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Review

Water modelling approaches and opportunities to simulate spatial water variations at crop field level

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ABSTRACT

Considerable spatial variability in soil hydraulic properties exists within a field, even in those considered homogeneous. Spatial variability of water as a major driver of crop heterogeneity gains particular relevance within the context of precision agriculture, but modelling has devoted insufficient efforts to scale up from point to field the associated ‘cause-effect’ relations of water spatial variations. Seven crop simulation models (WOFOST, DSSAT, APSIM, DAISY, STICS, AquaCrop and MONICA) and five hydrologic models (HYDRUS-1D, HYDRUS-2D, SWAP, MIKE-SHE and SWIM) were selected and their water modelling approaches were systematically reviewed for comparison. Crop models rely mainly on ‘discrete’ and empirical approaches for modelling soil water movement while hydrologic models emphasize more ‘continuous’ and mechanistic ones. Combining both types of models may not be the best way forward as none of the models consider all of the processes which are relevant for the simulation of spatial variations. Hydrologic models pay more attention to spatially variable water processes than crop simulation models, although their focus is on scales higher than the field which is the relevant scale for assessing the influence of such variations on crop behaviour. Opportunities for progress in the spatial simulation of water processes at field level will probably come from two different directions. One implying a stronger synergism between both model families by using continuous-type approaches to simulate some mechanisms in existing crop models, and the other through the integration of lateral flows in the simulation of discrete water movement approaches.

1. Introduction

An inherent action of biological sciences is the conceptual representation of systems through hierarchical levels (De Wit, 1982; Loomis et al., 1979). In agronomy related studies, it implies different levels of complexity determined by the nature of the issue addressed (Ahuja et al., 2019). Over the last 60 years, crop scientists have dedicated particular attention to modelling in an attempt to mathematically represent the functioning of agricultural systems at different levels of complexity, and to simulate their response to multiple factors in an ‘easy-fast’ and ‘low-cost’ way (Carberry, 2003; Fischer and Connor, 2018; Jin et al., 2018; Jones et al., 2017a; Lobell et al., 2009).

Conceptually, models can be divided into ‘functional-empirical’ or ‘mechanistic’ and distinguished according to their spatial scale, being classified as ‘point-based’ or ‘distributed’ (ASCE, 1982; Passioura, 1996; Thomas and Smith, 2003). While ‘engineering-oriented’ models tend to be classified as functional-empirical, 'science-oriented' models are mostly considered mechanistic (or process-based). While point-based scales ignore spatial variability by averaging or using ‘dominant’ characteristics to model an area of interest, distributed scales consider the spatial distribution of resources and the consequent crop response. Functional-empirical models have shown potential to support benchmarking, decision and policy making at different temporal-spatial scales (Boote et al., 1996; García-Vila et al., 2009; Mateos et al., 2002; Passioura, 1973). Mechanistic models have been mostly used to assist plant breeding for specific environments (Fischer and Connor, 2018; Struik, 2016; Yin and Struik, 2007), the identification of global yield-gaps (Byerlee et al., 2014; Boogaard et al., 2013; Grassini et al., 2015); (http://www.yieldgap.org/), and for agro-ecological resource management (Boote et al., 1996; Booker et al., 2015; Fischer et al., 2002; Thorp et al., 2008).

The extraordinary advances in computer engineering and programming languages, particularly over the last three decades, have intensified the modelling processes contributing to an increased

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adoption of such tools for many applications (Jones et al., 2017a; Passioura, 1996; Seidel et al., 2018; Thorp et al., 2012). The use of models in large cooperative efforts (such as The Agricultural Model Intercomparison and Improvement Project; www.agmip.org) has intensified recently, too, partially in response to new needs (Asseng et al., 2014). However, recent advances have not yet succeeded to scale up mechanisms from point to field level in crop models (Ahuja et al., 2019; Fischer and Connor, 2018). Such limitation may be leading to an impasse in modelling, compromising the adoption of these tools, mostly in the context of precision agriculture (Jones et al., 2017b). In fact, while significant advances have been made in the engineering aspects of precision agriculture, such as increasing spatial resolution, variable rate technologies and automation, much less effort has been devoted to understand the crop mechanisms in response to spatial variations (Cassman, 1999; McBratney et al., 2005; Monzon et al., 2018).

As considerable spatial variability in soil hydraulic properties exists within a field, even in those considered homogeneous (Nielsen et al., 1973), the accurate modelling of crop heterogeneity requires assessing the spatial variability of water as it affects crop behaviour (Ritchie, 1981; Sadras et al., 2016; Verhagen and Bouma, 1997). This aspect is considered a serious limitation in current crop models but it has received limited attention (Ahuja et al., 2014; Jones et al., 2017b).

In the modelling of water, two 'families' of models can be distinguished: crop models and hydrology based models. Both families have been widely used worldwide and different arguments are employed to promote the adoption of each one depending on the specifications of each case-study (Ahuja et al., 2014; Devia et al., 2015; Jones et al., 2017b). While crop models are centered on the growth and development as affected by the environment, hydrological modelling emphasizes mostly systems' water dynamics at different scales. In this sense, and in regard to water-related processes, crop models tend to be more empirically-based while hydrologic models are more mechanistic. In relation to spatial scales, while crop models are limited to point-based scales, some hydrological models distribute partially water processes. However, practically all distributed models have in fact 'discrete characteristics' (e.g. input parameters, boundary conditions) and follow non-linear relations for multi-dimensional representations that lead to important trade-offs between accuracy and data requirements that must be considered (Passioura, 1996). Just as distributed models rely partially on discrete characteristics, the distinction between mechanistic and empirical models is not clear-cut in this case, as there is a continuum between the two approaches as well, with mechanistic models having always some empirical components.

Essentially, if crop models are to be used to improve water management in precision agriculture, they may greatly benefit from spatial water modelling approaches capable of accurately represent and simulate within-field variation of water-related processes. It is important to reflect if this will be more likely achieved by distributing water processes in crop models (i.e. identifying conceptual gaps in the water balance structure) or by coupling both families.

Contemporary reviews on crop modelling (Ahuja et al., 2019; Boote et al., 2013; Bouman et al., 1996; de Wit et al., 2018; Holzworth et al., 2015; Jin et al., 2018; Jones et al., 2017a,b; Whisler et al., 1986) have tended to cover most main variables governing crop growth and development (at point-based scales), models structure and software details, but do not dwell on the modelling approaches with sufficient detail to be able to identify the main conceptual gaps that constrain the use of models for spatial variable applications. Also, most reviews focus on one or only a few models without reaching out to other different types of models (Boote et al., 1996; de Wit et al., 2018; Holzworth et al., 2015; van Ittersum et al., 2003). Rarely, a single variable, such as water, has been the subject of specific analyses in crop modelling reviews.

In our case, we have focused solely on water because it is a major determinant of spatial heterogeneity in the field (Nielsen et al., 1973, 1987; Ritchie, 1981; Ahuja et al., 1984; Sadler and Russell, 1997; Wallor et al., 2018). In an effort to assist in the scaling up of crop simulation models, we have carried out a systematic review of the approaches taken to simulate water in a number of selected crop and hydrologic models.

2. Methodology

2.1. Review approach

Since most of the selected models are based on similar fundamentals, this review followed a 'process-based' structure to avoid repetitive comparisons among models. The analysis was carried out in three consecutive steps: (1) selection of models based on a literature search of recent reviews; (2) identification and description of plant-soil-water processes addressed by the selected models; (3) compilation of results and a comparative analysis.

2.2. Model selection and soil-plant water processes description

The first step consisted of conducting a web search of the last ten years of published reviews on modelling that were either crop-based or hydrologic-based. Priority was given to 'multiple-species' and 'comprehensive' models since we focused on models complying with the following two criteria: (1) related literature is accessible and clear regarding fundamentals, equations and assumptions; and (2) the calibration and parameterization for multiple field crops is possible. A total of 42 articles were found, out of which 34 were rejected because they were focused on topics different than a crop model/s review. Eight documents were selected: one technical report (Kirby et al., 2013) and seven scientific papers (Donatelli et al., 2017; Holzworth et al., 2015; Jin et al., 2018; Jones et al., 2017a,b; Rauff and Bello, 2015; Shaw et al., 2013). The following seven 'crop-based' models were selected: WOFOST, DSSAT, APSIM, DAISY, STICS, AquaCrop and MONICA. An equivalent approach was followed to select the hydrology-based models. The initial search yielded a total of 99 results out of which 90 were also rejected for a similar reason as to the crop models. The final nine documents selected (Devia et al., 2015; Dwarakish and Ganasri, 2015; Gao and Li, 2014; Golden et al., 2014; Hallouin et al., 2018; Kauffeldt et al., 2016; Salvadore et al., 2015; Song et al., 2015; Sood and Smakhtin, 2015) referred to 12 models from which a final sample of five models was chosen based on the intended scale of analysis (i.e. small catchment plot or crop field level) and the potential to be coupled with 'crop-based' models in regard to water processes. The models are: HYDRUS-1D, HYDRUS-2D, SWAP, MIKE-SHE and SWIM.

Once models were selected, we proceeded with the identification of all processes where water moves along the soil-plant-atmosphere system, called here soil-plant water processes. Subsequently, a description of the modelling approaches followed by the selected models was obtained from the literature going back to the initial publication of each model. Soil-plant water processes were structured following the fate of water in a hypothetical hydrological unit: (1) pre-infiltration, (2) infiltration, (3) surface-water flow, (4) evaporation, (5) root water uptake and transpiration, (6) internal drainage, (7) capillary rise, (8) subsurface lateral flows, and (9) solute transport.

