MODELING N CONCENTRATION AND UPTAKE FOR MAIZE HYBRIDS UNDER GROWTH STAGE-BASED DEFICIT IRRIGATIONS

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ABSTRACT. *Current maize hybrids have lower critical aboveground biomass nitrogen (N) concentration (TCNP) and grain N concentration (GNC) compared to older hybrids, but few crop models have incorporated this trend. The objective of this study was to evaluate alternative algorithms for calculating TCNP (biomass-based method) and GNC (grain N demand based on N dilution curve) for predicting crop N concentration and N uptake for a current maize hybrid in the CERES-Maize model as implemented in the Root Zone Water Quality Model (RZWQM). Experimental data were obtained from a field study on maize irrigated to meet various percentages (40% to 100%) of evapotranspiration demand at both vegetative and reproductive stages in 2012 and 2013 in Greeley, Colorado. The original RZWQM showed little response of aboveground N concentration (AGBNC) to the irrigation treatments and overpredicted GNC in both years. As a result, crop N uptake was generally overpredicted, with root mean square error (RMSE) values of 28 to 60 kg N ha*$^{-1}$ *for the two years. Adjusted coefficients in the original TCNP and GNC algorithms (RZWQM_ADJ) effectively reduced the overpredicted GNC but with less improvement in response to the irrigation treatments in 2013 compared with the original RZWQM simulations. The RZWQM with modified TCNP and GNC algorithms simulated lower GNC and AGBNC than the original version, significantly improved the responses to the irrigation treatments, and captured the variations in measured GNC among seasons. The corresponding crop N uptake simulations improved more in 2012 than in 2013, with lower RMSE values of 16 to 32 kg N ha*$^{-1}$ *than the original and RZWQM_ADJ versions. The better-predicted grain N uptake by the alternative algorithms could be helpful to making better crop N management decisions under different deficit irrigation conditions.*

Keywords. *CERES-Maize, Crop N concentration, Crop N demand, Crop N uptake, Deficit irrigation, Maize hybrid, RZWQM.*

Crop nitrogen (N) uptake is a critical component affecting crop growth and soil N balance, such as soil residual N and N losses to the environment (leaching and emissions) in agricultural systems (Ma et al., 2007a), and is influenced by crop growth and soil N and water status (Fageria and Baligar, 2005). The concept of critical N concentration, defined as the minimum N concentration in aboveground biomass (AGB) required for maximizing growth (Greenwood et al., 1990), is an important indicator of better crop N management (Justes et al., 1994; Herrmann and Taube, 2004; Errecart and Agnusdei, 2014).

The critical N concentration in plant tops (TCNP) is estimated differently in different crop models (Jeuffroy et al., 2002), e.g., as a function of growth stage (AFRCWHEAT2, Porter, 1993; APSIM, Keating et al., 2003; CERES-Maize, Jones et al., 1986), fraction of the crop cycle, akin to growth stage (EPIC, Williams et al., 1989), degree days (DAISY, Hansen et al., 1991), and AGB (CropSyst, Stöckle et al., 2003; STIC, Brisson et al., 2003). These TCNP estimation methods were compared within different crop models for predicting crop N concentration and N uptake in response to different N fertilizer application rates (e.g., Stöckle and Debaeke, 1997; Zhao et al., 2014). The researchers found that the ability of these models to predict measured results collected from different climatic, soil, and management conditions varied substantially. Recently, Yakoub et al. (2017) compared the biomass-based and growth stage-based TCNP estimation methods using the maize model CSM-IXIM in DSSAT. They found that the biomass-based TCNP estimation method generally improved the simulations of crop yield, biomass, and N uptake under a

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range of N management treatments compared with the current growth stage-based method in IXIM. These studies did not investigate the performances of these TCNP estimation methods under different crop water stress levels, which is important for selecting TCNP methods to accurately predict crop N uptake under various climate and soil conditions.

Models also vary in their approach to estimating grain N uptake. Some crop models, such as AFRCWHEAT2 (Porter, 1993) and CropSyst (Stöckle et al., 2003), estimate grain N demand based on a declining grain N concentration (GNC), which is consistent with experimental and simulation results for wheat (Pan et al., 2006) and maize (Plénet and Lemaire, 2000). CERES-Wheat (Ritchie et al., 1998) and APSIM-Wheat (Asseng, 1998) estimate grain N demand using grain number, thermal time, and potential grain N filling rate, which poorly predicted GNC and N uptake under extreme drought conditions (Weiss and Moreno-Sotomayer, 2006). CERES-Maize estimates grain N demand based on the optimal N concentration for daily growth of grain, which is assumed constant (1.7%) under optimal conditions. The empirical calculation method generally produces GNC values of about 1.7% at maturity under optimal (no water and N stresses) conditions, which does not reflect the lower measured GNC levels for current maize hybrids in U.S. (Ciampitti and Vyn, 2012, 2013; Haegele et al., 2013) and in China (Chen et al., 2013). These changes in GNC from previous to current maize hybrids are not accounted for in most crop models, which were developed using data from prior maize cultivars (e.g., CERES-Maize). For example, Yakoub et al. (2017) compared the relationship between GNC and shoot N uptake based on Ciampitti and Vyn (2013) with the original GNC estimation method in the CSM-IXIM maize model and found that the Ciampitti and Vyn (2013) method significantly improved GNC simulations and crop N uptake under a range of N fertilizer treatments at Lleida in northeast Spain.

Soil water stress can reduce crop yield and N uptake in grasses (Lemaire et al., 1996), wheat (Sadras et al., 2004), and maize (Pandey et al., 2000) and the TCNP in shoots of tall fescue (Lemarie and Salette, 1984a, 1984b; Errecart et al., 2014). For grain N uptake, water stress can increase N remobilization and GNC with reduced grain yield for wheat, maize, and rice (Palta et al., 1994; Ciampitti and Vyn, 2012, 2013; Haegele et al., 2013). Chen et al. (2013) found that current maize hybrids also had higher remobilization efficiency and higher photosynthetic N use efficiency than previous maize cultivars in China. These characteristics of crop N redistribution and N use efficiency in response to water stress for new maize hybrids need to be accounted for in crop models. Many crop models, such as STIC, DNDC, and DayCent (Sansoulet et al. 2014), showed poor accuracy in predicting crop N uptake under water stress conditions. The RZWQM (Root Zone Water Quality Model) under- or over-predicted crop N uptake even when the crop yield was simulated accurately in the North China Plain (Fang et al., 2008) and in Iowa (Ma et al., 2007b).

The objective of this study was to propose and evaluate alternative algorithms for TCNP and GNC calculations in the CERES-Maize module incorporated in RZWQM for predicting crop N concentration and N uptake in current maize hybrids under a range of deficit irrigation conditions.

MATERIAL AND METHODS

EXPERIMENTAL SITE, IRRIGATION TREATMENTS, AND MEASUREMENTS

Data for this study were collected during a field experiment conducted in 2012 and 2013 at the USDA-ARS Limited Irrigation Research Farm near Greeley, Colorado (40.45° N, 104.64° W). The majority of the field experimental area contains Olney fine sandy loam soil. The soils are classified predominately as sandy loams with some areas and layers of sandy clay loams and loamy sands. Weather data were recorded on-site with a standard Colorado Agricultural Meteorological Network (http://ccc.atmos.colostate.edu/~coagmet/) evapotranspiration weather station (station GLY04), from which daily reference evapotranspiration (ET) was calculated.

The field was divided into two sections; maize was grown in the west section in 2012 and in the east section in 2013. Each section was divided into four replicated blocks, and each block was divided into twelve 9 m × 44 m plots, each with 12 north-south oriented rows on 0.76 m spacing. Twelve irrigation treatments were randomly assigned to the plots within each block (randomized complete block). The irrigation treatments were designed to meet various target percentages of full crop water requirement (CWR) during the vegetative (V7 to VT, $V_{7\text{-}T}$) and late reproductive (R4 to R6, $R_{4\text{-}6}$) growth stages and full CWR during the early reproductive stage (R1 to R3, $R_{1\text{-}3}$). The target percentages of full CWR were 40% to 100% at the $V_{7\text{-}T}$ and $R_{4\text{-}6}$ stages for these irrigation treatments (e.g., 65/40 indicates 65% of full CWR during $V_{7\text{-}T}$ and 40% of full CWR during $R_{4\text{-}6}$). Crop N concentration and uptake were measured from seven of the twelve treatments (100/100, 100/50, 80/80, 80/40, 65/65, 65/40, and 40/40).

Full CWR for the maize crop was determined and irrigations were applied based on daily reference ET and crop coefficients (FAO-56 methodology; Allen et al., 1998) and verified by observation of soil water content. Irrigations were applied every four or five days through surface drip irrigation tubing placed adjacent to each plant row (Trout and DeJonge, 2017). Soil water content was measured in each plot two or three times each week near the plant row with a portable time domain reflectometry (TDR) soil water meter for the 0-0.15 m soil layer and with a neutron attenuation soil water meter between 0.15 and 2.0 m below the soil surface at 0.3 m intervals. The measured soil water contents in the 0-1.2 m depth were used for model calibration and estimating the soil water balance considering maize root distributions within the 0-1.2 cm depth. Soil water uptake was not measured below 120 cm depth.

