Expansion and evaluation of two coupled root–shoot models in simulating CO₂ and H₂O fluxes and growth of maize

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Abstract
Leaf water pressure head (\(\Psi_{\text{leaf}}\)) and more specifically its critical thresholds (\(\Psi_{\text{threshold}}\)) characterize stomatal control of transpiration, particularly for C₄ plants, but this physiological process has rarely been integrated into dynamic crop models at the field scale. We further extended two coupled models with Feddes root water uptake (RWU) and Couvreur RWU models by adding the C₄ photosynthesis model in order to be applicable to a maize (Zea mays L.) crop growing under field conditions. The Feddes RWU model relates RWU and plant stress directly to the root zone water hydraulic potential, whereas the Couvreur model explicitly represents hydraulic signals between soil and stomata. Model performance was evaluated with a comprehensive dataset including stomatal conductance, \(\Psi_{\text{leaf}}\), sap flow, gross assimilation rate (GAR), soil water content (SWC), dry biomass, and leaf area index (LAI) from a two-season maize experiment under contrasting environments and water regimes. For the Couvreur model, the RWU and dry biomass were more sensitive to the root hydraulic conductance parameters than to \(\Psi_{\text{threshold}}\) and root growth parameters. The agreement index (\(I\)) for the Couvreur model after calibration was 0.91, 0.80, 0.81, and 0.69 for biomass, LAI, RWU, and GAR, respectively. The Feddes model performed similarly for the same metrics. The Feddes model simulated accurately the plant water stress in the first 45 d of the growing season, whereas the Couvreur model inaccurately predicted water stress, which resulted in lower agreement with observations (i.e., RMSEs of biomass simulated by Feddes and Couvreur model averaged from four validated plots were 0.171 and 0.214 kg m\(^{-2}\), respectively). The Feddes model showed the potential to be used for maize under water stress whereas the Couvreur model needs to be further evaluated and improved with an adequate estimation of root hydraulic conductance. A dynamic parameterization of normalized root system conductance and/or more accurate assimilate allocation to the roots, especially under drought stress, should be considered in order to apply this model in future studies to maize.

Abbreviations: ABA, abscisic acid; DAS, day after sowing; ETP, potential evapotranspiration; GAR, gross assimilation rate; LAI, leaf area index; RWU, root water uptake; SWC, soil water content; VPD, vapor pressure deficit.

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1 INTRODUCTION

Maize (Zea mays L.) is a major staple crop throughout the world. Drought stress, which negatively affects crop growth and yield production, is increasingly affecting several important maize cultivating regions (Daryanto et al., 2016). Increases in frequency and severity of drought events due to climate change (IPCC, 2021) have been recently reported. Maize is an important staple crop for global food security. Thus, field observations and modeling studies on how maize responds to water stress are necessary to produce robust predictions of crop growth, yield, and water use by crop models (Hammer et al., 2009).

Maize has various responses to water stress, which are determined by the plant cultivar as well as the intensity, duration, and rate of progression of the imposed stress (Pinheiro & Chaves, 2011). This includes leaf rolling (Baret et al., 2018), change in root architecture such as reduced lateral root branching (A. Zhan et al., 2015), or increasing root/shoot ratio (Q. Cai, Zhang, et al., 2017). Stomatal control is considered an early and effective response to water stress under field conditions to prevent excessive water loss and desiccation (Brodríbb & McAdam, 2011; Tyree & Sperry, 1988). Maize has been described as isohydric plant, which closes its stomata to maintain leaf pressure head ($\Psi_{leaf}$) above critical levels (Tardieu & Simonneau, 1998). Note that the hydraulic heads refer to total water potentials expressed in length units (i.e., meters) and pressure heads to hydraulic heads minus the gravitational potential or elevation (i.e., $-1$ MPa equal to $-100$ m). An alternative strategy is found in anisohydric plants, which have a looser stomatal control with the result that $\Psi_{leaf}$ will decrease in response to soil drying and/or increasing evaporative demand. Consequently, $\Psi_{leaf}$ in anisohydric plants experiencing drought stress will be considerably lower than in well-watered plants (Tardieu & Simonneau, 1998). A continuum exists in the degree to which stomata regulate the $\Psi_{leaf}$ for trees (Domec & Johnson, 2012; Franks et al., 2007; Klein, 2014; Meinzer et al., 2016) or in grapevines (Vitis vinifera L.) (Schultz, 2003). Also, cultivars of grapevine show large differences in minimum $\Psi_{leaf}$ indicating differing degrees of isohydric behavior (Coupe-Ledru et al., 2014). Comparing different herbaceous species, Turner et al. (1984) showed that there was a range from isohydric to increasingly anisohydric behavior in terms of the response to increasing vapor pressure deficit (VPD) under sufficient soil moisture. The $\Psi_{leaf}$ from eucalyptus (Eucalyptus gomphocephala DC.), a plant rather characterized as having anisohydric behavior, can decrease to very low values and vary with the fluctuations of soil moisture, whereas the difference between soil water pressure head and midday $\Psi_{leaf}$ is maintained constant over a season, which is defined as “isohydrotodynamic” (Franks et al., 2007).

Several underlying mechanisms are involved to explain those stomatal controls, which are still in debate (Tardieu, 2016; Martínez-Vilalta & Garcia-Forner, 2017; Meinzer, 2002). Differences in abscisic acid (ABA) signaling of stomatal closure could be the source of the difference between isohydric and anisohydric (Tardieu & Simonneau, 1998). Stomatal closure responded to a decrease of leaf-specific hydraulic conductance and vice versa (Schultz, 2003). The increase in cavitation resistance (thus reduces hydraulic loss) maintained higher leaf water pressure head under water stress in maize (Cochard, 2002). Hydraulic differences between grapevine cultivars could explain the variability in stomatal regulations. However, the environment (well-watered or limited water conditions and hydraulic properties of soil) also plays a dominant role compared with the genotypes (Hochberg et al., 2018).

Stomatal conductance can be modeled in many ways (Damour et al., 2010), at different scales (Table 1). Earlier empirical models related the effects of $\Psi_{leaf}$ to stomatal conductance with a multiplicative approach (Jarvis type of equation [Jarvis, 1976]) (Jensen et al., 1993, for spring barley [Hordeum vulgare L.]; Olioso et al., 1996 with soybean [Glycine max (L.) Merr.]), which requires a high number of parameters to capture different environmental conditions (Damour et al., 2010). The semiempirical Ball–Berry–Leuning equation (Ball et al., 1987; Leuning, 1995) related photosynthesis and stomatal conductance. However, this model initially did not consider the water stress or effects of $\Psi_{leaf}$ on stomatal conductance. The Ball–Berry–Leuning models were further improved through inclusions of the “water stress factor” on the slope of photosynthesis and stomatal conductance relationship. The water stress factors were calculated from soil water content (SWC) (Y. Wang & Leuning, 1998) or soil water pressure head (Oleson et al., 2013), which is often used in dynamic crop models and many land surface models (Damour et al., 2010; Verhoef & Egea, 2014).

Core Ideas
- A C₄ photosynthesis was introduced into two root–shoot models (Feddes and Couvreur models).
- Both coupled models were compared with a comprehensive dataset from field-grown maize.
- Effects of crop properties were evaluated by a mechanistic Couvreur model.
- The Feddes model simulated water stress well, whereas the Couvreur model had less agreement with observations.
- Future use of the Couvreur model requires accurate estimates of root system conductance.
TABLE 1 Summary of some common stomatal conductance models and their application scales

| Order | Approaches                          | Water relation underlying mechanism                                                                 | Applied scales                    | References (first use in plants)                                                                 |
|-------|-------------------------------------|--------------------------------------------------------------------------------------------------------|-----------------------------------|-------------------------------------------------------------------------------------------------|
| 1     | Multiplicative model, environmental factors are independent | Hydraulic signal: $\Psi_{\text{leaf}}$, constant $K_{\text{plant}}$                                    | Plant, field, landscapes          | Jarvis (1976) (spruce and Douglas fir); Jensen et al. (1993) (barley); Olioso et al. (1996) (soybean) |
| 2     | Hydraulic model                     | Hydraulic signal: $\Psi_{\text{leaf}}$, $K_{\text{plant}}$, and SWP                                  | Plant                             | Tyree and Sperry (1988); Jones and Sutherland (1991) (trees)                                  |
| 3     | Turgor regulation of guard cell (hydromechanical model)   | Hydraulic signal: SWP and guard cell water potential                                                   | Cell and leaf                     | Gao et al. (2002); Buckley et al. (2003)                                                       |
| 4     | Hydraulic and chemical ABA control  | Hydraulic and chemical signals: $\Psi_{\text{leaf}}$ and ABA                                          | Plant and pot                     | Tardieu and Davies (1993); Tardieu and Simonneau (1998); Tardieu et al. (2015) (maize)         |
| 5a    | Hydraulic and chemical ABA control  | Hydraulic and chemical signals: $\Psi_{\text{leaf}}$ and ABA                                          | Theoretical modeling studies      | Huber et al. (2014)                                                                            |
| 6     | Coupled photosynthesis– stomatal conductance ($A_{s}-g_{s}$) model | No water stress was considered                                                                       | Plant, field                      | Ball et al. (1987) (soybean) Leuning (1995) (Eucalyptus grandis)                           |
| 7     | Modified ($A_{s}-g_{s}$) model with water stress functions of SWC or SWP | Water stress functions of SWC or SWP, neither $\Psi_{\text{leaf}}$ nor $K_{\text{plant}}$ or ABA        | Plant, field, landscapes          | Oleson et al. (2013); Kucharik and Brye (2003) (varieties of trees, plant functional types); Rodriguez et al. (2001) (spring wheat); Wang and Leuning (1998) (wheat) |
| 8     | Modified ($A_{s}-g_{s}$) model with water stress functions from $\Psi_{\text{leaf}}$ | Hydraulic signals: water stress functions of $\Psi_{\text{leaf}}$, constant $K_{\text{plant}}$ | Theoretical modeling study with homogenous soil; field | Tuzet et al. (2003) (the applied crop was not specified)                                         |
| 9     | Modified ($A_{s}-g_{s}$) model with water stress functions from $\Psi_{\text{leaf}}$ and ABA | Hydraulic and chemical signals: Water stress functions of $\Psi_{\text{leaf}}$ and ABA, constant $K_{\text{plant}}$ | Leaf, theoretical modeling studies | Dewar (2002); Ahmadi et al. (2009); Verhoeff and Egea (2014) (tomato); Gutschick and Simonneau (2002) (sunflower); Huntingford et al. (2015) (tree) |
| 10    | Modified ($A_{s}-g_{s}$) model with water stress function ($T_{s}/T_{p}$) | Hydraulic signal: $\Psi_{\text{leaf}}$, dynamic $K_{\text{plant}}$ based on root length | Field                             | Nguyen et al. (2020) (winter wheat)                                                             |

Note. $A_{s}$, net photosynthesis rate; $g_{s}$, leaf stomatal conductance; ABA, acid abscisic; $K_{\text{plant}}$, whole plant hydraulic conductance; $T_{s}$, actual transpiration; $T_{p}$, potential transpiration; SWC, soil water content; SWP, soil water pressure head; $\Psi_{\text{leaf}}$, leaf pressure head. The modified $A_{s}-g_{s}$ models in the 7th, 8th, 9th, and 10th approaches were originated from the coupled $A_{s}-g_{s}$ model in the 6th approach (so-called Ball–Berry–Leuning model).

*This approach simulated transpiration reductions factor rather than explicitly simulated the $g_{s}$.