Following a basic description of all models, every water process was described in detail as simulated in each of the models. The fundamentals of the modelling approaches were described based on a literature search that was not limited by any time-frame. All results were synthesized in a table for a comparison among models (Appendix A). The tabled results are fully integrated with the text, following the same nomenclature and acronyms. Considering our sample ($N = 12$ models), a descriptive statistical analysis was conducted to explore differences among models in regard to the degree of spatial components and an association plot was produced to justify our discussion.

3. Modelling soil-plant water processes

3.1. The pre-infiltration phase

The pre-infiltration phase involves all water processes taking place above the soil surface (i.e. precipitation, irrigation, surface run-on, canopy or mulch interception, and gravitational flow through plant surfaces, commonly called stem-flow). This phase determines the amount of water supplied from precipitation (P), including outflows from the snowpack (DAISY, MONICA, HYDRUS-1D/2D, SWAP, MIKE-SHE) and irrigation (I) after subtracting the evaporated fractions of intercepted water by canopy and other surfaces (e.g. mulches). Some models operating at catchment scale (i.e. MIKE-SHE), consider superficial inflow (SIF) from run-on as a supply form, too (DHI, 2017b).

Precipitation is taken as an input (Beaudoin et al., 2009; Hansen et al., 1990; Jones et al., 2003; Keating et al., 2003; Nendel et al., 2011; Raes et al., 2009a; Simunek et al., 2008; van Dam et al., 1997; van Van Diepen et al., 1989; Verburg et al., 1996), which can be represented at point- or field-scale, depending on the spatial variability of rainfall and the availability of spatially distributed data (Basso et al., 2001; Thorp et al., 2008; Zhou and Zhao, 2019).

Irrigation, when considered (DSSAT, APSIM, DAISY, STICS, AquaCrop, MONICA, HYDRUS, SWAP, SWIM), must be previously set up within a management module that can be activated when necessary (Boote et al., 1996; García-Vila and Fereres, 2012; Hussein et al., 2011). Irrigation water supply is taken as a net inflow, either assuming no losses (DSSAT, APSIM, DAISY, AquaCrop, MONICA, HYDRUS, SWAP, SWIM) or by subtracting the corresponding application losses (STICS). Four irrigation methods may be considered: (1) Surface; (2) Sprinkler; (3) Drip; and (4) Subsurface drip. Irrigation applications may be simulated in three different ways: (1) a calendar defined by the user; (2) a planned irrigation schedule applying constant or variable rates once a threshold of soil water content is reached; (3) a planned schedule based on multiple-criteria (e.g. crop phenological stage, soil water content, water availability constraints).

The method influences whether irrigation is applied above canopy (i.e. sprinkler pivot) or below (i.e. furrow or drip irrigation). Irrigation applied above canopy implies the simulation of pre-infiltration processes such as canopy or mulch interception and evaporation from plant surfaces (STICS, HYDRUS, SWAP). Some models allow users to define the fraction of soil surface wetted by irrigation (AquaCrop).

The fraction of water intercepted by the canopy may be simulated by an analogy of the 'Beer-Lambert law' (B-L) (Murphy and Knoerr, 1975). Some models (APSIM) use the B-L approach to simulate 'rainfall attenuation', i.e. interception of rainfall or irrigation water applied over the canopy. The fraction of intercepted water by the canopy (or mulch) may be assumed as part of a direct evaporation 'pool' (Murphy and Knoerr, 1975) or recovered into the 'infiltration pool' (i.e. the amount reaching the soil surface) in form of stem flow down to the soil surface. For the recovered fraction, Brisson et al. (2003) proposed the simulation of stemflow (SF) as a function of LAI, light extinction coefficient (k) and an empirical crop coefficient (SF_{MAX}) that depends on the architecture and wettability of plant surfaces (Wang et al., 2015) and the total water supply, i.e. irrigation (I) and/or precipitation (P) according to:

$$\mathrm{SF} = \mathrm{SF}_{\mathrm{MAX}}[1 - e^{(-\mathrm{k\,LAI})}](P + I) \tag{1}$$

Alternatively, the method proposed by Braden (1985) and von Hoyningen-Huene (1981) can also be used to estimate the fraction of intercepted water (e.g. HYDRUS, SWAP):

$$\mathrm{INT} = \mathrm{a\,LAI}\left[1 - \left(1 + \frac{b\mathrm{AbC}_{\mathrm{pool}}}{\mathrm{a\,LAI}}\right)^{-1}\right] \tag{2}$$

where LAI is leaf area index, a is an empirical coefficient (assumed as 0.25 by default), b is the soil cover fraction (assumed as 0.33 of LAI), and AbCpool is the 'above canopy pool'.

Other models (DAISY, STICS) represent the effects of mulch residues on the modelling of water interception dynamics (Brisson et al., 2003; Hansen et al., 2012). Such advancements have focused on the development of empirical equations that estimate the quantity of soil cover with time (e.g. STICS). According to the calibration of Scopel et al. (1998), the effect can be represented by a negative logarithmic relation that determines the decomposition rate of the mulch type with time.

Some models (DAISY, MONICA, HYDRUS-1D/2D, SWAP, MIKE-SHE) integrate snow accumulation and melting processes within the pre-infiltration phase. As described by Abrahamsen and Hansen (2000), these processes can be determined as a function of precipitation, air temperature, global radiation, ground heat flux, albedo and depth of the snowpack. Water losses from the snowpack, occur in the form of evaporation, sublimation and percolation (when the retention capacity is exceeded), and evaporation tends to have priority over sublimation.

In this sense, the INFpool (expressed in units of length per time, as mm day^{-1} or cm day^{-1} in case of daily time-steps) can be calculated as the sum of non-intercepted water from rainfall (P), irrigation (I), and when considered, also superficial inflow from run-on (SIF) and stem-flow (SF). All contribute eventually as an input to a snow pack module (SPM), if considered, from which the melted fractions recover, counting as an input on the estimation of infiltration in the subsequent time-step. Non-recovered fractions through SF are likely to be lost through direct evaporation. The INFpool is therefore the amount of available water at soil surface to be infiltrated.

3.2. Infiltration

Effective infiltration (INFeff) is the fraction of INFpool that infiltrates into the soil at a given time step. The remaining fraction is considered a surface water surplus, that may originate water ponding (leading to accumulation, evaporation or infiltration in following time-steps) and surface runoff depending on the surface conditions and topographic characteristics of the area (Allen, 1991).

The simplest approach to estimate INFeff applies a simple capacity model (CAP) in which maximum infiltration capacity is defined as the difference between the soil saturation water content (θSAT) and actual water content (θ), expressed as a fraction of a volume. In this case, the infiltration capacity is defined as the maximum amount of INFpool that infiltrates in a given soil under specific conditions (WOFOST and MONICA; Appendix A).

An alternative and widely adopted approach (DSSAT, APSIM, STICS, AquaCrop; Appendix A) is the USDA curve number method (CN-method). As discussed in detail by Allen (1991), this 'infiltration-loss based method', calculates INFeff as a function of the potential maximum retention (S). S (expressed in mm) is defined according to the curve number (CN), which is an empirical parameter, determined from tabled empirical values, according to land cover and soil hydrological group (Cronshey, 1986; Rallison, 1980; Woodward et al., 2003):

$$S = 254\left(\frac{100}{\mathrm{CN}} - 1\right) \tag{3}$$

The soil hydrologic group classification is based on probability distribution curves of measured infiltration rates related to soil antecedent conditions (Allen, 1991; Cronshey, 1986). Therefore, CN is not a constant but varies from event to event. The robustness of this method is related to the vast quantity of field measurements that support it. However, it reveals some weakness when surface runoff (SRn) is a small fraction of the INFpool (i.e. arid or semi-arid conditions), a situation where a wider range of CN is observed (Allen, 1991). According to the CN-method, INFeff can be calculated as:

$$\mathrm{INFeff} = \mathrm{INFpool} - \left[\frac{(\mathrm{INFpool} - \chi S)^2}{\mathrm{INFpool} + (1 - \chi)S}\right] \tag{4}$$

where the subtracted fraction corresponds to SRn and χS corresponds to the 'initial abstraction' which is the initial fraction of S that can infiltrate before starting surface runoff (Allen, 1991). More mechanistic approaches compute infiltration according to the formulations of Richards (1931) and Richardson (1922) for transient flow conditions (DAISY, HYDRUS-1D/2D, SWAP, MIKE-SHE, SWIM; Appendix A). INFeff can be defined by unsaturated soil water movement, which is estimated through numerical solutions of the Richards equation (Buchan, 2003):

$$\text{INFeff} = \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta)\frac{\partial \psi}{\partial z} - K(\theta)\right] \tag{5}$$

where θ is the volumetric water content of the soil top layer (expressed as a fraction of a volume), t is time, z is the vertical coordinate (expressed in units of length), positive when water flows downwards, K is the unsaturated hydraulic conductivity as a function of θ, and ψ is capillary pressure head relative to atmospheric pressure (unit of length). While the space z and time t are independent variables, ψ and θ are dependent variables.