Maize (Dekalb DKC52-04RIB) was planted at an average rate of 81,000 seeds ha^{-1} in early May of 2012 and 2013. Nitrogen as urea ammonium nitrate (UAN 32%) was applied (side-dressed) uniformly to all treatments at planting (41 kg N ha^{-1}). During the vegetative stage, additional fertilizer (UAN 32%) injected into the irrigation water (fertigation) was applied as needed to meet estimated plant requirements for the 100/100 treatment. Estimated plant N requirements were based on projected yield (13 Mg ha^{-1}), soil tests at the beginning of the season, and N concentration in the irrigation

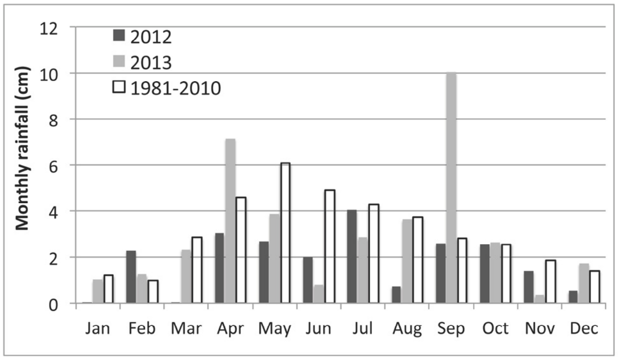

Figure 1. Monthly rainfall at the experimental site for 2012 and 2013 and long-term (1981-2010) average monthly rainfall.

water (25 ppm N). Total N application was 290 and 250 kg N ha^{-1} in 2012 and 2013, respectively.

Figure 1 shows the monthly rainfall for the two years and long-term average values for 1981 to 2010. The monthly rainfall was generally comparable with the long-term average conditions, except for June and August in 2012 with lower rainfall amounts, and April and September in 2013 with higher than the long-term average rainfall. Although the irrigation amounts were adjusted for rainfall, rainfall may have some effect on the soil water availability during periods of targeted deficits, and excessive rainfall may temporarily increase crop ET to be greater than the target CWR.

Actual crop ET (ET_c) was estimated from the soil water balance. Water runoff from the relatively flat sandy loam soil was assumed to be zero in the water balance calculation of ET_c (Fang et al., 2014). Deep percolation was estimated based on precipitation that exceeded the soil water storage deficit and verified by increases in soil water content in soil layers below the root zone. Deep percolation losses were small (<5% of irrigation plus precipitation) in both years due to precise irrigation scheduling and efficient application by drip irrigation.

From 2012 to 2013, aboveground biomass (dry weight) was measured at maturity for two 5-plant row sections, and grain yield was collected and measured from four 20 m long rows in the center of each plot. The N concentrations in the aboveground plant and grain were determined with a TruSpec CHN analyzer (LECO Corp., St. Joseph, Mich.) from biomass subsamples of ground plant material that passed through a 40 mesh sieve. A sample of approximately 0.10 g was placed in tinfoil and ignited in a furnace at 950°C within an oxygen environment inside a quartz combustion tube (Sweeney, 1989).

SOIL WATER AND CROP N UPTAKE SIMULATION PROCESSES IN RZWQM

RZWQM (ver. 2.6) is a comprehensive agricultural system model for process-level simulations of soil water, soil temperature, plant growth, pesticide fate, and soil C and N dynamics as influenced by various agricultural management practices (Ahuja et al., 2000). Specifically, RZWQM uses the Green-Ampt equation to estimate infiltration and the Richards equation to estimate soil water redistribution. The modified Brooks-Corey equations are used to describe the soil water retention curve (Brooks and Corey, 1964; Ahuja et al., 2000). The Brooks-Corey parameters for water retention can be estimated from the soil water content at 33 kPa ($\theta_{1/3}$) and 1500 kPa (θ_{15}), saturated water content (θ_s), and soil type for each soil layer (Fang et al., 2010b; Ma et al., 2012). The saturated hydraulic conductivity (K_{sat}) is estimated based on effective porosity ($\theta_s - \theta_{1/3}$) (Ahuja et al., 1989).

The updated DSSAT 4.5 crop models (e.g., CERES-Maize and CERES-Wheat) incorporated into RZWQM can be used to simulate crop growth, water use, and N uptake, while RZWQM provides soil water, soil temperature, and nutrient information for the crop models (Ma et al. 2006). The detailed processes of crop N uptake calculations in CERES-Maize (Jones et al., 1986) as implemented in RZWQM are shown in figure 2. The daily maize N uptake by a single plant is based on the minimum value of daily crop N demand (NDEM) and potential daily N supply to roots in soil layers (TRNU). NDEM is calculated from stover (aboveground stalks and leaves) N demand (TNDEM) and root N demand (RNDEM), and TRNU is estimated based on soil nitrate-N and NH_4-N contents and root length density in each soil layer (fig. 2). As shown in figure 2, if NDEM (TNDEM + RNDEM) is greater than TRNU, then crop N uptake is set as TRNU (i.e., TNDEM + RNDEM = TRNU); otherwise, crop N uptake is equal to NDEM. The stover and root N uptake (STOWTN or ROOTN) is divided by stover and root weight to calculate actual N concentration in stover (TANC) and in root (RANC), respectively (fig. 2).

As shown in figure 2, the key parameters for calculating crop N demand (NDEM) are the critical N concentrations in stover (TCNP) and roots (RCNP, with a default of 1.06% for maize in the model). The TCNP is also used to estimate crop N stress index (NFAC) along with TANC. In the original model (fig. 2), the TCNP was estimated based on crop growth stage (e.g., STAGE = 1 at end of juvenile to 6 at maturity), maximum level for critical tissue N concentration (CTCNP1, default value is 1.52), and a coefficient for change in TCNP with growth stage (CTCNP2, default value is 0.16), as follows:

$$\text{TCNP} = \text{EXP}^{(\text{CTCNP1} - \text{CTCNP2} \times \text{STAGE})} / 100 \tag{1}$$

Some other models use a biomass-based method (N dilution curve) to estimate TCNP for AGB (stover and ear), such as STIC and CropSyst. The N dilution curve (eq. 2) from Plénet and Lemaire (2000) was tested with AGB levels below 22 Mg ha^{-1} and has been evaluated in Germany (Herrmann and Taube, 2004) and Canada (Ziadi et al. 2008). Recently, the relationship (eq. 2) was further evaluated for higher AGB levels of 27 Mg ha^{-1} by Ciampitti et al. (2012) and 40 Mg ha^{-1} by Yakoub et al. (2017), which demonstrated its validity for a wide range of biomass levels (up to 40 Mg ha^{-1}). The method was incorporated into the model and compared with the growth stage-based method (eq. 1 vs. eq. 2 in fig. 2):

$$\text{TCNP} = \begin{cases} 0.034 & \text{if AGB} < 1 \\ 0.034 \times \text{AGB}^{-0.37} & \text{if AGB} \geq 1 \end{cases} \tag{2}$$

The response of estimated TCNP to these coefficients in

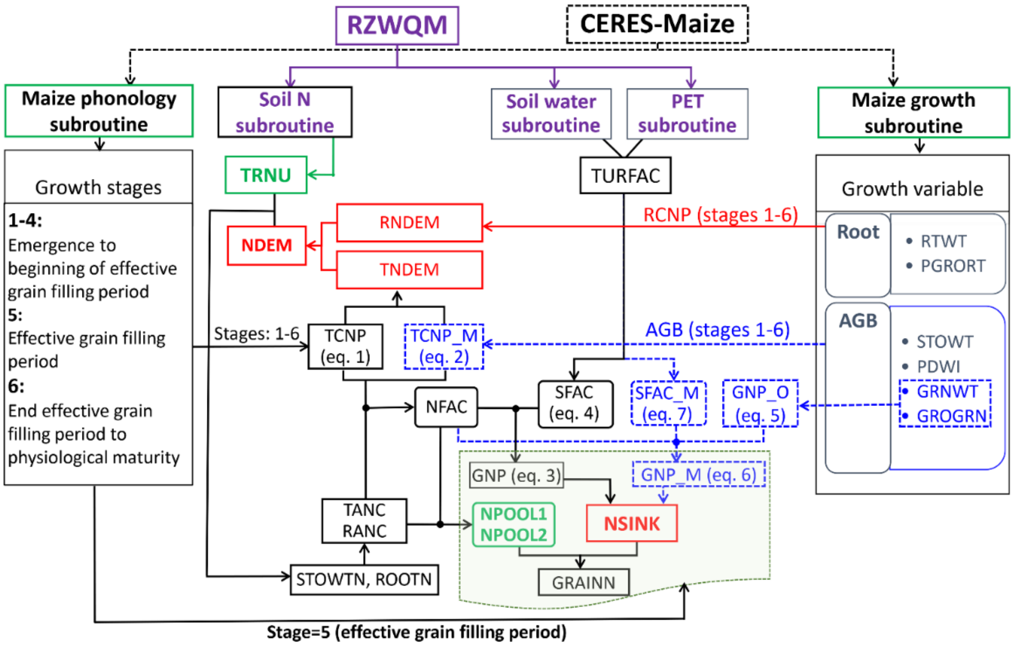

Figure 2. Flowchart for calculating maize N demand and N uptake using the original algorithms (eqs. 1, 3, and 4; Jones et al., 1986) or the alternative algorithms (eqs. 2, 5, 6, and 7) in CERES-Maize as incorporated into RZWQM:

AGB = aboveground biomass (Mg ha^{-1}).
GNP = N concentration in daily growth of grain (g N g^{-1}) (eq. 3).
GNP_O = optimal (no stress) N concentration in daily growth of grain (g N g^{-1}) (eq. 5).
GNP_M = modified N concentration in daily growth of grain (g N g^{-1}) (eq. 6).
GRAINN = daily grain N uptake during grain filling period (g N plant^{-1} d^{-1}).
GRNWT = grain weight (Mg ha^{-1}).
GROGRN = daily growth of grain (Mg ha^{-1} d^{-1}).
NDEM = crop N demand (g N plant^{-1}).
NFAC = crop N stress index (1 = no stress, 0 = maximum stress).
NPOOL1 = stover N available for translocation to grain (g N g^{-1}).
NPOOL2 = root N available for translocation to grain (g N g^{-1}).
NSINK = daily grain N demand (g N plant^{-1} d^{-1}).
PDWI = potential increment in daily shoot growth (g plant^{-1} d^{-1}).
PET = daily potential evapotranspiration (mm d^{-1}).
PGRORT = daily potential root growth (g plant^{-1} d^{-1}).
RANC = actual N concentration in root (g N g^{-1}).
RCNP = critical N concentration root (g N g^{-1}, a default of 1.06% is used).
RNDEM = root N demand (g N plant^{-1})
RTWT = root weight (g plant^{-1}).
SFAC = water stress factor on grain N demand (eq. 4).
SFAC_M = modified water stress factor on grain N demand (eq. 7).
STOVWT = stover (stem plus leaf) weight (g plant^{-1}).
TANC = actual N concentration in stover (g N g^{-1}).
TCNP = critical N concentration in stover (g N g^{-1}) (eq. 1).
TCNP_M = modified critical N concentration in stover (g N g^{-1}) (eq. 2).
TFAC = temperature stress factor on grain N demand.
TNDEM = stover (stalks and leaves) N demand (g N plant^{-1}).
TRNU = potential N supply with roots in soil layers (g N plant^{-1}).
TURFAC = soil water stress effect on expansion (1 = no stress, 0 = maximum stress).

equations 1 and 2 during the growth season are shown in figures 3a and 3b. For the growth stage-based method (eq. 1), coefficients CTCNP1 and CTCNP2 controlled the initial TCNP level and its decrease with time, respectively (fig. 3a). Similarly, for the biomass-based method (eq. 2), the coefficient values of 0.034 and -0.37 controlled the initial TCNP level and its decrease rate as biomass (AGB) increased (fig. 3b). The adjusted coefficients in equations 1 and 2 produced higher or lower TCNP values but had had little effect on grain N concentration under the experimental conditions with no N stress (data not shown).

