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Perspective

Improved descriptions of soil hydrology in crop models: The elephant in the room?

Nicholas Jarvis *, Mats Larsbo, Elisabet Lewan, Sarah Garré

Department of Soil and Environment, Swedish University of Agricultural Sciences, Box 7014, 750 07 Uppsala, Sweden

HIGHLIGHTS

- Models are powerful tools to assess impacts of management and climate on water balance, solute transport and crop yields.
- The use of empirical models of water flow in soil-crop models limits their applicability and will increase prediction error.
- This empiricism is unnecessary as physics-based flow models are at least as parsimonious and not difficult to parameterize.
- Longer run times are not a good enough reason to neglect the physics of water flow in the soil-crop system.
- Parameter uncertainty remains a challenge for both empirical and physics-based models and is too often ignored.

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ABSTRACT

Soil-crop simulation models are widely used to assess the impacts of soil management and climate change on soil water balance, solute transport and crop production. In this context, it is important that hydrological processes in the soil-crop system are accurately modelled. We suggest here that empirical treatments of soil water flow, water uptake by plant roots and transpiration limit the applicability of crop models and increase prediction errors. We further argue that this empiricism is to a large extent unnecessary, as parsimonious physics-based descriptions of these water flow processes in the soil-crop system are now available. Recent reviews and opinion articles, whilst strongly advocating the need for improvements to crop models, fail to mention the significant role played by accurate treatments of soil hydrology. It seems to us that empirical models of soil water flow have become the elephant in the room.

1. Introduction

Soil-crop simulation models are potentially powerful tools to assess the impacts of soil and crop management and climate on water balance, crop production and the environment (Fig. 1; Jones et al., 2017; Keating and Thorburn, 2018; Stöckle and Kemanian, 2020). In particular, they can be used to "add value" to long-term field experiments by identifying plausible explanations for observed treatment effects and by filling in gaps in the data with respect to variables that were not measured. Once calibrated against experimental data, soil-crop models can be used predictively to analyze, for example, the likely effects of changes in climate and land use and management on crop production and the environment (Nendel et al., 2018). In this context, it is important that water flows in the soil-crop system are described reliably, not only in studies focusing on soil water balance components and the environmental impacts of agriculture (e.g. agrochemical losses in surface runoff or leaching to groundwater; Keating and Thorburn, 2018), but also for simulations of crop growth since drought is known to be a major cause of reductions in crop yields (e.g. Ray et al., 2015; Daryanto et al., 2016).

In their recent review, Stöckle and Kemanian (2020) noted that multi-model comparisons have shown significant variability in simulation outputs among models even after calibration and that these uncertainties tend to increase when they are used predictively for future climates. Multi-model ensembles have been proposed as a way to improve the reliability of predictions in the face of uncertainty in process descriptions. However, in recent reviews, Silva and Giller (2020), Stöckle and Kemanian (2020) and Keating (2020) suggested that it would be better to focus efforts on identifying and correcting model deficiencies. The reasons for model errors are many and varied, as the

* Corresponding author.
E-mail address: nicholas.jarvis@slu.se (N. Jarvis).

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Fig. 1. Accurate descriptions of hydrological processes in crop models are needed for reliable predictions of climate change impacts on water balance, crop production and the environment (drawing by Miel Vandepitte).

soil-crop system is complex, replete with both known and unknown unknowns (Boote et al., 2013; Tardieu et al., 2018). However, in this perspective paper, we argue that many soil-crop models are neglecting what we already know (i.e. "known knowns") by employing over-simplified empirical descriptions of soil hydrological processes even though parsimonious physics-based approaches are now available that are more generally applicable. In ongoing efforts to improve crop models, we suggest that this "low-hanging fruit" should be picked first. A convergence among models for these processes for which the basic physical understanding has been in place for some years should lead to significant reductions in the variation of model predictions (Stöckle and Kemanian, 2020).

2. Modelling hydrological processes in the soil-crop system: empiricism vs. physics

Some crop models use a physics-based approach, Richards' equation, to describe water flow and storage in the soil. However, more often, crop models employ, in varying forms, empirical tipping bucket or capacity models for this purpose that neglect the role of water potentials in driving water flow in soil. Model comparison exercises have repeatedly shown that although the differences are sometimes small, models based on Richards' equation generally perform better (e.g. Diekkrüger et al., 1995; Maraux et al., 1998; Vanclooster and Boesten, 2000; Herbst et al., 2005; Wegehenkel et al., 2008; Kröbel et al., 2010; Soldevilla-Martinez et al., 2014; Guest et al., 2017; McBean et al., 2020; Groh et al., 2022). One main reason for this is that the conceptual basis of a tipping bucket flow model does not allow for upward water flows, which control both evaporation at the soil surface as well as capillary rise from groundwater into the root zone to maintain crop transpiration during dry summer periods (McBean et al., 2020; Longo et al., 2021; Jarvis et al., 2022). Empirical fixes and 'work-arounds' have been introduced in an attempt to overcome this limitation (e.g. Maraux et al., 1998; Wegehenkel et al., 2008; Longo et al., 2021), but the additional parameters introduced are difficult to estimate from direct measurements because their physical basis is very weak. In contrast, by adopting a suitable bottom boundary condition, Richards' equation is readily applicable to a wide range of hydrological settings to reflect, for example, critical differences in the hydrology of free-draining soils and soils with shallow water tables (Longo et al., 2021).

