Simulation of stomatal conductance and water use efficiency of tomato leaves exposed to different irrigation regimes and air CO2 concentrations by a modified "Ball-Berry" model

Wei, Zhenhua; Du, Taisheng; Li, Xiangnan; Fang, Liang; Liu, Fulai

Simulation of Stomatal Conductance and Water Use Efficiency of Tomato Leaves Exposed to Different Irrigation Regimes and Air CO₂ Concentrations by a Modified "Ball-Berry" Model

Zhenhua Wei [1,2], Taisheng Du [1]*, Xiangnan Li [2,3], Liang Fang [2] and Fulai Liu [2]*

[1] Center for Agricultural Water Research in China, China Agricultural University, Beijing, China, [2] Department of Plant and Environmental Sciences, Faculty of Science, University of Copenhagen, Taastrup, Denmark, [3] Northeast Institute of Geography and Agroecology, Chinese Academy of Sciences, Changchun, China

Stomatal conductance (g_s) and water use efficiency (WUE) of tomato leaves exposed to different irrigation regimes and at ambient CO₂ (a[CO₂], 400 ppm) and elevated CO₂ (e[CO₂], 800 ppm) environments were simulated using the "Ball-Berry" model (BB-model). Data obtained from a preliminary experiment (Exp. I) was used for model parameterization, where measurements of leaf gas exchange of potted tomatoes were done during progressive soil drying for 5 days. The measured photosynthetic rate (P_n) was used as an input for the model. Considering the effect of soil water deficits on g_s, an equation modifying the slope (m) based on the mean soil water potential (Ψ_s) in the whole root zone was introduced. Compared to the original BB-model, the modified model showed greater predictability for both g_s and WUE of tomato leaves at each [CO₂] growth environment. The models were further validated with data obtained from an independent experiment (Exp. II) where plants were subjected to three irrigation regimes: full irrigation (FI), deficit irrigation (DI), and alternative partial root-zone irrigation (PRI) for 40 days at both a[CO₂] and e[CO₂] environment. The simulation results indicated that g_s was independently acclimated to e[CO₂] from P_n. The modified BB-model performed better in estimating g_s and WUE, especially for PRI strategy at both [CO₂] environments. A greater WUE could be seen in plants grown under e[CO₂] associated with PRI regime. Conclusively, the modified BB-model was capable of predicting g_s and WUE of tomato leaves in various irrigation regimes at both a[CO₂] and e[CO₂] environments. This study could provide valuable information for better predicting plant WUE adapted to the future water-limited and CO₂ enriched environment.

Keywords: CO₂, alternative partial root-zone irrigation, model simulation, stomatal conductance, water use efficiency, tomato

INTRODUCTION

Plant stomata aperture play a predominant role in modulating the diffusion of CO_2 and H_2O vapor between leaf and atmosphere (Buckley and Mott, 2013), and optimizing photosynthetic and transpiration rates, hereby the water use efficiency (*WUE*) at leaf scale (Liu et al., 2009). It is well-established that both reduced irrigation regimes, especially alternate partial root-zone irrigation (PRI) and elevated atmospheric CO_2 environment ($e[CO_2]$) could induce partial stomatal closure and synergistically enhance *WUE* (Pazzagli et al., 2016). Therefore, a better understanding of how to model stomatal conductance for water vapor (g_s) is essential for the accurate prediction of leaf transpiration and improvement of plant *WUE* in response to the future water limited and CO_2 enriched environments.

A number of approaches has been tested for modeling g_s under well-watered conditions (Gutschick and Simonneau, 2002). Among those, the Ball-Berry model (BB-model) describing the linear coupling relation of g_s to photosynthetic rate (P_n), relative humidity (h_s), and CO_2 concentration (C_s) on the leaf surface (Ball et al., 1987) has been broadly adopted and utilized from leaf to plant scale due to its apparent accuracy and simplicity (Miner et al., 2017). However, the P_n-g_s relationship of BB-model would be changed under water stress (Damour et al., 2010), hence modified model is needed for simulating g_s, for instance, by incorporating empirical functions coupling with abscisic acid (ABA), leaf water potential or soil water potential (Sala and Tenhunen, 1996; Gutschick and Simonneau, 2002; Bauerle, et al. et al., 2004; Damour et al., 2010).

For drought-prone areas, more efficient irrigation techniques need to be developed and implemented in order to achieve optimal crop yield and quality (Du et al., 2015). PRI strategy has been demonstrated to save considerable amount of irrigation water without significantly reducing yield as compared to full irrigation (FI) (Kang and Zhang, 2004; Wei et al., 2016). It is well-known that reduced plant water consumption under PRI is resulted from a decreased g_s, which is primarily regulated by the root-to-shoot ABA signaling triggered in the roots exposed to drying soil (Davies et al., 2002; Liu et al., 2006). A modified BB-model based on the temporal and spatial change of soil water potential (Ψ_s) in the soil columns has been reported to be capable of predicting g_s and *WUE* of PRI treated potato leaves, indicating an enhancement of *WUE* for PRI in relation to FI plants (Liu et al., 2009).

Plants grown at $e[CO_2]$ generally possess an increased P_n but decreased g_s, resulting in a greater *WUE* as compared to those growth at $a[CO_2]$ (Pazzagli et al., 2016). An better understanding of the coordination between g_s and P_n in response to $e[CO_2]$ is crucial for simulating the *WUE* at leaf level. The magnitude of $e[CO_2]$ effect on g_s is modulated substantially together with other environmental variables, if g_s is independently acclimated to $e[CO_2]$ from P_n, this would alter the sensitivity of g_s to $[CO_2]$, P_n, and/or h_s, and thereby requiring re-parameterization of the BB-model for plants grown under different CO_2 environment (Ainsworth and Rogers, 2007). As lower g_s and higher *WUE* are anticipated under both $e[CO_2]$ and reduced irrigation strategies, and a synergic interaction of those two factors would further decrease g_s and enhance *WUE* (da Silva et al., 2017). However, this will complicate the influence of $e[CO_2]$ associated with PRI regime on the prediction of g_s and *WUE* using the BB-model.

To date, the change of g_s and *WUE* of tomato leaves in response to PRI strategy at $e[CO_2]$ have not been depicted by any model. Therefore, the objective of this study was to examine whether g_s is independently acclimated to $e[CO_2]$ and if the BB-model is capable of predicting leaf g_s and *WUE* of tomato leaves exposed to different irrigation regimes in combination with two CO_2 growth conditions. Such modeled g_s might provide
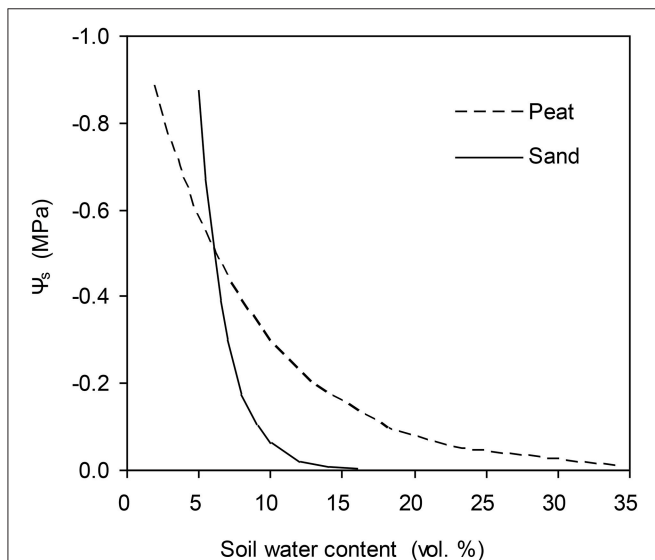

FIGURE 1 | Water retention curves of the peat substrate used in experiment one and of the sandy soil used in experiment two.
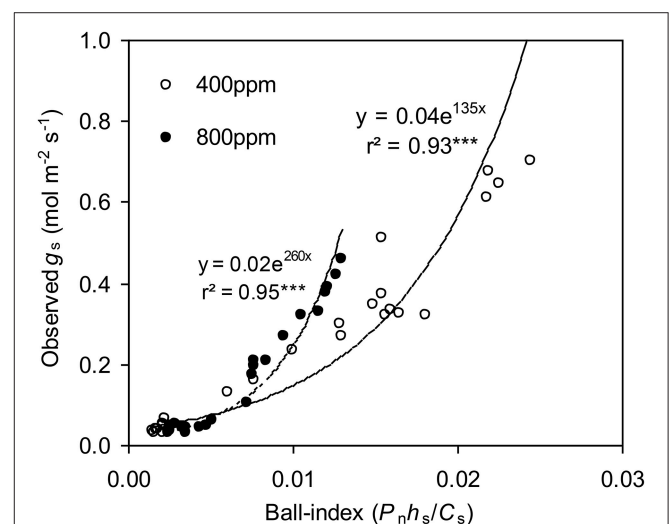

FIGURE 2 | Relationship between the observed stomatal conductance (g_s) and Ball-index ($P_n h_s / C_s$) of a tomato leaf during progressive soil drying at $[CO_2]$ concentration of 400 and 800 ppm, respectively in experiment one.

an effective way for estimating transpiration rate at canopy scale and optimizing WUE of tomato plant in the future drier and CO_2 enriched environment.