A comparison between the two methods (eqs. 1 and 2) for estimating TCNP in AGB is shown in figure 3c. The dilution N curve (eq. 2) generally produced lower TCNP in AGB during most of the crop season but reached similar final TCNP levels in AGB as the growth stage-based method (eq. 1). Comparing the highest (100/100) and lowest (40/40) irrigation treatments, the growth stage-based method produced similar TCNP levels for both treatments, but the dilution N curve (eq. 2) produced higher TCNP levels for the 40/40 treatment than for the 100/100 treatment at the middle and late growth stages, mainly due to the lower simulated AGB for the 40/40 treatment. This simulated trend with equation 2 was consistent with the measured AGB N concentration (AGBNC) for the 100/100 and 40/40 treatments. The adjustment of CTCNP1 and CTCNP2 in equation 1 produced similar TCNP for the two treatments because the growth stage-based method is only related to growth stage.

After flowering (STAGE = 5 for effective grain filling period, fig. 2), the grain N accumulation is supplied from two sources considered in the CERES-Maize model: one is stover N available for translocation to grain (NPOOL1), and the other is root N available for translocation to grain (NPOOL2), both of which are further adjusted by the crop N stress factor (NFAC), as shown in figure 2. The grain N demand for daily growth of a single plant (NSINK) is calculated from daily growth of grain (GROGRN) and its N concentration (GNP). If the daily grain N supply (NPOOL1 + NPOOL2) is less than the daily grain N demand (NSINK), then NSINK is set equal to the grain N supply (NSINK = NPOOL1 + NPOOL2); otherwise, NSINK is first supplied from NPOOL1 and then, if NSINK > NPOOL1, from NPOOL2.

The key variable of GNP for grain N demand and GNC

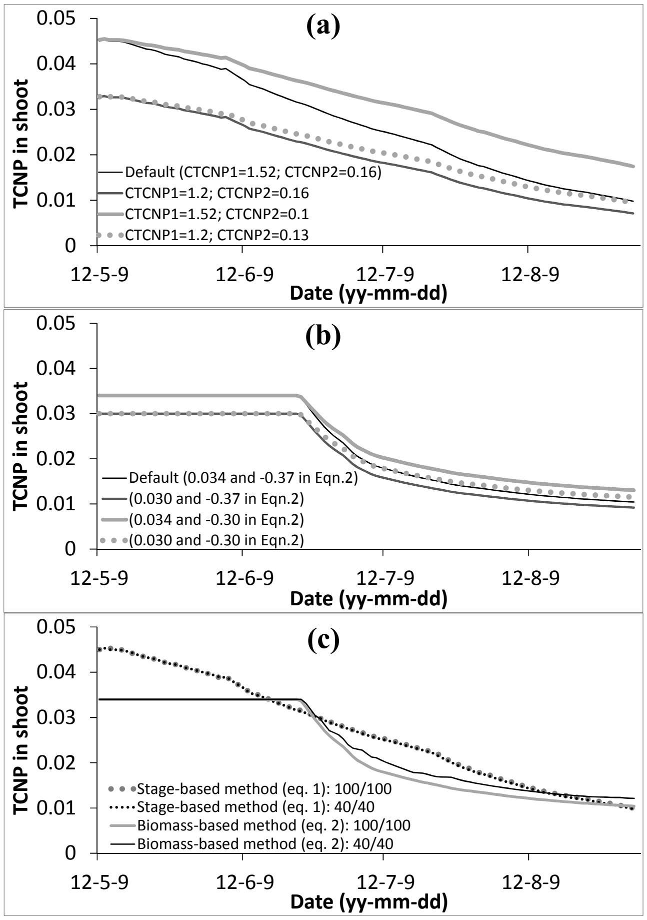

Figure 3. Response of calculated critical N concentration (TCNP, g N g^{-1}) in shoots to the coefficients for (a) the growth stage-based method (CTCNP1 and CTCNP2 in eq. 1) and (b) the biomass-based method (eq. 2), and (c) the estimated TCNP for the highest irrigation (100/100) and lowest irrigation (40/40) treatments using the above two methods (eqs. 1 and 2) in RZWQM.

is estimated by the following equations in CERES-Maize:

$$GNP = (0.004 + 0.013 \times NFAC) \times \max(SFAC,\ TFAC) \quad (3)$$

$$SFAC = 1.125 - 0.125 \times TURFAC \quad (4)$$

where SFAC (range 1 to 1.125) and TFAC (range 0.8 to 1.02 in this study) are water and temperature stress factors, respectively; NFAC (range 0 to 1) is crop N stress index (NFAC = 1 indicates no stress, and NFAC = 0 indicates maximum stress); and TURFAC (range 0 to 1) is soil water stress effect on expansion (1 is no stress, and 0 is maximum stress) calculated based on the ratio of potential daily root water uptake in the soil profile (TRWUP) and potential plant transpiration (EP).

According to equation 3, an optimal constant GNP level of 0.017 g N g^{-1} (1.7%) is obtained during the grain filling period under no N and water stress conditions (e.g., NFAC = 1, SFAC =1, and TFAC ≤ 1), which results in an overall GNC of 0.017 g N g^{-1} at maturity (Appendix 1). This GNC level is generally higher than the measured GNC at maturity for the current maize hybrids in U.S. (Djaman et al., 2013; Haegele et al., 2013; Setiyono et al., 2010) and in China (Chen et al., 2013). Based on the literature (e.g., Chen et al., 2013; Ciampitti and Vyn, 2012, 2013; Haegele et al., 2013), the GNP estimation from equation 3 under no stress condition needs to be reduced (e.g., decrease the coefficients values of 0.004 and 0.013 in eq. 3) to better predict the low GNC levels at maturity for the new maize hybrids.

An alternative way to estimate the optimal GNP under no stress condition was based on the exponential relationship between maize biomass or grain yield and its N concentration in previous studies (e.g., Greenwood and Barnes, 1978; Plénet and Lemaire, 2000; Ciampitti and Vyn, 2013). The optimal (no stress) N concentration in daily growth of grain (GNP_O, fig. 2) during grain filling can be estimated from the simulated GRNWT (Mg ha^{-1}) and daily growth of grain (GROGRN, Mg ha^{-1}) based on equation 5 (detailed information on developing eq. 5 is shown in Appendix 2):

$$GNP\_O = \frac{0.023\left(GRNWT^{1-0.25} - (GRNWT - GROGRN)^{1-0.25}\right)}{GROGRN} \quad (5)$$

The above equation to estimate optimal GNP under the no stress condition can be further adjusted by crop N and water stress factors (e.g., NFAC and SFAC in eq. 3) for actual GNP under non-optimal conditions at any day during the grain filling period, as follows:

$$GNP = \frac{0.023\left(GRNWT^{1-0.25} - (GRNWT - GROGRN)^{1-0.25}\right)}{GROGRN} \times NFAC \times \max(SFAC,\ TFAC) \quad (6)$$

The model using equation 6 predicted grain N concentrations at maturity that were similar to the measured data for the 100/100 treatment (no crop N and water stresses were simulated during the grain filling period; 1.23% vs. 1.19% in 2012 and 1.30% vs. 1.32% in 2013), while the original algorithms (eq. 3) resulted in high GNC levels at maturity of 1.7% for both years.

