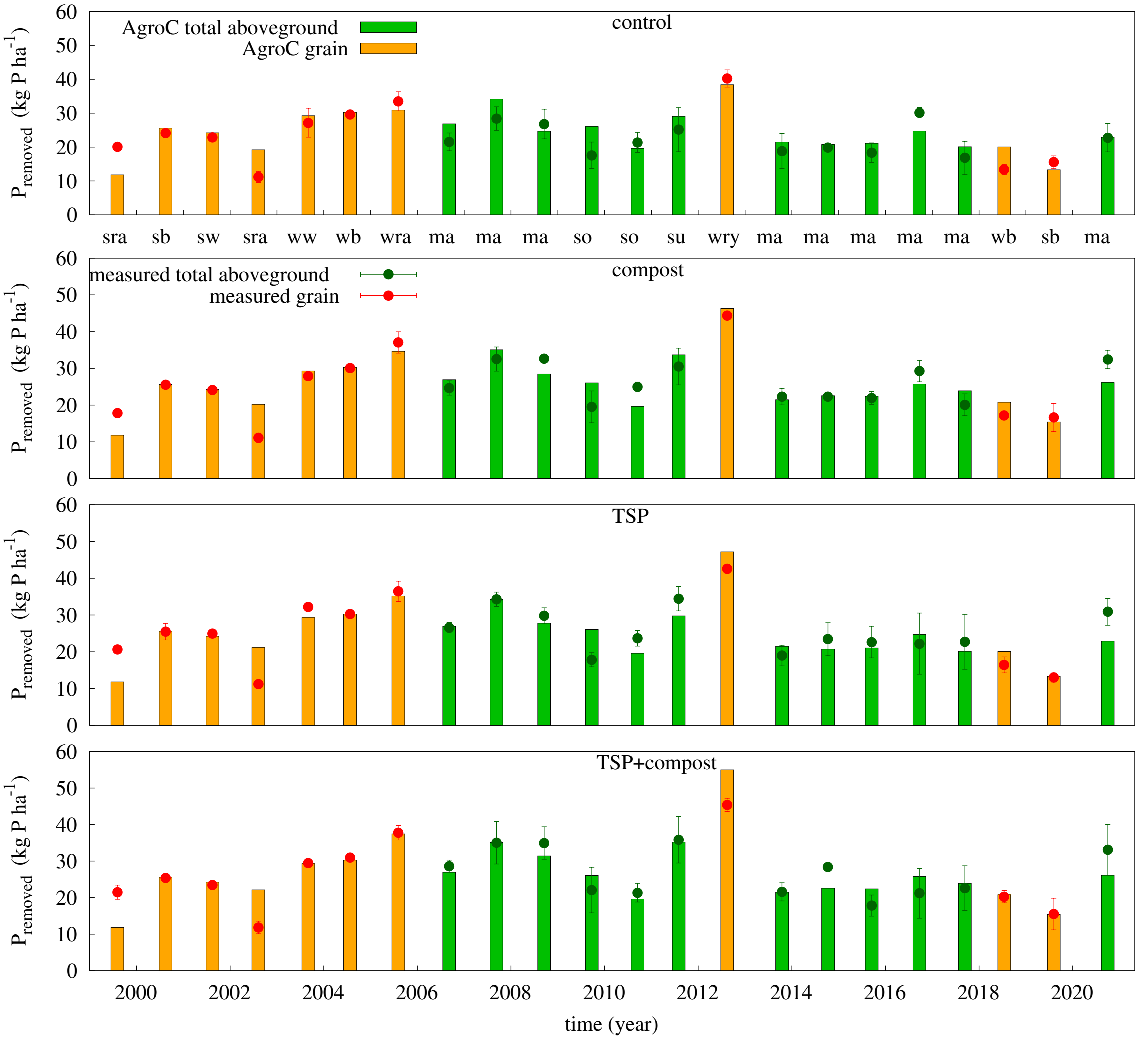

FIGURE 2 | Simulated (bars) and measured (points ± standard deviation) phosphorus removed by harvest for control, compost, TSP (triple superphosphate), and TSP + compost treatment. Crop rotation is indicated in the uppermost panel, where sra = spring rape, sb = spring barley, sw = spring wheat, ww = winter wheat, wb = winter barley, wra = winter rape, ma = maize, so = sorghum, su = sunflower, and wry = winter rye.

Calibration of the model with DGT-P data for the surface soil only caused considerable deviation of subsoil DGT-P data from simulated values, as indicated by a rather poor R^2 of 0.48 for all sampling depths (Figure 4).

3.3 | Plant-Available P Over Time

Figure 5 shows the temporal evolution of DGT-P and simulated P_{PA} for the 0–30 cm layer over the 22-year experimental period. Independent of the P fertilization treatment, a general trend of decreasing DGT-P could be observed over the first ~12 years of the experiment. This was basically reproduced by the simulation of P_{PA} with AgroC. A *t*-test (at error probability < 0.05) reveals that the measured DGT-P is significantly lower for each treatment from 2010 onwards than for the first measurement of this treatment in 1999.

The insert of Figure 5 shows that simulations for the different treatments were close to each other in the first 4 years of the LTE, approximately. Thereafter, the models diverged, and toward the end of 2021, the largest amount of P_{PA} was found in the TSP + compost treatment. The findings were corroborated by the DGT-P measurements. The relative differences between the treatments over time were also consistent between simulated and measured data (see insert Figure 5).

3.4 | Effect of P Availability on Yield

To investigate the response of yield to P availability as characterized by a specific P pool or fraction, the relative yield is commonly plotted against a P pool/fraction. Subsequently, an exponential function is fitted, assuming a Mitscherlich-type response. The upper panel of Figure 7 shows this relation between DGT-P and the relative yield for the Rostock field LTE. Treatment-specific relative yield was computed based on the assumption that the TSP + compost treatment yield represents the maximum potential yield at the site. According to Menzies et al. (2005) and Mason et al. (2010), nutrient deficiency is indicated if the relative yield does not exceed 90% of the potential one, that is, if the respective scaling factor is lower than 0.9. For the TSP treatment, the relative yield was lower than 0.9 in 3 years (maize in 2008, 2013, and 2014), but remained rather close to this threshold. The