Tuzet et al. (2003) introduced an empirical water stress factor on the Ball–Berry–Leuning stomatal conductance model. The water stress factor was below 1 if the simulated $\Psi_{\text{leaf}}$ was below the reference $\Psi_{\text{leaf}}$. The reference $\Psi_{\text{leaf}}$ in Tuzet’s study was defined as the value of $\Psi_{\text{leaf}}$ below which the stomatal conductance begins to decrease drastically (Jones & Sutherland, 1991; Olioso et al., 1996; Tuzet et al., 2003). Plants with a high stomatal sensitivity to $\Psi_{\text{leaf}}$ were then modeled with a higher reference $\Psi_{\text{leaf}}$ ($-1.2$ MPa) ($-1$ MPa $= -100$ m). For species that are more tolerant to water stress, a lower reference $\Psi_{\text{leaf}}$ was used (i.e., $-1.9$ or $-2.6$ MPa) (Tuzet et al., 2003). However, the $\Psi_{\text{leaf}}$ was simulated with the assumed constant whole-plant hydraulic conductance. Moreover, the model from Tuzet did not separate the different canopy layers (i.e., sunlit and shaded leaves), which can be the important feature when simulating CO$_2$ and H$_2$O gas exchange (de Pury & Farquhar, 1997; Y. Wang & Leuning, 1998). Additionally, Tuzet’s model considered soil profile as a single layer with homogeneous soil characteristics and a uniform root distribution, which is not the case under field conditions (van Dam, 2000; Vereecken et al., 2016). Tardieu and Davies (1993) proposed a stomatal conductance model involving $\Psi_{\text{leaf}}$ and xylem ABA. Abscisic acid is produced in the dehydrated roots and transported to the leaf, where it regulates stomatal closure. Consideration of either hydraulic signal combined with ABA or only ABA allowed the model to simulate anisohydric and isohydric behavior (Tardieu & Simonneau, 1998; Tardieu et al., 2015). The models with hydraulic and chemical...
signals from Tardieu and Davies (1993) were later simplified to a water stress factor or function, and then introduced into the slope of the coupled Ball–Berry–Leuning model (Dewar, 2002). A sensitivity analysis was conducted afterwards, showing that varied values of ABA and critical Ψ_leaf could mimic the range of stomatal responses of anisohydric and isohydric stomatal behaviors (Huber et al., 2014). The consideration of hydraulic or chemical signals for extending the Ball–Berry–Leuning equation has mainly been applied at the leaf scale (Ahmadi et al., 2009; Dewar, 2002; Gutschick & Simonneau, 2002) or in theoretical studies (Huntingford et al., 2015; Verhoeff & Egea, 2014) (Table 1). To our knowledge, modeling studies and performance evaluation of these models on simulating stomatal conductance, CO₂ and H₂O gas flux exchange, and crop growth processes are rarely done at the field scale.

Further improvements consider that water stress is calculated from leaf hydraulic head and/or xylem ABA concentration, thus replacing the more empirical approaches often based on SWC or soil water pressure head (i.e., theoretical modeling study; Verhoeff & Egea, 2014) and recent modeling studies under the field-grown condition in winter wheat (Triticum aestivum L.) (G. Cai et al., 2017, 2018; Nguyen et al., 2020; Sulis et al., 2019). Nguyen et al. (2020) coupled the HILLFLOW soil water balance model (Bronstert & Plate, 1997), crop model LINTULCC2 (Rodriguez et al., 2001), and root growth model SLIMROOT with Feddes’s root water uptake (RWU) model (Feddes et al., 1978) and Couvreur’s RWU model (Couvreur et al., 2012, 2014). The Feddes RWU model, which does not consider the plant hydraulic conductance, is commonly used in hydrological models. The Couvreur model explicitly calculates the root hydraulic conductance (Kₛ) based on the total length of the root system below a unit of surface area (i.e., cm⁻²). Leaf pressure head (Ψ_leaf) was explicitly simulated via extending Kₛ to whole-plant hydraulic conductance (Kₚ). The RWU approach by the Couvreur model is based on hydraulic principles that represented water dynamics within the root system. The model includes a stomatal regulation algorithm, which assumes that stomatal conductance is not influenced by Ψ_leaf as long as the Ψ_leaf is above a critical leaf pressure head threshold (Ψ_threshold). The Ψ_leaf is kept constant by changing stomatal conductance when the Ψ_threshold values are reached. In theory, the coupled model with Couvreur’s RWU model allows the reproduction of the different stomatal regulations by letting Ψ_threshold vary. The coupled model with Couvreur RWU predicted better water stress than the Feddes model (Nguyen et al., 2020). The coupled model with Couvreur RWU also was able to simulate Kₚ gross photosynthesis, transpiration, and soil water dynamics for winter wheat. However, the water response dynamics and model comparisons for Couvreur-coupled and Feddes-coupled models have not been parameterized and evaluated for maize. It is necessary to test the models for more crops and different weather conditions to build up larger experimental support for the models. We hypothesized that the coupled model with the Couvreur RWU model is generic enough to simulate the effects of soil water availability on the CO₂ and H₂O gas fluxes and crop growth of maize with varying weather conditions (including different levels of evaporative demand or potential evapotranspiration [ETP] and VPD). The objectives of this study were (a) to analyze the sensitivity of aboveground biomass growth and RWU of maize to changing plant-water-related parameters (semitransmplant hydraulic conductance parameters); and (b) to compare the predictive capacity of the coupled models with and without the inclusion of Kₚ (Couvreur and Feddes RWU models) in simulating maize crop growth, CO₂, and H₂O gas fluxes under different water regimes and contrasting weather conditions at the field scale. We used a comprehensive field dataset comprising measurements of CO₂ and H₂O gas flux from soil to leaf and dynamic crop growth (biomass and leaf area index [LAI]).

## 2 MATERIALS AND METHODS

### 2.1 Location and setup of the field experiments

The field experiments were located in a field near Jülich, western Germany (50°52' N, 6°27' E). The site is characterized by stony soil (hereby F1) with approximately 50–60% gravel by weight in the 10-cm topsoil. The study site was divided in two rainfed plots (P1 and P2) and one irrigated plot (P3). Maize was grown during two seasons (2017 and 2018). Silage maize cultivar Zoey was sown on 4 May and 8 May during the 2017 and 2018 season, respectively, with a plant density of 10.66 seeds m⁻² for all treatments and soil types (Figure 1a; Table 2). In 2018, the irrigated plot (F1P1) was seeded two weeks later, on 22 May (Figure 1a). Because the objective of this study was to analyze the performance of the coupled root–shoot model under different soil water conditions and evaporative demands, we selected datasets from irrigated and rainfed plots for two growing seasons, named 2017F1P3, 2017F1P2, 2018F1P3, 2018F1P2, and 2018F1P1. Detailed information on crop management is described in Table 2.

### 2.2 Weather conditions and irrigation management

The experimental site was characterized by temperate climate conditions with an average annual temperature of 9.9 °C and average annual precipitation of 698 mm (Prolingheuer et al., 2017). The regional climate is characterized by warm winters and cool summers. The average temperature during the growing season (May–October) is approximately 17 °C. The average annual precipitation is around 1000 mm with a peak in the summer months. The soil at the study site is classified as a loamy sand (CLG), with a thickness of approximately 90 cm. The soil texture is clay loam with a high gravel content (50–60%). The field is characterized by a temperate climate with mild winters and warm summers. The average temperature during the growing season (May–October) is approximately 17 °C. The average annual precipitation is around 1000 mm with a peak in the summer months. The soil at the study site is classified as a loamy sand (CLG), with a thickness of approximately 90 cm. The soil texture is clay loam with a high gravel content (50–60%).
| Variable                  | 2017       |          | 2018       |          |          |
|---------------------------|------------|----------|------------|----------|----------|
|                           | Normal     | Late     | Normal     | Late     | Late     |
| Sowing date               | 4 May 2017 | 8 May 2018 | 22 May 2018 | 26 May 2018 |
| Phenology                 |            |          |            |          |          |
| Emergence date            | 9 May 2017 | 13 May 2018 | 26 May 2018 | 21 July 2018 |
| Tasseling date            | 9 July 2017 | 9 July 2018 | 21 July 2018 | 21 July 2018 |
| Silking date              | 14 July 2017 | 11 July 2018 | 23 July 2018 | 23 July 2018 |
| Harvest date              | 12 Sept. 2017 | 22 Aug. 2018 | 2 Sept. 2018 | 2 Sept. 2018 |
| Plot names                | 2017F1P3   | 2018F1P2 | 2018F1P3   | 2018F1P2 | 2018F1P1 |
| Growing season, d<sup>a</sup> | 136        | 136      | 107        | 107      | 104      |
| Days without rain         | 66         | 66       | 77         | 77       | 71       |
| Water treatments          | Irrigated  | Rainfed  | Irrigated  | Rainfed  | Rainfed  |
| Cumulative rainfall, mm<sup>b</sup> | 248.7      | 248.7    | 91.3       | 91.3     | 81.9     |
| Irrigation, mm            | 130        | 0        | 257.6      | 66       | 66       |
| Fertilizer application, ha<sup>−1</sup> | 9 May 2017: 100 kg N + 40 kg P<sub>2</sub>O<sub>5</sub> | 22 May 2018: 100 kg N | 22 May 2018: 100 kg N | 22 May 2018: 100 kg N |
|                           | 6 July 2017: 80 kg N + 40 kg K<sub>2</sub>O | 30 May 2018: 40 kg P<sub>2</sub>O<sub>5</sub> + 40 kg K<sub>2</sub>O | 30 May 2018: 40 kg P<sub>2</sub>O<sub>5</sub> + 40 kg K<sub>2</sub>O | 30 May 2018: 40 kg P<sub>2</sub>O<sub>5</sub> + 40 kg K<sub>2</sub>O |
| Cultivar                  | Zea mays cv. Zoey |          |            |          |          |
| Sowing density            | 10.66 plants m<sup>−2</sup> or 75 x 12.5 cm |          |            |          |          |

<sup>a</sup>From sowing to harvest.

<sup>b</sup>For rainfall for whole growing season.
In 2017, the maize crop received 248.7 mm of rainfall during the growing period (136 d) (Table 2). Seasonal average, minimum, and maximum daily seasonal temperatures during were 17.6, 8.3, and 25.3 °C, respectively. The irrigation demand was estimated based on the precipitation collected from the rain gauge nearby the field (Table 2). Irrigation in the irrigated plots was carried out by dripper lines (T-Tape 520-20-500, Wurzelwasser GbR), which were installed at 0.3-m intervals parallel to the crop rows. In the irrigated plots, water was applied (10 times, 13 mm per irrigation event) from mid-June to the end of August for the irrigated plot (2017F1P3) (Table 2). No irrigation was applied in the rainfed plots in 2017. With an exceptionally hot and dry condition during the summertime, the 2018 can be classified as an extreme year for crop growth in our experiments (Buras et al., 2020). Crop received only 91.3 and 81.9 mm of rainfall in the early and late sowing plots in 2018, respectively (Table 2). Seasonal average, minimum, and maximum daily temperatures were 19.2, 10.9, and 27.3 °C, respectively. A total irrigation volume of 257.6 mm was applied (split into 13 applications) from mid-June to mid-August in the irrigated plot (2018I). The two rainfed plots (2018F1P1 and 2018F1P2) were watered four times (13, 22, 13, and 18 mm each time) to prevent the plants from dying due to severe drought.
2.3 Measurements

2.3.1 Soil water and root growth measurement

In each soil depth at 10, 20, 40, 60, 80, and 120 cm, time-domain reflectometer (TDR) probes and tensiometers (T4e UMS) and dielectric water potential sensors (MPS-2 matric potential, Decagon Devices) were installed to measure hourly SWC and soil water potential (see Figure 1b). Soil water measurements were described in detail in G. Cai et al. (2016) and Nguyen et al. (2020). Soil physical parameters of the stony soil (saturated hydraulic conductivity, saturated and residual SWC, and empirical coefficients affecting the shape of the van Genuchten hydraulic functions) were selected from G. Cai et al. (2018). Root growth was observed biweekly using a Bartz MR Camera system (VSI/Bartz Technology Corporation) from both left and right sides along 18 mini-rhizotubes in each plot. The image size of the camera was 16.5 mm long × 23.5 mm wide. The clear acrylic glass mini-rhizotubes (7 m long) were horizontally installed (Morandage et al., 2021) at six different depths of 10, 20, 40, 60, 80, and 120 cm below the soil surface in each water treatment. The root growth observation and root data processing were described in detail in Morandage et al. (2021). Only root growth data of two plots in 2017 (2017F1P3 and 2017F1P2) were shown in this study.