The methods used to solve Richards' equation are an important issue in hydrological research (van Dam, 2000a; van Dam et al., 1997). Many alternative mathematical solutions have been proposed (e.g. geometric means, arithmetic means, iterative methods), but the parabolic form of this equation in combination with the strong non-linearity of the soil hydraulic functions (i.e. functions relating water content, soil pressure head and hydraulic conductivity) makes it a non-consensus and difficult task. According to van Genuchten (1980) and Mualem (1976), the soil hydraulic functions can be represented as:

$$\theta(h) = \theta_{\mathrm{PWP}} + \frac{\theta_{\mathrm{SAT}} - \theta_{\mathrm{PWP}}}{(1 + |\alpha h|^{n})^{\frac{n-1}{n}}} \tag{6}$$

$$K(\theta) = K_{\mathrm{SAT}}\left(\frac{\theta - \theta_{\mathrm{PWP}}}{\theta_{\mathrm{SAT}} - \theta_{\mathrm{PWP}}}\right)^{\lambda}\left[1 - \left[1 - \left(\frac{\theta - \theta_{\mathrm{PWP}}}{\theta_{\mathrm{SAT}} - \theta_{\mathrm{PWP}}}\right)^{\frac{n}{n-1}}\right]^{\left(\frac{n-1}{n}\right)}\right]^{2} \tag{7}$$

where θ is the volumetric soil water content as a function of the soil pressure head (h), θ_{PWP} is the volumetric soil water content at permanent wilting point, θ_{SAT} is the volumetric soil water content at saturation point, α and n are empirical shape factors (respectively, expressed in units of length and unitless), K_{SAT} is the saturated hydraulic conductivity (expressed in units of length per time), and h is expressed in units of length. When INFpool increases at a higher rate than the maximum infiltration capacity (i.e. $K(\theta) = K_{\mathrm{SAT}}$), water accumulates at soil surface (DAISY, HYDRUS-1D/2D, SWAP, MIKE-SHE). The ponded infiltration can be modeled through a solution of Darcy's equation (DAISY) or according to the Green-Ampt approach (HYDRUS-1D/2D, SWAP, MIKE-SHE, Appendix A), which is based on Darcy's equation for continuous saturated conditions and considers the wetting front as the reference elevation, where gravitational head is zero (Green and Ampt, 1911). The decreasing hydraulic gradient caused by the wetting front drives the drop in infiltration rate over time, which can be mathematically represented as:

$$\text{INFeff} = K\left(\frac{L_f + H_0 + H_F}{L_f}\right) \tag{8}$$

where K represents the hydraulic conductivity, L_f is the thickness of the soil being considered (i.e. the depth of the wetting front), H_0 is the pressure head at soil surface and H_F is the pressure head at the wetting front (H_0 and H_F, both assumed to be constant). Despite being originally developed for flat land conditions, the Green-Ampt approach has also been applied to sloping surfaces (Chen and Young, 2006).

The INFeff estimation approaches that are based on the hydraulic conductivity of the top soil layer assume that after infiltrating into the soil, water is stored in successive layers downward according to a physical constraint that is imposed by the drainage ability of the soil (APSIM, STICS, AquaCrop).

3.3. Surface-water flow

Surface-water flow can be classified as a loss flow (i.e. when represented as SRn), a re-distribution flow (i.e. when represented as a lateral flow affecting the water balance of neighbouring hydrological units) or as a channel flow (i.e. for furrow irrigation simulation applications, as described by van Dam (2000a) and van Dam et al. (1997). However, in most of the selected models (i.e. all except MIKE-SHE), surface water flow is only represented as SRn and therefore considered as an outflow of the system. It is therefore relevant to discuss SRn in some detail below.

According to Ponce and Hawkins (1996), SRn can be distinguished into different forms (Appendix A): Hortonian overland flow (HRTf), saturation overland flow (SATf), throughflow (THRf), the direct channel interception flow (DCIf) and surface phenomena flow (SURf). Hortonian overland flow is the water flow occurring when rainfall or irrigation (or the combination of both by analogy with INFpool) exceeds soil infiltration capacity (i.e. typically the case of a rainfall storm). Saturation flow occurs when the profile gets saturated. While Hortonian flow is a 'pre-infiltration' process, saturation flow is a 'post-infiltration' one. Throughflow is the horizontal water flow beneath the land surface, usually when the soil is saturated. The direct channel interception flow is a type of runoff that refers to the spatial redistribution of rainfall directly intercepted by channels. This is an important type of flow in high dense and humid channel areas where channel interception may be the main source of surface-water flow, as reported by Hawkins (1973), who assessed watersheds characterized by frequent storm precipitation events, hilly landscapes and large areas of stream channels, where direct interception occurs in great extents. Under flat conditions, typical rice landscapes in the Philippines or channelled plots in the Netherlands can be taken as an example of these areas, too. Surface phenomena flow is all the flow driven by crust development, hydrophobic layers and frozen ground that do not allow vertical flow to occur. While some models simulate SRn (mostly in forms of HRTf, SATf, THRf) trough empirical approaches based on the CN-method (DSSAT, APSIM, STICS, AquaCrop), others derive SRn from Richards' based approaches (DAISY, HYDRUS-1D/2D, SWAP, SWIM). 'Overland flow models' such as MIKE-SHE dedicate particular attention to the simulation of SRn by dividing it into HRTf, SATf, SURf, THRf estimated through a 'diffusive wave' approach which considers a Manning's type roughness coefficient, and through the St. Venant equations (Saint-Venant, 1871), as explained in detail by DHI (2017a,b).

3.4. Evaporation

Evaporation (E) modelling has three different components: direct evaporation of water intercepted by the crop canopy (Ec), from the soil surface (Es), and from mulches (Em).

$$E = \mathrm{Ec} + \mathrm{Es} + \mathrm{Em} \tag{9}$$

However not all models calculate the three E components separately (DSSAT, MONICA), because, depending on the calculation procedure, evaporative demand may include all components together. The estimation of evaporation is conceptually divided into two steps for most of the selected models (WOFOST, APSIM, AquaCrop, DAISY, HYDRUS, SWAP): (1) the calculation of evaporative demand (ED_e), i.e. mass transfer based on latent heat; and (2) a 'partitioning' according to the corresponding evaporative surface area (i.e. fraction of crop canopy, fraction of uncovered soil, fraction of mulch).

The main formulations used to calculate the evaporative demand (ED_e) are based on the energy balance (Penman, 1948, 1956), which evolved as the PM equation (Allen et al., 1998; Monteith, 1976;

Monteith and Unsworth, 1990; Eq. (10); WOFOST, DSSAT, APSIM, DAISY, STICS, AquaCrop, MONICA, HYDRUS-1D/2D, SWAP). Other approaches used in the selected models are the Priestley-Taylor (PT) (Priestley and Taylor, 1972; Eq. (11); DSSAT, APSIM, STICS, MONICA), and Hargreaves (HG) (Hargreaves and Samani, 1982; Eq. (12); DAISY, HYDRUS-1D/2D) equations. The formulations of the equations are:

$$\mathrm{ED}_e = \frac{0.408\Delta(\mathrm{Rn} - G) + \left(\frac{\varphi \times 900}{T + 273}\right)U_2(\mathrm{es} - \mathrm{ea})}{\Delta + \varphi(1 + 0.34U_2)} \tag{10}$$

$$\mathrm{ED}_e = \frac{\Delta(\mathrm{Rn} - G)}{\Delta + \varphi}\alpha_{\mathrm{PT}} \tag{11}$$

$$\mathrm{ED}_e = C_H\,\mathrm{Ra}\sqrt{(T_{\mathrm{MAX}} - T_{\mathrm{MIN}})}(T_{\mathrm{MEAN}} + 17.8) \tag{12}$$

where Δ is the he slope of the saturation vapor pressure function versus temperature (kPa°C^{-1}), Rn is the daily net radiation at the soil surface (i.e. incoming minus reflected radiation expressed in MJ m^{-2} day^{-1}), G is the soil heat flux (MJ m^{-2} day^{-1}), φ is the psychrometric constant that is calculated according to the altitude (set by default as 66 Pa K^{-1}), T represents the mean temperature of the air (measured at 2 m height and expressed in °C), U_2 represents the wind speed (also measured at 2 m height and expressed in m s^{-1}), es represents the saturation vapor pressure, ea the air vapor pressure (the difference of both equals vapour pressure deficit – VPD), both expressed in kPa, α_{PT} is an empirically derived factor that depends on the season and location in relation to large water bodies (Castellvi et al., 2001) and varies from 1.26 (Priestley and Taylor, 1972) in minimal advection conditions, to maximum reported values that vary from 1.74 to 3.12 (Eaton et al., 2001; Jensen et al., 1990; Viswanadham et al., 1991), C_H is a constant parameter, assumed as 0.0023 according to Hargreaves and Samani (1982), Ra is the extraterrestrial solar radiation (MJ m^{-2} d^{-1}), and T_{MAX} and T_{MIN} are respectively maximum and minimum air temperatures (both expressed in °C).