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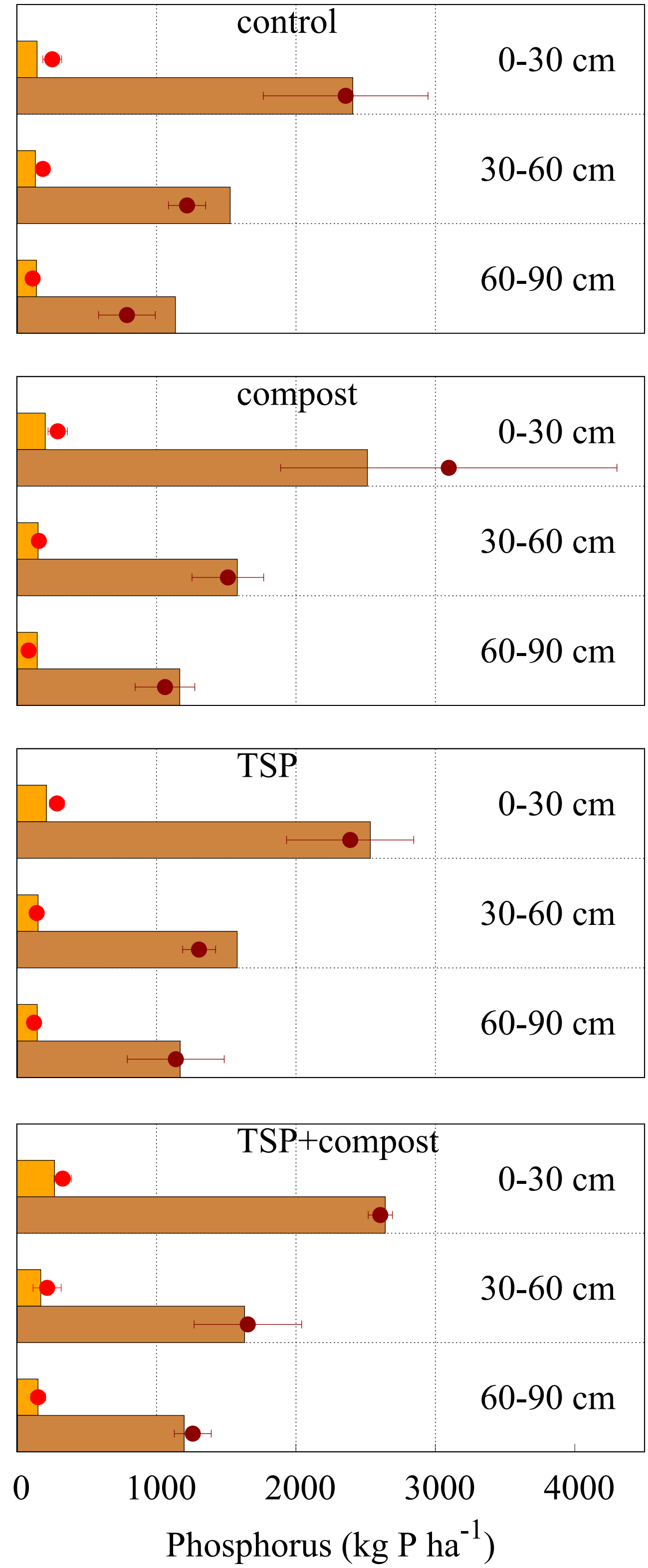

FIGURE 3 | Simulated intermediate (orange bars) and steady (brown bars) P pool vs. corresponding sequential P-fractions, that is, $NaHCO_3$-P (red points ± standard deviation), and NaOH-P plus H_2SO_4-P (brown points ± standard deviation) for three soil depths on April 29, 2015.

relative yield criterion of 0.9 was also not met three times for the compost treatment. It was lower for summer rape in 1999 and in 2002, and for winter rye in 2018. The lowest value of 0.82 was observed for the compost treatment for the first year of the LTE in 1999. In contrast, the control treatment showed nine relative yield values below 0.9.

The measured yield of the control plots was significantly lower (at error probability < 0.05) than for the TSP + compost treatment in 9 out of 22 harvests. Significantly lower yield was almost exclusively observed for maize as well as for spring rye and spring wheat in 2000 and 2001, respectively.

3.5 | Phosphorus Balance

The measured P balance indicates a gain of 491 kg P ha^{-1} after 22 experimental years for the TSP + compost treatment, small losses for the TSP and compost treatment, and a loss of about −530 kg P ha^{-1} for the control. This gain/loss pattern over the treatments was reproduced by the model. The P gain calculated for the TSP + compost treatment of 8% was only slightly underestimated by the AgroC counterpart, with a simulated gain of 6.5% (Table 4). For the TSP and compost treatment, the P gain was almost equal to P losses, which was also reflected in the model, with a remaining uncertainty of about 50 kg P over 22 years.

The AgroC model can be used to answer the question of how much fertilization is required to perfectly balance the soil P stocks. The model for the TSP + compost treatment was inverted such that the amount of TSP fertilization is inversely estimated to guarantee a zero gain in the soil P balance. The analyses show that a reduction to 56% of the originally TSP amount (=12.2 kg P ha^{-1} until 2013, 16.8 kg P ha^{-1} from 2014 onwards) in combination with the original compost amendments would have ensured a perfectly balanced budget.

4 | Discussion

4.1 | Harvest Biomass and P Exports

Simulated average maize annual P exports by harvest are close to the observations. For maize and wheat, Smolders et al. (2021) reported mean annual total aboveground P of 35 kg ha^{-1} under non-limiting conditions for experimental sites in Belgium. The respective value of 26.3 kg ha^{-1} observed for maize in this study is lower, which might be explained by the on average less favorable water availability conditions of the loamy sand soil of the Rostock site. The order of treatments in terms of P removal was reproduced correctly by AgroC. The differences in P exports by harvest between the treatments were also well reflected (Table 4). For instance, the difference measured over the entire observation period between the TSP + compost treatment with the highest and the control treatment with the lowest sum of total exported P by harvest is 68 kg ha^{-1} (584 minus 516 kg ha^{-1}). The respective value estimated with the AgroC models is 55 kg ha^{-1} (589 minus 534 kg ha^{-1}).

Wang et al. (2014), who used the APSIM model to cover a range of crops including wheat and maize, obtained an R^2 of 0.87 and 0.84 for total aboveground biomass and grain yield related to the measurements, respectively. Comparable values were

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TABLE 3 | Model agreement indices for harvested biomass, P removed by harvest, P pools over depth measured on April 29, 2015, and measured diffusive gradient thin-films P (DGT-P).