2.3.2 Crop growth and gas fluxes measurement

Because of the limited number of plants in each plot, two maize plants were sampled biweekly to determine the LAI and aboveground dry biomass during the entire growing seasons (Figure 1b) (in total seven and nine observations [including harvest]) in 2017 and 2018, respectively. Green and brown leaf area was measured using a leaf area meter (LI-3100C, Licor Biosciences). At harvest, in addition to the sampling of two plants, five separate replicates (1 m² each) were harvested to determine the aboveground dry biomass and leaf area. The aboveground dry biomass was measured using the oven drying method (Nguyen et al., 2020).

Hourly leaf stomatal conductance and leaf pressure head ($\Psi_{\text{leaf}}$, m) (−100 m equivalent to −1 MPa) were measured every 2 wk under clear and sunny conditions (7–10 measured days, from 8:00 a.m. to 5:00 p.m.). Stomatal conductance ($g_s$) of two sunlit leaves (uppermost fully developed leaves) and one shaded leaf was measured at steady-state using a LICOR 6400 XT device (Licor Biosciences) with a reference CO₂ concentration of 400 μmol mol⁻¹, flow rate of 500 μmol s⁻¹, and using real-time records of photosynthetic active radiation, VPD, and leaf temperature provided by the instrument. The leaves were quickly detached by a sharp knife to measure $\Psi_{\text{leaf}}$ with a digital pressure chamber [SKPM 140/(40-50-80), Skye Instrument] with the working air pressure with a range of 0–3,500 kPa. In 2018, to capture the full diurnal course, $\Psi_{\text{leaf}}$ was determined from predawn at hourly intervals to 7:00 p.m. on 3 d (2 d before irrigation and 1 d after irrigation). Based on the LAI measurement, the sunlit leaf area ($\text{LAI}_{\text{su}}$) was calculated based on measured LAI, coefficient of light extinction (CoLi), and solar zenith angle (SoZe) (Equations 1 and 2) (Moreshet et al., 1990). Solar zenith angle (SoZe) is the angle between the sun’s ray and the vertical.

$$\text{LAI}_{\text{su}} = \left(1 - e^{-\text{CoLi} \times \text{LAI}}\right)/\text{CoLi}$$

(1)

$$\text{CoLi} = \frac{1}{2 \cos(\text{SoZe})}$$

(2)

Canopy pressure head ($\Psi_c$, m) was computed as leaf area-weighted average of sunlit and shaded leaf pressure heads (Moreshet et al., 1990, 1996) assuming that both leaves are transpiring (Petersen et al., 1991) (Equation 3):

$$\Psi_c = \Psi_{\text{su}} \frac{\text{LAI}_{\text{su}}}{\text{LAI}} + \Psi_{\text{sh}} \left(1 - \frac{\text{LAI}_{\text{su}}}{\text{LAI}}\right)$$

(3)

where $\Psi_c$ is canopy pressure head (m); $\Psi_{\text{su}}$ is pressure head of sunlit leaf (m); $\Psi_{\text{sh}}$ is pressure head of shaded leaf (m); LAI is measured leaf area index (–); LAI$_{\text{su}}$ is leaf area index of sunlit leaf (–).

In 2017, 15 sap flow sensors (SGA13, SGB 16, and SGB 19 types) based on stem diameter size were installed on maize plants from 7 July until harvest (five sensors in each plot) (Figure 1b). For the 2018 growing season, the same number of sensors were installed from 28 June until the harvest. The plant stem diameter and associated physical indices of each sensor type were entered into data loggers so that the sap flows were automatically calculated by the standard Dynamax program (Dynamax, 2009). The 10-min sap flow rate of a single plant (g h⁻¹) was aggregated to hourly intervals then upscaled to canopy transpiration rate (mm h⁻¹ or mm d⁻¹) based on the plant density per square meter. The standard deviation of the sap flow measurements in different maize stems was calculated.

We calculated the plant hydraulic conductance according to Ohm’s law by dividing the hourly sap flow by the difference between effective root zone hydraulic head and canopy pressure head (Nguyen et al., 2020). The effective root zone hydraulic head was computed based on hourly measured soil water hydraulic head and measured root length density (cm cm⁻²) at six depths (10, 20, 40, 60, 80, and 120 cm) in the soil profile (Section 2.3.1) following Equations 6 and 11 (see Section 2.4.3.4, the Couvreur RWU model). During one
measurement day, four hourly values of the plant hydraulic conductance were obtained from measurements between 11:00 a.m. and 2:00 p.m. The average and standard deviation of these hourly measurements were calculated for each measurement day.

The manually closed chamber system (Langensiepen et al., 2012) was used to measure the hourly canopy gas exchange on the same day with the measurement of the leaf pressure head by another customized LICOR 6400 XT (Licor Biosciences) (Figure 1b). Simultaneously, soil respiration was measured manually by LI-8100 (Licor Biosciences) with three replicates in each treatment. Because we focused on the comparison of the hourly instantaneous gross assimilation rate, which was simulated by the crop model, the measured soil respiration was subtracted from the instantaneous canopy CO₂ exchange rate.

2.4 Model description

2.4.1 Overview of the two coupled root: Shoot models

We used two coupled root–shoot models: “HILLFLOW 1D-Feddes RWU model-SLIMROOT-LINTULCC2” and “HILLFLOW 1D-Couvreur RWU model-SLIMROOT-LINTULCC2” within the modeling framework SIMPLACE (www.simplace.net). These two coupled models were used for winter wheat and described in Nguyen et al. (2020). The HILLFLOW 1D is the physically based water balance model (Bronstert & Plate, 1997), which contains Feddes RWU model (hereafter, Feddes model) (Feddes et al., 1978) and Couvreur RWU model (hereafter, Couvreur model) (Couvreur et al., 2012, 2014). The SLIMROOT is the root growth model. The LINTULCC2 shoot growth model simulates phenology, photosynthesis, assimilation partitioning, and leaf growth. In the current study, the shoot growth models have been modified by an additional subroutine for the C₄ photosynthesis pathway (Figure 2a). The rest of modeling subroutines were kept the same as in Nguyen et al. (2020).

2.4.2 Implementation of C₄ photosynthesis parameterization for maize

LINTULCC2 (and the coupled root–shoot models in Nguyen et al., 2020), originally developed for wheat, calculates CO₂ uptake for sunlit and shaded leaves based on the Farquhar approach for C₃ photosynthesis. (Farquhar et al., 1980). It uses a numerical iteration approach (Leuning, 1995), which initially assumes that intercellular CO₂ concentration (Ci) equals 0.7 times the ambient atmospheric CO₂ concentration (Cab) (Jones, 1992; Rodriguez et al., 2001). A mechanistic photosynthesis model for maize (C₄ plant) was developed (Collatz et al., 1992; von Caemmerer & Furbank, 2003; Yin & Struik, 2009) and introduced into LINTULCC2. The parameters and model variables, as well as sequential equations to mimic the CO₂ pathway in C₄, are described in detail in Appendix A and Appendix B. The C₄ models have rarely been implemented into crop models (Yin & Struik, 2009; Yin & van Laar, 2005) because of the complex equations and requirement of high temporal resolution input data at leaf scale (Yin & Struik, 2009). The C₄ model can be solved either by numerical iteration approach (i.e., Leuning, 1995) or analytical solution (i.e., solving cubic equations; Collatz et al., 1992; Yin & Struik, 2009; X. Zhan et al., 2003). For the C₄ implementation into the modeling framework (SIMPLACE) (Figure 2a), we used the numerical iteration approach. We assumed the initial Cᵢ was 0.4 times the C₄ (Jones, 1992; Vico & Porporato, 2008; Wong et al., 1979). For the sake of simplification, we used bundle sheath cell conductance of 3 mM m⁻² s⁻¹ (von Caemmerer, 2000).

2.4.3 Description of other modeling subroutines

Potential evapotranspiration and transpiration

The ETP (mm h⁻¹) was calculated based on the Penman–Monteith equation (see Nguyen et al., 2020) (Figure 2a). The potential transpiration (Tpot) was calculated by Equation 4:

\[
T_{pot} = \text{ETP} \left(1 - e^{-kLAI}\right) \tag{4}
\]

where \(k\) is the light extinction coefficient. The light extinction coefficient varies depending on maize genotypes, leaf properties, and leaf arrangements. We used the \(k = 0.6\) in this study for maize (Hay & Porter, 2006). The potential transpiration \(T_{pot}\) (mm h⁻¹) implies that the transpiration of the crop is not limited by the root zone water hydraulic head (Figure 2a).

Root growth model

The maize root system of maize is composed of primary, seminal, crown, and lateral roots. Crown roots could have greater water uptake due to their higher axial conductivity in the proximal parts as compared with younger seminal roots (Ahmed et al., 2018). For simplification, the crown roots (nodal roots) were not explicitly included in the root growth model (SLIMROOT) used in our study. SLIMROOT simulates the vertical extension of the seminal roots and the distribution of lateral roots within soil profiles (Williams & Izaurralde, 2005). Lateral roots are simulated when the assimilates supplied by the shoot to the roots is greater than the assimilate demand of seminal roots. Thus, the omission of explicit growth of crown roots in SLIMROOT is compensated by larger amount of simulated lateral roots. The extension of lateral and seminal roots...
FIGURE 2  Description of (a) the coupled root–shoot models, which have been modified with \(C_4\) photosynthesis in this study (adopted from Nguyen et al., 2020), and (b) modeling workflow, used water treatments, simulation outputs, and related parameters. The orange arrow in (a) illustrates the feedbacks from the hourly simulations to daily simulation, whereas the gray arrow describes the feedbacks from daily simulations to the hourly simulations. The dashed black arrows denote the weather input and parameters to the modeling subroutines. The continuous black arrows in (a) indicate the linkages among the subroutines. The water treatments, variables names, and parameters in (b) are explained in the Table 3 and Figure 1, and in the text. TBASE, base temperature; MinTTANTH, minimum thermal time requires for anthesis; GFDUR, thermal time of grain filling duration.
was simulated based on the root biomass, the soil bulk density, the SWC from the HILLFLOW water balance model, and the computed soil temperature from STMPsim (Nguyen et al., 2020) (Figure 2a). Maize roots start to die after silking.