MATERIALS AND METHODS

The BB-Model and Its Modification

The BB-model (Ball et al., 1987) describes the relationship between leaf stomatal conductance (g_s) and photosynthetic rate (P_n), relative humidity (h_s) and CO_2 concentration (C_s) on the leaf surface:

$$g_s = mP_n \frac{h_s}{C_s} + g_0 \quad (1)$$

where g_0 is the residual stomatal conductance if P_n is zero, m is the slope of relation between g_s and $P_n h_s/C_s$ (the Ball-index), also called the stomatal sensitivity factor. Under well-watered condition, the m is a constant and this model is a simple linear correlation between g_s and Ball-index. However, under soil water deficits, m could be varied largely, and the relationship between g_s and $P_n h_s/C_s$ becomes curvilinear (Sala and Tenhunen, 1996). Accounting for the effect of soil water deficits on leaf g_s, numerous approaches have been used to adjust the m. The modified m could be based on an exponential function related to the ABA concentration in the xylem sap (Gutschick and Simonneau, 2002). Our earlier studies found that plant ABA could be empirically expressed as a linear function of the mean soil water potential (Ψ_s) in the root zone (Liu et al., 2008). Hereby, in this study, the xylem sap ABA was replaced by Ψ_s:
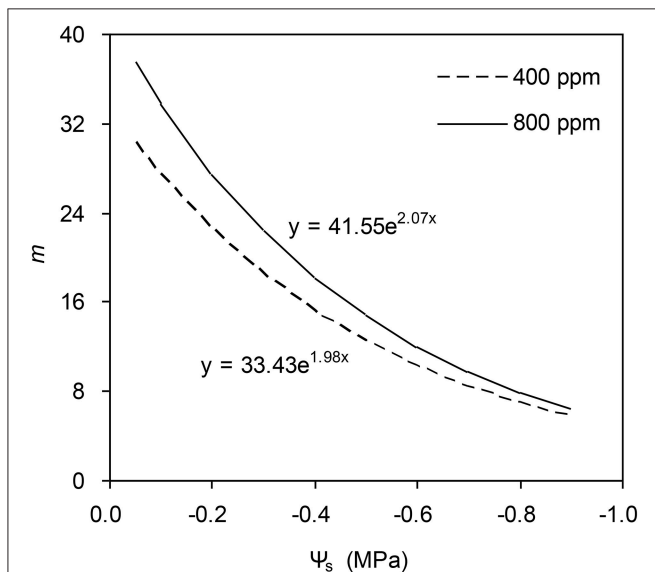
$$m = m_i e^{-\beta \psi_s} \quad (2)$$

FIGURE 3 | Simulation results of the effect of soil water deficits on the slope of the BB-model for a tomato leaf at [CO_2] concentration of 400 and 800 ppm, respectively (details see Equation 2). Data is from experiment one ($n = 25$).

where m_i is the initial slope of the BB-model without soil water deficits, β is a constant.

In Equation (1), C_s was calculated as:

$$C_s = C_a - P_n \frac{1.37}{g_b} \quad (3)$$

where C_a is the atmospheric CO_2 concentration (i.e., 400 or 800 ppm in this study); g_b is the boundary layer conductance and shown to be 9.29 mol m^{-2} s^{-1} in the leaf chamber according to the manufacture's directions. The h_s is computed as the ratio of two partial pressures of water vapor at the leaf surface and in the leaf internal space of stomata, e_s/e_i. The e_s was obtained by Equation (4) as shown by Gutschick and Simonneau (2002):

$$g_s(e_i - e_s) = g_b(e_s - e_a) \quad (4)$$

By rearranging Equation (4), h_s was calculated as:

$$h_s = \frac{e_s}{e_i} = \frac{(e_a/e_i + g_s/g_b)}{(1 + g_s/g_b)} \quad (5)$$

where e_a is the partial pressure of water vapor in the air and is obtained during gas exchange measurement. e_i could be computed by Equation (5) from the leaf temperature (T, °C).

$$e_i = 6.11 e^{\left(\frac{7.5 \ln(10)T}{T+237.3} \right)} \quad (6)$$

It is necessary to notice that g_s is used as an input variable for computing h_s (Equation 5). The g_s could be obtained by rearranging the BB-model as:

$$g_s = \frac{mP_n(e_a/e_i + g_s/g_b)}{C_s(1 + g_s/g_b)} + g_0 \quad (7)$$

Equation (7) could then be elaborated as a quadratic equation of g_s:

$$(C_s/gb)g_s^2 + (C_s - g_0 C_s/g_b - mP_n/g_b)g_s + (-(g_0 C_s + mP_n e_a/e_i)) = 0 \quad (8)$$

g_s was solved as:

$$g_s = \frac{-B + \sqrt{(B)^2 - 4AC}}{2A} \quad (9)$$

where A $= (C_s/g_b)$, B $= (C_s - g_0 C_s/g_b - mP_n/g_b)$ and C $= -(g_0 C_s + mP_n e_a/e_i)$. By applying PROC NLIN (SAS 9.4 Ins. Inc.) of g_s on the remaining variables, the parameters g_0 and m were derived. Here, m could be replaced by Equation (2) to consider the effect of soil water deficits on g_s.

After estimating g_s by Equation (9), leaf transpiration rate (T_r) could be calculated as:

$$T_r = \frac{(e_i - e_a)}{P_a(1/g_s + 1/g_b)} \quad (10)$$

where P_a is the air pressure (1013 hPa). WUE of tomato leaves was then computed as:

$$WUE = \frac{P_n}{T_r} = \frac{P_n P_a(1/g_s + 1/g_b)}{(e_i - e_a)} \quad (11)$$

The aim of this study was to examine the capability of the BB-model in predicting g_s and *WUE* for tomato leaves at $e[CO_2]$ in combination with different irrigation regimes as this has not been done up to date; therefore, we have taken the observed P_n as an input for the BB-model rather than developing a coupled model for P_n. Moreover, we compared the performance of the original BB-model (without m modification) and the modified BB-model (with m modification by Equation 2) in simulating g_s and *WUE* in order to evaluate the importance of soil water deficits on the model performance under different irrigation regimes and CO$_2$ enriched environment.

Data

The data for this study are from two pot experiments conducted in a climate-controlled greenhouse at the experimental farm of the Faculty of Science, University of Copenhagen, Taastrup, Denmark. The experimental setups have been detailed elsewhere (Yan et al., 2017; Wei et al., 2018) and are only summarized here. In both experiments, the tomato seeds (*Solanum lycopersicum* L., cv. Elin) were sown on 26th Sept. 2016. Half of the plants were grown in a greenhouse cell with ambient CO$_2$ concentration of 400 ppm ($a[CO_2]$), and another half were grown in a cell with elevated CO$_2$ concentration of 800 ppm ($e[CO_2]$). In the first experiment (Exp. I), plants were grown in 1.5 L pots filled with peat substance. Since 31st Oct., plants were subjected to progressive soil drying by withholding irrigation from the pots for 5 days when the g_s decreased to ca. 10% of that on 31st Oct. (i.e., when pot weight ca. 320 g). Gas exchange measurements (P_n and g_s) were made at midday around 10:00 h with a portable photosynthetic system (LiCor-6400XT, LI-Cor, NE, USA). Measurements were performed on one leaf per plant at 20°C chamber temperature and 1200 μmol m^{-2} s^{-1} photon flux density, and at a $[CO_2]$ of 400 ppm for $a[CO_2]$ and 800 ppm for $e[CO_2]$ treatment, respectively. The mean volumetric soil water content in the pots was monitored by weighing the pots daily. The mean Ψ_s was then obtained based on the water retention curve for the peat substance (**Figure 1**). Other environmental variables such as e_a and T were also obtained during gas exchange measurements. The data obtained from this experiment was used for parameterization.