		$kg\,ha^{-1}$	$kg\,ha^{-1}$			
Treatment	**Variable**	**MAE**	**RMSE**	**ME**	R^2	*n*
TSP + compost	Biomass	1499.9	2103.3	0.84	0.87	22
TSP + compost	Removed P	3.1	4.5	0.67	0.73	22
TSP + compost	P pools over depth	37.5	42.8	1.00	1.00	6
TSP + compost	DGT-P				0.65	22
TSP	Biomass	1132.4	1673.2	0.89	0.90	22
TSP	Removed P	3.3	4.4	0.67	0.69	22
TSP	P pools over depth	93.0	130.9	0.97	0.99	6
TSP	DGT-P				0.68	22
Compost	Biomass	1390.5	1916.6	0.88	0.89	22
Compost	Removed P	3.0	3.8	0.73	0.75	22
Compost	P pools over depth	152.4	247.7	0.95	0.97	6
Compost	DGT-P				0.70	22
Control	Biomass	1506.7	2248.5	0.75	0.87	22
Control	Removed P	3.5	4.3	0.58	0.63	22
Control	P pools over depth	149.7	197.7	0.94	0.96	6
Control	DGT-P				0.69	22

Abbreviations: MAE = mean absolute error; ME = model efficiency; *n* = number of observations; R^2 = coefficient of determination; RMSE = root mean square error; TSP = triple superphosphate.

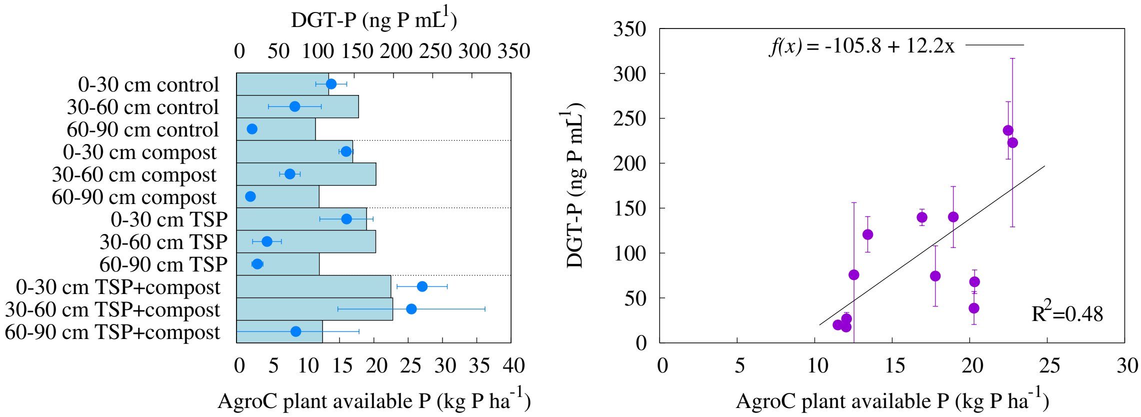

FIGURE 4 | Depth-specific DGT-P (points ± standard deviation) and corresponding simulated plant-available P (bars) for April 29, 2015.

determined in this study (Table 3). Further, Wang et al. (2014) report slightly lower R^2 of 0.75 and 0.73 with respect to the P uptake for total aboveground P uptake and grain P, respectively. In our study, slightly lower coefficients of determination were also found for P removal than for the biomass simulation (Table 3). The lowest R^2 of 0.63 was found for the control treatment. However, the model performance regarding biomass and P uptake was generally acceptable and comparable to the performance of other models reported in the literature (Wang et al. 2014; Mohammed et al. 2024).

4.2 | P Pools Over Depth

The Hedley fractionation scheme was criticized for imperfect identification of P fractions (Barrow et al. 2021). It was used for comparison to the simulation with respect to the intermediate and steady P pools. However, in this study, the original Hedley fractions were massively aggregated (see Equations 5 and 6) such that any potential misidentification of fractions with comparable sorption/desorption properties for comparison with model pools may be less evident. Despite the high

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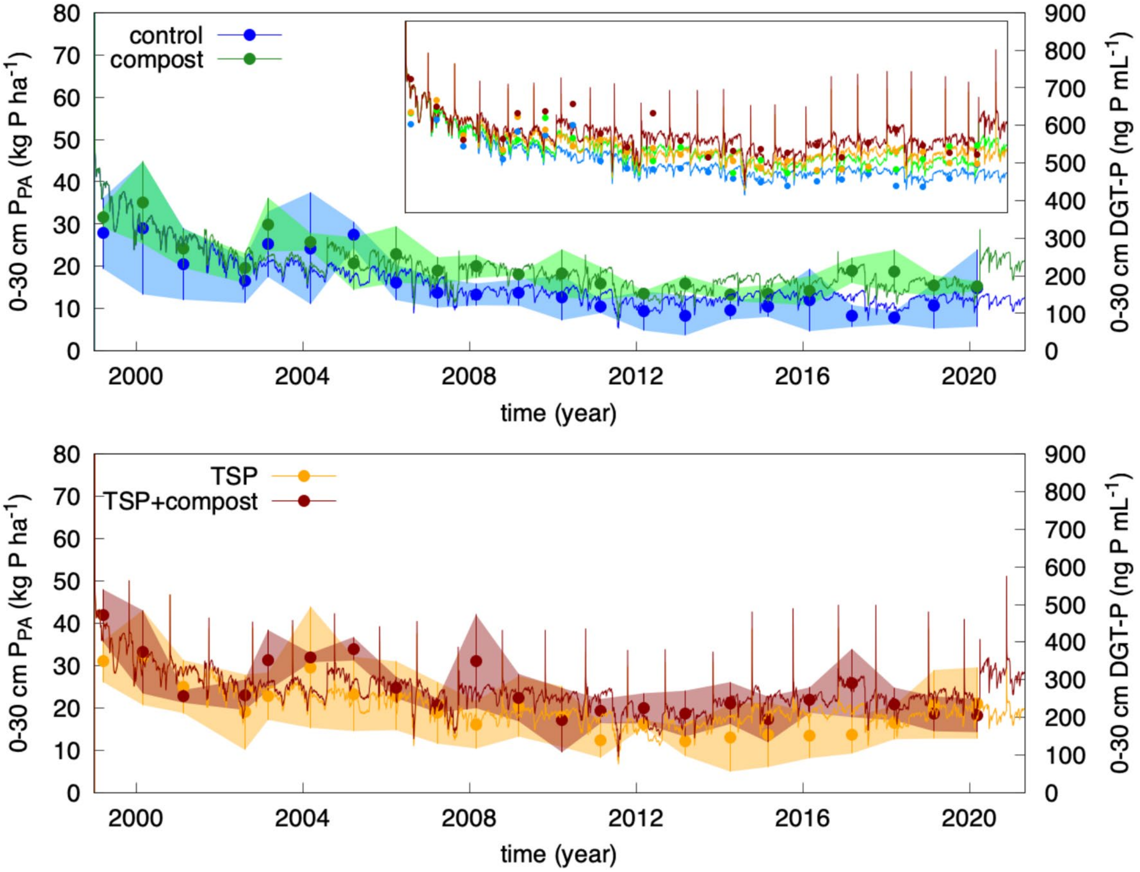

FIGURE 5 | Measured DGT-P (points, standard deviation indicated by colored areas) and corresponding simulated plant-available P (lines) for control, compost, TSP (Triple Superphosphate), and TSP + compost treatment. The figure insert shows the simulated plant-available P of all treatments against the measured average DGT-P value. Axis scaling of the figure insert is identical to the large figures.