Once EDe is estimated (expressed in units of length per time, as mm day^{-1}), some models follow a Beer-Lambert type approach (INT-BL) using LAI and the extinction coefficient (k) to calculate an evaporation coefficient (K_e) to estimate Es (WOFOST, DSSAT, APSIM, DAISY, STICS, MONICA, HYDRUS-1D/2D, SWAP, SWIM), while others follow a soil-cover based method (SC-M), whether using soil cover (SC) instead (AquaCrop, HYDRUS-1D/2D, SWAP, MIKE-SHE, SWIM). Some models deliver the option to follow both approaches. The two approaches are expressed as follows:

$$\mathrm{Es} = \sum (\mathrm{ED}_{\mathrm{e}i}K_e \times e^{-\mathrm{kLAI}_i}) \tag{13}$$

$$\mathrm{Es} = \sum [\mathrm{ED}_{\mathrm{e}i}K_e(1 - \mathrm{SC}_i)] \tag{14}$$

where the subscript i corresponds to the model time-step (e.g. hourly, daily), and Ke is the evaporation coefficient for wet surfaces set by default as 1.10 according to Allen et al. (1998). Alternative approaches derive both daily crop (Ec$_i$) and soil water evaporation (Es$_i$) directly from an adaptation of the original Penman's equation (PE) (Penman, 1963) as function of the fraction of uncovered soil (DSSAT):

$$E = \mathrm{Ec}_i + \mathrm{Es}_i = R_{\mathrm{s}i}[(4.88 \times 10^{-3}) - (\mathrm{GS}_i 4.37 \times 10^{-3})](T_i + 29) \tag{15}$$

where T_i is the daily air temperature (°C), Rs$_i$ is daily solar radiation (MJ m^{-2}) and GS$_i$ is a ground surface correction factor defined according to the light extinction coefficient (k) and daily values of leaf area index (LAI$_i$) as following:

$$\mathrm{GS}_i = (0.1e^{-\mathrm{kLAI}_i}) + [0.2(1 - e^{-\mathrm{kLAI}_i})] \tag{16}$$

Similar approaches can be followed to estimate Em (STICS). However, in the case of inert mulching, the extinction coefficient decreases in time due to the decomposition of those residues as well as soil cover fraction (Scopel et al., 1998).

In addition to the previous methods, some models (MIKE-SHE, SWIM, DAISY, STICS) estimate E through soil vegetation atmosphere transfer schemes (SVAT, Appendix A). The SVAT approach (Brisson et al., 2003; Hansen et al., 2012; van der Keur et al., 2001; Verburg et al., 1996; Verburg, 1996) is based on the aerodynamic transfer of water vapor and integrates the effect of the aerodynamic resistance to water vapour transport (r_a), the soil-vegetation-atmosphere pathways components resistance (r_c), the saturated vapour pressure at canopy temperature (es$_{(\mathrm{Tc})}$), the vapour pressure in the overlying air boundary (e_{ref}), the air density, the ratio of the molecular mass of water vapour to that of dry air (ρ_ε) and the canopy pressure (ρ_s) as follows:

$$E = \frac{\rho_\varepsilon}{\rho_s}\left(\frac{\mathrm{es}_{(T_c)} - e_{\mathrm{ref}}}{r_a + r_c}\right) \tag{17}$$

where the calculation of E accounts for the different evaporation pathways. These approaches are also called networks of resistances (Campbell, 1985; Koster and Suarez, 1994). Some models divide soil evaporation in two consecutive stages (APSIM, STICS, AquaCrop, SWAP, MIKE-SHE, SWIM), others integrate it into a single formulation (e.g. WOFOST, DSSAT, DAISY, MONICA, HYDRUS, SWAP). Models integrating one single formulation apply directly to EDe a 'Beer-Lambert' type integrated approach (INT-BL) whether using LAI (see Eq. (13)) or a soil-cover based method (SC-M) if using SC (see Eq. (14)).

The 'two-stage method' (2-stage-M) proposed by Ritchie (1972) and based on Philip and De Vries (1957), considers that evaporation occurs in two consecutive stages: the first limited by the energy available, and the second, limited by water availability. While in the first stage, the evaporative rate is a function of the potential evaporative demand (EDe), in the second stage, a falling response takes place since the surface soil water content decreases with time and Es depends on the flow of water to the soil surface which decreases exponentially with time.

The '2-stage-M' approach may be integrated into a single formulation considering a reduction factor that equals 1 for the first stage, and decreases to 0 during the second stage (AquaCrop):

$$\mathrm{Es} = (1 - \mathrm{SC})K_r K_e \mathrm{ED}_e \tag{18}$$

When the second stage starts, K_r is calculated through an exponential relation that depends on a decline factor (f_k) related to the relative soil water content (W_{rel}) (AquaCrop):

$$K_r = \frac{e^{f_k \times W_{\mathrm{rel}}} - 1}{e^{f_k} - 1} \tag{19}$$

where W_{rel} is a relative weighting factor, estimated according to Raes et al. (2017). For a given soil type, the second stage evaporation can also be empirically related to the square root of an independent variable, such as time (APSIM):

$$\mathrm{Es}_{\mathrm{stage-II}} = \eta\sqrt{t} \tag{20}$$

where η represents a parameter related to the soil type and t is time; Others use an empirical parameter (A) as following (STICS):

$$\mathrm{Es}_{\mathrm{stage-II}} = \sqrt{(2A\sum \mathrm{ED}_i) + A^2} + A \tag{21}$$

where parameter (A) depends on the aerodynamic resistance, the latent heat of vaporization, the water vapour pressure, air temperature, and a diffusion coefficient that is related to the bulk density of the evaporative soil layer and the surface temperature (Brisson and Perrier, 1991); The second stage Es rate can still be modeled as a function of soil water flow (q). This tends to be the case of approaches operating at smaller time-steps (SWAP, MIKE-SHE). In this sense, Es gets boundary limited by the maximum upward flow, modelled through a numerical solution of Richards' equation that is simplified in the following form (van Dam and Feddes, 2000):

$$\mathrm{Es}_{\mathrm{stage-II}} < -K_{1/2}\left[\frac{(h_{\mathrm{atm}} - h_1) - z_1}{z_1}\right] \tag{22}$$

where $K_{1/2}$ represents the average hydraulic conductivity in the top soil evaporative layer (expressed in units of length per time), z_1 corresponds to the thickness of the top soil evaporative layer (expressed in units of length), $h_{\text{atm}} - h_1$ is the pressure gradient between atmospheric and top layer pressure (expressed in units of length).

3.5. Transpiration and root water uptake

Crop transpiration (T) is determined by the atmospheric-evaporative demand (EDt) and limited by root water uptake. Atmospheric conditions govern EDt while root water uptake is a function of both soil water availability and resource capture dynamics (Passioura, 1983). In general, models estimate first potential transpiration demand and then actual T rates according to canopy and root water uptake related factors, as well as to soil water status. Despite the atmospheric demand for transpiration (EDt) being conceptually the same as the evaporative demand (EDe), some models have the possibility to treat them separately as two different calculation procedures depending on different approaches and methods (DSSAT, APSIM, DAISY, STICS, AquaCrop, MONICA, HYDRUS-1D/2D). For this reason, we represent atmospheric demand for transpiration as EDt and evaporative demand for evaporation as EDe (Appendix A).

Similarly to EDe, EDt is estimated by the selected models according to one of the following approaches: Penman-Monteith (WOFOST, DSSAT, APSIM, DAISY, STICS, AquaCrop, MONICA, HYDRUS-1D/2D, SWAP), Priestley-Taylor (DSSAT, APSIM, STICS and MONICA as well), Hargreaves (DAISY, HYDRUS-1D/2D) or a SVAT scheme (MIKE-SHE, SWIM, DAISY and STICS as well). In order to estimate potential crop transpiration (Tc), some models multiply EDt by a crop specific coefficient (Kc) (MONICA), while others use a transpiration coefficient that is equivalent to the crop basal coefficient (Kc_b) (AquaCrop). While Kc includes both soil evaporation and crop transpiration, the Kc_b is a specific parameter representing the transpiration fraction and a residual diffusive evaporation component supplied beneath vegetation (Allen et al., 1998, 2005; Raes et al., 2017). Tc is then adjusted to the transpiration surface through a 'Beer-Lambert type' integrated approach (INT-BL) using LAI (MONICA) or through a green canopy soil cover based method (SC-M) (AquaCrop), both equivalent to the evaporation approaches and respectively expressed as:

$$T_c = \text{ED}_t\text{Kc}(1 - e^{-\text{kLAI}_i}) \quad (23)$$

$$T_c = \text{ED}_t\text{Kc}_b\text{SC} \quad (24)$$

where SC is the green canopy soil cover adjusted for micro-advective effects. According to van Dam et al. (1997), an alternative Tc approach depending on the ratio between the daily amount of intercepted precipitation and the evaporation rate of water intercepted by the canopy (β) is used (SWAP). This approach assumes that Tc is reduced by the water evaporation from the wet canopy (Ec), since part of the latent heat flux is 'consumed' on leaf evaporation processes. The canopy transpiration through the leaf stomata gets maximum when β gets equal to zero (i.e. when Ec equals zero).

Actual transpiration (Ta) can be reduced in multiple stress situations: soil saturation, low soil moisture, salinity, and excessive temperatures inducing stomata closure (Hsiao, 1973). This can be modeled through the use of stress coefficients (Ks), which are calculated as (AquaCrop):

$$\text{Ks} = 1 - S_{\text{rel}} \quad (25)$$

$$\text{Ks} = 1 - \left[\frac{e^{S_{\text{rel}}\text{fshape}} - 1}{e^{\text{fshape}} - 1}\right] \quad (26)$$

$$\text{Ks} = \frac{S_n S_x}{S_n + (S_x - S_n)e^{-r(1 - S_{\text{rel}})}} \quad (27)$$

where S_{rel} is the relative stress level and f_{shape} is the curve shape factor, S_n and S_x are respectively the relative stress level at the lower and upper threshold and r is a rate factor (Raes et al., 2009b). AquaCrop is the only of the selected models which appears to use both transpiration coefficients equivalent to crop basal coefficients (Kcb) and multiple stress coefficients (Ks). For this specific case, Ta is estimated as:

$$T_a = \text{ED}_t\text{Kc}_b\text{SC Ks} \le S_i \quad (28)$$

where Ks varies from 0 to 1 according to three main different approaches.