In equation 4, the water stress factor (SFAC) was assumed to increase with TURFAC from 1 under the no stress condition (TURFAC = 1) to 1.125 under the highest stress condition (TURFAC = 0). This range is much lower than the range of measured GNC at the different water stress levels in this experiment (1.12% to 1.42% for 2012 and 1.32% to 1.61% for 2013). Little experimental data are available to develop a response of GNC to water stress. In Nebraska, Djaman et al. (2013) measured an increase in GNC from 1.4% under full irrigation to 1.6% under rainfed conditions. In Queensland, Australia, Kamoshita et al. (1998) also measured higher GNC values for sorghum hybrids under rainfed conditions (2.25% to 2.75%) than under irrigated conditions (1.5% to 2.0%). The above results and current field measurements suggest a larger increase in GNC and GNP as crop water stress increases, so the coefficient values of 1.25 and 0.125 in equation 4 were empirically adjusted to 1.5 and 0.5 in equation 7 with a higher SFAC range from 1 for no water stress (TURFAC =1) to 1.5 for the highest water stress (TURFAC = 0):

$$SFAC\_M = 1.5 - 0.5 \times TURFAC \quad (7)$$

A comparison of GNP calculated from the original and alternative algorithms in response to the variables in these equations is shown in figure 4. The original GNP algorithm (eq. 3) showed no response to grain accumulation under optimal conditions (no water, N, or temperature stress), whereas the alternative GNP algorithm (eq. 6) resulted in reduced GNP with accumulation of grain yield during grain filling (fig. 4a). This result was consistent with the decline in measured GNC during the grain filling period (Plénet and Lemaire, 2000). In figure 4b, with the increase in crop water stress (decrease in TURFAC), the alternative SFAC algorithm (eq. 7 vs. eq. 4) simulated greater GNP increase than the original algorithm. When the simulated average TURFAC for the grain filling period decreased from 1 for the 100/100 treatment to about 0.7 to 0.8 for the 40/40 treatment, the corresponding GNC value at maturity increased by about 21% (fig. 4b), which was comparable with the measured GNC increases of 19% in 2012 and 23% in 2013. For the response of GNP to increased N stress (decreased NFAC) (fig. 4c), a slightly smaller decrease in GNP was calculated by the alternative algorithm (eq. 6) compared with the original algorithm (eq. 3), mainly due to the higher GNP with lower grain yield (eq. 5) caused by higher N stresses. As both crop water and N stress increased (fig. 4d), GNP showed a quadratic decrease with the new algorithm (eq. 6) and a linear decrease with the original algorithm (eq. 3), mainly due to the pronounced increase in GNP due to high water stress in the alternative algorithm (eq. 7 vs. eq. 4). However, under field conditions, the soil N and water stresses would likely be more complex than is shown in figure 3d.

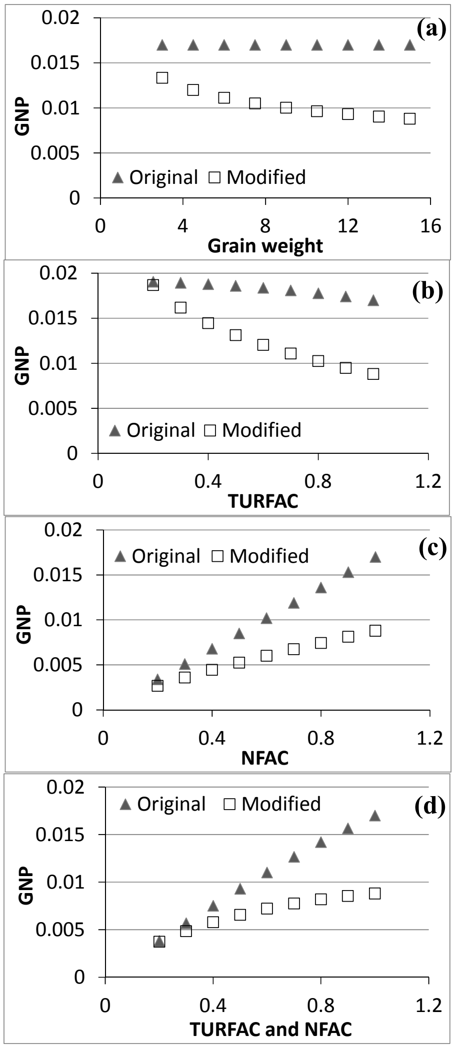

Figure 4. Comparisons of N concentration in daily grain growth (GNP, g N g^{-1}) in response to (a) grain weight (Mg ha^{-1}) under optimal conditions, (b) crop water stress (TURFAC), (c) nitrogen stress (NFAC), and (d) both stresses as estimated with the original (eqs. 3 and 4) and modified (eqs. 6 and 7) GNP algorithms. High values of TURFAC or NFAC indicate low water or N stress levels, respectively. When analyzing the response of GNC to a factor (e.g., TURFAC), other factors were assumed optimal (e.g., NFAC = 1).

Based on the above modifications to the algorithms for calculating TCNP and GNP in the CERES-Maize module, the RZWQM version with the original equations 1, 3, and 4 (RZWQM_OLD) and the modified version with the alternative equations 2, 6, and 7 (RZWQM_MOD) were compared and evaluated for their ability to prediction crop yield, AGB, GNC, AGBNC, and N uptake in AGB and grain under the various growth stage-based irrigation treatments from 2012 to 2013. Prior to these comparisons, we manually adjusted the coefficient values in equations 1, 3, and 4 in the calibrated RZWQM_OLD based on the information in figures 3a, 4a, and 4b and the measured data from the irrigation treatments to test if the simulated GNC and AGBNC could be improved for these irrigation treatments. The final selected coefficient values were respectively 1.45 and 0.13 in equation 1, 0.002 and 0.011 in equation 3, and 1.5 and 0.5 in equation 4. The RZWQM version with the above adjusted coefficients in equations 1, 3, and 4 is called RZWQM_ADJ.

MODEL CALIBRATIONS AND EVALUATIONS

In this study, the original RZWQM using equations 1, 3, and 4 (RZWQM_OLD) was first calibrated and validated for simulating soil water balance and crop production of the irrigation treatments. The three versions of RZWQM (RZWQM_OLD, RZWQM_ADJ, and RZWQM_MOD) with the calibrated parameters from RZWQM_OLD were then evaluated for their simulations of crop production, plant N concentrations, and N uptake under the growth stage-based irrigation treatments.

The automatic parameter estimation software (PEST; Doherty, 2010) was used to calibrate RZWQM_OLD using measured data (end-of-season crop yield and aboveground biomass, soil water content in the 0-120 cm depth, and growth stage data, including emergence, anthesis, and maturity) from the full irrigation (100/100) and lowest irrigation (40/40) treatments in both 2012 and 2013. Other treatments with different irrigation levels during the $V_{7\text{-}T}$ and $R_{4\text{-}6}$ stages (100/50, 80/80, 80/40, 65/65, and 65/40) were used for model evaluation. The measured crop N concentration and N uptake data from all treatments were used for evaluating and comparing the model's performance before and after the modifications described above.

In a previous study at the experimental site, Ma et al. (2015) found that an average of the measured field capacity (FC) values was adequate for model simulation. In this study, we also used an average of measured FC values ($\theta_{1/3}$)

for each soil layer from the 28 sets (7 treatments × 4 replicates) for each year because the maize was planted in different field sections in 2012 (west section) and 2013 (east section) (table 1). The permanent wilting point (soil residual water content) was set as 0.035 cm^3 cm^{-3} in the model according to the soil texture. These parameter values were similar to the calibrated parameter values (0-1.2 m depth) from Ma et al. (2012) based on the 2008-2011 experimental data (table 1) but produced better simulations of soil water content and ET$_c$ across these irrigation treatments for the two years than the simulations using the parameters from Ma et al. (2012).

The maize cultivar parameters were initialized for PEST optimization based on previous simulation studies with a different maize cultivar used at the experimental site from 2008 to 2011 (Ma et al., 2012; Fang et al., 2014), and the parameter ranges for PEST optimization were also set according to previous simulation studies in the region (DeJonge et al., 2011; Ma et al., 2012). As shown in table 2, the final calibrated maize cultivar parameters were close to the previous calibration results for the same local area from DeJonge et al. (2011).

To evaluate the model performance, statistical criteria were used, including mean difference (MD), root mean square error (RMSE), Nash-Sutcliffe efficiency (NSE; Nash and Sutcliffe, 1970), and coefficient of determination (R^2), along with measured versus simulated data plots:

$$\text{MD} = \frac{1}{n}\sum_{i=1}^{n}\left(P_i - O_i\right) \tag{8}$$

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(P_i - O_i\right)^2} \tag{9}$$

$$\text{NSE} = 1.0 - \frac{\sum_{i=1}^{n}\left(O_i - P_i\right)^2}{\sum_{i=1}^{n}\left(O_i - O_{avg}\right)^2} \tag{10}$$

$$\text{R}^2 = \left\{\frac{\sum_{i=1}^{n}\left(O_i - O_{avg}\right)\left(P_i - P_{avg}\right)}{\left[\sum_{i=1}^{n}\left(O_i - O_{avg}\right)^2\right]^{0.5}\left[\sum_{i=1}^{n}\left(P_i - P_{avg}\right)^2\right]^{0.5}}\right\}^2 \tag{11}$$

where P_i is the ith estimated value, O_i is the ith observed value, O_{avg} and P_{avg} are the average of observed and simulated values, respectively, and n is the number of data pairs.

RESULTS AND DISCUSSIONS

Similar soil water content, ET$_c$, and crop water and N stress values were simulated by the three RZWQM versions (RZWQM_OLD, RZWQM_ADJ, and RZWQM_MOD) for each irrigation treatment and each year. The simulated crop yields and AGB were almost the same for the three versions, with similar MD, RMSE, NSE, and R^2 values (table 3). We only present the simulation results from RZWQM_OLD for the above outputs, compared with measured data. The crop N concentration and N uptake simulations were compared for all the three model versions, along with measured data.

SOIL WATER STORAGE AND SEASONAL CROP ET$_C$

When RZWQM was calibrated with the 100/100 and

Table 1. Averaged soil water content at 33 kPa ($\theta_{1/3}$) from measured field capacity in the field and estimated saturated hydraulic conductivity (K_{sat}) by RZWQM for 2012 and 2013.