**Physically based soil water balance model**

The water balance model HILLFLOW 1D (Bronstert & Plate, 1997) calculates SWC and water fluxes by numerically solving the Darcy equation for unsaturated water flow in porous media (Bronstert & Plate, 1997). To express the relations between soil water pressure head, SWC, and hydraulic conductivity, the Mualem–van Genuchten models were used (van Genuchten, 1980) (Section 2.3.1). In this study, the soil profile with a depth of 1.5 m was vertically discretized into 50 layers. The mixed upper boundary condition represents the flux at the soil surface by the precipitation and evaporation rates as long as the soil pressure heads are not higher or lower critical heads. For the bottom boundary, free drainage was implemented.

**Feddes’ and Couvreur’s RWU models**

The Feddes RWU model (Feddes et al., 1978) was implemented in the HILLFLOW 1D (Bronstert & Plate, 1997). The RWU of each soil layer is calculated from normalized root length density (NRLD) in that layer and a water stress function α, which depends on the soil water pressure head (ψ, m) in that soil layer and potential transpiration rate $T_p$ (mm h$^{-1}$) (Feddes et al., 1978):

$$\text{RWU}_i = \alpha(\psi_i, T_p) T_p \text{NRLD}_i \Delta z_i$$

(5)

where RWU$_i$ (m d$^{-1}$) is RWU in the soil layer $i$. The NRLD$_i$ (m$^{-1}$) is computed from the root length density, RLD ($\text{cm}^{-3}$) and discretized soil thickness, $\Delta z_i$ (m):

$$\text{NRLD}_i = \frac{\text{RLD}_i}{\sum_{i=1}^{N} \text{RLD}_i \Delta z_i}$$

(6)

The parameters of the α stress functions for specific crops like maize were selected from (Wesseling et al., 1991). The approach to estimate root hydraulic conductance and the Couvreur RWU model from winter wheat was implemented for maize. The root hydraulic conductance ($K_{\text{rs, doy}}$, d$^{-1}$) and the root system conductance for compensatory water uptake ($K_{\text{comp, doy}}$, d$^{-1}$) were computed based on the total length of the root system below a unit surface area TRLD$_{doy}$ (cm$^{-2}$) (Equation 7) at a given day of the year (DOY), which is the output from SLIMROOT (Figure 2):

$$\text{TRLD}_{doy} = \sum_{i=1}^{N} \text{RLD}_i \Delta z_i$$

(7)

where RLD$_i$ is root length density at layer $i$ (cm$^{-3}$) and $\Delta z_i$ is the thickness of the layer (cm). The normalized root hydraulic conductance $K_{\text{rs, normalized}}$ (d$^{-1}$ cm$^{-1}$ cm$^2$) was taken from Nguyen et al. (2020) and G. Cai et al. (2018) to calculate the daily root hydraulic conductance:

$$K_{\text{rs, doy}} = K_{\text{rs, normalized}} \text{TRLD}_{doy}$$

(8)

The original model from Couvreur et al. (2014) considered the hydraulic conductance from the roots to the plant collar by assuming that the hydraulic resistance from plant collar to leaf was minor and could be neglected as compared with the root system resistance. The shoot hydraulic resistance could be large as reported in some crop plants (Gallardo et al., 1996) or trees (Domec & Pruyn, 2008). To simulate the leaf pressure head, the whole-plant hydraulic conductance ($K_{\text{plant}}$) needs to be estimated. The whole-plant hydraulic conductance can be estimated from different plant organs (soil to root, stem to leaf, for instance in the study from Saliendra et al. [1995]), or a more complex approach based on plant architecture in Janott et al. (2011). The hydraulic conductance data from plant collar to leaf, which depends on environmental conditions and plant species, are often rare and difficult to obtain (Chunfang et al., 1999; Meunier et al., 2018; Sunita et al., 2014). We followed the simple approach in (Nguyen et al., 2020), the root hydraulic conductance ($K_{\text{rs, doy}}$) (d$^{-1}$) was used to calculate the whole plant hydraulic conductance ($K_{\text{plant, doy}}$) based on a constant fraction β ($\beta = 0.55$) (Equation 9):

$$K_{\text{plant, doy}} = \beta K_{\text{rs, doy}}$$

(9)

where β (unitless) is a fraction to upscale root hydraulic conductance to whole-plant hydraulic conductance ($K_{\text{plant, doy}}$).

The Couvreur RWU model is based on a mechanistic description of water flow in the coupled soil–plant system. The RWU in a certain soil layer is related to the water potentials and RWU in other soil layers so that compensatory uptake is considered in this model. The RWU (mm h$^{-1}$) in a certain soil layer $i$ is obtained from

$$\text{RWU}_i = T_{\text{plant, doy}} \text{NRLD}_i \Delta z_i + K_{\text{comp, doy}} (\psi_i - \psi_{sr}) \text{NRLD}_i \Delta z_i$$

(10)

where $\psi_i$ (m) is the hydraulic head in layer $i$, $\psi_{sr}$ (m) is the average hydraulic head in the root zone, $K_{\text{comp, doy}}$ (d$^{-1}$) is root system conductance for compensatory water uptake, and NRLD (unitless) is normalized root length density. The average root zone hydraulic head is calculated as the weighted average of the hydraulic heads in the different soil layers as

$$\psi_{sr} = \sum_{i=1}^{N} \psi_i \text{NRLD}_i \Delta z_i$$

(11)
The plant transpiration rate is the minimum of the potential transpiration rate $T_p$ (mm h$^{-1}$) and the transpiration rate $T_{\text{threshold}}$ (mm h$^{-1}$) when the pressure head in the canopy reaches a threshold value, $\psi_{\text{threshold}}$, which triggers stomatal closure:

$$T_{\text{plant}} = \max \left[0, \min(T_p, T_{\text{threshold}})\right]$$  \hspace{2cm} (12)

$T_{\text{threshold}}$ is calculated from the difference between the root zone pressure head and the threshold pressure head of the canopy that is multiplied by the plant hydraulic conductance, $K_{\text{plant}}$, as

$$T_{\text{threshold}} = K_{\text{plant}} \left(\psi_{\text{sr}} - \psi_{\text{threshold}}\right)$$  \hspace{2cm} (13)

Both coupled models use a water stress index ($f_{\text{wat}}$, Equation 14) as the ratio of $T_{\text{plant}}$ and potential transpiration to consider the downregulation effects of water stress on maximum carboxylation rate and stomatal conductance (Appendix A and Appendix B):

$$f_{\text{wat}} = \frac{T_{\text{plant}}}{T_p}$$  \hspace{2cm} (14)

where $f_{\text{wat}}$ is the water stress factor ($-$); $T_{\text{plant}}$ and $T_p$ are the actual and potential transpiration rate, respectively (mm h$^{-1}$).

The photosynthesis and stomatal conductance, water balance, RWU, and Penman–Monteith subroutines run at the hourly resolution, whereas the remaining subroutines calculate in a daily time step (Figure 2a). For a further description of the water balance model, root growth model, Feddes’ and Couvreur’s RWU models, crop model, Penman–Monteith subroutines, and modeling configuration we refer the readers to the detailed model description and parameterization from Nguyen et al. (2020). In summary, we will compare the performance of two coupled root–shoot models with two different RWU subroutines in simulating CO$_2$ and H$_2$O fluxes and crop growth of maize (Figure 2a):

- HILLFLOW1D-Couvreur’s RWU-SLIMROOT-LINTULCC2 (Couvreur)
- HILLFLOW1D-Feddes’ RWU-SLIMROOT-LINTULCC2 (Feddes)

### 2.5 Modeling workflow

#### 2.5.1 Model sensitivity analysis

Before performing the sensitivity analysis, the Feddes and Couvreur models were calibrated with maize phenology parameters. The base temperature was set to 8 °C, whereas the minimal temperature sum from sowing to anthesis were varied from 500 to 900 °C d (see Table 3, phenology parameters) until the simulated anthesis date is matched to the observed silking date. The model was further calibrated by changing the temperature sum from anthesis to harvest parameter to fit the simulated and the observed harvest dates (see Table 3; Figure 2b).

In our work, the crop-water-related parameters in the Couvreur model ($K_{\text{rs,normalized}}$ and critical canopy pressure head threshold $[\Psi_{\text{threshold}}]$) and SLIMROOT root growth model were adopted from the literature. However, the parameters for maize such as $K_{\text{rs,normalized}}$ are rarely reported. G. Cai et al. (2017, 2018) reported that $K_{\text{rs,normalized}}$ ranges from 0.03 × 10$^{-5}$ to 0.48 × 10$^{-5}$ d$^{-1}$ cm$^{-1}$ cm$^2$ for winter wheat. The $\psi_{\text{threshold}}$ characterizes the specific stomatal behavior. The isohydric response was initially defined at the species level (Tardieu & Simonneau, 1998), nevertheless, this behavior shows a continuum even within species (Franks et al., 2007; Klein, 2014; Schultz, 2003). The use of $\psi_{\text{threshold}}$ and its values are different among modeling approaches. The $\psi_{\text{threshold}}$ of −260 m was the reference leaf pressure head for species with insensitive stomatal regulation such as anisohydric (Tuzet et al., 2003). In contrast, the reference leaf water pressure head for isohydric was −120 m (Tuzet et al., 2003). Various authors used the $\psi_{\text{threshold}}$ of −160 m for both winter wheat and maize (G. Cai et al., 2018; Couvreur et al., 2012, 2014). Moreover, the root growth parameters can vary among maize cultivars and soil types. In SLIMROOT, parameters such as specific weight for lateral root (WLROOT, g m$^{-1}$), and specific weight for seminal root (WSROOT, g m$^{-1}$) are required. Because the specific weights of roots in cereal crops vary with the soil strength (Colombi et al., 2017; Hernandez-Ramirez et al., 2014), we selected the specific weights of roots for the stony soil from the range that was reported by van Noordwijk and Brouwer (1991) for the modeling sensitivity analysis for maize.