The actual crop transpiration (Ta) is limited by an extraction sink term (Ta < Si), which, in the case of multi-layer models, is computed separately for each individual soil layer. According to Ritchie (1972, 1981) and Feddes et al. (1978), Si can be calculated as a linear function (LIN) of soil moisture content (θ) or pressure head (h) and the maximum extraction rate (S_{MAX}):

$$S_i = \alpha(h)S_{\text{MAX}}(z) \quad (29)$$

where S_{MAX} depends on the vertical rooting depth and $\alpha(h)$ is a coefficient that depends linearly on h in three different phases: (1) h is considered to increase linearly from 0 to 1, between a h-minimum threshold (i.e. saturation conditions) and an intermediate h-threshold; (2) h equals 1 for an intermediate interval of h (i.e. optimal soil moisture content pressure head for plant uptake); and (3) h decreases linearly from 1 to 0 (i.e. at permanent wilting point). The coefficient α can also be represented as a function of soil water content (Raes et al., 2017; van Genuchten, 1980). This approach can be employed in both 'discrete' or 'continuous' representation schemes of the vadose zone. 'Discrete' schemes determine $S_{\text{MAX}}(z)$ as the product of Ta and a root density term (D_{root}), which can be computed separately for each individual layer (APSIM, STICS, AquaCrop, MONICA) or for the whole root zone (DSSAT, WOFOST), abbreviated as following:

$$S_{\text{MAX}} = T_a D_{\text{root}} \quad (30)$$

where D_{root} represents the fraction of total root density in each layer, when computed individually for multiple layers, or the rooted fraction of a single layer depth, when computed for the whole root zone. On the other hand, some 'continuous' schemes (DAISY, SWAP, SWIM) define S_{MAX} through an integral equation (from root depth to soil surface) that can be simplified as:

$$S_{\text{MAX}} = \left[\frac{T_a \pi_{\text{root}}}{\int_{-\text{Droot}}^{0} \pi_{\text{root}}\,\partial z}\right] \quad (31)$$

where π_{root} is the root length density (expressed in mm mm^{-3}), defined as function of both space and time (van Dam et al., 1997). Space can be represented in one ($\pi_{\text{root}}(z, t)$) or two dimensions ($\pi_{\text{root}}(x, z, t)$) as respectively described by van Dam et al. (1997) and Simunek and Hopmans (2009).

An alternative approach (APSIM) describes Si through an exponential relation (EXP):

$$S_i = [1 - e^{\text{kl}(t - \text{tc})}]S_{\text{MAX}} \quad (32)$$

where k is a diffusivity constant (expressed in cm^2 day^{-1}), l is the root length density (equivalent to π_{root} but here expressed in cm of root per cm^3 of soil), t is time and tc is the beginning time of water extraction (Passioura, 1983; Tinker, 1976). According to DHI (2017b), an alternative to this relation is to simplify the root depth as a linear function of time while assuming root length density as constant (MIKE-SHE).

According to van Genuchten (1987), an osmotic pressure term (h_ϕ) can be included in the calculation of α (Eq. (29)) that becomes a non-linear function (HYDRUS-1D/2D, SWIM), also time dependent $\alpha(h, h_\phi, z, t)$ (Simunek et al., 2018a; van Genuchten, 1987). For the specific case of HYDRUS-2D, a horizontal coordinate is also incorporated into the $\alpha(h, h_\phi, x, z, t)$ extraction function (Simunek and Hopmans, 2009), and Si is calculated as:

$$S_i = \int_{\Omega R} [\alpha(h, h_\phi, x, z, t)\frac{L_t}{L_x L_z}]T_a \quad (33)$$

where L_x is the width of the root zone (ΩR), L_z is the depth of ΩR, and L_t is the soil surface associated with the transpiration process, all expressed in units of length (Simunek and Hopmans, 2009).

Apart from the three general modelling approaches described for Si calculation, some models (HYDRUS-1D/2D) also include a module for compensatory mechanisms (Appendix A) regulating root water extraction (Simunek and Hopmans, 2009). This enables the simulation of physiological responses at the root level under spatially distributed stress conditions (Bouten, 1995; Hsiao, 1973; Li et al., 2001). In these cases, a root adaptability factor, defined as the threshold value above which reduced root water (or nutrient) uptake in water (or nutrient) stressed parts of the root zone, is fully compensated by increased uptake in other root zones that are less stressed.

3.6. Redistribution and drainage

Modelling drainage processes has been a central issue in hydrology for centuries (Skaggs and Chescheir, 1999). For point-based models, drainage is represented as a vertical flow (Chescheir, 2003), generally simulated in two main ways (Appendix A): with a 'tipping-bucket' approach (TBA), or based on Darcy's or Richards' equations.

The TBA, as described by Emerman (1995), implicitly considers that macropore water flow is the only mechanism of water transport between each 'tipping bucket' (i.e. soil layer). Each 'bucket' is boundary defined by a lower and an upper limit; the θ_{PWP} (when empty) and the θ_{FC} (when full). If water content exceeds θ_{FC}, water excess flows vertically downwards to the next layer for a given time-step. The TBA models (WOFOST, DSSAT, APSIM, STICS, AquaCrop, MONICA) are simple and fully discrete in time (constant conditions are assumed for a certain time interval). A notable limitation of the TBA approach is the fact that the chosen time step is critical for an accurate prediction of the observation (Emerman, 1995). The minimum effective time step is the minimum period over which an appropriate fraction of the soil water excess (when $\theta > \theta_{FC}$) drains down to the next unit. The fundamental equation describing internal drainage (D) under TBA is:

$$D = \alpha(\theta - \theta_{FC}) \tag{34}$$

where α is the drainage coefficient and $\theta > \theta_{FC}$ (Emerman, 1995; Ritchie, 1984).

Modelling approaches based on Darcy's and Richards' equations allow a continuous representation of soil water movement, for saturated and unsaturated conditions. While Darcy's is used for steady-state flow modelling (Buchan and Cameron, 2003), Richards' is used for transient flows (Buchan, 2003; Richards, 1931; Simunek and van Genuchten, 2008). The model formulations are dependent on the spatial-scale, as the flow term (q) can be defined as a one, two or three dimensional vector (Buchan, 2003), leading to different calibration requirements and computation times.

Soil water movement also depends on the wetting/drying history of the soil, a phenomenon called hysteresis (Hillel, 1980). In general, hysteresis retards water movement, while preferential flow enhances water movement. In all crop models described here, hysteresis is ignored since only one curve is used to describe the $h(\theta)$ relationship (WOFOST, DSSAT, APSIM, DAISY, STICS, AquaCrop, MONICA). This is mostly due to the time and cost associated with the inclusion of hysteresis in the calibration of this relationship. However, this might lead to considerable uncertainties regarding the simulation of infiltration and lateral flow rates, mostly at larger time-steps (van Dam, 2000b). However, soil water hysteresis effects can be simulated using the Scott's scaling method (SCOTS), which requires only the calibration of the main drying and wetting water retention curves to calculate the scanning curves (Scott, 1983). The scanning curves are derived by linear scaling of the main curves as follows (HYDRUS-1D/2D, SWAP):

$$\frac{\theta_{SAT}^{*} - \theta_{res}}{\theta_{SAT} - \theta_{res}} = \frac{\theta_{act} - \theta_{res}}{\theta_{md} - \theta_{res}} \tag{35}$$

where θ_{SAT}* is the adapted θ_{SAT}, θ_{act} is the actual water content, θ_{md} is the water content of the main drying curve at the actual soil water pressure head, and θ_{res} is the residual water content of the wetting scanning curve (Kroes et al., 2017b).

3.7. Capillary rise

Quantification of capillary rise (CR) is of great importance for the accurate simulation of the water balance, particularly in areas with shallow groundwater tables (Kroes et al., 2017a). However, not all selected models conceptually consider CR on the calculations of the water balance. Those following a 'tipping-bucket approach' TBA and considering CR, either take it as an input (STICS, MONICA), or simulate it (DSSAT, AquaCrop) according to relations (soil texture specific) between water table depth, soil hydraulic properties and actual soil water content (or pressure head) of the unsaturated receiving layers (Raes et al., 2017). For the first case (STICS, MONICA), CR is defined by a Neumann type lower boundary condition (i.e. flux is a function of time, as CR depends on a defined calendar). For the second case (DSSAT, AquaCrop), both a Dirichlet type (i.e. CR as a function of soil water content) and a Cauchy type condition (i.e. CR flux as a function of groundwater level) are considered (Raes et al., 2017; Ritchie, 1998). However, none of these cases (DSSAT, STICS, AquaCrop, MONICA), simulate the feedback between the vadose zone and the water table (i.e. the water table depth is not updated).

Models using Richards' equation (DAISY, HYDRUS-1D/2D, SWAP, MIKE-SHE, SWIM), have different approaches to simulate CR flow while updating water table depth (Hansen et al., 2012; Simunek et al., 1999; van Dam, 2000a; van Dam and Feddes, 2000; Verburg, 1996). In the selected models there are four different types (Appendix A): (1) models that do not-consider CR (X) (WOFOST, APSIM); (2) models with predefined CR ($D - \mathrm{CR}$) (STICS, MONICA); (3) models simulating CR but without updating water table depth ($\mathrm{SnU} - \mathrm{CR}$) (DSSAT, AquaCrop), and (4) models simulating CR and updating water table depth ($\mathrm{SU} - \mathrm{CR}$) (DAISY, HYDRUS-1D/2D, SWAP, MIKE-SHE, SWIM).