		Current Study				Ma et al.(2012)	
Soil Depth (m)	Soil Bulk Density (g cm^{-3})	$\theta_{1/3}$ for 2012 (cm^3 cm^{-3})	$\theta_{1/3}$ for 2013 (cm^3 cm^{-3})	K_{sat} for 2012 (cm h^{-1})	K_{sat} for 2013 (cm h^{-1})	$\theta_{1/3}$ for 2008-2011 (cm^3 cm^{-3})	K_{sat} for 2008-2011 (cm h^{-1})
0.00-0.15	1.492	0.2510	0.2741	3.02	1.95	0.262	4.26
0.15-0.30	1.492	0.2332	0.2555	4.08	2.79	0.249	3.55
0.30-0.60	1.492	0.2029	0.2192	6.44	5.08	0.220	4.33
0.60-0.90	1.568	0.1958	0.1756	4.68	6.31	0.187	4.02
0.90-1.20	1.568	0.1907	0.1667	5.06	7.14	0.173	4.08
1.20-1.50	1.617	0.2068	0.1671	2.86	5.46	0.162	0.85
1.50-2.00	1.617	0.2460	0.1918	1.30	3.71	0.198	0.19

Table 2. Initial, minimum-maximum (range), and final values of crop cultivar genetic parameters for calibrating CERES-Maize model as implemented in RZWQM with the parameter estimation software (PEST; Doherty, 2010).[a]

Parameter	Description	Initial	Range	Final	DeJonge et al. (2011)
P1	Degree-days (base temperature of 8°C) from seedling emergence to end of juvenile phase (thermal degree days).	245.6	230-270	262	265
P2	Day length sensitivity coefficient, the extent (days) that development is delayed for each hour increase in photoperiod above the longest photoperiod (12.5 h) at which development proceeds at maximum rate.	0.1562	0.10-0.5	0.14	0.4
P5	Degree-days (base temperature of 8°C) from silking to physiological maturity (thermal degree days)	704.4	550-890	570.9	589
G2	Potential kernel number	994.1	850-1150	1060	908
G3	Potential kernel growth rate (mg kernel^{-1} d^{-1})	6.239	4-15	12	10
PHINT	Degree-days required for a leaf tip to emerge (phyllochron interval) (thermal degree days)	52.89	40-55	48.2	45

[a] The initial values and range of crop cultivar parameters used for PEST were based on previous studies at the experimental site (Ma et al., 2012; Fang et al., 2014) or from the local area (DeJonge et al., 2011).

Table 3. Statistical results for grain yield (GY, kg ha^{-1}), aboveground biomass (AGB, kg ha^{-1}), N concentration in grain (GNC, %) and AGB (AGBNC, %), and N uptake by grain (GYNup, kg N ha^{-1}) and AGB (AGBNup, kg N ha^{-1}) for all treatments simulated by RZWQM without or with adjusting the coefficients in equations 1, 3, and 4 (RZWQM_OLD or RZWQM_ADJ) and by the modified version with the new equations 2, 6, and 7 (RZWQM_MOD).[a]

		2012						2013					
Model Version	Variable	Meas. Mean	Sim. Mean	MD	RMSE	R^2	NSE	Meas. Mean	Sim. Mean	MD	RMSE	R^2	NSE
All versions	GY	10881	11484	603	1343	0.67	-0.14	9452	9133	-319	1063	0.69	0.56
	AGB	20649	21690	1041	2023	0.77	0.50	18254	19353	1099	2016	0.69	0.45
RZWQM_OLD	AGBNC	1.01	1.19	0.17	0.19	0.21	-3.93	1.18	1.08	-0.10	0.15	0.49[b]	-3.35
	AGBNup	207	257	50	60	0.66	-16.29	214	209	-4	28	0.53	-0.73
	GNC	1.32	1.71	0.39	0.40	0.55	-22.52	1.46	1.71	0.25	0.27	0.91	-4.31
	GYNup	143	196	54	60	0.40	-38.75	136	156	20	31	0.45	-3.96
RZWQM_ADJ	AGBNC	1.01	1.06	0.04	0.09	0.83	-0.01	1.18	0.97	-0.21	0.23	0.60[b]	-9.68
	AGBNup	207	212	5	24	0.64	-1.81	214	173	-41	46	0.51	-3.79
	GNC	1.32	1.34	0.02	0.06	0.55	0.37	1.46	1.33	-0.13	0.16	0.90	-0.81
	GYNup	143	153	10	21	0.40	-3.96	136	121	-15	22	0.44	-1.64
RZWQM_MOD	AGBNC	1.01	1.01	0.00	0.05	0.76	0.67	1.18	0.97	-0.21	0.21	0.97	-8.26
	AGBNup	207	217	10	20	0.63	-0.99	214	187	-27	32	0.50	-1.33
	GNC	1.32	1.31	-0.01	0.06	0.57	0.54	1.46	1.38	-0.08	0.09	0.83	0.91
	GYNup	143	149	6	16	0.39	-1.77	136	125	-12	17	0.48	-0.59

[a] MD is mean difference, RMSE is root mean square error, R^2 is coefficient of determination, and NSE is Nash-Sutcliffe efficiency.

[b] Indicates a negative relationship between measured and simulated data.

40/40 treatments from 2012 and 2013 (fig. 5), the simulated soil water storage (SWS) in the 0-120 cm depth matched the measured data reasonably well, with overall RMSE and R^2 values of 2.50 cm and 0.67 in 2012 and 2.75 cm and 0.64 in 2013, respectively. The simulated SWS values tended to be higher than the measured values, with MD values of 1.60 cm (100/100) and 0.40 cm (40/40) in 2012, while SWS was under-simulated in 2013, with MD values of -1.23 cm (100/100) and -1.16 cm (40/40). Better simulations of SWS (lower RMSE and high R^2) were obtained for the 40/40 treatment than for the 100/100 treatment across the two years (fig. 4). These simulation errors were generally comparable with those from previous studies at the same experiment site (Ma et al., 2012; Fang et al., 2014) and in the North China Plain (Fang et al., 2010a).

Similar SWS simulation results were obtained for model evaluations with the other five treatments, with RMSE values between 1.46 and 2.51 cm and R^2 values between 0.30 and 0.68 (fig. 5). The overall RMSE and R^2 values for the five treatments were 2.22 cm and 0.58 in 2012 and 2.48 cm and 0.39 in 2013, respectively. These simulation errors were also comparable with previous simulation results from Ma et al. (2012), with RMSE = 3.7 cm for 0-200 cm soil depth at the same experiment site, and Fang et al. (2010a), with RMSE values between 2.85 and 3.83 cm for 0-120 cm soil depth in the North China Plain. The model underpredicted SWS for most of these evaluation treatments, except for the 100/50 treatment in 2012 and the 65/65 treatment in 2013 (fig. 5). One possible reason may have been the incomplete lateral distribution of 2-D flow for drip irrigation. Measurements of SWS were taken near the drip line and may have given higher readings than the modeled SWS based on a homogeneous one-dimensional layer.

Although the field estimated ET_c was not used for model calibrations, the simulated seasonal ET_c values (ranging from 43.5 to 68.2 cm) were close to the field estimated ET_c values from the soil water balance (ranging from 42.5 to 68.4 cm) across the treatments, with RMSE and R^2 values of 1.72 cm and 0.97 in 2012 and 2.42 cm and 0.91 in 2013, respectively. Across the two years, the field estimated ET_c and simulated ET_c both showed a decrease with irrigation level from 100/100 to 40/40, and the overall RMSE and R^2 values for simulated ET_c were 2.10 cm and 0.92, respectively, which was comparable with previous RZWQM applications at the site (Fang et al., 2014; RMSE=5.65 cm and R^2=0.81) and with an irrigated wheat-maize cropping system in the North China Plain (Fang et al., 2010a; RMSE = 4.15 cm and R^2 = 0.83).

SIMULATED DAILY CROP WATER AND N STRESS

The RZWQM-simulated daily water stress generally increased (decreased TURFAC values) from the 100/100 to 40/40 treatments at both the $V_{7\text{-T}}$ and $R_{4\text{-}6}$ stages across the two years, mainly due to decreased water input (irrigation plus rainfall) (fig. 6). For model calibrations with the 100/100 and 40/40 treatments, crop water stress was not simulated (TURFAC =1) in either year during the early reproductive stage, as was intended by the treatments. For the 40/40 treatment, substantial stress was simulated for both the $V_{7\text{-T}}$ and $R_{4\text{-}6}$ stages in both years. For the 100/100 treatment, no water stress was simulated in 2012 (fig. 6a), but some stress (lower TURFAC values) was simulated at the $V_{7\text{-T}}$ stage in 2013 (fig. 6b). This result was mainly associated with high early-season evaporative demand and inadequate water input (rainfall plus irrigation) during the early stage ($V_{7\text{-T}}$) in 2013 (fig. 6b). For evaluations with the other five treatments, the model simulated higher crop water stress (lower TURFAC values) at the $V_{7\text{-T}}$ stage in 2013 than in 2012 but lower crop water stress (higher TURFAC values) at the $R_{4\text{-}6}$ stage in 2013 than in 2012, except for the 80/80 treatment (fig. 6). Little or no water stress during the $R_{4\text{-}6}$ stage was simulated for the 100/50 treatment, even with the decreased SWS during this period simulated by the model (fig. 5), which was partly due to the over-simulated soil water content in the top soil layers (0-60 cm depth) and under-simulated soil water in the deep layers (60-120 cm depth) (data not shown).

Under the experimental conditions, the simulated daily N stress (NFAC) values were high and stable (0.98 to 1) among the irrigation treatments for the two years (data not shown).