ME values, there were also some systematic errors. The intermediate P pool of the AgroC model tends to be smaller than indicated by the $NaHCO_3$-P fraction of the sequential P-fractionation.

For German Cambisols, Gocke et al. (2021) reported average P_{tot} stocks to a depth of 100 cm of 7139 ± 780 kg P ha^{-1}, which is slightly larger than observed in this study. This may be partly due to the fact that we related P stocks to 0–90 cm only, but not to the top 1 m of soil. Nevertheless, the magnitude is quite close to the stocks measured and simulated in our study for the TSP + compost treatment, which is closest to the common farming practice.

The DGT method provides reliable estimates of plant-available P (Siebers et al. 2021). The 0–30 cm DGT-P variation over the treatments coincided well with the simulated pools and is also in the range reported by Lychuck et al. (2021) for the labile P pool. For the 30–60 and the 60–90 cm layers, P_{PA} was clearly overestimated by the model, except for the TSP + compost treatment (Figure 4). The TSP + compost treatment was calibrated with the DGT-P time series by adjusting the PSP parameter for the 0–30 cm layer. However, the PSP values of the layers underneath were as initially chosen. For 30–90 cm depth, the initial values of the labile and active pools for all treatments were those derived from the spin-up equilibrium runs based on the TSP + compost treatment.

4.3 | Plant-Available P Over Time

The decline of P_{PA} following the start of the LTE observed for all four treatments was probably related to the previous management that included larger amounts of P fertilization. In AgroC, this resulted in elevated stocks of the labile and active P pool. In general, agreement of the temporal evolution of AgroC P_{PA} and DGT-P can be stated, proven by R^2 ranging between 0.65 and 0.70 over the four treatments (Table 3). The R^2 between simulated data of AgroC P_{PA} and the measured ones via DGT-P across all treatments was 0.72. Figure 6 also shows that no single treatment model systematically deviated from this overall picture. An exception was the period 2003 to 2005, when DGT-P stocks increased for all treatments, which was not captured by the model P_{PA}. We attribute the elevated DGT-P for this period to the fact that soil sampling was performed in spring while winter crops were grown. Continued microbial activity over the winter, with increased mineralization of organic P (Hu et al. 2022; Pätzold et al. 2020), likely contributed to the elevated DGT-P stocks. Generally, at the time of sampling for DGT analyses in February/March, a crop was not present.

The PSP value defines the fraction of P that remains dissolved in the liquid phase, that is, the fraction that is not sorbed to the active P pool (Equation 2). The PSP value usually ranges from 0.05 to 0.75 (Williams and Izaurralde 2008). The PSP value of 0.078 determined inversely for the plough horizon was clearly

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TABLE 4 | Simulated and measured phosphorus balance from 1999 to 2021, estimated from P removed by harvest products, leaching, and fertilization.

	1999	Harvest		Leaching	Fertilization			Balance		Gain %	
kg P ha^{-1}	AgroC	AgroC	Measured	AgroC	Mineral	Organic	Total	AgroC	Estimated	AgroC	Estimated
TSP + compost	6141	−589	−584	−4.8	537	546	1083	401.8	491.1	6.54	8.00
TSP	6141	−554	−561	−4.8	537	0	537	−79.7	−21.5	−1.30	−0.35
Compost	6141	−570	−565	−4.8	0	546	546	−65.9	−22.2	−1.07	−0.36
Control	6141	−534	−516	−4.8	0	0	0	−546.3	−530.1	−8.90	−8.63

Note: The gain percentage was computed as the relative increase to the initial P stocks assumed for the AgroC model runs. Positive numbers indicate input to the agroecosystem, negative numbers indicate loss.
Abbreviation: TSP = triple superphosphate.

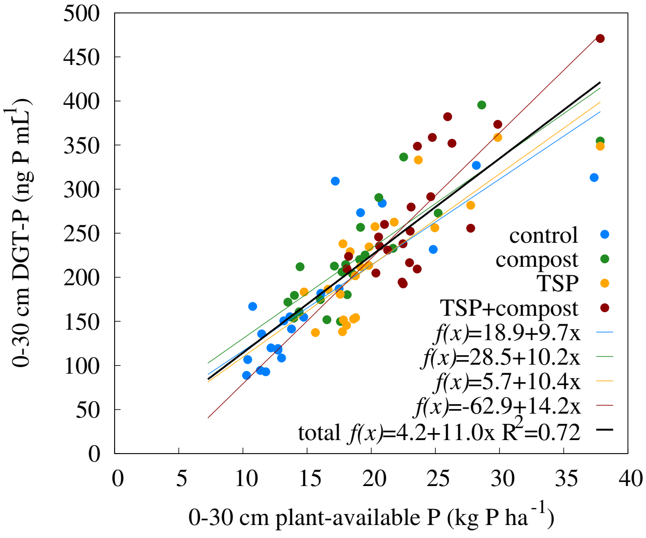

FIGURE 6 | 0–30 cm measured DGT-P vs. simulated plant-available P over the entire observation period. Lines represent corresponding linear fits for control, compost, TSP (triple superphosphate), TSP + compost treatment, and full data set.