The models were then validated by data obtained from another experiment (Exp. II). In this experiment, tomato plants were grown in pots with roots divided into two equal compartments. The pots (10 L) were filled with a sandy soil. The

water retention curve of the sandy soil is shown in **Figure 1**. Three weeks after transplanting, plants were subjected to three irrigation regimes: (1) full irrigation (FI), in which both soil columns were irrigated daily to 18% (vol.); (2) alternative partial root-zone drying (PRI), in which only one soil column was watered daily to 70% irrigation amount of FI while the other was allowed to dry until the soil water content had decreased to ca. 6%; then the irrigation was shifted; (3) deficit irrigation (DI), in which the same amount of water for PRI was irrigated evenly to the two soil columns. The irrigation treatments lasted 40 days and each soil compartment of the PRI plants had experienced five drying/wetting cycles. The mean soil water content of each soil column was determined by TDR (Time Domain R ctometry; TRASE, Soil Moisture Equipment Corp., USA). The P_n and g_s and other environmental variables were obtained in the same way as for experiment I.

Statistics

The performance of the original and the modified BB-model was compared by evaluating the coefficient of determination (r^2), the mean absolute error (MAE) and the root mean square of error (RMSE) of the linear regressions between the measured and the observed values of g_s and *WUE*. Analysis of covariance (ANCOVA) (SAS 9.4 Ins. Inc.) was performed to reveal the regression lines between vapor pressure deficit (*VPD*) in the atmosphere and leaf *WUE*.

RESULTS

Model Parameterization

The data from experiment I was used for model parameterization. In brief, during the 5 days of soil drying Ψ_s decreased from -0.01 to -0.53 MPa and -0.01 to -0.61 MPa, g_s decreased from 0.61 to 0.03 mol m^{-2} s^{-1} and 0.39 to 0.03 mol m^{-2} s^{-1}, and P_n decreased from 15.3 to 1.54 mmol m^{-2} s^{-1} and 18.3 to 3.77 mmol m^{-2} s^{-1}, for the plants grown at $[CO_2]$ concentration of 400 and 800 ppm, respectively.

To calculate the slope (m) of the BB-model, we first calculated h_s by using the observed g_s values. The Ball-index, viz. $P_n h_s / C_s$ was then computed. By plotting the observed g_s against the Ball-index, an exponential, rather than a linear relationship between the two variables was found in both $a[CO_2]$ and $e[CO_2]$ (400 and 800 ppm) environment (**Figure 2**). Thus, m was not a constant indicating that g_s is not linearly correlated with P_n and h_s.

TABLE 1 | Parameters of the original and modified BB-models at $[CO_2]$ concentration of 400 and 800 ppm obtained from the multi-regression (Equation 9) over the data of experiment one.

Treatment	Model	Slope (m or m_i)	Intercept (g_0) (mol m^{-2} s^{-1})	β (MPa^{-1})
400 ppm	Original BB-model	26.85 (23.53 ~ 30.17)	-0.024 (-0.069 ~ 0.021)	Not relevant
	Modified BB-model	33.43 (29.57 ~ 37.29)	0.019 (-0.013 ~ 0.051)	-1.98 (-2.86 ~ -1.10)
800 ppm	Original BB-model	37.62 (33.96 ~ 41.29)	-0.085 (-0.112 ~ -0.057)	Not relevant
	Modified BB-model	41.55 (37.02 ~ 46.07)	-0.004 (-0.035 ~ 0.026)	-2.07 (-3.21 ~ -0.93)

The original BB-model has a constant slope, m; while the modified BB-model has an initial slope, m$_i$ and which is reduced exponentially by soil water deficits (Equation 2). Values in the parentheses are 95% confidence intervals of the parameters (n = 25).

Accordingly, the effects of soil water deficits on m (i.e., Equation 2) must be taken into account. This was done by incorporating Equation (2) into Equation (9). The simulation results show that the initial slope of the BB-model (i.e., m_i) was 33.43 and 41.55 at $a[CO_2]$ and $e[CO_2]$, respectively; while the both of actual slope (m) decreased exponentially with declining Ψ_s (**Figure 3**; **Table 1**). Also, the m_i was significantly greater for plants grown under $e[CO_2]$ than under $a[CO_2]$. From **Figures 4**, **5** it can be seen that the modified BB-model significantly improved the g_s and *WUE* simulations as compared with the original BB-model due to the higher r^2, lower MAE and RMSE values in both $a[CO_2]$ and $e[CO_2]$ environment.
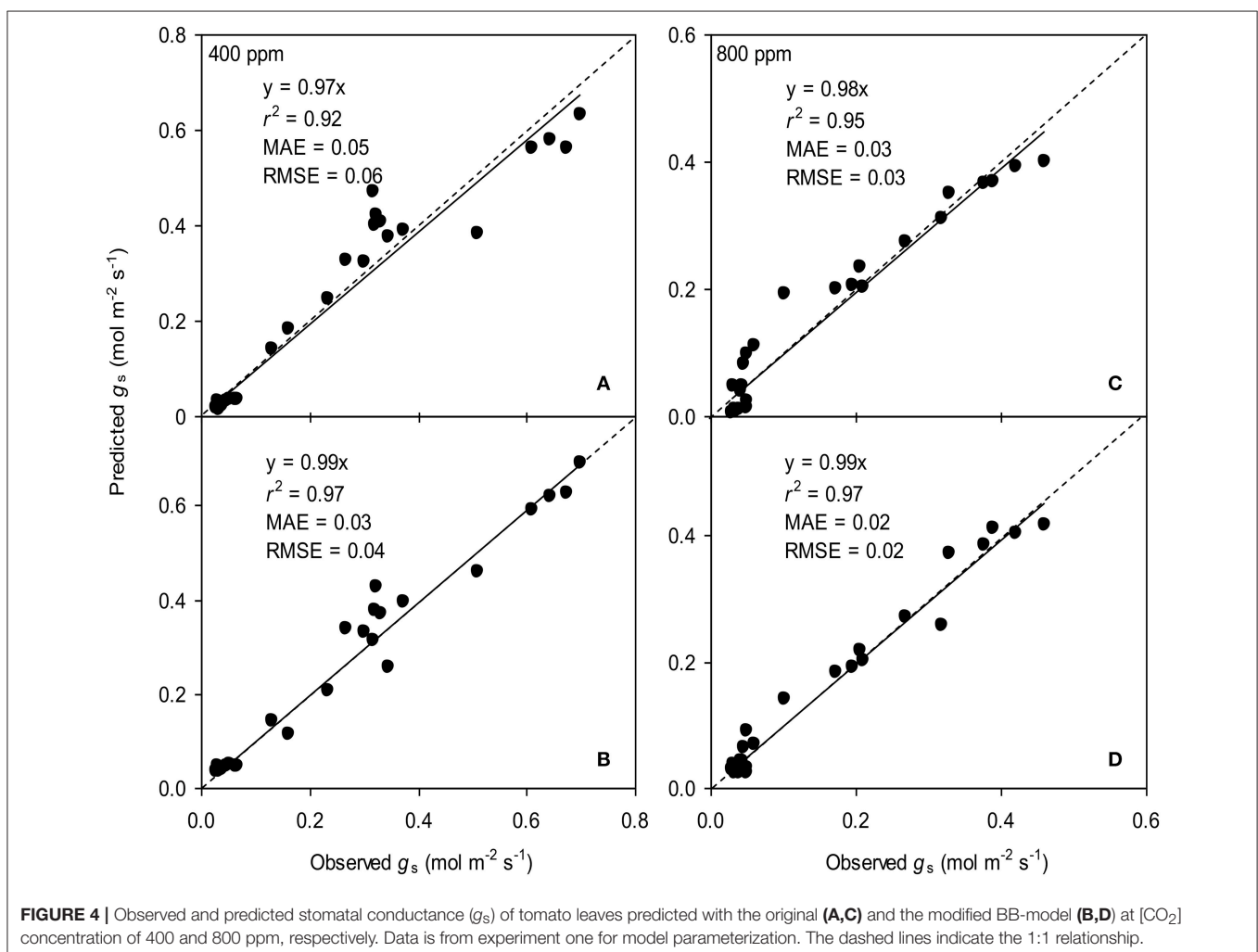
Model Validation