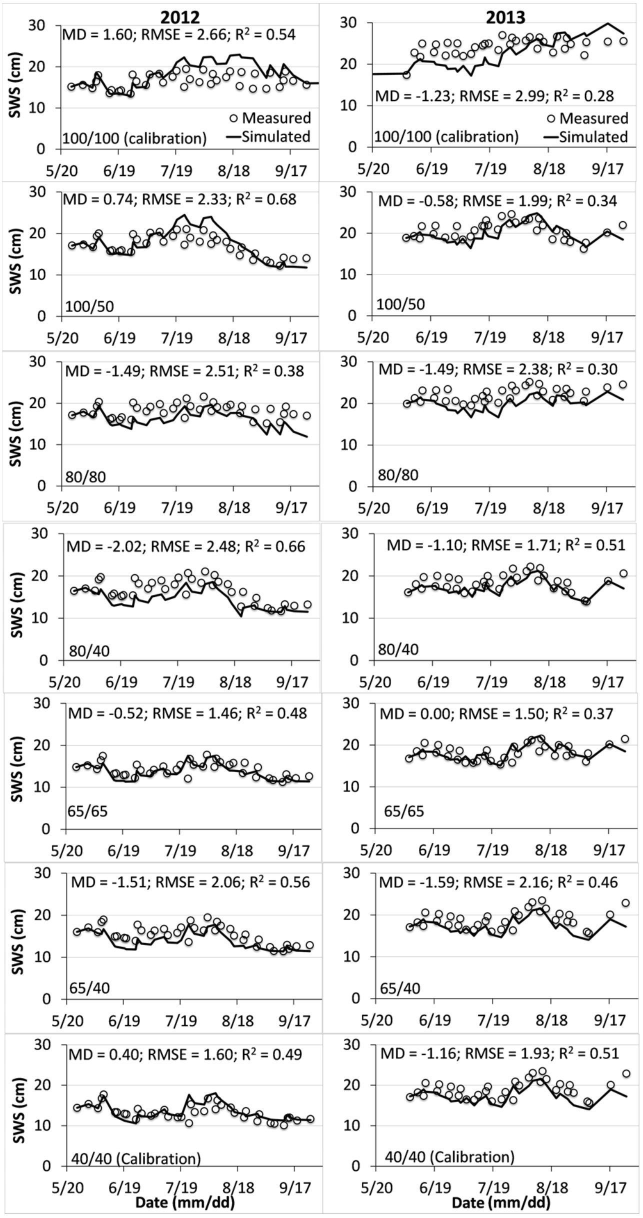

Figure 5. Measured and simulated soil water storage (SWS, 0-120 cm) for 2012 and 2013 maize seasons by RZWQM (the 100/100 and 40/40 irrigation treatments were used for calibrations, and the other treatments were used for evaluations).

The simulated high NFAC values (little or no crop N stress) are consistent with the intended N fertilizer input for adequate N supply for maize growth in the experiment. Crop water stress is the main factor influencing crop growth, N concentration, and N uptake under these experimental conditions.

GRAIN YIELD AND ABOVEGROUND BIOMASS

For RZWQM calibration with the 100/100 and 40/40 treatments from 2012 to 2013, the RMSE and MD values were 587 and -71 kg ha^{-1} for grain yield and 1200 and 648 kg ha^{-1} for AGB, respectively. This result was comparable with previous RZWQM simulation results at the same experiment site (RMSE = 354 kg ha^{-1} for grain yield and 1203 kg ha^{-1} for AGB; Fang et al., 2014). However, the model evaluation results with the other five treatments from 2012 to 2013 were slightly worse than the calibration results, with RMSE and MD values of 1384 and 227 kg ha^{-1} for grain yield and 2265 and 1239 kg ha^{-1} for AGB, respectively.

As shown in figures 7a and 7d and figures 8a and 8d, both measured and simulated grain yield and AGB decreased from the highest to lowest irrigation treatments for the two years, with overall RMSE values of 1211 kg ha^{-1} for grain yield and 2007 kg ha^{-1} for AGB across all seven treatments. However, the model overpredicted grain yield and AGB by 19.9% to 29.4% for the 100/50 treatment across the two years when no crop water stress was simulated for the R_{4-6} stage (figs. 6a and 6b). On the other hand, the model underpredicted grain yield for the 80/40 (13.7%) and 65/40 (12.5%) treatments in 2013, when high crop water stress was simulated for the V_{7-T} stage (fig. 6b) due to the underpredicted soil water contents for the two treatments in 2013 (fig. 5). The simulations of AGB and grain yield were comparable, with similar RMSE and R^2 values between the two years (table 3). Compared with the previous RZWQM simulation results for 2008 to 2011 deficit irrigation treatments with uniform water stress throughout the growing season (Ma et al., 2012; Fang et al., 2014), these poorer simulations indicate a need for model improvements to better respond to water stress at the different growth stages of maize.

AGB N CONCENTRATION AND N UPTAKE

RZWQM_OLD, using the original algorithms for TCNP and GNP (eqs. 1, 3, and 4), overpredicted AGBNC for all irrigation treatments in 2012 (fig. 7b) but underpredicted AGBNC for most treatments in 2013 (fig. 7e), with MD values of 0.17% in 2012 and -0.10% in 2013 (table 3). The corresponding RMSE values for the simulated AGBNC were 0.19% in 2012 and 0.15% (12.7%) in 2013. An inverse response of simulated AGBNC compared to measured AGBNC for the irrigation treatments was obtained in 2013 (R^2 = 0.49; table 3). The negative NSE values for simulated AGBNC across the two years indicated that the measured mean was a better estimator than the model. RZWQM_OLD generally overpredicted AGB N uptake for all treatments except for 40/40 in 2012, with MD and RMSE values of 50 and 60 kg N ha^{-1}, respectively (table 3 and fig. 7c), which was mainly caused by the overpredicted AGBNC (table 3 and fig. 7b). In 2013, however, the AGB N uptake was better predicted, with lower MD and RMSE values for these treatments (fig. 7f), mainly due to compensation between the overpredicted AGB (MD = 1099 kg ha^{-1}) and underpredicted AGBNC (MD = -0.10%) (figs. 7d and 7e; table 3).

RZWQM_ADJ (with adjusted coefficients in eqs. 1, 3, and 4) simulated lower AGBNC levels compared to the RZWQM_OLD simulations. The AGBNC levels were underpredicted for all treatments in 2013 (MD = -0.21% in table 3; fig. 7e) and overpredicted for most treatments (100/100, 100/50, 80/80, 80/40, and 65/40) in 2012 (MD = 0.04% in table 3; fig. 7b). Compared with the RZWQM_OLD simulations (fig. 7b and table 3), improved AGBNC simulations were obtained in 2012, with lower RMSE (0.09% vs. 0.19%) and higher R^2 (0.83 vs. 0.21). However, in 2013 (fig. 7e), poorer AGBNC predictions were obtained with higher RMSE for RZWQM_ADJ (0.23%) than for RZWQM_OLD (0.15%). Measured and

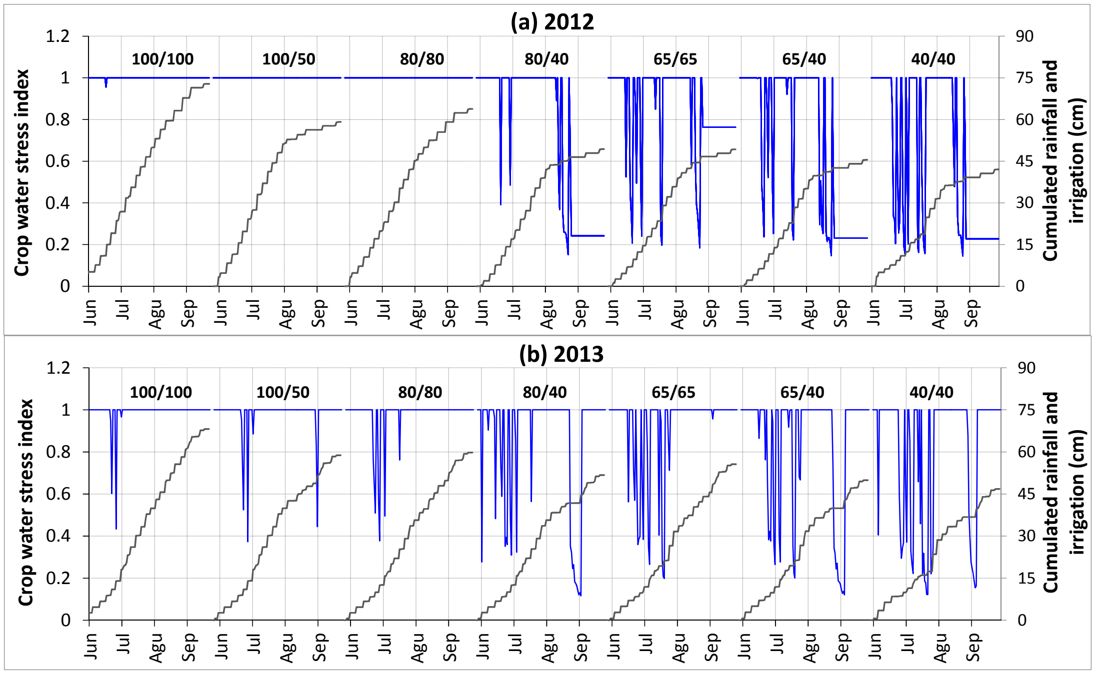

Figure 6. RZWQM-simulated daily crop water stress index (TURFAC, blue line) and cumulative rainfall plus irrigation (gray line) for the different growth stage-based irrigation treatments for (a) 2012 and (b) 2013. TURFAC is a ratio of potential daily root water uptake in the soil profile (TRWUP, cm d^{-1}) and potential plant transpiration (EP, cm d^{-1}); a higher TURFAC value means lower crop water stress.

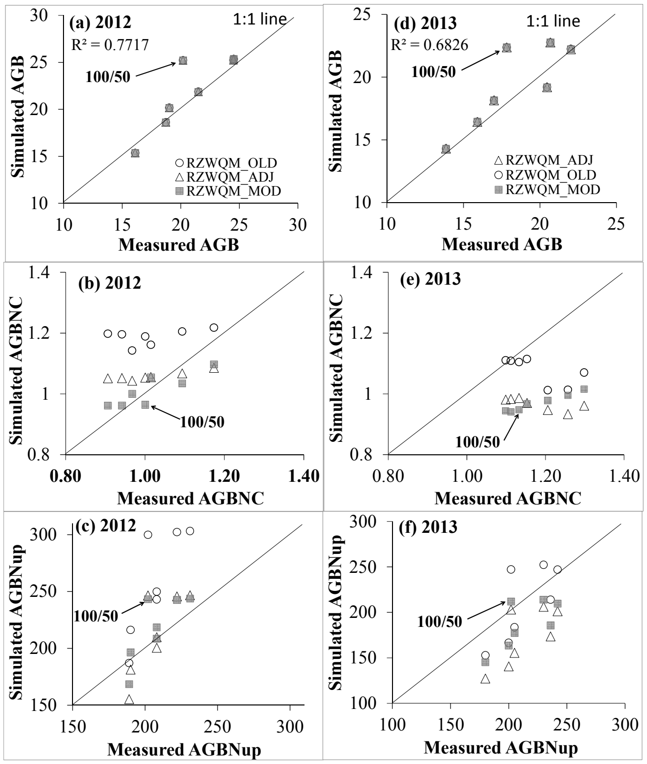

Figure 7. Response of aboveground biomass (AGB, Mg ha^{-1}), AGB N concentration (AGBNC, %), and AGB N uptake (AGBNup, kg ha^{-1}) to different growth stage-based irrigation treatments for 2012 and 2013 simulated by RZWQM versions without or with adjusting the coefficients in equations 1, 3, and 4 (RZWQM_OLD or RZWQM_ADJ) and by the modified version with equations 2, 6, and 7 (RZWQM_MOD).