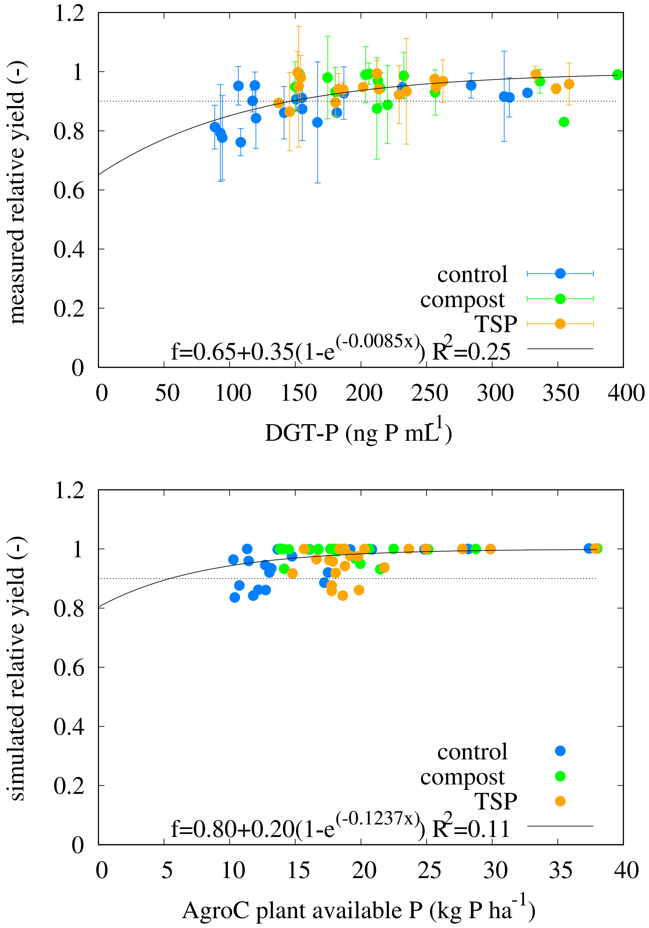

FIGURE 7 | DGT-P against measured relative yield and simulated plant-available P against simulated relative yield for control, TSP (Triple Superphosphate), and compost treatment.

in the lower range of PSP values reported elsewhere (Sharpley et al. 1984; Knisel et al. 1993; Williams and Izaurralde 2008). On one hand, this low PSP can partially be explained by the

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soil characteristics in terms of soil pH, clay content, organic C content, and labile P level (Sharpley et al. 1984) at test site Stover Acker. On the other hand, it can be explained by the original inorganic P pool concept of Jones, Cole, et al. (1984) as implemented in EPIC, for example, and in which the labile pool consists of soluble plus surface-sorbed mineral P (McGechan and Lewis 2002). In the AgroC model, the labile pool P_{lab} solely represents the water-soluble P. This results in lower labile P and higher active P pool masses, which in turn requires lower PSP values.

4.4 | Effect of P Availability on Yield

The rather heterogeneous response of yield to P limitation for the control treatment might be explained by the fact that crop species, and even specific traits, are expected to differ in their sensitivity to P limitation (Smolders et al. 2021; Khan et al. 2023). Further, other limiting factors like soil water availability (Das et al. 2022) play a role in the response of yield in dependence on specific crop/drought combinations occurring in some years. In summary, 22 years after the LTE started, there was a distinguishable P deficiency for the control treatment without any P amendment and a moderate P deficiency for the other two trials. This trend was also reflected by the AgroC modeling. As depicted in the lower panel of Figure 7, the simulated relative yield response to plant-available P showed a similar response to the measured ones using DGT-P as reference. The model confirmed the P deficiencies for the control treatment and the smaller deficiencies observed for the TSP and compost treatments. The coefficient of determination for the exponential fits in Figure 7, however, was low, reflecting the limited systematic variation in the yield data. In relation to the TSP-compost treatment, measured yield was significantly lower for the control plot in 9 out of 22 cases, which was mainly observed for maize. This again points to crop-specific sensitivities to P limitation. Further, it is probably a consequence of the soil P stocks at the beginning of the experiment being so large that the soil could compensate for the lack of P fertilization in the control treatment for a substantial period.

4.5 | Phosphorus Balance

As indicated in Section 3.1, there was basically agreement between the simulated and measured P removal by harvest. The largest discrepancy was observed for the control, where a removal of 18 kg P ha^{-1} was not predicted by AgroC, which already explains minor final deviations between simulated and measured P balance. Likely, additional processes contribute to the slightly larger P uptake by harvest in the control, like P provisioning via arbuscular mycorrhizal fungi (George et al. 1995; Vogel et al. 2024), not yet covered in the model design of AgroC. Besides, there is an imperfect initialization of plant-available P at model start, as this was largely based on the TSP + compost treatment. Notably, the overall simulated and measured P balance is in agreement with respect to gains and losses of P over the 22 years of duration of the LTE.

4.6 | Model Evaluation and Parameter Sensitivity

Crop growth parameters, crop-specific P demand, and P sorption and uptake parameters determined for the TSP + compost treatment were used to predict P balances and P uptake stress for the other three treatments (control, compost, and TSP). The model validation criteria for those three treatments point to a positive evaluation of the model assumptions.

After calibration of PSP for the 0–30 cm layer, agreement with the temporal evolution of P_{PA} according to the DGT method was given. AgroC is based on a slightly modified definition of the labile pool as part of the mineral P pool concept according to Jones, Cole, et al. (1984), such that the use of literature methods (Sharpley et al. 1984) to estimate PSP is not entirely valid. Instead, in this study, PSP was calibrated based on the TSP + compost treatment and was applied in a forward manner to the other three treatments. This procedure indicates that a site-specific calibration, and probably also a depth-specific calibration as discussed above, is required. Once PSP is calibrated, the benefits of combining model estimates with the DGT method can be exploited for use in an Agricultural digital twin. A major limitation of DGT-P tests is the fact that due to the disturbed sampling, and because the experiments are performed at water holding capacity (Degryse et al. 2009) with an unknown water content, a plant-available P stock in kg ha^{-1} is not attainable. This would, of course, be very helpful to calculate P balances and support decision-making with respect to P fertilization amounts. However, in conjunction with a process-based model that is calibrated using the DGT-P measurements over time, this issue can be solved. Following this procedure, quantitative P fertilization recommendations can be given.

In addition to PSP, the stable to active pool ratio $Q_{STAB/ACT}$ was also adjusted to match the experimentally determined stocks of total P. With a value of 7.4, $Q_{STAB/ACT}$ is higher than the default value of 4 suggested by Jones, Cole, et al. (1984). This parameter is implemented as a fixed value in many models. For the estimation of P_{PA}, the $Q_{STAB/ACT}$ ratio eventually has little effect, but it is required to match the measured conditions with respect to the slow/stable mineral P pools. Departing from the simplified model assumption of a $Q_{STAB/ACT}$ at equilibrium equal to 4 is necessitated, assuming that a site-specific amount of slow/stable mineral P pools in dependence on the historic P fertilization scheme, soil parent material, and properties resulting from pedogenesis is given (Cross and Schlesinger 1995; Holford 1997). The reverse rate modifier R_{rev} (default value = 0.1) was not modified, as well as the computation of the b_0 parameter controlling the sorption/desorption rate between the active and the stable mineral P pool (Equation 3). Both parameters showed little effect on P_{PA} in this study.