A failure to consider the physics of water flow in soil also has important consequences for modelling water balance components. For example, field drains cannot be incorporated into capacity water flow models in any realistic way, while empirical "curve numbers" are used as a simple empirical work-around to generate surface runoff as a function of daily rainfall and surface soil moisture contents. In contrast, physics-based treatments of drainage are compatible with water flow models based on Richards' equation, while soil evaporation and surface runoff can be incorporated into the surface boundary condition without recourse to additional empirical parameters. In reality, water potential acts as the link between soil and plant water status (Manzoni et al., 2013; de Swaef et al., 2022; Jarvis et al., 2022). As capacity models of soil water flow cannot predict water potential, many crop models employ empirical approaches to describe water uptake and transpiration, most often based on simple threshold functions of the total plant available water in the root zone (e.g. Brisson et al., 2003). This approach can work well under conditions of monotonic drying (e.g. Robertson and Fukai, 1994), but it may fail to match crop water uptake rates and patterns during complex wetting and drying cycles in the field (e.g. van den Berg et al., 2002; Guswa, 2005; Akuraju et al., 2017).

Early soil-crop models based on Richards' equation for soil water flow also made use of purely empirical functions for root water uptake (e.g. Feddes et al., 1976). In recent years, simple physics-based models of water uptake and transpiration suitable for use in conjunction with Richards' equation have been proposed (e.g. de Jong van Lier et al., 2008, 2013; Couvreur et al., 2012; Javaux et al., 2013; Sulis et al., 2019). These developments were stimulated by a growing understanding of the limitations of the earlier empirical models, especially their inability to account for the physical mechanisms of "compensation", whereby water uptake increases from sparsely rooted wetter soil layers when the more densely rooted surface soil layers become dry (e.g. Jarvis, 2011; Jarvis et al., 2022). Model benchmarking studies (de Willigen et al., 2012; Heinen, 2014; dos Santos et al., 2017) and comparative tests against field data (Cai et al., 2017, 2018) have shown that these simple physics-based models generally perform better than empirical descriptions of root water uptake. They are also parsimonious, requiring no more parameters than empirical models. These parameters are also easier to estimate since they have a stronger physical basis (de Willigen et al., 2012; Javaux et al., 2013).

We do not want to give the impression that soil-crop models based on Richards' equation are necessarily free from their own deficiencies and problems. One example is that the hydraulic functions commonly used as input to Richards' equation ignore the presence of soil macropores that significantly affect saturated hydraulic conductivity (e.g. Jarvis et al., 2013) and therefore the partitioning of rainfall between surface runoff and infiltration, as well as drainage rates and soil water storage (Or, 2019). However, rather than a reason to abandon physics altogether, this should be taken as a challenge to strengthen the physical basis of hydrological models. In this spirit, modified soil hydraulic functions that account for the effects of soil macropores have been developed, along with methods to estimate the additional parameters required (e.g. Huth et al., 2012; Jarvis et al., 2013; Fatichi et al., 2020).

3. Why do crop models still employ empirical descriptions of hydrological processes?

Models based on Richards' equation usually give more accurate simulations of the soil water balance for a wider range of soil types than empirical capacity models. It therefore seems relevant to consider why empirical models were employed to describe soil water flow in crop models originally developed more than 30 years ago and whether one or more of these reasons may still be valid. One reason may simply have been that most of them were developed by teams of crop scientists and agronomists with little, if any, input from soil physicists and hydrologists. Many plant scientists today are also likely to be unfamiliar with soil physics theory, in the same way that soil physicists may not possess much expertise on the processes driving plant growth. We feel that these boundaries between topic areas should not be allowed to limit the application of state-of-the-art process understanding in soil-crop models. Instead, the complex nature of interacting processes in the soil-crop system should be recognized by including all relevant specialisms in multi-disciplinary modelling teams.

Another practical issue is that physics-based models of soil water flow run more slowly, as they require short (sub-daily) time steps to ensure numerical stability and convergence (Farthing and Ogden, 2017). However, computing power has increased enormously in recent decades, so that this should no longer be critical, not even for calibration exercises or spatial applications of models at the regional scale. Speed is still a relevant issue in such modelling applications, but in our opinion saving computing time is not an acceptable reason for employing model process descriptions that depart too far from physical realism.

Another reason often advanced for using empirical models of soil water flow is that models based on Richards' equation require data on soil water retention and hydraulic conductivity functions that makes their parameterization more difficult. We contend that this is less of an issue than is often claimed. It is certainly the case that there are some significant pitfalls in the parameterization of soil hydrological models, but this is the case for both capacity models and models based on Richards' equation. A typical implementation of Richards' equation requires at most six parameters to describe the soil hydraulic functions. Empirical capacity models vary in the number of parameters, but typically they employ at least seven (porosity, field capacity, wilting point, runoff curve number, one or two parameters reflecting hydraulic conductivity and two parameters controlling soil evaporation). If a workaround "fix" for capillary rise is also introduced into the model, then the number of parameters increases further. Both types of model include parameters that control hydraulic conductivity, but whereas the parameter in Richards' equation has a clear physical basis connected to Darcy's law, the corresponding parameter in empirical capacity models does not, which makes its estimation more difficult.