The BB-models (with or without m modifications) were validated by the data obtained from the experiment II (Wei et al., unpublished). Shortly, for the FI plants Ψ_s was kept above -0.001 MPa; for the DI plants, Ψ_s ranged between -0.001 and -0.112 MPa; for the PRI plants, Ψ_s of the wet soil column was maintained above -0.001 MPa while that of the dry soil column ranged from -0.001 to -0.398 MPa during the treatment period. The model simulations indicated that
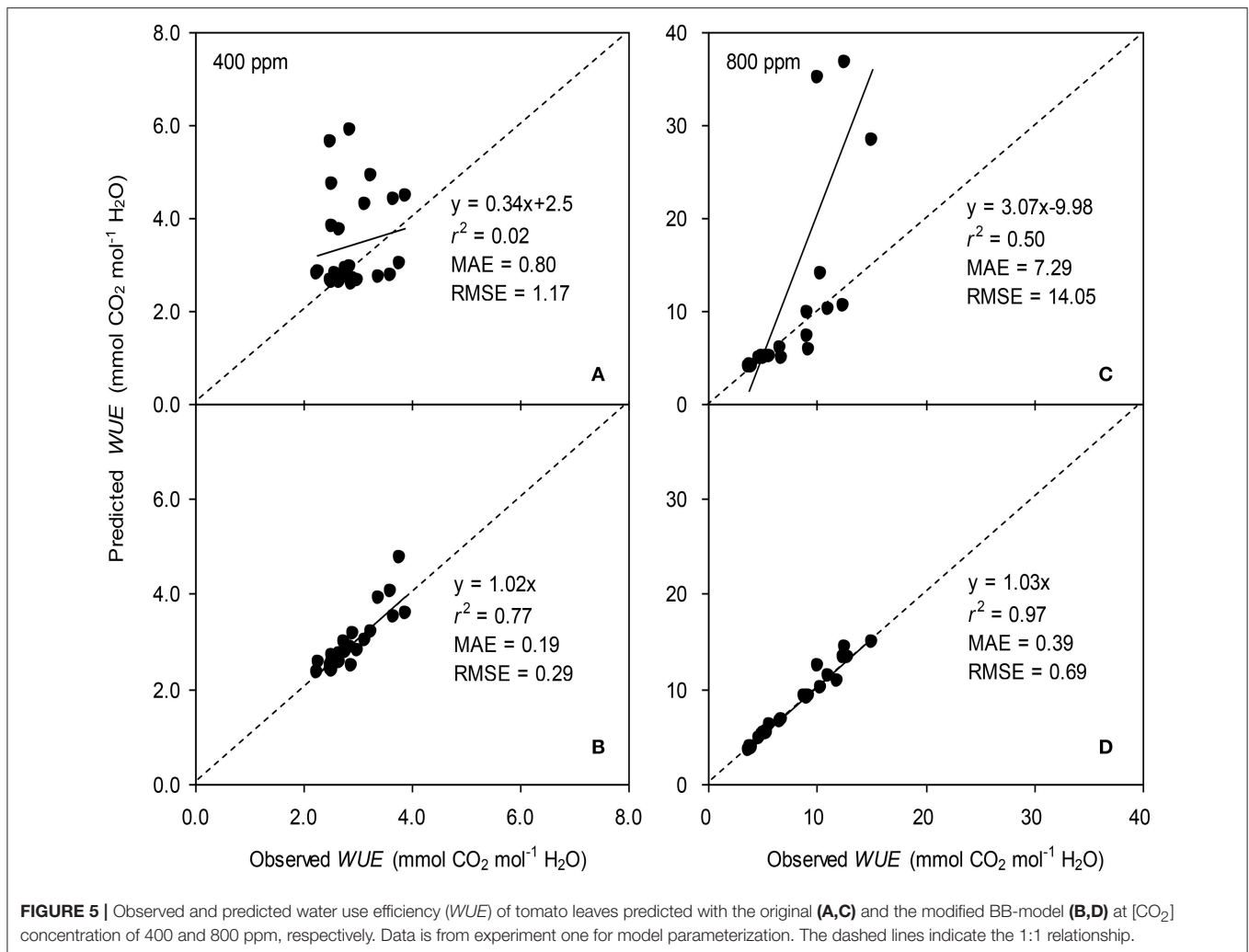
both models were able to explain more than 71% of the variation in g_s; for any FI, DI or PRI tomato plant, the modified BB-model was obviously superior to the original BB-model in predicting leaf g_s owing to its equal or higher r^2, lower MAE and RMSE values at both $a[CO_2]$ and $e[CO_2]$ (**Figures 6**, **7**).

The original model showed poor predictability for *WUE* ($0.21 < r^2 < 0.64$) of tomato leaves (**Figures 8**, **9**). The modified BB-model performed better in predicting leaf *WUE* than did the original BB-model for any FI, DI or PRI tomato plant owing to its greater r^2 ($0.46 < r^2 < 0.75$), lower MAE and RMSE values in both $a[CO_2]$ and $e[CO_2]$ conditions. **Figure 10** shows there was a negative relationship between *VPD* and *WUE*. The correlation between predicted *VPD* and *WUE* was not different among the FI, DI, and PRI treatments under the same BB-model and $[CO_2]$ environment (**Table 2**).

DISCUSSION

In the two pot experiments, the simulation of the BB-model in predicting g_s and *WUE* of tomato leaves grown in $a[CO_2]$

FIGURE 4 | Observed and predicted stomatal conductance (g_s) of tomato leaves predicted with the original **(A,C)** and the modified BB-model **(B,D)** at $[CO_2]$ concentration of 400 and 800 ppm, respectively. Data is from experiment one for model parameterization. The dashed lines indicate the 1:1 relationship.

FIGURE 5 | Observed and predicted water use efficiency (*WUE*) of tomato leaves predicted with the original **(A,C)** and the modified BB-model **(B,D)** at [CO$_2$] concentration of 400 and 800 ppm, respectively. Data is from experiment one for model parameterization. The dashed lines indicate the 1:1 relationship.

and e[CO$_2$] environment under different irrigation regimes was performed. For both a[CO$_2$] and e[CO$_2$] plants, the original and modified BB-model could explain more than 71% of the observed variation in g_s for all irrigation regimes; the modified BB-model was notably superior to the original model in predicting g_s and *WUE*, although the two models showed relatively poor simulation in *WUE* of tomato leaves ($r^2 < 0.75$) under different irrigation treatments.

It is well-known that partial stomatal closure leading to decrease in leaf g_s during progressive soil drying was mainly induced by the increased root-to-shoot chemical signaling (ABA) in moderate soil moisture deficit (Liu et al., 2005). Moreover, changes in environmental conditions especially h_s or *VPD* might mediate ABA action and influence leaf gas exchange (Wilkinson and Davies, 2002). A high h_s or lowered *VPD* may decrease the delivery and concentration of ABA in the guard cells, resulting in minimal increase in g_s and carbon assimilation without greater increase in transpiration (Speirs et al., 2013). In the current study, mostly the parameters e_i and e_a in the BB-model could well characterize the alteration in h_s or *VPD* and modulation on ABA catabolism in relation to the growth environment of the plants. In

addition, the modulation of CO$_2$ concentration in combination with *VPD* and soil water deficits on the ABA signaling and its regulation on g_s has not been well illustrated and needs further investigations (Yan et al., 2017).