Within this study, the blueprint for an agricultural digital twin with respect to P availability and the resulting yield response evolved. Data on plant organ-specific biomass, P removal by harvest, plant-available P at 0–30 cm depth as determined by DGT, and sequential fractionation over soil depth flowed into the digital model, where the parameters A_{max}, XPC_{tot}, $Q_{STAB/ACT}$, and PSP were inversely estimated for an optimum match to the physical entity. According to Purcell and Neubauer (2023), this

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unidirectional information flow into the model created a partially integrated digital twin, which is referred to as a "digital shadow." Full integration would require a bidirectional information flow. For example, if the model-derived optimum P fertilization rate was passed back to the real world and implemented as the future P fertilization practice. In practice, that is, not at an LTE site as in this study, less site-specific soil information will be available.

5 | Conclusions

The DGT-P results and the model agree that after 22 years without P addition, the plant-available P is about half of what would be available for the common organic and mineral P fertilization strategy. AgroC and the measured harvest biomass reveal a moderate effect of P availability on crop performance 22 years after discontinuing P fertilization. From the P balances, we conclude that the current P fertilization rate, either by organic or mineral amendment, generates an almost optimal P supply to the crops. The treatment with both organic and mineral fertilization and two times the amount of P fertilization leads to an increase in soil P stocks, which potentially causes negative side effects.

The AgroC model and the DGT-P method indicate that a new plant-available P equilibrium will be established in dependence on the new P management. The desorption rate from the stable P pools, in combination with the P fertilization, will finally determine the new equilibrium level of plant-available P. For the investigated test site near Rostock, we found a time lag of about 12 years for this process. However, this can be different at other sites, as different soil, climatic, and P fertilization conditions prevail there.

The establishment of a digital shadow (Purcell and Neubauer 2023) demonstrates how P test data can inform a process-based model of P availability. In a real-world application of an agricultural digital twin, less measured information is likely to be available, which will inevitably deteriorate model quality. Nevertheless, it appears to be an appropriate tool to avoid unwanted system states, like P limitation to crop growth or groundwater exposure to P leaching. It has the potential to reduce risks when farmers make decisions. In this study, the combination of the DGT-based determination of plant-available P with a sequential fractionation scheme allowed for an approximation of the P cycle with the slightly modified pool concept of Jones, Cole, et al. (1984). Since basically all available P tests have proven relevance to some degree, any combination of a P cycle model with a P test can work in this respect if, as demonstrated in this study, links between model pools and P test results can be established.

Author Contributions

Michael Herbst: conceptualization, formal analysis, investigation, methodology, visualization, writing – original draft. **Gihan Mohammed:** investigation, formal analysis, methodology. **Bettina Eichler-Löbermann:** data curation, formal analysis, writing – original draft. **Wulf Amelung:** conceptualization, formal analysis, writing – original draft. **Jan Vanderborght:** conceptualization, writing – original draft. **Nina Siebers:** data curation, funding acquisition, project administration, resources, writing – original draft.

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Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

References

Allen, R. G., L. S. Pereira, D. Raes, and M. Smith. 1998. "Crop Evapotranspiration. Guidelines for Computing Crop Water Requirements." In *FAO Irrigation and Drainage Paper No. 56*, 300. Food and Agriculture Organization of the United Nations (FAO).

Barrow, N. J., A. Sen, N. Roy, and A. Debnath. 2021. "The Soil Phosphate Fractionation Fallacy." *Plant and Soil* 459: 1–11. https://doi.org/10.1007/s11104-020-04476-6.

Bauke, S. L., C. von Sperber, F. Tamburini, et al. 2018. "Subsoil Phosphorus Is Affected by Fertilization Regime in Long-Term Agricultural Experimental Trials." *European Journal of Soil Science* 69: 103–112.

Brogi, C., J. A. Huisman, M. Herbst, et al. 2020. "Simulation of Spatial Variability in Crop LAI and Yield Using Agro-Ecosystem Modelling and Geophysics-Based Quantitative Soil Information." *Vadose Zone Journal* 19: e20009. https://doi.org/10.1002/vzj2.20009.

Coleman, K., and D. S. Jenkinson. 2008. "RothC-26.3. A Model for the Turnover of Carbon in Soil." Model Description and Windows Users Guide. IACR-Rothamsted, 47. https://www.rothamsted.ac.uk/sites/default/files/RothC_guide_WIN.pdf.

Cross, A. F., and W. H. Schlesinger. 1995. "A Literature Review and Evaluation of the Hedley Fractionation: Applications to the Biogeochemical Cycle of Soil Phosphorus in Natural Ecosystems." *Geoderma* 64: 197–214.

Das, B. T., S. Schmidt, J. Biggs, D. W. Lester, N. Bourne, and N. I. Huth. 2022. "Simulating Long-Term Phosphorus, Nitrogen, and Carbon Dynamics to Advance Nutrient Assessment in Dryland Cropping." *Field Crops Research* 285: 108590. https://doi.org/10.1016/j.fcr.2022.108590.

Degryse, F., E. Smolders, H. Zhang, and W. Davison. 2009. "Predicting Availability of Mineral Elements to Plants With the DGT Technique: A Review of Experimental Data and Interpretation by Modelling." *Environmental Chemistry* 6: 198–218. https://doi.org/10.1071/EN09010.

Eichler-Löbermann, B., T. Zicker, M. Kavka, et al. 2021. "Mixed Cropping of Maize or Sorghum With Legumes as Affected by Long-Term Phosphorus Management." *Field Crops Research* 265: 108120. https://doi.org/10.1016/j.fcr.2021.108120.

George, E., H. Marschner, and I. Jakobsen. 1995. "Role of Arbuscular Mycorrhizal Fungi in Uptake of Phosphorus and Nitrogen From Soil." *Critical Reviews in Biotechnology* 15: 257–270. https://doi.org/10.3109/07388559509147412.

Gocke, M. I., A. Don, A. Heidkamp, F. Schneider, and W. Amelung. 2021. "The Phosphorus Status of German Cropland—An Inventory of Top- and Subsoils." *Journal of Plant Nutrition and Soil Science* 184: 51–64. https://doi.org/10.1002/jpln.202000127.

Groenendijk, P., and J. G. Kroes. 1999. "Modelling the Nitrogen and Phosphorus Leaching to Groundwater and Surface Water ANIMO 3.5." Report 144, DLO Winand Staring Centre.