If direct measurements are not available, the soil hydraulic parameters can be determined by model calibration against measurements of soil water contents or fluxes in the field. In such cases, great care should be exercised, as different parameter combinations may result in equally good fits to the measurements (i.e. non-unique solutions or "equifinality", Beven, 2006). This will not be apparent to the model user if parameter values are adjusted by "trial and error", which is still the case in many applications of crop models (Seidel et al., 2018). Thus, even though a hydrological model can be calibrated to match field data satisfactorily, it may be doing so for the wrong reasons, which means that model predictions of soil water balance and crop production in a future climate could be seriously in error (e.g. Kersebaum et al., 2007, 2015; Bellocchi et al., 2010). In particular, crop models are often calibrated against measurements of soil water content made in the field at only one or a few depths in a soil profile. In some studies, the depth-distribution of soil water contents is ignored and the model is only compared to the total store of water in the soil profile or crop root zone. With such limited calibration data, satisfactory fits with model simulations cannot be taken as evidence that the model parameterization is reasonable. Sonkar et al. (2019) showed that data on soil water contents alone is not enough to properly constrain a hydrological model of the soil-crop system based on Richards' equation. They concluded that data on another component of the water balance (i.e. deep drainage or evapotranspiration) is needed in addition to water contents in order to uniquely identify parameters describing soil hydraulic properties and crop root distribution. The extent to which models based on capacity flow concepts also suffer from this kind of 'equifinality' has not been tested to our knowledge, but they are likely to be at least as susceptible, as they contain several parameters that cannot be directly measured.

Parameterization of soil hydrological models is even more of a challenge for large-scale applications, although this has been greatly facilitated in recent decades by the development of regional and global soils databases and associated pedotransfer functions for soil water contents at field capacity and wilting point as well as some of the more widely used soil hydraulic functions (Vereecken et al., 2010). The data support is admittedly still limited for some widespread soil types, particularly for tropical soils, many of which have physical and hydraulic properties that are quite distinct from soils developed in temperate climates (Minasny and Hartemink, 2011). Nevertheless, robust pedotransfer functions to support applications of both empirical capacity flow models as well as hydrological models based on Richards' equation have been specifically developed for tropical soils (e.g. van den Berg et al., 1997; Hodnett and Tomasella, 2002; Minasny and Hartemink, 2011).

4. Conclusions

It is not a problem per se that empirical components are incorporated into simulation models. Indeed this is almost always unavoidable, especially in models designed for practical use, either because mechanistic understanding of some processes is lacking, or because it would be too impractical to implement in the model. However, *unnecessary* empiricism should be avoided in our opinion. When a physics-based approach is just as easy to use as a corresponding (more) empirical approach, then it should be preferred. In this respect, we cannot see any convincing reasons to still use empirical models of soil water flow more than 30 years on from their development. This issue appears to be discussed much less now than in the past. None of the recent reviews and opinion articles calling for improvements to crop models that we cited in the introduction explicitly mention hydrological processes. It seems that empirical models of soil water flow have become "the elephant in the room".

Concepts and definitions

We define an empirical (or phenomenological) model as a model that describes natural phenomena in a way which is intended to be consistent with reality, but which is not directly derived from fundamental theory. In other words, as opposed to a physics-based model, an empirical or phenomenological model is not derived from first (physical) principles. From a philosophical point of view, all models have an empirical basis, even physics-based ones, since ultimately all models are derived from observations. However, we use the terms physical law and physical first principles when the model derived from these initial observations proves its generality by passing repeated tests against later measurements.

Capacity or tipping bucket models of soil water flow can be classified as phenomenological as they attempt to mimic the physical process of water flow without directly addressing the physical forces driving the flow, nor the soil hydraulic properties that control it.

Richards' equation is obtained by combining a fundamental physical principle (the law of conservation of mass) with Darcy's law for soil water flow. Darcy developed this flow equation empirically through experimentation. However, it should be considered as a physics-based model, since it can also be derived from first principles (Whitaker, 1986). Hence, we classify models based on Richards' equation as physics-based. In practice, however, the solution of Richards' equation for transient soil water flow involves a mix of fundamental physical theory and some empiricism. Two linked soil hydraulic functions are required to solve Richards' equation: a water retention function describing the relationship between water potential and water content and a function describing the variation of hydraulic conductivity with either water content or potential. Both functions reflect the underlying soil pore size distribution. Models used to describe these soil hydraulic properties combine empirical functions for soil water retention with physics-based models of water flow at the pore-scale.

Data availability

No data was used for the research described in the article.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could influence the opinions reported in this paper.

Data availability

No data was used for the research described in the article.

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