3.8. Subsurface lateral flow

Among the models, subsurface (water) lateral flow (SSLF) is simulated only by Richards' equation based models. However, most of these models (DAISY, HYDRUS-1D, SWAP, MIKE-SHE, SWIM) limit SSLF simulations to lateral drainage processes, such as lateral out flows between the simulated plot and neighbouring drainage canals (Simunek et al., 2018b; Simunek et al., 1998; van Dam, 2000a; van Dam et al., 1997; Verburg, 1996). For these cases (Appendix A), lateral flow to drains (q_{drain}) is represented by the Hooghoudt equation (Ritzema, 1994) which can be simplified as follows:

$$q_{drain} = \frac{\phi_{WL} - \phi_{drain}}{\gamma_{drain}} = \frac{8K_{SAT}^{h} d\Delta h_{tot} + 4K_{SAT}^{h} d\Delta h_{tot}^{2}}{L^2} \tag{36}$$

where ϕ_{WL} (cm) represents mean groundwater level, ϕ_{drain} is the drain level (cm), and γ_{drain} is the resistance to drainage (cm day^{-1}); q_{drain} (cm d^{-1}) is the drain discharge rate, K_{SAT}^{h} (cm d^{-1}) is the horizontal saturated hydraulic conductivity, d (cm) is the equivalent depth, which is a reduced value of the impermeable layer depth below the drain level, Δh_{tot} (cm) is the total hydraulic head difference between the drain level and the phreatic level at midpoint, and L (cm) is the drain spacing. This approach is not considered fully distributed since q_{drain} is assumed as a system water loss but not as a re-distributive process. An alternative approach is used in HYDRUS-2D, which considers SSLF within the water balance calculation by adding a horizontal term to the Richards' equation as follows:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta)\frac{\partial \psi}{\partial z} - K(\theta)\right] + \frac{\partial}{\partial x}\left[K(h)\frac{\partial h}{\partial x}\right] \tag{37}$$

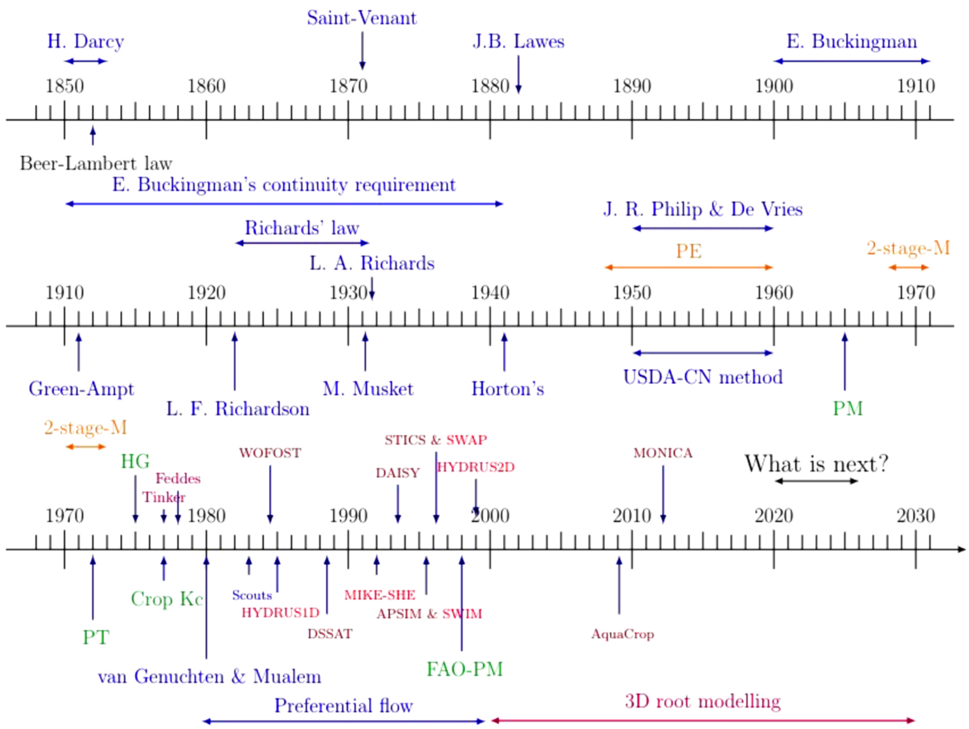

Fig. 1. Chronological evolution of modelling approaches and theoretical fundamentals; in blue: methodological approaches related to infiltration processes and soil-water movement; in orange: related to evaporation; in green: to transpiration; in dark-purple: plant-root water uptake; in dark-red: crop growth simulation models; in dark-pink: hydrology based models. PE means Penman equation, 2-stage-M corresponds to the 2 stage method proposed by Ritchie (1972), PT means Priestley and Taylor, HG represents the Hargreaves equation and PM is Penman-Monteith. FSPM means 'functional structural plant modelling. The Beer-Lambert Law, which embraces a wider scope than crop-hydrological issues but it has influenced many modelling approaches of evaporation and transpiration is represented in black color. All horizontal arrows refer to the time-scale below, except in the case of 'preferential flow' and '3D root modelling'.

where the hypothetical horizontal gradient of both hydraulic conductivity and pressure head is added to the 1-D vertical formulation. For this case, a 'Galerkin finite-element method' is used to convert the differential equation into a discrete type problem (Mohsen, 1982; Simunek et al., 1999). A similar approach is proposed by van Dam et al. (1997) for introducing 'Neumann-type' conditions in the SWAP model to define the lower boundary in the calculations of capillary rise (CR) through Richards' equation.

3.9. Solute transport

Within the scope of this review, and considering the existing relations between solute concentration and root water uptake (e.g. salinity, co-limitation as discussed by Cossani and Sadras (2003)), we included a general description of solute transport processes. We limited our analysis to identify whether salts and nutrient transport processes are addressed by the selected models.

In AquaCrop, particular attention is given to the salt balance and consequently, to crop yield response to salinity (Raes et al., 2009a,b). According to Raes et al. (2012), incoming and outgoing salt fluxes can be simulated with downward (i.e. vertical leaching) and upward water movement (i.e. flow of saline water through capillary rise from a shallow water table). Conceptually, the salinity concentration for a given layer (σ_k) can be updated at each time step, every time water moves in ($\Delta\theta_{\text{in}}$) or moves out ($\Delta\theta_{\text{out}}$). For these cases, the salt balance of a given layer is determined for a particular time step as:

$$\frac{\partial\sigma_k}{\partial t} = \frac{(\sigma_k\theta_k) + (\sigma_{\text{in}}\Delta\theta_{\text{in}}) - (\sigma_{\text{out}}\Delta\theta_{\text{out}})}{\theta_k + \Delta\theta_{\text{in}} - \Delta\theta_{\text{out}}} \tag{38}$$

where σ_k is the specific layer salt content (expressed in g) and θ_k is the actual water content (expressed in mm) of layer k. Other models, based on Richards' equation (e.g. HYDRUS, SWAP, SWIM), use differential equations based on the convective-dispersive transport (C-D) theory, which can be simplified as:

$$\frac{\partial c_\theta}{\partial t} = \left[\frac{\partial}{\partial z}\theta D\frac{\partial c}{\partial z}\right] - \frac{\partial q_c}{\partial z} \tag{39}$$

where c_θ (mg L^{-1}) is the solute concentration (i.e. salts and nutrients in inorganic form) in soil solution, θ is the soil volumetric water content (cm^3 cm^{-3}), q is the water flux (cm day^{-1}) and D is the dispersion coefficient which, according to (Kersebaum, 1989), can be estimated as:

$$D = D_0\tau^{-1} + D_v\left(\frac{q}{\theta}\right) \tag{40}$$

where D_0 is the solute diffusion coefficient (which can be assumed as 2.14 cm day^{-1} for the case of nitrate), τ represents the tortuosity and D_v is the standard dispersion factor (assumed as 25 cm for the case of nitrate). According to van Genuchten (1985), solute adsorption effects can be incorporated by considering the adsorbed concentrations as a linear function of solute concentrations. This has great importance for nutrient transport modelling as following:

$$\frac{\partial}{\partial t}(\theta_{\text{ci}} + \rho S_i) = \frac{\partial}{\partial z}\left(D\frac{\partial c_i}{\partial z} - qC_i\right) - \mu_{\text{wi}}\theta_{\text{ci}} - \mu_{\text{si}}\rho S_i \tag{41}$$

where c_i is the solute concentration (g cm^{-3}), S_i is the adsorbed concentration (mg mg^{-1} or %), θ is the volumetric water content (%), q the volumetric flux (cm day^{-1}), D is the dispersion coefficient (cm^2 day^{-1}), ρ the porous medium bulk density (g cm^{-3}), z is distance (cm), and t is time (day); the subscript i delineates the i^{th}chain member. The coefficients w_i and s_i correspond to rate constants for the first-order decay in the liquid and solid phases of the soil respectively. Units can be adjusted to multiple temporal scales.

4. Crop and hydrologic models: what sets them apart?

The diversity found in the employed methods to simulate the role of water varied among models and among the different processes, which is partly related to the historical development of the models, as shown in the chronological map of modelling approaches presented in Fig. 1 . Note that while hydrologic models have their foundations mostly on research that started in the XIX Century, crop models are sustained by more recent approaches, whose fundamentals evolved from the 1950–60s (Jin et al., 2018; Jones et al., 2017a). After the publication of Darcy's equation and Beer-Lambert law (Fig. 1), we note that hydrologists devoted most of their subsequent efforts to the development of modelling approaches of soil-water movement (e.g. infiltration, capillary forces, drainage processes). However, crop plants were still excluded from the hydrologic system at the time, with modelling prioritizing the representation of soil-water processes without focusing on related plant processes such as transpiration and root water uptake.