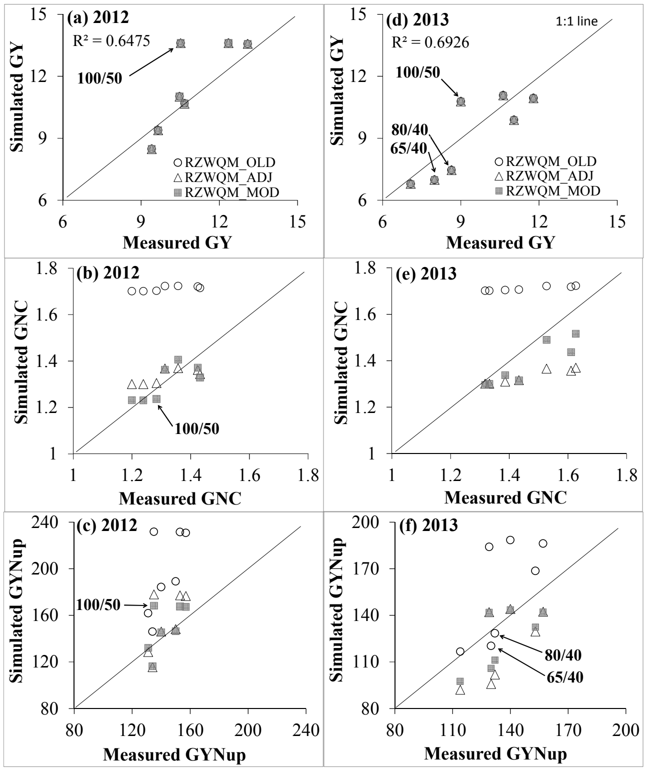

Figure 8. Response of grain yield (GY, Mg ha^{-1}), grain N (GNC, %), and grain N uptake (GYNup, kg ha^{-1}) to the different growth stage-based irrigation treatments for 2012 and 2013 simulated by RZWQM versions without or with adjusting the coefficients in equations 1, 3, and 4 (RZWQM_OLD or RZWQM_ADJ) and by the modified version with the new equations 2, 6, and 7 (RZWQM_MOD).

RZWQM_ADJ-simulated AGBNC also showed an inverse response to irrigation treatments in 2013 (R^2 =0.60 in table 3; fig. 7e). Similar to the AGBNC simulations, the simulated AGB N uptake was also improved in 2012, with reduced RMSE (24 vs. 60 kg N ha^{-1}) and MD (5 vs. 50 kg N ha^{-1}). Poorer prediction of AGB N uptake occurred in 2013, with increased RMSE and MD values, compared with the RZWQM_OLD simulations (figs. 7c and 7f; table 3).

RZWQM_MOD, using the alternative TCNP and GNP algorithms (eqs. 2, 6, and 7), predicted lower AGBNC levels for all irrigation treatments compared to the RZWQM_OLD simulations (figs. 7b and 7e). The response of RZWQM_MOD-simulated AGBNC to the irrigation treatments was much improved from the RZWQM_OLD simulations, with R^2 increased from 0.21 to 0.76 in 2012 and from 0.49 (negative relationship) to 0.97 in 2013 (table 3). The NSE for AGBNC also increased to positive (0.67) in 2012 but was negative in 2013 with underpredicted AGBNC (table 3 and fig. 7e). The corresponding RMSE values decreased from 0.19% to 0.05% in 2012 and increased from 0.15% to 0.21% in 2013 (table 3). The AGB N uptake simulated by RZWQM_MOD was also improved, with lower MD and RMSE values in 2012 (table 3 and fig. 7c) but was comparable (similar RMSE values in table 3) to the RZWQM_OLD simulations in 2013, mainly because RZWQM_MOD simulated lower AGBNC in 2013 (fig. 7e). In 2012, the AGB N uptake was more poorly simulated by RZWQM_MOD for the 100/50 treatment than for the other treatments (fig. 7c), mainly due to the overpredicted AGB for the treatment (fig. 7a). In 2013, RZWQM_MOD simulated AGB N uptake better for the 100/50 treatment than for other treatments (fig. 7f), mainly due to the overpredicted AGB (fig. 7d) and underpredicted AGBNC (fig. 7e) for the treatment. Therefore, better crop N uptake simulation may not always relate to better simulation of both crop yield and crop N concentrations, which should be considered when using crop N uptake for calibration.

All the three model versions underpredicted AGBNC in 2013, and only RZWQM_MOD captured the increase in AGBNC as water stress increased ($R^2 = 0.97$ for 2013 in table 3 and fig. 6e). The other two versions simulated AGBNC responses to water stress levels that were inverse to the measured responses (table 3 and fig. 6e). Adjusting the parameters in equation 2 could increase the simulated AGBNC values in 2013 but would result in overpredictions of AGBNC in 2012. RZWQM_MOD underpredicted AGBNC for the 100/50 treatment in 2012 and 2013, which may be partly associated with the overpredicted AGB (figs. 7a and 7d) when using the AGB-based TCNP estimation method (eq. 2). The underpredicted AGBNC in 2013 for the higher water stress treatments (65/65, 65/40, and 40/40) may be associated with the complexity of crop N remobilization among different organs in response to water stress that the model did not account for.

GNC AND GRAIN N UPTAKE

Similar to the simulated AGBNC, RZWQM_OLD predicted similar GNC values (1.70% to 1.72% in 2012 and 2013) and showed little response to the irrigation treatments for the two years (figs. 8b and 8e), which was expected based on the GNP calculation (eq. 3; fig. 4). However, the measured data showed high variability among these irrigation treatments (1.20% to 1.42% in 2012 and 1.32% to 1.61% in 2013). The corresponding RMSE and MD values for simulated GNC were 0.40% and 0.39%, respectively, in 2012, and 0.27% and 0.25%, respectively, in 2013. The overprediction of GNC resulted in overpredicted grain N uptake (MD = 54 kg N ha^{-1} in 2012 and 20 kg N ha^{-1} in 2013) for all irrigation treatments (figs. 8c and 8f) except for the 80/40 and 65/40 treatments in 2013 (fig. 8f), which was mainly due to the underpredicted grain yield for the treatments (fig. 8d). The overall RMSE and R^2 values for simulated grain N uptake were 60 kg N ha^{-1} and 0.40, respectively, in 2012 and 31 kg N ha^{-1} and 0.45, respectively, in 2013 (table 3).

RZWQM_ADJ predicted reduced GNC values for all irrigation treatments across the two years, with decreased RMSE values from 0.40% to 0.06% in 2012 and from 0.27% to 0.16% in 2013, compared to the RZWQM_OLD simulations (table 3; figs. 8b and 8e). As a result, the simulated grain N uptake was also lower than the RZWQM_OLD simulations (figs. 8c and 8f), with lower RMSE values of 21 kg N ha^{-1} in 2012 and 22 kg N ha^{-1} in 2013 (table 3). GNC was underestimated for all treatments in 2013 and was overpredicted for all treatments except 66/65 and 40/40 in 2012 (figs. 8b and 8e), which is consistent with the AGBNC simulations (figs. 7b and 7e). The RZWQM_ADJ-simulated GNC also varied less than the measured data among the irrigation treatments (1.30% to 1.37% in 2012 and 2013), suggesting a limited effect of changing the coefficients in equation 4 on GNC response to water stress. Further increasing the coefficients in equation 4 to 1.75 and 0.75 resulted in little difference from the simulation with coefficient values of 1.5 and 0.5 (data not shown). Adjusting these coefficients in equations 1, 3, and 4 also did not improve predictions of the difference in measured GNC between the two years (e.g., 1.42% vs. 1.61% for the 100/100 treatment), where very similar GNC values were simulated for the two years (1.36% for the 100/100 treatment; figs. 8b and 8e). The higher measured GNC and AGBNC values in 2013 than in 2012 may be partly due to lower measured grain yield and AGB in 2013 than in 2012, as expected from the N dilution curve (eq. 2). Adjustment of these coefficients in equations 1, 3, and 4 can help to identify the more sensitive parameters in simulating GNC and AGBNC in CERES-Maize, which could potentially be made adjustable parameters for detailed calibration with measured data under different conditions.

RZWQM_MOD (eqs. 2, 6, and 7) simulated lower GNC values but with higher variations (1.23% to 1.42% in 2012 and 1.30% to 1.52% in 2013) across the treatments and showed better response to the irrigation treatments, with higher NSE values of 0.54 in 2012 and 0.91 in 2013, compared with the RZWQM_OLD simulations (figs. 8b and 8e; table 3). The corresponding MD and RMSE values were reduced to -0.01% and 0.06%, respectively, in 2012 and to -0.08% and 0.09%, respectively, in 2013 (table 3). As a result, the grain N uptake was generally better simulated, with lower MD and RMSE values of 6 and 16 kg N ha^{-1}, respectively, in 2012 and -12 and 17 kg N ha^{-1}, respectively, in 2013, compared with the RZWQM_OLD simulations (table 3). These results suggest that the modifications to the TCNP and GNP calculations (eqs. 2, 6, and 7) effectively simulated the GNC response to various water stress conditions. The consistently higher measured and simulated GNC values for these treatments in 2013 than in 2012 (figs. 8b and 8e; table 3) suggest that the modified GNP calculations also respond better to variations among crop seasons. The RZWQM_MOD version can be further improved by adjusting the coefficients in the new algorithms (eqs. 2, 6, and 7) based on measured crop N concentrations.