For the Couvreur model, the sensitivity of cumulative RWU and total aboveground dry biomass at harvest was tested with the step-wise change of four plant–water relation parameters ($K_{\text{rs,normalized}}$; specific weight of seminal and lateral root, and $\psi_{\text{threshold}}$), whereas the photosynthesis parameters of maize (Table 3, “before calibration”) were the same for all simulations. In the first set of simulations, the $K_{\text{rs,normalized}}$ was sequentially changed to 0.008, 0.04, 0.15, 0.185, 0.2554, 0.372, 0.48, 0.59, and 0.81 × 10$^{-5}$ d$^{-1}$ cm$^{-1}$ cm$^2$. For the second part, the specific weight of seminal roots varied sequentially to 0.005, 0.0075, 0.01, 0.0125, 0.015, 0.0175, 0.02, 0.0225, and 0.025 g m$^{-1}$, whereas the specific weight of lateral roots was the same (0.0061 g m$^{-1}$) for all simulations. For the third set of simulations, the specific weight of seminal roots was kept at 0.02 g m$^{-1}$, whereas the specific weight of lateral roots was sequentially changed to 0.001, 0.002,
| Subroutines | Parameters | Explanation (unit) | Sources | Maize (2017F1P3) | Default (before calibration) | After calibration |
|-------------|-----------|--------------------|---------|------------------|-----------------------------|-------------------|
| Assimilation | maxSLA | Maximum specific leaf area (m² g⁻¹) | Amanullah et al. (2007); Miner and Bauerle (2019); Zhou et al. (2020) | | 0.03 | 0.04 |
| | VCMAX25 | The maximum carboxylation rate of Rubisco at 25 °C (μM m⁻² s⁻¹) | Miner and Bauerle (2019); Perdomo et al. (2016); von Caemmerer (2000) | | 30 | 41 |
| | Vₚₘₙₙ | The maximum phosphoenolpyruvate carboxylase (PEP) carboxylation rate (μM m² s⁻¹) | Miner and Bauerle (2019); Perdomo et al. (2016); Massad et al. (2007) | | 80 | 120 |
| | a₁ | Slope of coupled photosynthesis and stomatal conductance model (–) | Oleson et al. (2013); Wang and Leuning (1998) | | 6 | 4.5 |
| Couvreur RWU model | Kᵥₚₙ₉₉normalized | Normalized root hydraulic conductance (cm d⁻¹) | G. Cai et al. (2018) | | 0.2554 × 10⁻⁵ | 0.37 × 10⁻⁵ |
| | Ψₜₚₚₚₚ | Canopy water potential threshold (m) | Cochrard (2002); Tuzet et al. (2003); Tardieu and Simonneau (1998) | | −200 | |
| | β | Fraction to upscale from Kᵥₚₚₚₚ to Kₚₚₚₚₚ (–) | Nguyen et al. (2020) | | 0.55 | |
| Feddes RWU model | hlim1 | Soil water pressure head at anaerobic limit (m) | Wesseling et al. (1991); Šimůnek et al. (2009) | | 0 | |
| | hlim2 | Upper limit of pressure head range for optimal transpiration (m) | | | −0.03 | |
| | hlim3h | Lower limit of pressure head range for optimal transpiration for high transpiration rate, Ṭₚₒₜₒₜₒₜ (m) | | | −3.25 | |
| | hlim3l | Lower limit of pressure head range for low transpiration rate, Ṭₚₒₜₒₜₒₜ (m) | | | −6 | |
| | hlim4 | Soil water pressure head at wilting point (m) | | | −80 | |
| | Ṭₒₜₒₜₒₜ | High transpiration rate (m d⁻¹) | | | 0.0048 | |
| | Ṭₒₜₒₜₒₜ | Low transpiration rate (m d⁻¹) | | | 0.00096 | |
| Root growth | MaxDEP | Maximum root depth (m) | | | 1.5 | |
| | RINPOP | Number of emerged plant per square meter (no. m⁻²) | | | 10.66 | |
| | RSROOT | Maximum elongation rate of seminal root (m d⁻¹) | Watt et al. (2006) | | 0.03 | |
| | NRSPP | Number of seminal root per plant (no. plant⁻¹) | Lynch (2013) | | 3 | |
| | WLROOT | Specific weight for lateral root (g m⁻¹) | Nguyen et al. (2020) | | 0.0061 | |
| | WSROOT | Specific weight for seminal root (g m⁻¹) | Nguyen et al. (2020) | | 0.02 | |

*Note: RWU, root water uptake.*
0.003, 0.0035, 0.004, 0.005, 0.0061, 0.007, and 0.008 g m\(^{-1}\).
In the last set of simulations, the critical leaf pressure head (\\(\Psi_{\text{threshold}}\)) was changed between -120 and -290 m.

2.5.2 Model calibration, validation, and comparison

**Criteria for model evaluation.** The model performance in simulating aboveground dry biomass, LAI, actual transpiration (also referred to as RWU), gross assimilation rate, and SWC in different soil depths was assessed via (a) the root mean square errors (RMSE) (Equation 15); (b) correlation coefficients (\(r\)) (Equation 16); and (c) index of agreement (\(I\), the degree to which simulated values approached the observations) (Willmott, 1981; Willmott et al., 1985) (Equation 17). This value varies from 1 (for perfect agreement) to 0 (for no agreement);

\[
\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n} (\text{Sim}_i - \text{Obs}_i)^2}{n}}
\]

(15)

\[
r = \frac{\sum_{i=1}^{n} (\text{Sim}_i - \text{Sim}) (\text{Obs}_i - \text{Obs})}{\sqrt{\left[\sum_{i=1}^{n} (\text{Sim}_i - \text{Sim})^2\right] \left[\sum_{i=1}^{n} (\text{Obs}_i - \text{Obs})^2\right]}}
\]

(16)

\[
I = 1 - \frac{\sum_{i=1}^{n} (\text{Sim}_i - \text{Obs}_i)^2}{\sum_{i=1}^{n} \left(\left|\text{Sim}_i - \text{Obs}\right| + \left|\text{Obs}_i - \text{Obs}\right|\right)^2}
\]

(17)

where \(\text{Sim}\) and \(\text{Obs}\) are simulated and measured variables, respectively; \(i\) is the index of a given variable; \(\text{Sim}\) and \(\text{Obs}\) are the mean of the simulated and measured data, respectively; and \(n\) is the number of observations.

**Model calibration.** We used the irrigated plots in 2017 (2017F1P3) for calibration. We calibrated the Feddes and Couvreur model by varying the following parameters: specific leaf area (SLA, m\(^2\) g\(^{-1}\)), maximum carboxylation rate of Rubisco at 25 °C (VCMAX25, \(\mu\)mol m\(^{-2}\) s\(^{-1}\)), maximum phosphoenolpyruvate carboxylase (PEP) carboxylation rate (\(V_{\text{pmax}}\), \(\mu\)mol m\(^{-2}\) s\(^{-1}\)), the slope of coupled photosynthesis and stomatal conductance model (\(a_1\), –), and \(K_{\text{r,s,normalized}}\) (Table 3; Figure 2). The RMSE (Equation 15), correlation efficiency (\(r\)) (Equation 16), and \(I\) (Equation 17) were calculated using the R software (R Core Team, 2018) and used to compare the simulated and observed LAI, gross assimilation rate, aboveground dry biomass, and actual transpiration. The best parameter set was identified manually by choosing a simulation with the lowest RMSE and the highest \(r\) and \(I\). The chosen parameters and associated output results are referred to as “after calibration” (FA and CA for Feddes and Couvreur models, respectively; Figure 2b). The calibrated parameters and the default parameters are listed in Table 3.

**Modeling validation and comparison.** The parameter set from the “after calibration” step was used for model validation and comparing the Couvreur and Feddes models (Table 3; Figure 2b). Based on the criteria for model evaluation (\(r\), RMSE, and \(I\)), we examined the model capacity for simulating the aboveground dry matter, LAI, RWU, SWC, and gross assimilation rate for the remaining water treatments. The remaining treatments were used for this last stage: the rainfed plot in 2017 (2017F1P2), the irrigated plot with normal sowing date in 2018 (2018F1P3), the rainfed plot with normal sowing date in 2018 (2018F1P2), and the rainfed plot with a late sowing date in 2018 (2018F1P1) (cf. Table 2; Figure 1a; Figure 2b).

3 RESULTS AND DISCUSSION

3.1 Model sensitivity analysis

The sensitivity of RWU and biomass to the changing \(K_{\text{r,s,normalized}}\), specific weights of the seminal and lateral root, and critical pressure head \(\Psi_{\text{threshold}}\) were illustrated in Figure 3. The change of \(K_{\text{r,s,normalized}}\) and specific weight of seminal and lateral roots directly affects total root hydraulic conductance (thus whole-plant hydraulic conductance, \(K_{\text{plant}}\)) because they depend on total root length and hydraulic conductance of root segments. The reduction of \(K_{\text{r,s,normalized}}\) leads to a stronger decrease in RWU and biomass in 2018 as compared with 2017. This is due to less soil water availability in 2018 than those in 2017. However, the increased \(K_{\text{r,s,normalized}}\) by the same magnitude had a smaller relative effect on RWU and biomass than decreasing values of \(K_{\text{r,s,normalized}}\). A larger increase of RWU and biomass was observed in the more severe water stress plots (i.e., the two rainfed plots in 2018) as compared with the other less severe water stress plots (i.e., irrigated and rainfed plots in 2017). This indicates that increasing water uptake capacity by plants would increase the uptake of water and crop growth in maize.

Decreasing the specific weight of lateral and seminal roots increases the total root length, thus the whole-plant hydraulic conductance that resulted in increase in RWU and biomass, especially in 2018. In contrast, RWU and biomass decreased because the total root length was reduced through increasing specific weight of roots. A larger change of RWU and biomass was observed with the change of specific of seminal root as compared with the change of lateral root. Use of \(\Psi_{\text{threshold}}\) at -120 and -140 m resulted in a substantial
Relative changes of (a, c, e, g) simulated cumulative root water update (RWU) and (b, d, f, h) simulated aboveground biomass to the reference of cumulative RWU and aboveground biomass at harvest by changing normalized root hydraulic conductance ($K_{rs,\text{normalized}}$), specific weights of seminal (WSROOT) and lateral (WSLROOT) roots, and canopy pressure head threshold ($\Psi_{\text{threshold}}$) in the irrigated plot in 2017 (2017F1P3), rainfed plot in 2017 (2017F1P2), irrigated plot with normal sowing date in 2018 (2018F1P3), rainfed plot with normal sowing date in 2018 (2018F1P2), and rainfed plot with late sowing date (2018F1P1). The reference of simulated cumulative RWU and biomass (vertical lines) for each treatment is based on the plant water relation parameters ($K_{rs,\text{normalized}} = 0.185 \text{ d}^{-1} \text{ cm}^{-1} \text{ cm}^{2}$, WSROOT = 0.02 g m$^{-1}$, WSLROOT = 0.0061 g m$^{-1}$, and $\Psi_{\text{threshold}} = -200$ m) from winter wheat (Nguyen et al., 2020) and $C_{4}$ photosynthesis parameters in Table 3 (“before calibration”). $\Psi_{c}$ is canopy pressure head.
reduction of RWU and biomass as compared with those \( \Psi_{\text{threshold}} \) values below −160 m (Figure 3g,h), especially in the rainfed plots in 2018. The use of a high \( \Psi_{\text{threshold}} \) leads to tight control \( \Psi_c \) and stomatal conductance that consequently reduces transpiration and photosynthesis because plants keep \( \Psi_c \) close to its threshold value (Olioso et al., 1996). An increase of the \( \Psi_{\text{threshold}} \) means that water stress occurs earlier, which finally causes more reduction of RWU and biomass. When \( \Psi_{\text{threshold}} \) varies from −160 to −200 m, the change in RWU and biomass is less pronounced as compared with changes in RWU and biomass by using of \( \Psi_{\text{threshold}} \) from −120 and −140 m (Figure 3g,h). The reason is the soil water availability, which becomes very small when the soil water pressure head considerably declined. When the soil is dry, there is no more water to be extracted in spite of further decreasing \( \Psi_{\text{threshold}} \). These findings are well corroborated with findings from Nguyen et al. (2020) where higher \( \Psi_{\text{threshold}} \) (i.e., −120 or −140 m) could overestimate water stress (thus lower biomass and RWU) in winter wheat.

### 3.2 Crop model calibration

There was a relatively large deviation in the observed aboveground dry biomass and LAI between two measured replicates, which indicates the crop heterogeneity within the treatment (Figure 4). The seasonally simulated growth curves of LAI and biomass were satisfactorily captured after calibration in both Couvreur and Feddes models (Figure 4a,b; Supplemental Material S1). The RMSE of the Feddes model before calibration was 0.97 kg m\(^{-2}\) and 1.72 (−) for biomass and LAI, respectively, whereas the corresponding RMSEs after calibration were 0.36 kg m\(^{-2}\) and 0.69 (Table 4). In the Couvreur model, the RMSE of biomass and LAI before calibration were 1.01 kg m\(^{-2}\) and 1.83, respectively, which got improved after calibration having the value of 0.24 kg m\(^{-2}\) and 0.66 for biomass and LAI, respectively (Table 4). The model simulated relatively well the plant hydraulic conductance (\( K_{\text{plant}} \)) after calibration (Appendix D). The mean of measured \( K_{\text{plant}} \) from 75 to 126 d after sowing (DAS) was 10.47 × 10\(^{-5}\) ± 3.26 × 10\(^{-5}\) d\(^{-1}\), whereas the simulated \( K_{\text{plant}} \) by Couvreur model in the same period was 9.04 × 10\(^{-5}\) d\(^{-1}\).