A better understanding of whether there is physiological acclimation of g_s to water stress and e[CO$_2$] is crucial for describing plant responses using the BB-model (Miner et al., 2017). The influence of soil water stress on the slope (*m*) has been contradictory. Misson et al. (2004) measured 350% variation in *m* of ponderosa pine during the developing season; similarly, Héroult et al. (2013) found that two eucalyptus species had significant reductions in *m* under drought. However, Xu and Baldocchi (2003) showed that *m* remains relatively constant for blue oak even under severe water stress. Hence, disparate proposals have been suggested to account for the effect of water deficit on *m* of the BB-model (Buckley and Mott, 2013). To emphasize the significance of the root-to-shoot ABA signaling in regulating g_s during mild soil drying, an ABA-based module was incorporated into the original BB-model to modify the *m* (Gutschick and Simonneau, 2002; Bauerle, et al. et al., 2004). The common point of those proposals for *m*
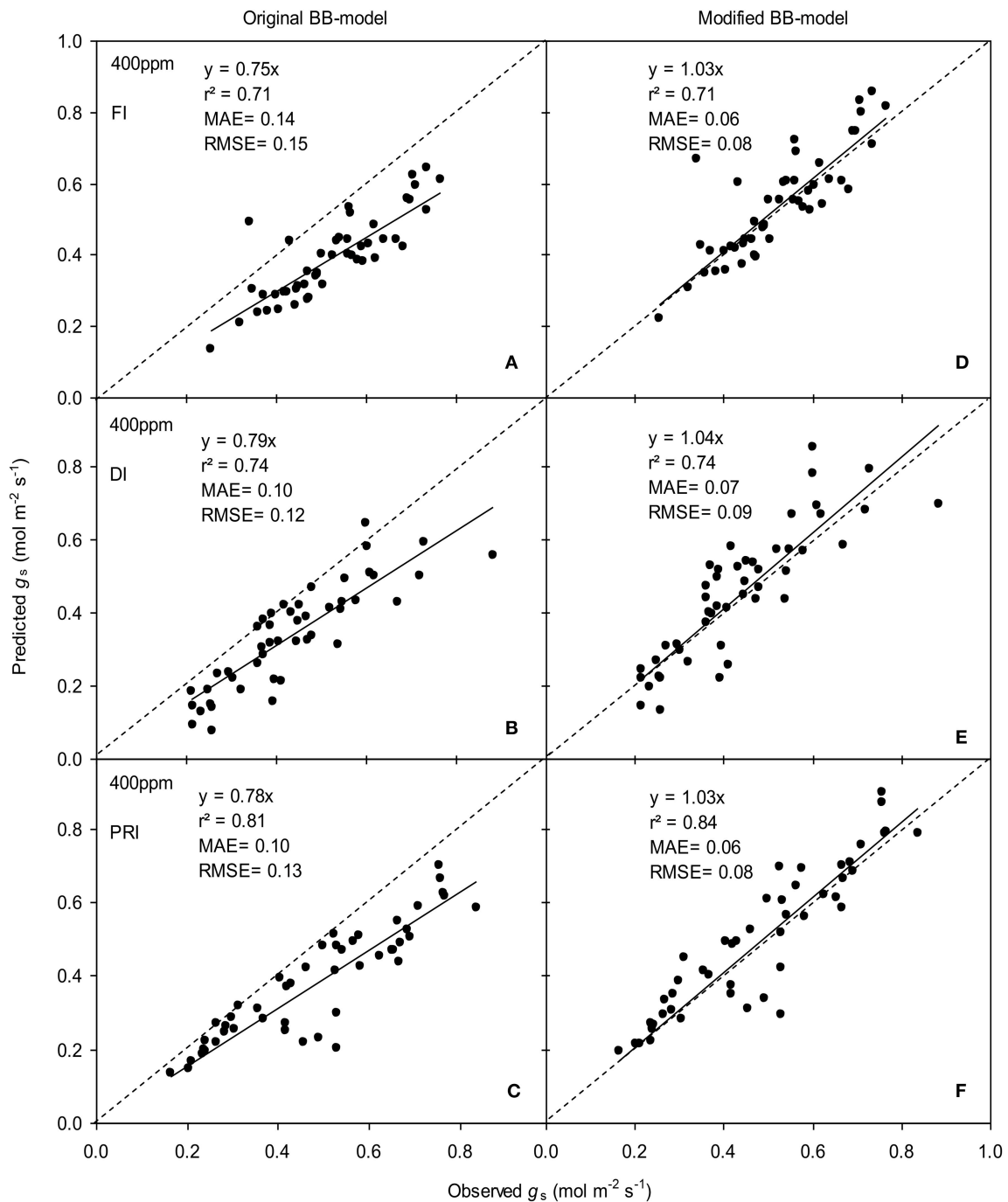
FIGURE 6 | Observed and predicted stomatal conductance (g_s) of experiment two data with the original **(A–C)** and the modified BB-model **(D–F)** of a tomato leaf under full irrigation (FI) **(A,D)** (n = 48), deficit irrigation (DI) **(B,E)** (n = 48) and alternative partial root-zone irrigation (PRI) **(C,F)** (n = 48), treatments at [CO$_2$] concentration of 400 ppm. The predictability of the models was compared by the coefficient of determination (r^2), the mean absolute error (MAE), and the root mean square of error (RMSE) of the linear regressions between the observed and predicted g_s. The dashed lines indicate the 1:1 relationship.

modification has been that the initial slope of the BB-model, i.e., m_i is scaled downward in response to progressive soil drying (Liu et al., 2009). In the present study, the modified m is related to soil water potential (Ψ_s) and it was found

that such modification remarkably improved the predictability of model especially for the drought stressed tomato leaves grown at either a[CO$_2$] and e[CO$_2$] environment (**Figures 4, 5**). Besides, the m obtained from the model parameterization
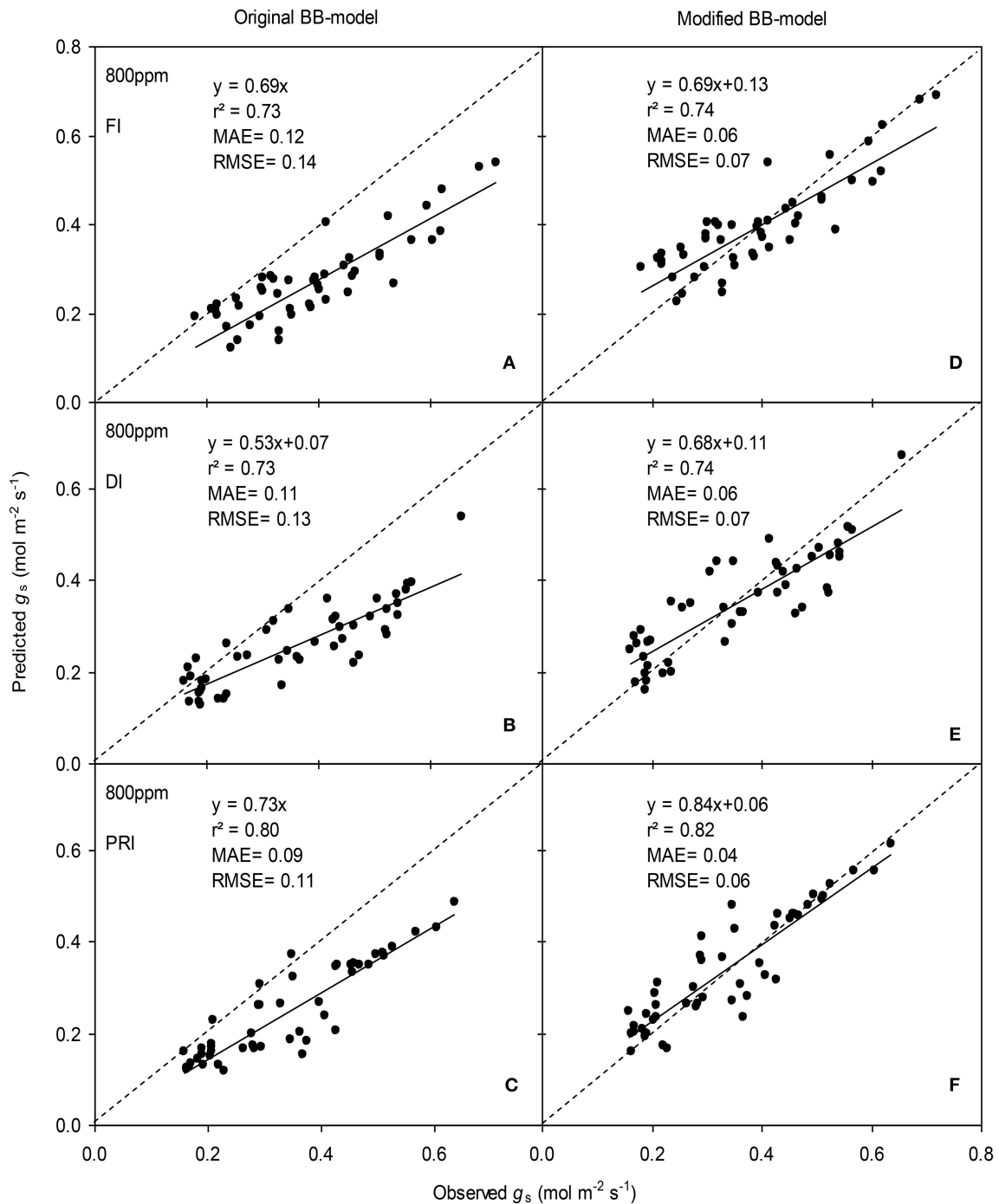
FIGURE 7 | Observed and predicted stomatal conductance (g_S) of experiment two data with the original **(A–C)** and the modified BB-model **(D–F)** of a tomato leaf under full irrigation (FI) **(A,D)** ($n = 48$), deficit irrigation (DI) **(B,E)** ($n = 48$) and alternative partial root-zone irrigation (PRI) **(C,F)** ($n = 48$), treatments at [CO$_2$] concentration of 800 ppm. The predictability of the models was compared by the coefficient of determination (r^2), the mean absolute error (MAE), and the root mean square of error (RMSE) of the linear regressions between the observed and predicted g_S. The dashed lines indicate the 1:1 relationship.