This paradigm changed substantially in the 1960s, when the pioneering works of some agronomists and physicists working on photosynthesis (de Wit, 1965; Duncan et al., 1967), broadened perspectives and brought biological variables into the water modelling context (Bouman et al., 1996; Jones et al., 2017a). In fact, the study of photosynthesis was at the root of the development of the first crop models, leading to an uniform approach where Appendix Amost crop models today are radiation driven. This common approach has oriented modelling towards the simulation of optimal conditions, not paying sufficient attention to the responses to environmental stress, thus limiting their use in crop management research (Loomis et al., 1979). The uncertainty regarding future climate scenarios (Hansen and Jones, 2000; Rosenzweig et al., 2014) and the growing demand for decision support tools within the context of precision agriculture (McBratney et al., 2005; Cassman, 1999) will very likely require additional efforts to improve crop modelling under water-limited conditions, i.e. to integrate more water-driven mechanisms in crop models or, as discussed by Passioura (1996), to transform source-limited approaches into sink-limited.

Regarding the diversity of employed methods among models, there is a higher diversity in the simulation approaches of pre-infiltration processes (Fig. 2). The number of components considered in the calculation of the infiltration pool varies substantially among models (Fig. 2). The main issues are related to the incorporation (or exclusion) of snow pack modules and calculation methods related to canopy interception and surface inflow (or outflow) from run-on (or runoff) processes (Fig. 2 and Appendix A). Such discrepancies might be the result of a longer scientific heritage, since it appears that more time has been dedicated to the study of infiltration-related processes than to other water balance processes (Fig. 1), promoting the observed diversification of methodologies and modelling approaches. Another case of methodological discrepancy among models is related to evaporation from soil, where several different methods are used: one or two stages, with the second stage limited either by time or by soil water flow, which can be modeled in several different forms (Section 3.4 and Appendix A).

The highest degree of concordance among models is related to the calculation of evaporative demand (Fig. 2). From the five methods identified (i.e. PE, PM, PT, HG and SVAT schemes; Appendix A), the large majority of models have adopted PM equation (Section 3.4), with the exception of MIKE-SHE and SWIM (Appendix A). Similarly, in most cases reviewed (Fig. 2), the root water uptake is based on a linear model relating relative uptake to soil water content between the upper and the lower limit (Section 3.5).

While evaporative demand is more or less uniformly treated, this is not the case for the partitioning of ET into evaporation and transpiration. Most models follow a Beer-Lambert type equation depending on the canopy extinction coefficient and leaf area index (Sections 3.4 and 3.5), but for some of the hydrologic models (HYDRUS-1D, HYDRUS-2D, SWAP, SWIM) an option is offered to use the soil cover method instead. In general, in the case of most crop models, there is a clear agreement on the use of Beer-Lambert formulation, but for hydrologic models both

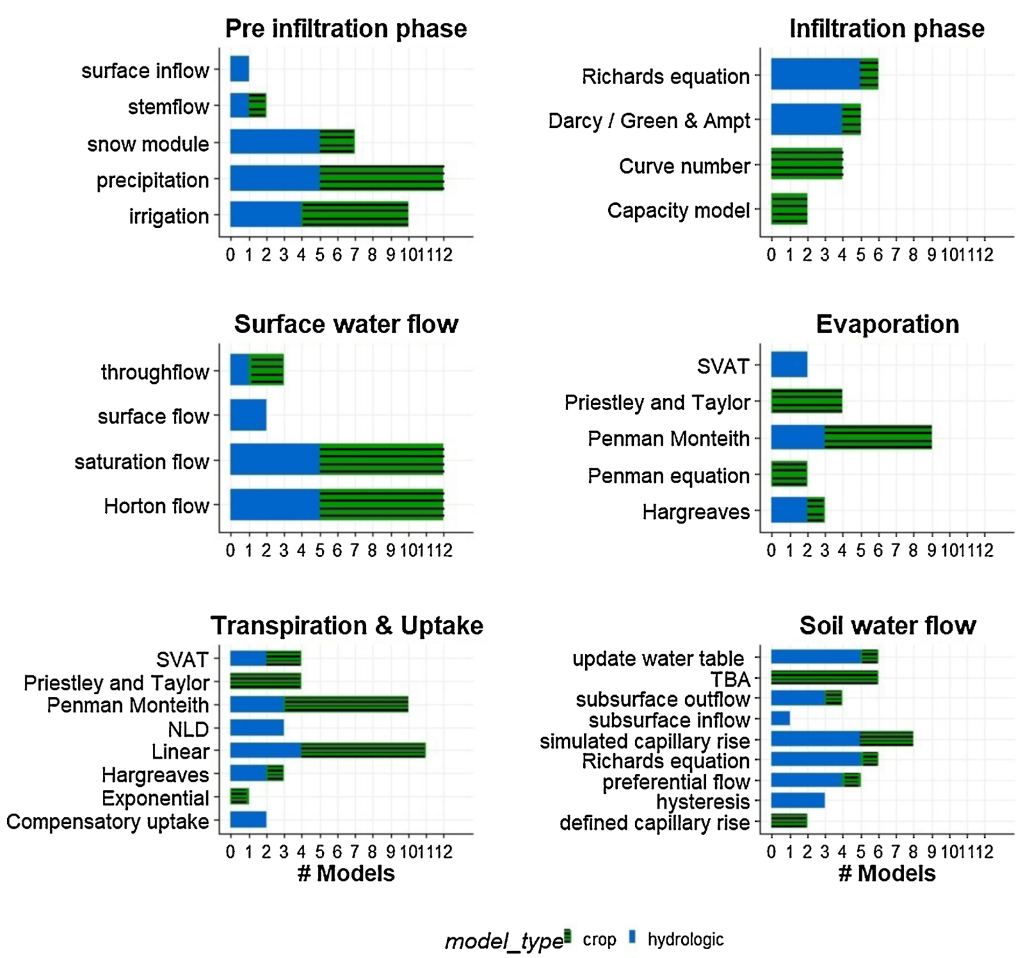

Fig. 2. Number of models simulating a specific process ($N = 12$), the most common modelling approaches used. The horizontal bars show the number of models that simulate (use) the corresponding process (approach). 'NLD' means that non-linear differential equations are used in the estimation of the extraction sink term (as an alternative to linear or exponential approaches).

options seem to be equally adopted (Appendix A).

While there is substantial agreement in the fundamental approaches of the reviewed models, there are also major differences among the two model families. The main differences found between crop and hydrologic models are related to temporal and spatial resolution of processes in the soil-plant-atmosphere continuum, and to the degree of mechanistic or empirical-based approaches used (Appendix A), implying considerable differences in terms of complexity as well. While the crop models (with the exception of DAISY) follow a TBA, hydrologic models are based on numerical solutions of Richards' equation (Section 3.6). Such a divergence implies structural differences between both families not only in terms of spatial resolution but also in terms of temporal scales.

The TBA limits models to a point-based scale where drainage is assumed to be a steady flow (Section 3.6), only vertical and discrete in time (resulting in longer time-steps, e.g. daily). The degree of empiricism involved in TBA based models (i.e. most crop models) is also higher (e.g. CN-method, drainage coefficients, capillary rise defined by Neumann type conditions). On the other hand, hydrologic models, based on numerical solutions of Richards, are capable of simulating the water balance at shorter time-steps (e.g. hourly) and of integrating some multi-dimensionality in the simulation of water flows by distributing partially water over the horizontal space.

5. Opportunities to simulate spatial water variation

The ability to simulate continuity and multi-dimensionality does not necessarily imply the simulation of a full distribution of water over space, as none of the hydrologic models (and none of the crop models) simulates all spatial processes that we have identified (Fig. 3). All spatial processes are covered by at least one model (Fig. 2), but none of these models covers all of them simultaneously (Fig. 3). Some models consider subsurface lateral flows but still ignore surface inflow from run-on (Fig. 3). Additionally, as more generally discussed (Passioura, 1996; Nielsen and Alemi, 1989), the apparent continuity associated with hydrologic models can also be a point of discussion as these models follow 'discrete characteristics' too (e.g. input parameters, boundary conditions, reduced dimensions through the Galerkin finite-element method, Scott's scaling method for simulating hysteresis), becoming eventually more stochastic rather than deterministic.

Regarding the simulation of water processes spatially at crop field level, some methodologies for geospatial simulation, visualization and validation of models (e.g. geospatial interpolation of point based simulations, zonal statistics applied to mapped simulation results, integration of modelling with remote sensing) have been proposed (Basso et al., 2001; Booker et al., 2015; Campos et al., 2019; Casa et al., 2015; Droogers and Bastiaanssen, 2000; Er-Raki et al., 2007; Grassini et al., 2015; Han et al., 2019; Jégo et al., 2012; Jia et al., 2011; Lobell et al., 2015; Lorite et al., 2013; McBratney et al., 2005; Moiling et al., 2005; Silvestro et al., 2017; Shu et al., 2018; Ward et al., 2018). However, while most of these cases have been developed at regional scales, not addressing within-field spatial variation (Droogers and Bastiaanssen, 2000; Grassini et al., 2015; Han et al., 2019; Jia et al., 2011; Lobell and Azzari, 2017; Lobell et al., 2015; Lorite et al., 2013; Sadler and Russell, 1997; Shu et al., 2018; Zwart and Bastiaanssen, 2007), others, that reveal some promising advances in respect to the spatial simulation of water and vegetation, do still neglect spatial compensations of yield determining factors such as variations of the harvest index or root growth (Moiling et al., 2005; Booker et al., 2015; Ward et al., 2018). In addition, we acknowledge that the assimilation of remote sensing to quantify spatial variations is also problematic as ample variation can be observed when using reflectance signals to derive canopy structure parameters with implications on crop transpiration and photosynthetic activity (e.g. LAI, SC), as done by Campos et al. (2019), Casa et al. (2015), Er-Raki et al. (2007), Silvestro et al. (2017), requiring in-situ and crop specific calibration that is not straight forward (Gao et al., 2020).