13652389, 2025, 4, Downloaded from https://bsssjournals.onlinelibrary.wiley.com/doi/10.1111/ejss.70160 by Forschungszentrum Jülich GmbH Research Center, Wiley Online Library on [12/08/2025]. See the Terms and Conditions (https://onlinelibrary.wiley.com/terms-and-conditions) on Wiley Online Library for rules of use; OA articles are governed by the applicable Creative Commons License

Hedley, M. J., J. W. Stewart, and B. S. Chuhan. 1982. "Changes in Inorganic and Organic Soil Phosphorus Fractions Induced by Cultivation Practices and by Laboratory Incubations." *Soil Science Society of America Journal* 46: 970–976.

Herbst, M., H. J. Hellebrand, J. Bauer, et al. 2008. "Multiyear Heterotrophic Soil Respiration: Evaluation of a Coupled CO_2 Transport and Carbon Turnover Model." *Ecological Modelling* 214: 271–283.

Holford, I. C. R. 1997. "Soil Phosphorus: Its Measurement, and Its Uptake by Plants." *Soil Research* 35: 227–239.

Hu, Y., K. A. Jarosch, M. Kavka, and B. Eichler-Löbermann. 2022. "Fate of P From Organic and Inorganic Fertilizers Assessed by Complementary Approaches." *Nutrient Cycling in Agroecosystems* 124: 189–209. https://doi.org/10.1007/s10705-022-10237-x.

Jones, C. A., C. V. Cole, A. N. Sharpley, and J. R. Williams. 1984. "A Simplified Soil and Plant Phosphorus Model. I. Documentation." *Soil Science Society of America Journal* 48: 800–805.

Jones, C. A., A. N. Sharpley, and J. R. Williams. 1984. "A Simplified Soil and Plant Phosphorus Model: III. Testing." *Soil Science Society of America Journal* 48: 810–813.

Khan, F., A. B. Siddique, S. Shabala, M. Zhou, and C. Zhao. 2023. "Phosphorus Plays Key Roles in Regulating Plants' Physiological Responses to Abiotic Stresses." *Plants* 12, no. 15: 2861. https://doi.org/10.3390/plants12152861.

Klosterhalfen, A., M. Herbst, L. Weihermüller, et al. 2017. "Multi-Site Calibration and Validation of a Net Ecosystem Carbon Exchange Model for Croplands." *Ecological Modelling* 363: 137–156. https://doi.org/10.1016/j.ecolmodel.2017.07.028.

Klotzbücher, A., K. Kaiser, T. Klotzbücher, M. Wolff, and R. Mikutta. 2019. "Testing Mechanisms Underlying the Hedley Sequential Phosphorus Extraction of Soils." *Journal of Plant Nutrition and Soil Science* 182: 570–577. https://doi.org/10.1002/jpln.201800652.

Knisel, W. G., R. A. Leonard, and F. M. Davis. 1993. "GLEAMS Groundwater Loading Effects of Agricultural Management Systems." V2.1, Part 1: Nutrient Component Documentation. UGA-CPES-BAED Publication No. 5.

Koch, M., J. Kruse, B. Eichler-Löbermann, et al. 2018. "Phosphorus Stocks and Speciation in Soil Profiles of a Long-Term Fertilizer Experiment: Evidence From Sequential Fractionation, P *K*-Edge XANES, and ^{31}P NMR Spectroscopy." *Geoderma* 316: 115–126. https://doi.org/10.1016/j.geoderma.2017.12.003.

Kruse, J., M. Abraham, W. Amelung, et al. 2015. "Innovative Methods in Soil Phosphorus Research: A Review." *Journal of Plant Nutrition and Soil Science* 178: 43–88. https://doi.org/10.1002/jpln.201400327.

Lychuck, T. E., A. P. Moulin, R. L. Lemke, et al. 2021. "Modelling the Effects of Climate Change, Agricultural Inputs, Cropping Diversity, and Environment on Soil Nitrogen and Phosphorus: A Case Study in Saskatchewan, Canada." *Agricultural Water Management* 252: 106850. https://doi.org/10.1016/j.agwat.2021.106850.

Mason, S., A. McNeill, M. J. McLaughlin, and H. Zhang. 2010. "Prediction of Wheat Response to an Application of Phosphorus Under Field Conditions Using Diffusive Gradients in Thin-Films (DGT) and Extraction Methods." *Plant and Soil* 337: 243–258. https://doi.org/10.1007/s11104-010-0521-0.

McGechan, M. B., and D. R. Lewis. 2002. "Sorption of Phosphorus by Soil, Part 1: Principles, Equations and Models." *Biosystems Engineering* 82: 1–24. https://doi.org/10.1006/bioe.2002.0054.

Menzies, N. W., B. Kusumo, and P. W. Moody. 2005. "Assessment of P Availability in Heavily Fertilized Soils Using the Diffusive Gradient in Thin Films (DGT) Technique." *Plant and Soil* 269: 1–9.

Mohammed, G., N. Siebers, I. Merbach, S. J. Seidel, and M. Herbst. 2024. "Simulation of Soil Phosphorus Dynamics and Crop Yield for Organic and Mineral Fertilization Treatments at Two Long-Term Field Sites." *Science of the Total Environment* 957: 177517. https://doi.org/10.1016/j.scitotenv.2024.177517.

Nash, J. E., and J. V. Sutcliffe. 1970. "River Flow Forecasting Through Conceptual Models Part I—A Discussion of Principles." *Journal of Hydrology* 10: 282–290.

Nawara, S., T. V. Dael, R. Merckx, et al. 2017. "A Comparison of Soil Tests for Available Phosphorus in Long-Term Field Experiments in Europe." *European Journal of Soil Science* 68: 873–885. https://doi.org/10.1111/ejss.12486.

Nelder, J. A., and R. A. Mead. 1965. "A Simplex Method for Function Minimization." *Computer Journal* 7: 308–313.

Pätzold, S., M. Leenen, P. Frizen, T. Heggemann, P. Wagner, and A. Radionov. 2020. "Predicting Plant Available Phosphorus Using Infrared Spectroscopy With Consideration for Future Mobile Sensing Applications in Precision Farming." *Precision Agriculture* 21: 737–761. https://doi.org/10.1007/s11119-019-09693-3.

Pearse, S. J., E. J. Veneklaas, G. R. Cawthray, M. D. A. Bolland, and H. Lambers. 2006. "Carboxylate Release of Wheat, Canola and 11 Grain Legume Species as Affected by Phosphorus Status." *Plant and Soil* 288: 127–139. https://doi.org/10.1007/s11104-006-9099-y.