is higher (**Table 1**) than that observed mean value in C3 crops (Miner et al., 2017).

In soybean and wheat, the m significantly decreased when grown at e[CO$_2$] (Bunce, 2004; Tausz-Posch et al., 2013).

However, no change of m was noticed in five tree species (Medlyn et al., 2001) and soybean grown in a long-term free-air CO$_2$ enrichment (FACE) experiment (Leakey et al., 2006), suggesting that acclimation of g_S is mostly along with
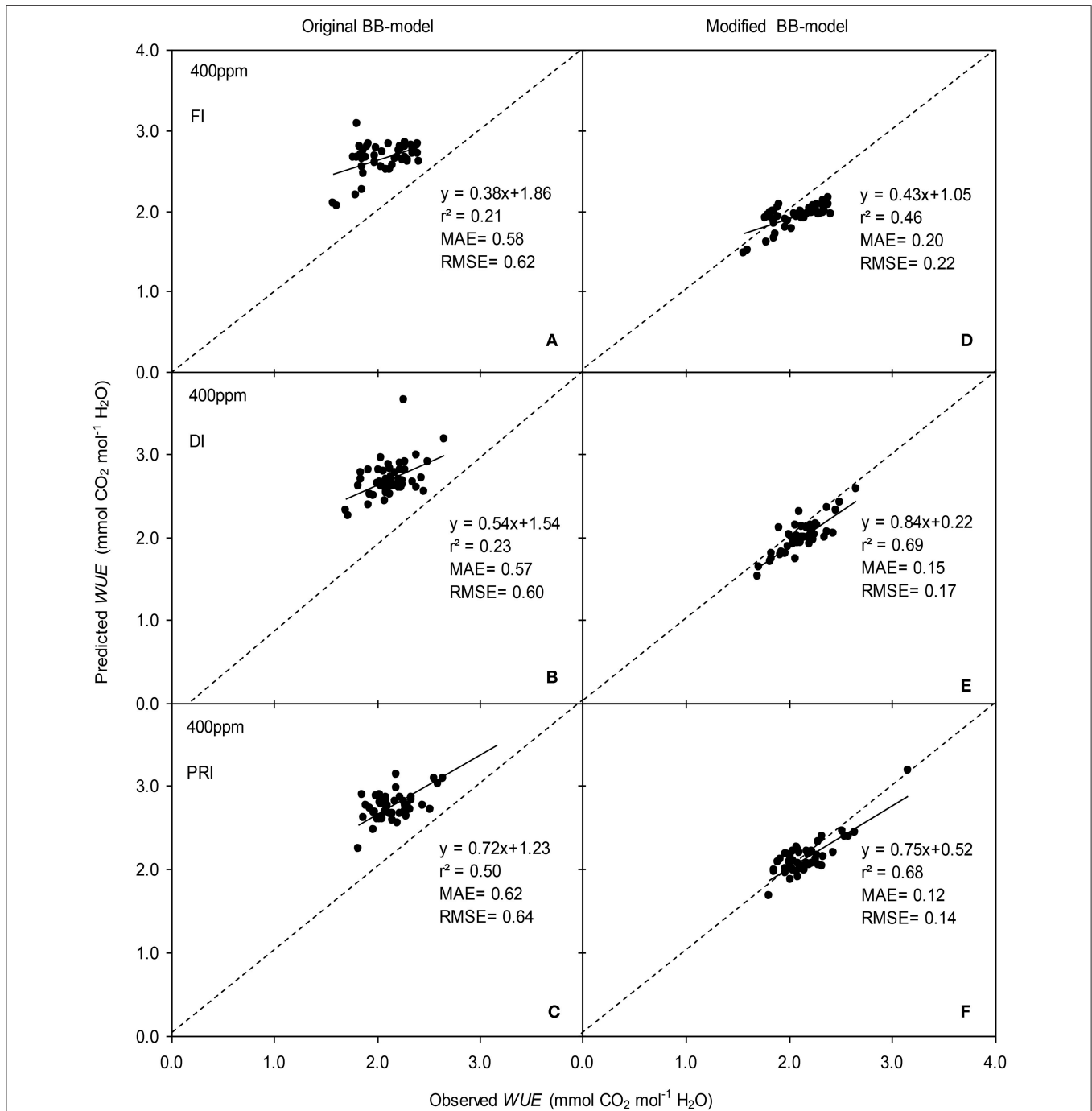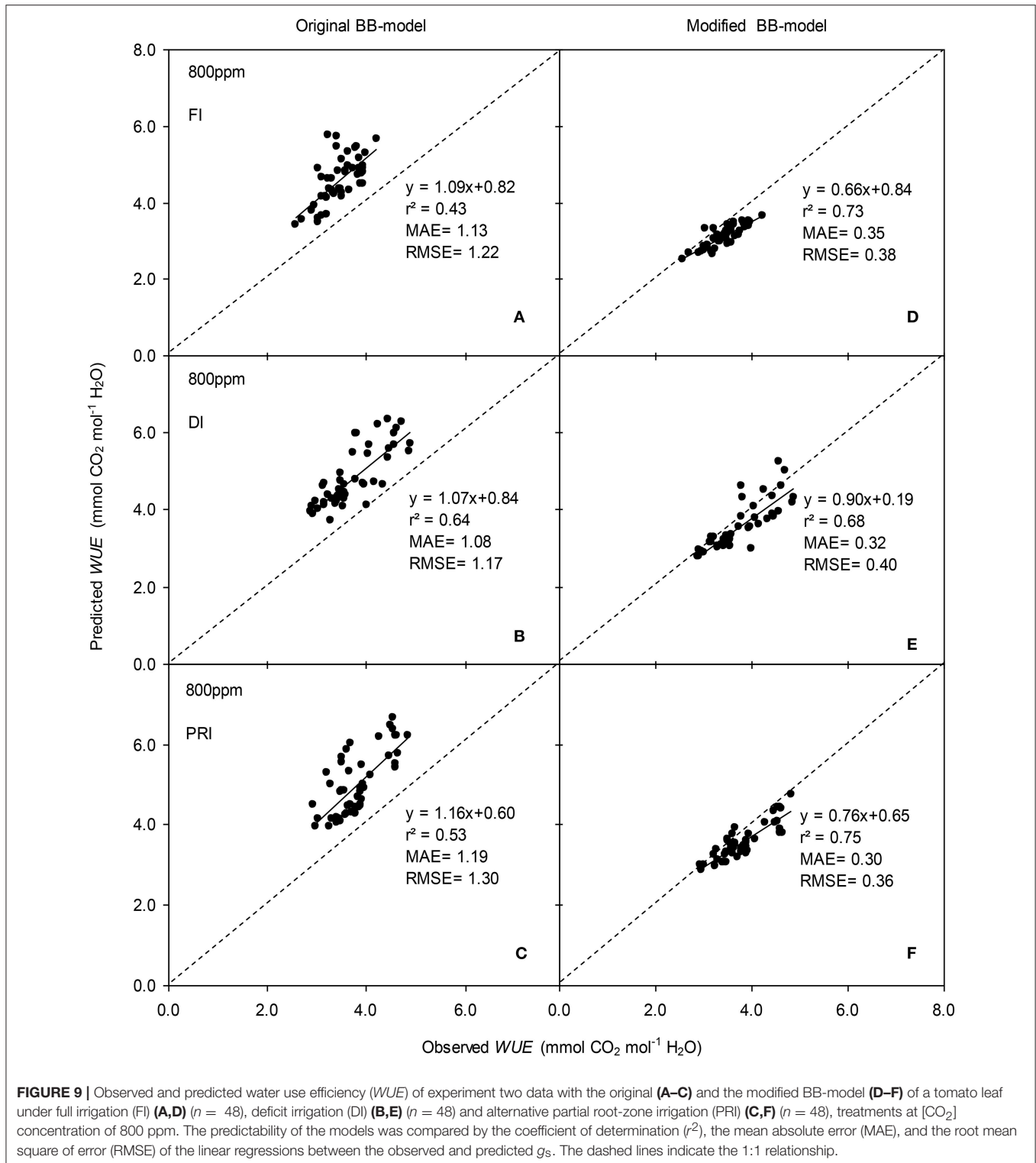
FIGURE 8 | Observed and predicted water use efficiency (*WUE*) of experiment two data with the original **(A–C)** and the modified BB-model **(D–F)** of a tomato leaf under full irrigation (FI) **(A,D)** (*n* = 48), deficit irrigation (DI) **(B,E)** (*n* = 48) and alternative partial root-zone irrigation (PRI) **(C,F)** (*n* = 48), treatments at [CO$_2$] concentration of 400 ppm. The predictability of the models was compared by the coefficient of determination (*r*^{2}), the mean absolute error (MAE), and the root mean square of error (RMSE) of the linear regressions between the observed and predicted *g*$_s$. The dashed lines indicate the 1:1 relationship.