The water supply (precipitation and irrigation), daily root water uptake (RWU or \( T_a \)), and SWC were displayed in Figure 5. Both models were able to represent the seasonal fluctuation of RWU and SWC (Figure 5a). After calibration, the Feddes model simulated higher RWU than the Couvreur model from sowing to 48 DAS, which was consistent with the lower estimated SWC of the Feddes model than the Couvreur model. After calibration, the simulated RWU of the Couvreur was almost similar to those from the Feddes model after 48 DAS. Both models underestimated RWU from 75 to 112 DAS that led to lower simulated cumulative RWU as compared with cumulative sap flow (Figure 5a; Appendix C; Supplemental Material S2). This is because both models underestimated potential transpiration. The correlation efficiency (\( r \) and \( I \) were relatively similar before and after calibration for both models. Both models slightly underestimated the SWC after calibration, especially in the later growing season at the 60- and 80-cm soil depths (Figure 5b; Supplemental Material S3).

The transpiration reduction was also shown in Figure 5c. Before calibration, water stress (\( \text{fwat} < 1 \)) appeared already from 8 to 68 DAS in the Couvreur model. Water stress also occurred in the period from 8 to 45 DAS for the Couvreur model after calibration. However, it was less pronounced as compared with the water stress before calibration. The water stress did not occur in the case of Feddes model in this period both after and before calibration, except on 15 and 16 DAS. This caused the lower simulated biomass and LAI in the Couvreur model as compared with the Feddes model. The Couvreur model simulated less transpiration reduction (less water stress) than in the Feddes model at the late growing season (after 68 DAS). This could explain the higher simulated biomass and LAI from the Couvreur model in comparison to the Feddes model after calibration.

Diurnal courses of RWU, \( \Psi_c \), \( g_s \), and gross assimilation rate (GAR) followed the observed values in the selected days (Figure 6). Root water uptake was slightly lower than measured sap flow in the morning (i.e., 9:00–10:00 a.m.) but the opposite was the case in the afternoon (4:00–6:00 p.m.) (Figure 6b; 74, 75, 90, and 104 DAS). Root water uptake
TABLE 4 Root mean square error (RMSE), coefficient of correlation ($r$), and agreement index ($I$) of aboveground dry biomass, leaf area index (LAI), daily root water uptake (RWU or $T_a$), and hourly gross assimilation rate (GAR) before and after modeling calibration for 2017F1P3 and modeling validation for 2017F1P2, 2018F1P3, 2018F1P2, and 2018F1P1 treatments (cf. Figure 1; Table 2)

| Parameter | Statistic | Before calibration | Validation |
|-----------|-----------|---------------------|------------|
|           |           | 2017F1P3 | 2017F1P2 | 2018F1P3 | 2018F1P2 | 2018F1P1 | Overall |
|           | C         | F         | C         | F         | C         | F         | C         | F         | C         | F         |
| Dry biomass | RMSE     | 1.01      | 0.97      | 0.24      | 0.36      | 0.31      | 0.28      | 0.52      | 0.55      | 0.19      | 0.25      | 0.15      | 0.18      | 0.29      | 0.32      |
|           | $r$       | 0.96      | 0.96      | 0.95      | 0.95      | 0.89      | 0.9       | 0.96      | 0.95      | 0.89      | 0.85      | 0.91      | 0.96      | 0.91      | 0.92      |
|           | $I$       | 0.67      | 0.66      | 0.9       | 0.91      | 0.93      | 0.92      | 0.85      | 0.83      | 0.93      | 0.83      | 0.88      | 0.79      | 0.90      | 0.84      |
|           | $n$       | 8         | 8         | 8         | 8         | 8         | 8         | 10        | 10        | 10        | 10        | 10        | 10        | 38        | 38        |
| LAI       | RMSE      | 1.83      | 1.72      | 0.66      | 0.69      | 0.75      | 0.63      | 0.94      | 0.96      | 0.87      | 0.84      | 0.65      | 0.53      | 0.80      | 0.74      |
|           | $r$       | 0.89      | 0.9       | 0.89      | 0.88      | 0.85      | 0.85      | 0.8       | 0.81      | 0.76      | 0.78      | 0.71      | 0.74      | 0.78      | 0.80      |
|           | $I$       | 0.6       | 0.73      | 0.89      | 0.88      | 0.83      | 0.85      | 0.76      | 0.75      | 0.85      | 0.85      | 0.74      | 0.78      | 0.80      | 0.81      |
|           | $n$       | 8         | 8         | 8         | 8         | 8         | 10        | 10        | 10        | 10        | 10        | 10        | 38        | 38        |           |
| RWU       | RMSE      | 1.62      | 1.41      | 0.67      | 0.78      | 0.54      | 0.38      | 1.27      | 1.29      | 1.17      | 1.13      | 0.92      | 0.91      | 0.98      | 0.93      |
|           | $r$       | 0.91      | 0.94      | 0.94      | 0.95      | 0.91      | 0.95      | 0.73      | 0.74      | 0.74      | 0.73      | 0.74      | 0.76      | 0.78      | 0.80      |
|           | $I$       | 0.81      | 0.85      | 0.96      | 0.94      | 0.94      | 0.97      | 0.85      | 0.84      | 0.72      | 0.77      | 0.72      | 0.74      | 0.81      | 0.83      |
|           | $n$       | 64        | 64        | 64        | 64        | 66        | 66        | 54        | 54        | 54        | 54        | 54        | 54        | 228       | 228       |
| GAR       | RMSE      | 12.85     | 12.59     | 7.83      | 7.96      | 7.35      | 7.44      | 7.55      | 7.38      | 8.29      | 8.15      | 8.21      | 8.20      | 7.85      | 7.79      |
|           | $r$       | 0.72      | 0.63      | 0.78      | 0.75      | 0.75      | 0.76      | 0.77      | 0.78      | 0.67      | 0.68      | 0.65      | 0.66      | 0.71      | 0.72      |
|           | $I$       | 0.48      | 0.6       | 0.81      | 0.82      | 0.72      | 0.7          | 0.68      | 0.69      | 0.72      | 0.74      | 0.64      | 0.64      | 0.69      | 0.69      |
|           | $n$       | 61        | 61        | 61        | 61        | 56        | 56        | 41        | 41        | 45        | 45        | 44        | 44        | 186       | 186       |

Note. The unit of RMSE for RWU (mm d$^{-1}$), GAR ($\mu$Mm$^{-2}$ s$^{-1}$), aboveground dry biomass (kg m$^{-2}$), and LAI (–); $n$ is the number of samples/measurement points. C, HILLFLOW1D-Couvreur’s RWU-SLIMROOT-LINTULCC2; F, HILLFLOW1D-Feddes’ RWU-SLIMROOT-LINTULCC2. 

*Average values from all validated plots (2017F1P2, 2018F1P3, 2018F1P2, and 2018F1P1).
started later than transpiration because the stored water in the plant is used for transpiration. The hydraulic capacitance can delay the change of $\psi_c$ that derives water uptake, which was not considered in our model. However, the differences between simulated RWU and sap flow in the morning and afternoon due to the plant hydraulic capacitance was canceled out when the hourly sap flow and RWU were aggregated. Both models were able to simulate the diurnal courses of transpiration, stomatal conductance of sunlit leaves, and gross assimilation rate (GAR) as used in Figure 6.

**Figure 5** Comparison between observed (Obs, red) and (a) daily actual transpiration (RWU or $T_a$), (b) soil water content at different soil depths, and (c) daily transpiration reduction factor ($f_{wat}$) simulated by Couvreur before calibration (CB), Couvreur after calibration (CA), Feddes before calibration (FB), and Feddes after calibration (FA) in the irrigated plot in 2017 (2017F1P3). The black and red bars in (a) denote precipitation (Prec) and irrigation (Irri), respectively. The error bars in (a) indicate standard error for five sap flow sensors. Vertical gray lines in (a, c) show days with the measured and simulated diurnal courses of root water uptake (RWU), canopy hydraulic head ($\psi_c$), stomatal conductance ($g_s$), and gross assimilation rate (GAR) as used in Figure 6.

**Figure 6** Diurnal courses of five selected measurement days: 5 July (62 DAS), 17 July (74 DAS), 18 July (75 DAS), 2 August (90 DAS), and 16 August 2017 (104 DAS). (a) Global radiation ($R_s$, black long dash lines) and vapor pressure deficit (VPD, cyan long dash lines), (b) actual transpiration (RWU or $T_a$), (c) canopy hydraulic head ($\psi_c$), (d) stomatal conductance to water vapor ($g_s$), and (e) gross assimilation rate (GAR) at the irrigated plot in 2017 (2017F1P3). The black dots denote the observed. The lines denote simulated output by Couvreur before calibration (CB, blue dotted lines), Couvreur after calibration (CA, blue solid lines), Feddes before calibration (FB, dark dotted lines), and Feddes after calibration (FA, black solid lines). Sap flow sensors were installed on 8 July 2017. Simulated stomatal conductance is from sunlit leaves. Vertical black bars in (b) represent the standard deviation of the flux measurements in the five different stems.

### 3.3 Crop model validation and comparison between the Feddes and Couvreur RWU models

#### 3.3.1 Aboveground dry biomass and LAI

The development of aboveground dry biomass and LAI when applying the calibrated model for different treatments are
The Couvreur model predicted lower biomass and LAI than the Feddes model in the early growth stages across all treatments in both years, whereas more biomass and LAI were simulated by the Couvreur model than the Feddes model at the later crop growth stages. The biomass from Feddes and Couvreur models was satisfactorily simulated in the rainfed plot in 2017 (2017F1P2), the rainfed plot with normal sowing date in 2018 (2018F1P2), and the rainfed plot with late sowing date (2018F1P1). In the 2018F1P3 plot, the biomass and LAI from both models have a good match with that observed before the silking time. However, afterward, the models underestimated biomass and LAI. The RMSEs of LAI were 0.94 and 0.96 for Couvreur and Feddes models, respectively, in this plot. In the drought plot (i.e., 2018F1P2), both models overestimated LAI from 65 DAS to harvest (Figure 7f) with RMSEs of 0.87 and 0.84, respectively. In these plots, leaves started rolling when the leaf pressure head was around \(-150\) m (equivalent to \(-1.5\) MPa), and complete curling and rolling occurred when the leaf pressure head was around \(-200\) m in our field coinciding with days having severe drought stress.
drought, high temperature, and high VPD. This was in agreement with another observation of leaf rolling at leaf pressure heads of \(-100\) m, with its maximum around \(-200\) m in a study on maize from Moulia (1994). Low leaf water pressure head could result in a reduction of leaf elongation rate and leaf area under water-limited conditions (Munns et al., 2000; Salah & Tardieu, 1997; Westgate & Boyer, 1985). Our leaf growth model is based on assimilate partitioning, specific leaf area parameters, and air temperature at a daily time scale; thus, it is not able to capture the instant effects of leaf water status on leaf area variability.

3.3.2 Transpiration reduction

The transpiration reduction (fwat) from the four validated plots was displayed in Figure 8. The Couvreur model displayed water stress in all plots at the beginning of growing seasons (8 to 45 DAS for the normal sowing plots and 17 to 52 DAS for the late sowing plot), which is opposite to the Feddes model. After this period, the Feddes model predicted more severe water stress than the Couvreur model. Both models were able to simulate the severe water stress during severe soil water depletion (from 56 to 105 DAS in 2018F1P2; from 60 DAS to the end of the growing season in 2018F1P1) (Figure 8c,d).