Purcell, W., and T. Neubauer. 2023. "Digital Twins in Agriculture: A State-of-the-Art Review." *Smart Agricultural Technology* 3: 100094. https://doi.org/10.1016/j.atech.2022.100094.

Pylianidis, C., S. Osinga, and I. N. Athanasiadis. 2021. "Introducing Digital Twins to Agriculture." *Computers and Electronics in Agriculture* 184: 105942. https://doi.org/10.1016/j.compag.2020.105942.

Requejo, M. I., and B. Eichler-Löbermann. 2014. "Organic and Inorganic Phosphorus Forms in Soil as Affected by Long-Term Application of Organic Amendments." *Nutrient Cycling in Agroecosystems* 100: 245–255. https://doi.org/10.1007/s10705-014-9642-9.

Sadukhan, D., Q. Zhiming, T. Zhang, C. S. Tan, M. Liwang, and A. A. Andales. 2019. "Development and Evaluation of a Phosphorus (P) Module in RZWQM2 for Phosphorus Management in Agricultural Fields." *Environmental Modelling & Software* 113: 48–58. https://doi.org/10.1016/j.envsoft.2018.12.007.

Sharpley, A. N., C. A. Jones, C. Gray, and C. V. Cole. 1984. "A Simplified Soil and Plant Phosphorus Model: II. Prediction of Labile, Organic and Sorbed Phosphorus." *Soil Science Society of America Journal* 48: 805–809.

Siebers, N., L. Wang, T. Funk, et al. 2021. "Subsoils—A Sink for Excess Fertilizer P but a Minor Contribution to P Plant Nutrition: Evidence From Long-Term Fertilization Trials." *Environmental Sciences Europe* 33: 60. https://doi.org/10.1186/s12302-021-00496-w.

Simunek, J., M. Sejna, H. Saito, and M. T. van Genuchten. 2013. *The HYDRUS-1D Software Package for Simulating the One-Dimensional Movement of Water, Heat, and Multiple Solutes in Variably-Saturated Media—Version 4.17*, 308. Department of Environmental Sciences, University of California Riverside.

Simunek, J., and D. L. Suarez. 1993. "Modeling of Carbon Dioxide Transport and Production in Soil 1. Model Development." *Water Resources Research* 29: 487–497. https://doi.org/10.1029/92WR02225.

Smolders, E., S. Nawara, E. De Cooman, et al. 2021. "The Phosphate Desorption Rate in Soil Limits Phosphorus Bioavailability to Crops." *European Journal of Soil Science* 72: 221–233.

Spitters, C. J. T., H. van Keulen, and D. W. G. van Kraalingen. 1989. "A Simple and Universal Crop Growth Simulator, SUCROS87." In *Simulation and Systems Management in Crop Protection. Simulation Monographs*, edited by R. Rabbinge, S. A. Ward, and H. H. van Laar, vol. 32, 147–181. PUDOC.

Tipping, E., C. J. Somerville, and J. Luster. 2016. "The C:N:P:S Stoichiometry of Soil Organic Matter." *Biogeochemistry* 130: 117–131. https://doi.org/10.1007/s10533-016-0247-z.

13652389, 2025, 4, Downloaded from https://bsssjournals.onlinelibrary.wiley.com/doi/10.1111/ejss.70160 by Forschungszentrum Jülich GmbH Research Center, Wiley Online Library on [12/08/2025]. See the Terms and Conditions (https://onlinelibrary.wiley.com/terms-and-conditions) on Wiley Online Library for rules of use; OA articles are governed by the applicable Creative Commons License

Vanclooster, M., P. Viaene, and J. Diels. 1994. *WAVE: A Mathematical Model for Simulating Water and Agrochemicals in the Soil and Vadose Environment: Reference and User's Manual, Release 2.0*, 154. Katholieke Universiteit Leuven.

Vereecken, H., M. Vanclooster, M. Swerts, and J. Diels. 1991. "Simulating Water and Nitrogen Behaviour in Soils Cropped With Winter Wheat." *Fertilizer Research* 27: 233–243. https://doi.org/10.1007/BF01051130.

Vogel, H. J., W. Amelung, C. Baum, et al. 2024. "How to Adequately Represent Biological Processes in Modeling Multifunctionality of Arable Soils." *Biology and Fertility of Soils* 60: 263–306. https://doi.org/10.1007/s00374-024-01802-3.

Wang, E., M. Bell, L. Zhongkui, P. Moody, and M. E. Probert. 2014. "Modelling Crop Response to Phosphorus Inputs and Phosphorus Use Efficiency in a Crop Rotation." *Field Crops Research* 155: 120–132.

Weihermüller, L., A. Graf, M. Herbst, and H. Vereeecken. 2013. "Simple Pedotransfer Functions to Initialize Reactive Carbon Pools of the RothC Model." *European Journal of Soil Science* 64: 567–575. https://doi.org/10.1111/ejss.12036.

Weihermüller, L., M. Herbst, M. Javaux, and M. Weynants. 2017. "Erratum to "Revisiting Vereecken Pedotransfer Functions: Introducing a Closed-Form Hydraulic Model"." *Vadose Zone Journal* 16: 1–2. https://doi.org/10.2136/vzj2008.0062er.

Weihrauch, C., and C. Opp. 2018. "Ecologically Relevant Phosphorus Pools in Soils and Their Dynamics: The Story So Far." *Geoderma* 325: 183–194. https://doi.org/10.1016/j.geoderma.2018.02.047.

Weynants, M., H. Vereecken, and M. Javaux. 2009. "Revisiting Vereecken Pedotransfer Functions: Introducing a Closed-Form Hydraulic Model." *Vadose Zone Journal* 8: 86–95. https://doi.org/10.2136/vzj2008.0062.

Williams, J., S. Dagitz, M. Magre, A. Meinardus, E. Steglich, and R. Taylor. 2015. *EPIC User's Manual Version 0810*. Blackland Research and Extension Center.

Williams, J. R., and R. C. Izaurralde. 2008. "The APEX Model." APEX_EPIC_BRCREPORT2008-02_2.pdf.

Zicker, T., S. von Tucher, M. Kavka, and B. Eichler-Löbermann. 2018. "Soil Test Phosphorus as Affected by Phosphorus Budgets in Two Long-Term Field Experiments in Germany." *Field Crops Research* 218: 158–170. https://doi.org/10.1016/j.fcr.2018.01.008.

Supporting Information

Additional supporting information can be found online in the Supporting Information section. **Data S1.** Supporting Information.

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