The improvement of RZWQM_MOD-simulated AGBNC in response to the deficit irrigation treatments was mainly contributed by both increased GNC (eqs. 6 and 7 for GNP; figs. 4a and 4b) and TCNP (eq. 2 and fig. 3c) as AGB and grain yield decreased with increased water stresses. In 2013, however, all the three model versions underpredicted AGBNC for most treatments (fig. 7e), even with overpredicted GNC by RZWQM_OLD or slightly underpredicted GNC by RZWQM_MOD (fig. 8e). This result indicates poorer simulation of stover N concentration and uptake under these water stress conditions, and further evaluation is needed of shoot N uptake from the soil and N remobilization from stover to grain in the model. The improvement in GNC simulation by RZWQM_MOD was mainly due to reduced GNP simulation as grain biomass accumulation under optimal conditions (resulting from increased N use efficiency, as shown in fig. 4a based on eq. 6) and substantial increase in GNP as water stress increased (eq. 7 and fig. 4b). Previous experimental results also reported higher N use efficiency and shoot N remobilization for current hybrid maize cultivars than for previous cultivars (e.g., Ciampitti and Vyn, 2012, 2013; Ciampitti et al., 2013; Haegele et al., 2013; Chen et al., 2013). Different from the original TCNP and GNP algorithms (eqs. 1 and 3), the modified algorithms (eqs. 2 and 6) estimate crop N concentration depending on crop growth simulations directly (e.g., AGB and grain yield are used in these equations). Therefore, the accuracy in simulating crop N concentration might be more influenced by the accuracy in predicted AGB and grain yield for RZWQM_MOD (eqs. 2 and 6) than for RZWQM_OLD (eqs. 1 and 2). These coefficients in the new algorithms (eqs. 2, 6, and 7) can be potentially considered cultivar parameters related to N uptake in CERES-Maize and be adjusted for local maize cultivars based on measured data.

CONCLUSIONS

Further improving crop model predictions, such as crop growth, water use, and N uptake, is required for making better decisions on agricultural water and N management under various conditions. In this study, we developed alternative algorithms for calculating crop N demand (TCNP and GNP) and compared these alternative algorithms with the original algorithms in the CERES-Maize model as implemented in RZWQM for predicting grain yield, crop N concentration, and N uptake for current maize hybrids under a wide range of water availability. In general, reasonable simulations of soil water content, crop water and N stress, and final crop aboveground biomass and grain yield were produced by the RZWQM versions with different crop N demand algorithms in CERES-Maize. The original model (RZWQM_OLD) overestimated crop N concentration in maize hybrids, but the prediction was significantly improved by adjusting the coefficients in the algorithms for crop N demand calculations (TCNP and GNP). However, even with the adjusted coefficients in the algorithms, the RZWQM_ADJ version could not successfully predict the crop N concentration response to the irrigation treatments or different crop seasons. The RZWQM_MOD version, with alternative algorithms for calculating crop N demand in CERES-Maize, produced better responses of crop N concentration to a wide range of irrigation treatments and to different crop seasons. The improved crop N concentration simulations by RZWQM_MOD generally resulted in better simulations of crop N uptake across the irrigation treatments when both crop aboveground biomass and grain yield were accurately predicted. However, reasonable simulations of crop N uptake were possible even with under- (or over-) predicted crop biomass or crop N concentration. Under this condition, crop biomass (grain yield) and crop N uptake should be used simultaneously for model calibration, avoiding the bias in properly simulating only two of the three variables of crop biomass, crop N concentration, and N uptake.

The modification to the shoot critical N concentration estimation method had little or no effect on grain N concentration simulations because the grain N supply was adequate for grain N demand under the non-N-limited experimental conditions. Because N availability was adequate and only final measured crop N concentrations were used in the study, the modifications to crop N demand calculations (eqs. 2 and 6) were not tested for the model's ability to simulate crop N concentration under inadequate N conditions.

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APPENDIX 1

During the grain filling period of maize under the no stress condition and defining the following variables: GNP_i is optimal N concentration of new grain growth at day i after grain filling (g N g^{-1}), GNC_i is optimal N concentration of grain at day i after grain filling (g N g^{-1}), and GROGRN_i is optimal new grain growth at day i after grain filling (g plant^{-1} d^{-1}), we have:

$$\text{GNC}_i = \frac{\text{total grain N uptake}}{\text{grain yield}} = \frac{\sum_{i=1}^{n}\left(\text{GNP}_i \times \text{GROGRN}_i\right)}{\sum_{i=1}^{n}\text{GROGRN}_i} \tag{12}$$

Under optimal conditions (no stress), GNP_i (i =1, n) at any day is consistent, with a value of 1.7% g N g^{-1}, based on the GNP algorithm in the CERES-maize model (eq. 3 in the text). Therefore, equation 12 can be written as:

$$\text{GNC}_i = \frac{\sum_{i=1}^{n}\left(\text{GNP}_i \times \text{GROGRN}_i\right)}{\sum_{i=1}^{n}\text{GROGRN}_i} = 0.017 \times \frac{\sum_{i=1}^{n}\text{GROGRN}_i}{\sum_{i=1}^{n}\text{GROGRN}_i} = 0.017 \tag{13}$$

This equation also showed that high grain N concentration (GNC) at maturity was related to high N concentration in new growth of grain (GNP) under optimal conditions.

APPENDIX 2

During the grain filling period of maize under the no stress condition and defining the following variables: GNP_i is optimal N concentration of new grain growth at day i after grain filling (g N g^{-1}), GNC_i is optimal N concentration of grain at day i after grain filling (g N g^{-1}), GROGRN_i is optimal new grain growth at day i after grain filling (g plant^{-1} d^{-1}), GRNWT_i is optimal grain weight at day i after grain filling (g plant^{-1}), NSINK_i is optimal N uptake of daily new grain growth at day i after grain filling (g N plant^{-1} d^{-1}), and GRAINN_i is optimal total N uptake of grain at day i after grain filling (g N plant^{-1}), we have:

$$\text{NSINK}_i = \text{GROGRN}_i \times \text{GNP}_i \tag{14}$$

$$\text{GRAINN}_i = \sum_{i=1}^{n}\text{NSINK}_i \tag{15}$$

$$\mathrm{GRNWT}_i = \sum_{i=1}^{n} \mathrm{GROGRN}_i \quad (16)$$

$$\mathrm{NSINK}_i = \mathrm{GRAINN}_i - \mathrm{GRAINN}_{i-1} \quad (17)$$

$$\mathrm{GRNWT}_{i-1} = \mathrm{GRNWT}_i - \mathrm{GROGRN}_i \quad (18)$$

$$\mathrm{GRAINN}_i = \mathrm{GRNWT}_i \times \mathrm{GNC}_i \quad (19)$$

Based on equations 14, 17, and 19, we have:

$$\begin{aligned} \mathrm{GNP}_i &= \frac{\mathrm{NSINK}_i}{\mathrm{GROGRN}_i} \\ &= \frac{\mathrm{GRAINN}_i - \mathrm{GRAINN}_{i-1}}{\mathrm{GROGRN}_i} \\ &= \frac{\mathrm{GRNWT}_i \times \mathrm{GNC}_i - \mathrm{GRNWT}_{i-1} \times \mathrm{GNC}_{i-1}}{\mathrm{GROGRN}_i} \end{aligned} \quad (20)$$

The optimal crop N concentration generally declines exponentially with biomass accumulation (e.g., Plénet and Lemaire, 2000; Greenwood and Barnes, 1978). Similarly, Plénet and Lemaire (2000) proposed a relationship between optimal ear N concentration (EARNC, g N g^{-1}) and ear weight (EARWT, Mg ha^{-1}) during the grain filling period for maize (i.e., EARNC = $0.023 \times \mathrm{EARWT}^{-0.25}$). Because the grain weight (GRNWT, Mg ha^{-1}) is the main component of the ear during the grain filling period, a similar relationship between GNC and GRNWT can exist during the grain filling period and was demonstrated by the measured data for maize grain yield and N uptake from about 2500 treatments worldwide (Ciampitti and Vyn, 2014). This relationship between GNC and GRNWT can be expressed as:

$$\mathrm{GNC}_i = 0.023 \times \mathrm{GRNWT}_i^{-0.25} \quad (21)$$

Converting the units (g plant^{-1}) of GRNWT_i, $\mathrm{GRNWT}_{i\text{-}1}$, and GROGRN_i in equation 20 to Mg ha^{-1} and combining equations 18, 20, and 21, the optimal GNP_i at day i after grain filling can be obtained from GRNWT_i and GROGRN_i as follows (eq. 5 in the text):

$$\begin{aligned} \mathrm{GNP}_i &= \frac{\left(\mathrm{GRNWT}_i \times 0.023 \times (\mathrm{GRNWT}_i)^{-0.25} - \mathrm{GRNWT}_{i-1} \times 0.023 \times (\mathrm{GRNWT}_{i-1})^{-0.25}\right)}{\mathrm{GROGRN}_i} \\ &= \frac{0.023 \times \left(\mathrm{GRNWT}_i^{1-0.25} - \mathrm{GRNWT}_{i-1}^{1-0.25}\right)}{\mathrm{GROGRN}_i} \\ &= \frac{0.023 \times \left(\mathrm{GRNWT}_i^{1-0.25} - (\mathrm{GRNWT}_i - \mathrm{GROGRN}_i)^{1-0.25}\right)}{\mathrm{GROGRN}_i} \end{aligned} \quad (22)$$