3.3.3 RWU and SWC

Simulated \(T_p\), RWU, and SWC were presented in Figure 9 for the rainfed plot in 2017 (2017F1P2) and the irrigated plot with a normal sowing date in 2018 (2018F1P3). The Couvreur model simulated lower RWU and SWC than the Feddes model in the earlier growing phases. However, it calculated slightly higher RWU and SWC than the Feddes model in the later growing period. Both models simulated fairly well the dynamics of RWU at the 2017F1P2 (Figure 9a,b) with RMSEs of 0.54 and 0.38 mm d\(^{-1}\) for the Couvreur and Feddes model, respectively. In the irrigated plot 2018F1P3, the simulated \(T_{act}\) and measured sap flow were much higher than those in 2017F1P2 (also in 2017F1P3). Such high sap flow values in the 2018F1P3 plot was consistent with the reported sap flow rates in maize in a semiarid climate and irrigated conditions in maize (Langensiepen et al., 2009). Note that the growing season 2018 can be classified as an extreme year for crop growth in our experiments with exceptionally hot and dry conditions during the summer. Our measured sap flow rates for some days at the irrigated plot (2018F1P3) reached up to 10.6 mm d\(^{-1}\) where the daily maximum VPD and maximum temperature were up to 3.8 kPa and 37 \(^\circ\)C, respectively. This could explain why our measured sap flow was higher than sap flow that were reported in previous studies in Germany (i.e., Heinlein et al., 2017; Langensiepen et al., 2009). The dynamics of predicted SWC from the two models followed the measured values over different soil depths for both water treatments (Figure 9b,d; Supplemental Material S3).

The comparison of simulated \(T_p\), RWU, and SWC from two models to the measured data at the remaining rainfed plots in 2018 with normal (2018F1P2) and late sowing dates (2018F1P1) was shown in Figure 10. Compared with the measured sap flow, both models overestimated RWU from 52 to 70 DAS at the 2018F1P2 and from 52 to 73 DAS at the 2018F1P1. The overestimated RWU by both models in these periods in two plots was consistent with their overestimated SWC at corresponding times at the topsoil layers (10-, 20-, and 40-cm depths). However, after these periods, the simulated RWU from the two models matched relatively well. Soil is a heterogeneous substrate, whereas it is also spatially different within the plot. Thus, it is rather difficult to find a representative set of soil characteristics valid for a whole plot in our study, which can explain the deviations of simulated RWU and SWC in two models.
FIGURE 9  Comparison between measured sap flow (Obs, red) and simulated (a, c) root water uptake (RWU or $T_a$) and potential transpiration ($T_p$), and (b, d) soil water content by Couvreur (C, blue line) and Feddes (F, black line) from sowing to harvest in the (a, b) rainfed plot with normal sowing date in 2017 (2017F1P2) and (c, d) irrigated plot with normal sowing date in 2018 (2018F1P3). Time series of precipitation (Prec) and irrigation (Irri) are given in the panels. Vertical red bars in (a) and (c) represent the standard deviation of the flux measurements in the five different stems.

3.4  Overall performance of the coupled models with Couvreur and Feddes RWU models

Numerous studies applied the common Feddes RWU model with HYDRUS water balance model (Šimůnek et al., 2009) in simulating soil water flux and nutrient flow under different water regimes (González et al., 2015), the interaction of water and salt content (He et al., 2017; Q. Wang et al., 2015), or nitrogen levels and irrigation methods (Tafteh & Sepaskhah, 2012). Few studies coupled crop models (i.e., WOFOST crop model) with the Feddes RWU model and HYDRUS model to simulate crop growth and water uptake in maize (Li et al., 2012; Yang et al., 2017). Note that the coupling of LINTULCC2 crop model with the Feddes RWU model in this study considers the more mechanistic $C_4$ assimilation routines and stomatal conductance model. Moreover, these subroutines link with soil water flux at the hourly step, which is not represented in the abovementioned studies. The coupled model with the Feddes RWU model simulated well the transpiration reduction, assimilate, RWU, and crop growth for maize in both years.

The modeling approach using $\Psi_{\text{threshold}}$ as a trigger for stomatal control and involving plant hydraulic conductance has received increasing attention in improvements and applications of the soil–plant–atmosphere model. However, most work so far investigates water response behavior in crops such as soybean (Olioso et al., 1996) or spring wheat (Jensen et al., 1993). Comparison of modeling performance between Feddes RWU model and Couvreur RWU model has been done in winter wheat (G. Cai et al., 2017, 2018; Nguyen et al., 2020). The Couvreur model uses a stomatal regulation model, which assumes that stomatal conductance is not influenced by $\Psi_c$ as long as the $\Psi_c$ is above $\Psi_{\text{threshold}}$. The $\Psi_c$ was kept constant by changing stomatal conductance when the $\Psi_{\text{threshold}}$ is reached. In fact, this is a perfectly isohydric system. Thus, from the theoretical point of view, this approach should be able to represent stomatal regulation of maize because it maintained its $\Psi_c$. 
FIGURE 10  Comparison between measured sap flow (Obs, red) and simulated (a, c) root water uptake (RWU or \( T_a \)) and potential transpiration (\( T_p \)), and (b, d) soil water content by Couvreur (C, blue line) and Feddes (F, black line) from sowing to harvest in the rainfed plots in 2018 with (a, b) normal sowing date (2018F1P2) and with (c, d) late sowing date (2018F1P1). Time series of precipitation (Prec) and irrigation (Irri) are given in the panels. Vertical red bars in (a) and (c) represent the standard deviation of the flux measurements in the five different stems at certain \( \Psi_{\text{threshold}} \) values (Cochard, 2002; Tardieu & Simonneau, 1998). To the best of our knowledge, this is the first study where the performance of the Couvreur RWU model is evaluated and compared with the Feddes model for maize under field scale. Our results showed that both models simulated rather similarly the crop growth, \( \text{CO}_2 \), and \( \text{H}_2\text{O} \) gas flux exchanges of maize in the main growing season.

The means of simulated \( K_{\text{plant}} \) by Couvreur model from 75 to 126 DAS in the irrigated and rainfed plots in 2017 were \( 9.33 \times 10^{-5} \) and \( 9.04 \times 10^{-5} \text{ d}^{-1} \), respectively (Appendix D). The small difference in simulated \( K_{\text{plant}} \) between irrigated and rainfed plots was due the small difference in simulated root length (Appendix E). The differences in the observed root lengths were also small between the two plots (Appendix E). Based on the measured root length, we would expect that there are only small differences in measured \( K_{\text{plant}} \) between the two plots. However, the differences in the average measured \( K_{\text{plant}} \) in 2017 were large with \( 10.47 \times 10^{-5} \pm 3.26 \times 10^{-5} \text{ d}^{-1} \) and \( 6.86 \times 10^{-5} \pm 3.04 \times 10^{-5} \text{ d}^{-1} \) for the irrigated and rainfed plots, respectively (mean values from 75 to 126 DAS). The smaller observed \( K_{\text{plant}} \) in the rainfed plot must be due to factors that are not considered in the model. It could be due to the higher resistance for water flowing from soil in the drier soil of the rainfed plot.

The Couvreur model displayed water stress in all plots during the initial growth stages (14 to 45 DAS in 2017, 3 to 45 DAS in the normal sowing plots in 2018, and 2 to 37 DAS for the late sowing plot in 2018). In contrast, the Feddes model simulated water stress only on few days (14 and 15 DAS in 2017 and 23 DAS at the normal sowing plots in 2018 and 8 DAS for the late sowing plot in 2018) during the initial growth stages. The inaccurate simulation of water stress in the Couvreur model could be related to the low simulated \( K_{\text{plant}} \) in the earlier growing period. This explains the slightly lower simulated biomass and LAI from the Couvreur model as compared with the Feddes model and the observed data in this period. After this period, the Couvreur model predicted water stress and crop growth better than the Feddes model when \( K_{\text{plant}} \) increased (Appendix E). The root and plant hydraulic conductance in the Couvreur model is a function of the total root length system. Because the Feddes model did not consider the root hydraulic property, it was not sensitive to the low
estimates of root system conductance (in the earlier growth of root), which is opposite to the Couvreur model. A sensitivity analysis was carried out by changing either $K_{\text{init,normalized}}$ or $\beta$ to examine the effect on transpiration reduction and biomass (data not shown). The increase of $K_{\text{init,normalized}}$ or $\beta$ improved the prediction of water stress at the earlier growth stage of the crop; however, it led to an underestimation of water stress (thus overestimation of RWU and biomass growth) at the later growth stage. The supply of assimilates from shoot to root is given by a partitioning table based on the thermal time. This approach probably was not sufficient to capture dynamic changes in carbon allocation to the root over the cropping season (thus dynamic root hydraulic conductance), especially under the condition of drought stress.

In this study, the coupled model was calibrated using data from the irrigated plot in 2017 based on the value ranges of parameters that were taken from other modeling studies and literature. The calibrated parameters worked fairly well for both the water-stressed and non-water-stressed plots. This could be related to the choice of initial parameter values. However, it is still questionable whether the derived parameters are suitable to describe water uptake and crop growth also under conditions of lower soil water availability. Further studies might be required to derive crop stress parameters from inverse modelling (i.e., in G. Cai et al., 2018) when data from water-stressed treatments are used for maize. Modeling and understandings the effect of varying soil moisture and evaporative conditions on crop growth, $\text{CO}_2$, and $\text{H}_2\text{O}$ gas flux exchange at field conditions often requires comprehensive and expensive measurements to capture the soil–plant–atmosphere continuum. The modeling study and the presented data, to the best of our knowledge, are unique. Due to the associated complex and expensive construction of underground rhizotrone facilities, the experimental sites did not allow to involve replicates in water treatments (Nguyen et al., 2020). The limited size of the subplot did not allow for a larger sample of biomass, leaf-cutting, and LAI, which can become noisy due to the soil and water heterogeneity within the subplots. The spatial variability of stomatal reactions over leaves, plants, and stands of plants can be large (Rochette et al., 1991). However, despite these shortcomings, the data illustrated the difference and variability among water regimes and two growing seasons that are still valid for model calibration, validation, and for comparing the two model approaches in the present study.

### 4 | CONCLUSION

We extended and evaluated two different RWU approaches within a coupled soil water balance and crop growth model for maize. One of the RWU models was the recently developed Couvreur RWU approach, which simulates the water potential gradient from soil to root and to leaves based on whole-plant hydraulic conductance, whereas the other approach was the commonly used Feddes model that does not explicitly include plant hydraulic conductance.

For the coupled model with the Couvreur RWU approach, the effect of the change of the root segment conductance, specific weight of roots, and the leaf pressure head threshold at which stomata close on RWU and aboveground biomass is amplified by the positive feedback between the aboveground biomass, the root biomass, the total root length, the root system hydraulic conductance, and plant hydraulic conductance. For instance, decreasing the specific weight of lateral and seminal roots increases the total root length, and thus the $K_{\text{plant}}$ that led to an increase in RWU and biomass. The coupled model, which considers plant hydraulic conductance and links root system properties to plant water uptake, water stress, and crop growth in a more mechanistic way, could be able to describe the effects of specific crop characteristics (change of root segment conductance, specific root lengths of seminal and lateral root, or leaf critical pressure head) on crop performance under different conditions of soil moisture and evaporative demand.