the photosynthetic acclimation, resulting in an unchanged *m* in *e*[CO$_2$] condition (Ainsworth and Rogers, 2007; Gimeno et al., 2016). In contrast to those, here the *m* in *e*[CO$_2$] was significantly greater than that in *a*[CO$_2$] environment (**Table 1**), implying *g*$_s$ was independently acclimated to *e*[CO$_2$] from *P*$_n$.

A greater *m* indicates a higher sensitivity of stomata to the plant growth environment (such as radiation, humidity, soil water availability, and CO$_2$ concentration). In this study, the intercept of the modified BB-model, i.e., *g*$_0$ for tomato leaves was relatively lower than that obtained in an earlier potato study by

FIGURE 9 | Observed and predicted water use efficiency (*WUE*) of experiment two data with the original **(A–C)** and the modified BB-model **(D–F)** of a tomato leaf under full irrigation (FI) **(A,D)** (*n* = 48), deficit irrigation (DI) **(B,E)** (*n* = 48) and alternative partial root-zone irrigation (PRI) **(C,F)** (*n* = 48), treatments at [CO$_2$] concentration of 800 ppm. The predictability of the models was compared by the coefficient of determination (*r*^{2}), the mean absolute error (MAE), and the root mean square of error (RMSE) of the linear regressions between the observed and predicted *g*$_S$. The dashed lines indicate the 1:1 relationship.

Liu et al. (2009), and was not statistically significant from zero. A decreased g_0 indicates a low stomatal conductance in the dark. It has been reported that at $e[CO_2]$ the simulated g_0 could be lower, greater or no change as compared with that at $a[CO_2]$ (Medlyn

et al., 2001; Bunce, 2004; Leakey et al., 2006). The BB-model not only requires environmental variables, also need the plant photosynthesis. Earlier studies have adopted the Farquhar's photosynthesis model (Farquhar et al., 1980) as an integrated
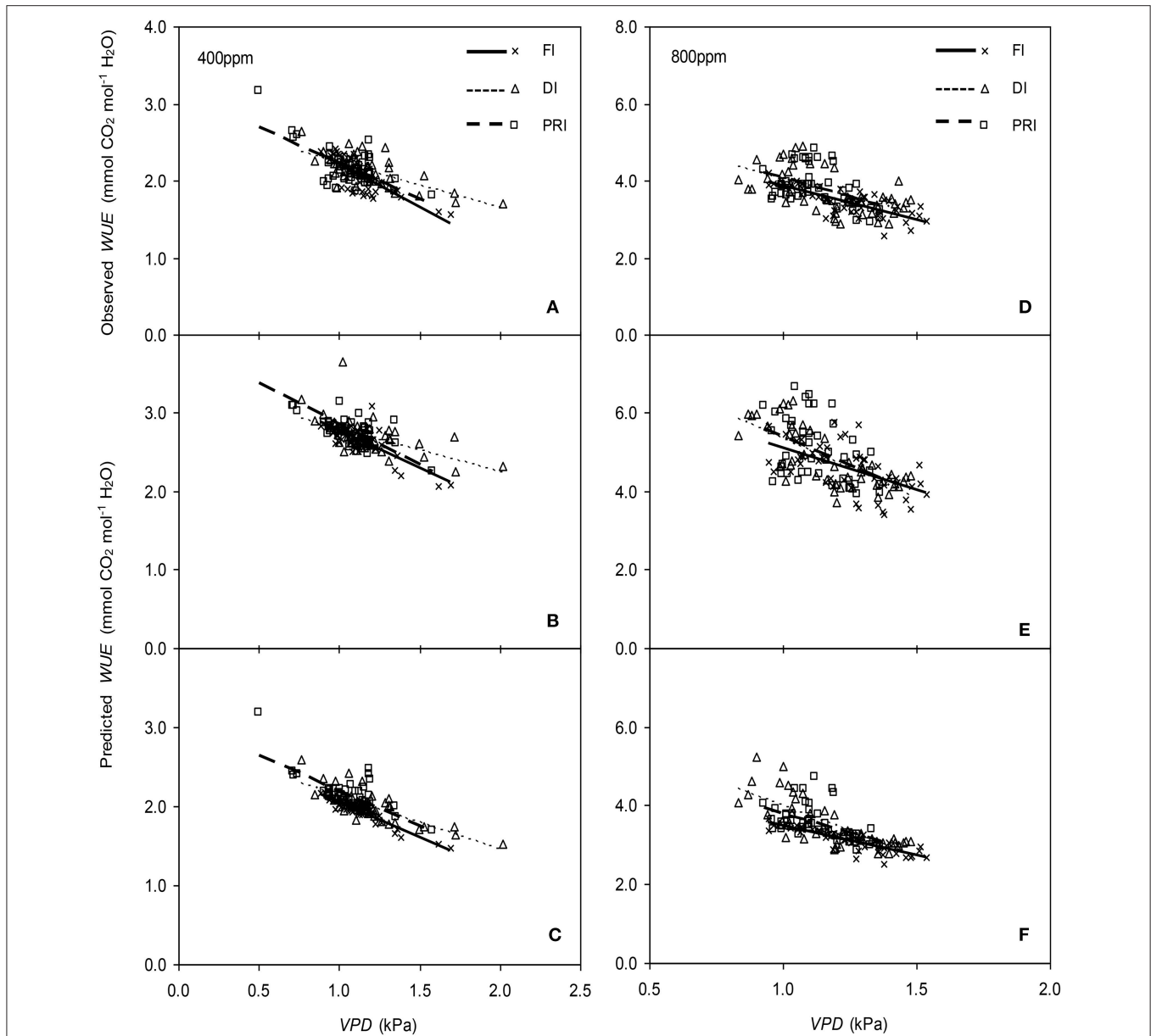
FIGURE 10 | Relationships between the vapor pressure deficit (*VPD*) of the atmosphere and the measured photosynthetic water use efficiency (*WUE*) **(A,D)**, and the simulated *WUE* by the original **(B,E)**, and the modified BB-model **(C,F)** of tomato leaves under full irrigation (FI), deficit irrigation (DI) and alternative partial root-zone irrigation (PRI) regimes at [CO$_2$] concentration of 400 and 800 ppm, respectively. The Comparison of regression lines under different irrigation treatments are seen in **Table 2**.

module in the BB-model for simulating leaf P_n (Gutschick and Simonneau, 2002; Bauerle, et al. et al., 2004; Misson et al., 2004). However, such model is largely apt to a model of the correlation between P_n and g_s resulted from the interdependence of those two factors, and it is useless for interpreting the causality (Liu et al., 2009). Numerous reports have confirmed that, applying the observed P_n as an input variable, the BB-model could performed successfully in predicting g_s over different species (Misson et al., 2004; Liu et al., 2009). In addition, accompanied with decreased g_s, leaf P_n would maintained or increased under PRI or e[CO$_2$] (Pazzagli et al., 2016), which

could complicate the simulation of P_n for plants grown under PRI strategy combined with e[CO$_2$] environment. Thus, in this study, the measured leaf P_n was used to improve the model's performance in predicting g_s across a wide range of soil water status.