We emphasize that in terms of water spatial distribution and its effects on crop growth and development, geostatistical methods applied to point-based (or partially distributed) water balances might smooth considerably the actual spatial heterogeneity, because lateral water movement and 'cause-effect' relations between neighbouring cells are still partly ignored (Fig. 3). This awareness is in line with the observations reported by Wallor et al. (2018). In addition to this, relying solely on geostatistics to deal with spatial heterogeneity does not resolve the existing knowledge gaps in regard to the driving mechanisms (McBratney et al., 2005). This was also raised by Nielsen and Wendroth (2003), who suggested that statistical methods should not replace research inventiveness in the assessment of spatial and temporal variations.

In order to distribute spatially water processes in crop models, further steps might be foreseen in two different directions. One implying a stronger synergism between both model families, that might result in the addition of spatial and continuous mechanisms to crop models, other through the integration of lateral flows in current TBA based discrete approaches. The specific processes and approaches that

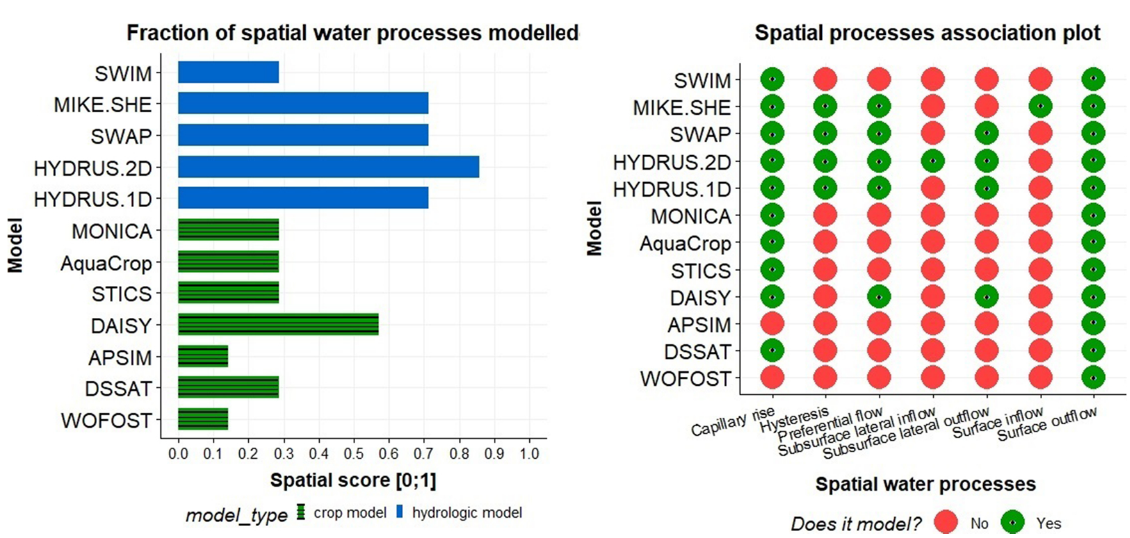

Fig. 3. 'Spatial scores' (left); spatial water processes considered in each model (right). Spatial scores represent the relative amount of spatial processes found in each model (expressed as the amount of spatial processes considered by a model, divided by the total amount of spatial processes that we identified).

hold the most promise for advances are related to the incorporation of surface inflow and subsurface lateral flows (Fig. 3), by using differential equations (Sections 3.3 and 3.8) or through novel water spatial partitioning relations that must be developed for TBA based discrete approaches.

The future will surely be determined by the existing trade-offs between models complexity and adoption. The excessive simulation time and the calculation complexity associated with mechanistic structures that was sometimes seen in the past as a constraint to adoption (Loomis et al., 1979; Nielsen and Alemi, 1989; Passioura, 1996), is very likely to be overcome by today's enormous computational capacity of alternative operational systems (Thorp et al., 2012). However, larger calibration and parameterization requirements associated to mechanistic approaches that depend on complex numerical and analytical solutions of nonlinear equations may not meet the small 'appetite for data' that we aim for in an attractive tool. Therefore, both ways imply important trade-offs between accuracy and data requirements that must be considered. In any case, we conclude that further steps are in need of experimental datasets for the calibration and validation of new upscaling efforts (as also raised by Sadler and Russell (1997)). Spatially distributed data related to subsurface soil texture and plant available water will be essential to achieve a better performance of modelling (Wallor et al., 2018). In this sense, crop modelers are strongly encouraged to come up with innovative databases, suitable for upscaling and spatially calibrating modelling tools at field level.

The success of precision agriculture and spatial management will surely benefit from new advances in the spatial modelling of water as we identify scope for conceptual improvements. Further (coordinated) research efforts are definitely needed, empowering linkages between researchers, farmers, sensing manufacturers and consultants is highly recommended in order to promote field experiments at 'real scales' capable of capturing satisfactory levels of spatial variation.

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Appendix A. Synthesis of soil-plant water processes

See Table 1.

Table 1

Synthesis of models. *Codes:* INFpool = Infiltration pool, INFeff = effective infiltration, INFponding = ponding infiltration, SRn = Forms of surface runoff (2: Horton and saturation flow; 3a: previous plus throughflow; 3b: previous plus surface flow; All: all described forms of SRn, P = precipitation, I = irrigation, SPM = snowpack module, SF = stemflow, INT = intercepted pool, SIF = surface inflow (from run on), CAP = capacity model, CN = curve number, G&A = Green and Ampt., PE = Penman equation, PM = Penman-Monteith, PT = Priestly and Taylor, HG = Hargreaves, SVAT = Soil vegetation atmosphere transfer scheme, CU = compensatory uptake, SSLF = subsurface lateral flow, PF = preferential flow, INT-BL = Integrated through Beer-Lambert equation, SC-M = Soil cover method, LIN = Linear, EXP = Exponential, NLD = Non-linear differential equations, ED_e (or ED_t) = Evaporation demand to estimate evaporation (or transpiration), TBA = Tipping bucket approach, D-CR = predefined CR, SnU-CR = simulated CR without updating water table, SU-CR = simulated CR and updated water table.

Model	WOFOST	DSSAT	APSIM	DAISY	STICS	AquaCrop	MONICA	HYDRUS-1D	HYDRUS-2D	SWAP	MIKE-SHE	SWIM
INFpool	P	P,I	P, I	P, I, SPM	P, I, SF	P,I	P, I, SPM	P, I, INT, SPM	P, I, INT, SPM	P, I, INT, SPM	P, I, INT, SPM, SIF	P, I, SPM
INFeff	CAP	CN	CN	Richards	CN	CN	CAP	Richards	Richards	Richards	Richards	Richards
INFponding	×	×	×	Darcy	×	×	×	G&A	G&A	G&A	G&A	×
SRn	2	2	2	3a	3a	2	2	2	2	2	All	3b
ED_e	PE,PM	PE,PT	PM,PT	PM,HG	PM,PT	PM	PM,PT	PM,HG	PM,HG	PM	SVAT	SVAT
ED_t	PM	PM,PT	PM,PT	PM,HG, SVAT	PM,PT,SVAT	PM	PM,PT	PM,HG	PM,HG	PM	SVAT	SVAT
2-stage	×	×	✓	×	✓	✓	×	×	×	✓	×	✓
Partitioning	INT-BL	INT-BL	INT-BL	INT-BL	INT-BL	SC-M	INT-BL	INT-BL,SC-M	INT-BL,SC-M	INT-BL,SC-M	SC-M	INT-BL,SC-M
K_s	×	✓	✓	×	✓	✓	×	×	×	×	×	×
S_i	LIN	LIN	LIN,EXP	LIN	LIN	LIN	LIN	LIN,NLD	LIN,NLD	LIN	LIN	NLD
CU	×	×	×	×	×	×	×	✓	✓	×	×	×
Drainage	TBA	TBA	TBA	Richards	TBA	TBA	TBA	Richards	Richards	Richards	Richards	Richards
CR	×	SnU-CR	×	SU-CR	D-CR	SnU-CR	D-CR	SU-CR	SU-CR	SU-CR	SU-CR	SU-CR
Hysteresis	×	×	×	×	×	×	×	✓	✓	✓	×	×
SSLF	×	×	×	*OUT*	×	×	×	*OUT*	*OUT*, *IN*	*OUT*	×	×
PF	×	×	×	✓	×	×	×	✓	✓	✓	✓	×

Main sources: (1) Boogaard et al. (2014); (2) Hoogenboom et al. (2017); (3) Verburg (1996), Keating et al. (2003); (4) Hansen et al. (1990), Abrahamsen and Hansen (2000), Hansen et al. (2012); (5) Brisson et al. (2003); (6) Steduto et al. (2009), Raes et al. (2009a, 2017); (7) Nendel et al. (2011); (8) Simunek et al. (1998), Simunek et al. (2018a); (9) Simunek et al. (1999); (10) van Dam et al. (1997), van Dam (2000c), Kroes et al. (2017c); (11) Abbott et al. (1986), DHI (2017b); (12) Verburg et al. (1996).

Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at https://doi.org/10.1016/j.agwat.2020.106254.

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