Overall, the biomass, leaf area development, SWC, canopy pressure heads, leaf stomatal conductance, and transpiration rate were relatively well predicted for maize by both models. However, the coupled Couvreur model simulated inaccurately water stress in the first 45 d of the crop season, resulting in slightly underestimated biomass and LAI, which was opposite to the results from the Feddes model. Nevertheless, the coupled Couvreur model simulated slightly better transpiration reduction, water uptake, assimilation, and crop growth than the Feddes model in the late growing period.

Future application of the more mechanistic Couvreur approach in predicting the crop responses to different soil water conditions should pay attention to an accurate estimate of $K_{\text{plant}}$. A root growth model, which considers changes in carbon allocation to the root system that are triggered by stress through a more mechanistic representation of root–shoot partitioning, would improve accuracies in the simulation of whole-plant hydraulic conductance in different growth stages. Using a dynamic parameterization of the normalized root system conductance (i.e., different $K_{\text{rs,normalized}}$) could further improve the estimation of whole-plant hydraulic conductance.

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AUTHOR CONTRIBUTIONS
Thuy Huu Nguyen: Conceptualization; Data curation; Formal analysis; Investigation; Methodology; Software; Validation; Visualization; Writing–original draft; Writing–review & editing. Matthias Langensiepen: Conceptualization; Funding acquisition; Methodology; Resources; Supervision; Writing–review & editing. Hubert Hüging: Data curation; Methodology; Resources; Writing–review & editing. Thomas Gaiser: Project administration; Resources; Software; Writing–review & editing. Sabine Seidel: Writing–review & editing. Frank Ewert: Conceptualization; Funding acquisition; Methodology; Project administration; Resources; Software; Supervision; Writing–review & editing.

CONFLICT OF INTEREST
We declare that we do not have any commercial or associative interest that represents a conflict of interest in connection with the work submitted.

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APPENDIX A
List of main variables used in the photosynthesis models and their units

| Variables | Explanation | Unit |
|-----------|-------------|------|
| VMAX     | Maximum carboxylation rate | μM m⁻² s⁻¹ |
| Jmax     | Maximum electron transport rate | μM electrons m⁻² s⁻¹ |
| J        | Electron transport rate | μM electrons m⁻² s⁻¹ |
| Ca       | Atmospheric CO₂ concentration | μM mol⁻¹ |
| Ci       | Intercellular CO₂ concentration | μM mol⁻¹ |
| Cm       | Mesophyll CO₂ concentration | μM mol⁻¹ |
| Cbs      | Bundle-sheath CO₂ concentration | μM mol⁻¹ |
| O₂       | Atmospheric O₂ concentration | mM mol⁻¹ |
| rCiCa    | Ratio of intercellular CO₂ to atmospheric CO₂ concentration | – |
| gbd      | Boundary layer conductance | m s⁻¹ |
| gs       | Stomatal conductance | mol m⁻² s⁻¹ |
| gbs      | Bundle-sheath conductance to CO₂ | mM m⁻² s⁻¹ |
| gm       | Mesophyll conductance to CO₂ | mol m⁻² s⁻¹ |
| g₀       | Residual stomatal conductance when irradiance approaches zero | mol m⁻² s⁻¹ |
| αm       | Fraction relates stomatal conductance and mesophyll conductance | – |
| DS       | Leaf to air vapor pressure deficit (VPD) | kPa |
| D₀       | Parameters reflect the sensitivity of stomatal conductance to VPD | kPa |
| Γ*       | CO₂ compensation point in the absence of day respiration | μM mol⁻¹ |
| a₁       | Empirical coefficient relates photosynthesis and stomatal conductance | – |
| R₀       | Day respiration rate | μM m⁻² s⁻¹ |
| Rm       | Mesophyll mitochondrial respiration rate | μM m⁻² s⁻¹ |
| KMC      | Michaelis–Menten constant for CO₂ | μM mol⁻¹ |
| KMO      | Michaelis–Menten constant for O₂ | mM mol⁻¹ |
| EAVCMX   | Energy activation for maximum carboxylation rate | J mol⁻¹ |
| Aₙ       | Net photosynthesis rate | μM m⁻² s⁻¹ |
| A₁       | Rubisco activity limited net photosynthesis rate | μM m⁻² s⁻¹ |
| A₂       | RuBp limited photosynthesis rate | μM m⁻² s⁻¹ |
| Lbs      | Rate of CO₂ leakage from bundle-sheath to mesophyll | μM m⁻² s⁻¹ |
| V₀       | The PEP carboxylation rate | μM m⁻² s⁻¹ |
| Vₚmax    | The maximum PEP carboxylation rate | μM m⁻² s⁻¹ |
| Kp       | The Michaelis-Menten constant for CO₂ of PEP | μM mol⁻¹ |
| Vpr      | The PEP regeneration rate | μM m⁻² s⁻¹ |
| I₂       | The absorbed irradiance | μM m⁻² s⁻¹ |
| θ        | Empirical curvature parameter of hyperbolic function | – |
| fwat     | Water stress index | – |

APPENDIX B
Description of photosynthesis approach for maize (C₄)
The CO₂ transfers along the path from atmospheric CO₂ concentration (Cₐ) to intercellular CO₂ concentration (Cᵢ) according to Fick’s law of diffusion:

\[ Cᵢ = Cₐ - Aₙ \left( \frac{1}{g_{bd}} + \frac{1}{g_s} \right) \]  \hspace{1cm} (A1)

where \( Cₐ \) and \( Cᵢ \) are atmospheric and intercellular CO₂ concentration (μmol mol⁻¹). The \( 1/g_{bd} \) and \( 1/g_s \) are boundary layer resistance and stomatal resistance, respectively. The width of sunlit and shaded maize leaves was assumed to be 0.01 m, and their boundary layer resistance was computed as follows (Campbell & Norman, 1998):

\[ \frac{1}{g_{bd}} = 300\sqrt{0.01/μ} \]  \hspace{1cm} (A2)
where $u$ is wind speed (m s$^{-1}$). Air diffusion from intercellular space to mesophyll cell is given as

$$C_m = C_i - A_n/g_m \quad (A3)$$

In addition to stomatal conductance, the nonstomatal limitations (here, mesophyll conductance) appear to be coregulated under water stress (Flexas et al., 2004). Stomatal conductance and internal conductance (or mesophyll conductance) were both proportionally decreased under soil water deficit (Warren, 2008). In our work, due to the absence of detailed data, we assumed that $g_m$ is proportional to $g_s$, namely, $g_m = \alpha_m g_s$. The proportionality differed among species so that $\alpha_m$ ranges from 0.77 to 2.31 (Ouyang et al., 2017; Warren, 2008).

Stomatal conductance was simulated based on the Leuning approach (Leuning, 1995) with consideration of water stress ($f_{wat}$), the effect of leaf to air vapor pressure deficit ($1 + DS/D_0$), intercellular CO$_2$ concentration ($C_i$), and $\Gamma^*$ being CO$_2$ compensation point in the absence of day respiration ($R_d$).

$$g_s = g_0 + \frac{a_1 A_n}{(C_i - \Gamma^*) (1 + DS/D_0)} f_{wat} \quad (A4)$$

Following the approach from Farquhar et al. (1980) and von Caemmerer (2000), the rubisco-limited rate of photosynthesis rate is given by

$$A_c = \frac{V_{\text{CMAX}} (C_{bs} - \Gamma^*)}{C_{bs} + \text{KMC} \left(1 + \frac{O_2}{K_MO}\right)} f_{wat} - R_d \quad (A5)$$

where $C_{bs}$ and $O_2$ are the CO$_2$ and O$_2$ concentration at the site of photosynthesis activities, which is bundle sheath cell in maize; $V_{\text{CMAX}}$ is the maximum catalytic activity of Rubisco at leaf temperature; $\Gamma^*$ is CO$_2$ compensation point at the absence of $R_d$; and KMC and KMO are Michaelis–Menten kinetics for CO$_2$ and O$_2$.

The photosynthesis can be limited by the RuBp regeneration rate, which is driven by ATP and NADPH that supplied by the electron transport rate $J$. The rate of RuBp-limited CO$_2$ assimilation was computed by

$$A_j = \frac{J}{4.5C_{bs} + 10.5\Gamma^*} - R_d \quad (A6)$$

where $C_{bs}$ is the CO$_2$ concentration at the bundle sheath cell. The electron transport $J$ was estimated based on the absorbed irradiance ($I_2$), an empirical curvature parameter of hyperbolic function ($\theta$) (von Caemmerer, 2000):

$$J = \frac{I_2 + J_{\text{max}} + \sqrt{(I_2 + J_{\text{max}})^2 - 4\theta I_2 J_{\text{max}}}}{20} \quad (A7)$$

The leaf net photosynthesis ($A_n$) was the function of both $A_c$ and $A_j$:

$$A_n = \min (A_c, A_j) \quad (A8)$$

C$_4$ photosynthesis involves both the mesophyll and bundle sheath cells of the leaves, which characterized a high CO$_2$ concentrating mechanism that allows Rubisco at this location to fix CO$_2$. This process inhibits the oxygenation reaction and reduces the photorespiration rate. The supply of CO$_2$ due to the PEP carboxylation ($V_p$) can be formulated as a function of CO$_2$ assimilation ($A$), the rate of CO$_2$ leakage from bundle-sheath to mesophyll ($L_{bs}$), and mitochondrial respiration ($R_m$):
APPENDIX C
Cumulative precipitation and irrigation (Prec+Irri), simulated ETP, potential transpiration ($T_p$), and actual transpiration (RWU or $T_a$) by Couvreur (C) and Feddes (F), and measured transpiration by sap flow sensors (Obs) (a) at the irrigated plot in 2017 (2017F1P3) for before calibration (2017F1P3_B) and after calibration (2017F1P3_A) and (b) at the rainfed plot in 2017 (2017R1), the irrigated plot with normal sowing date (2018F1P3), rainfed with normal sowing date (2018F1P2), and rainfed plot with late sowing date (2018F1P1). Data are shown from 8 July to harvest on 12 September in 2017, whereas they are from 29 June to 21 August in 2018.

APPENDIX D
Comparison of simulated whole-plant hydraulic conductance ($K_{plant}$) by the Couvreur model (C) from sowing to harvest in different water treatments in (a) 2017 and (b) 2018. The observed plant hydraulic conductance is shown for 2017 [solid and squared dots in (a)]. The vertical bars represent the standard deviation of four hourly plant hydraulic conductance values at around midday (11:00 a.m. to 2:00 p.m.). Two plots in 2017 were the irrigated (2017F1P3) and the rainfed plot (2017F1P2). Three plots in 2018 were the irrigated plot with normal sowing date (2018F1P3), rainfed plot with normal sowing date (2018F1P2), and the rainfed plot with late sowing date (2018F1P1) (Table 2; Figure 1). The simulated $K_{plant}$ in 2017F1P3 was from the Couvreur model before calibration (CB) and after calibration (CA). The $K_{plant}$ from the other treatments (2017F1P2, 2018F1P3, 2018F1P2, and 2018F1P1) were based on the simulations with the calibrated parameters (see Table 3).
APPENDIX E

Comparison between observed root length from rhizotubes (cm cm$^{-2}$) (cyan line with dots) and simulated root length density (RLD) (cm cm$^{-3}$) from 10-, 20-, 40-, 60-, 80-, and 120-cm soil depth (a, d) on 8 June 2017; (b, e) at silking on 13 July 2017; and (c, f) at harvest on 12 Sept. 2017 by the Couvreur (C, solid blue) and Feddes model (F, solid black) in the irrigated plot (2017F1P3, upper panel) and rainfed plot (2017F1P2, lower panel) in 2017.