Figures 6, **7** illustrated that the modified BB-model performed better than the original BB-model in predicting leaf g_s of the three irrigation treatments at each atmospheric [CO$_2$] concentration, especially for the PRI tomato plant with highest high r^2, lowest MAE and RMSE values. It is evident that a decreased g_s of leaf grown at e[CO$_2$] would affect plant water use and further

TABLE 2 | Comparison of the regression lines between vapor pressure deficit of the air (*VPD*) and the predicted *WUE* under different irrigation treatments at [CO$_2$] concentration of 400 and 800 ppm, respectively (**Figure 10**).

Treatment		Observed			Predicted by BB-model			Predicted by modified BB-model		
		Slope	Y-intercept	r^2	Slope	Y-intercept	r^2	Slope	Y-intercept	r^2
400 ppm	FI	−1.11 ± 0.13	3.32 ± 0.15a	0.77***	−0.93 ± 0.11	3.71 ± 0.13a	0.78***	−0.86 ± 0.04	2.91 ± 0.05a	0.96***
	DI	−0.58 ± 0.09	2.81 ± 0.11a	0.68***	−0.54 ± 0.12	3.34 ± 0.14a	0.56***	−0.68 ± 0.08	2.81 ± 0.09a	0.79***
	PRI	−0.92 ± 0.15	3.14 ± 0.16a	0.67***	−1.04 ± 0.14	3.89 ± 0.15a	0.75***	−0.90 ± 0.13	3.09 ± 0.14a	0.72***
800 ppm	FI	−1.74 ± 0.22	5.61 ± 0.27a	0.76***	−2.14 ± 0.46	7.23 ± 0.57a	0.57***	−1.52 ± 0.13	5.01 ± 0.17b	0.86***
	DI	−1.81 ± 0.37	5.85 ± 0.44a	0.58***	−3.03 ± 0.42	8.36 ± 0.50a	0.73***	−2.56 ± 0.33	6.52 ± 0.39a	0.76***
	PRI	−1.89 ± 0.56	5.96 ± 0.64a	0.44**	−2.92 ± 0.91	8.31 ± 1.03a	0.43**	−1.93 ± 0.47	5.73 ± 0.54ab	0.51***

*Each value is represented as values ± SE (Standard Error). Different letters within each of the Y-intercept column indicate significant different between the regression lines of the treatments at P < 0.05 level (ANCOVA). ** and *** indicate significance of the regression lines at P < 0.01 and < 0.001 levels, respectively.*

contribute to the varied Ψ_s (Kaminski et al., 2014). Likewise, the soil water heterogeneity induced by the PRI treatment could markedly altered the root-to-shoot ABA signaling involved in regulating g_s, and the physiological responses, including leaf g_s become more sensitive to the reduction of Ψ_s in the PRI than that in DI plant (Davies et al., 2002; Liu et al., 2008). Besides, previous study has revealed that xylem ABA concentration of PRI-treated potatoes is determined by Ψ_s and not by Ψ_s-dry (Liu et al., 2008), consistent with the results that the model performed much better when using mean Ψ_s in the whole root zone than using Ψ_s-dry to account for the effect of soil drying on g_s (Liu et al., 2009). Therefore, a modification of m using Ψ_s incorporating into the BB-model is desired and necessary for achieving a better prediction of PRI tomato g_s in the e[CO$_2$] environment.

In the present study, similar to that for g_s simulation, the modified BB-model also showed a better predictability for tomato *WUE* at leaf scale of all irrigation regimes in both [CO$_2$] concentration as compared to the original model, particularly for PRI-treated plant, although the improvement of the prediction was less significant (**Figures 8, 9**). This could be ascribed to the accumulated errors in several variables for calculating *WUE* from the modeled g_s. Nonetheless, regardless of the Ψ_s effect, the original and modified BB-model normally could not distinguish the influence of irrigation regimes on *WUE* of tomato leaves in either [CO$_2$] condition (**Figure 10**; **Table 2**), indicating a robust relationship between *WUE* and *VPD* among different soil moisture condition and atmospheric [CO$_2$] concentration. It is well-known that PRI combined with e[CO$_2$] plants could lead to an increase of P_n, and a decrease of stomatal aperture,

hence synergistically enhancing leaf *WUE* (Pazzagli et al., 2016). Thus, a greater *WUE* is expected for the PRI plant grown in e[CO$_2$] environment as simulated by the modified g_s and BB-model.

Collectively, tomato g_s was independent acclimation to e[CO$_2$] environment from P_n. Introducing Ψ_s of whole root zone into the BB-model could improve the model predictability of the model on g_s and *WUE* of tomato leaves under combinations of different irrigation regimes and CO$_2$ environments. This information is useful for better predicting *WUE* of tomato plant in a future drier and CO$_2$ enriched environment.

AUTHOR CONTRIBUTIONS

ZW: Done the experiment and finished the first manuscript; TD: The corresponding author, the work was supervised by him; XL: Help to do the experiment; LF: Help to do the experiment; FL: The corresponding author, the work was supervised by him.

ACKNOWLEDGMENTS

REFERENCES

Ainsworth, E. A., and Rogers, A. (2007). The response of photosynthesis and stomatal conductance to rising [CO$_2$]: mechanisms and environmental interactions. *Plant Cell Environ.* 30, 258–270. doi: 10.1111/j.1365-3040.2007.01641.x

Ball, J. T., Woodrow, I. E., and Berry, J. A. (1987). "A model predicting stomatal conductance and its contribution to the control of photosynthesis under different environmental conditions," in *Progress in Photosynthesis Research, Vol. 4, Proceedings of the 7th International Congress on Photosynthesis*, ed J. Biggins (Dordrecht: Martins Nijhoff), 221–224.

Bauerle, W. L., Toler, J. E., and Wang, G. G. (2004). Stomatal conductance of *Acer rubrum* ecotypes under varying soil and atmospheric water conditions: predicting stomatal responses with an abscisic acid-based model. *Tree Physiol.* 24, 805–811. doi: 10.1093/treephys/24.7.805

Buckley, T. N., and Mott, K. A. (2013). Modelling stomatal conductance in response to environmental factors. *Plant Cell Environ.* 36, 1691–1699. doi: 10.1111/pce.12140

Bunce, J. A. (2004). Carbon dioxide effects on stomatal responses to the environment and water use by crops under field conditions. *Oecologia* 140, 1–10. doi: 10.1007/s00442-003-1401-6

Damour, G., Simonneau, T., Cochard, H., and Urban, L. (2010). An overview of models of stomatal conductance at the leaf level. *Plant Cell Environ.* 33, 1419–1438. doi: 10.1111/j.1365-3040.2010.02181.x

da Silva, J. R., Patterson, A. E., Rodrigues, W. P., Campostrini, E., and Griffin, K. L. (2017). Photosynthetic acclimation to elevated CO₂ combined with partial rootzone drying results in improved water use efficiency, drought tolerance and leaf carbon balance of grapevines (*Vitis labrusca*). *Environ. Exp. Bot.* 134, 82–95. doi: 10.1016/j.envexpbot.2016.11.007

Davies, W. J., Wilkinson, S., and Loveys, B. (2002). Stomatal control by chemical signalling and the exploitation of this mechanism to increase water use efficiency in agriculture. *New Phytol.* 153, 449–460. doi: 10.1046/j.0028-646X.2001.00345.x

Du, T. S., Kang, S. Z., Zhang, J., and Davies, W. J. (2015). Deficit irrigation and sustainable water-resource strategies in agriculture for China's food security. *J. Exp. Bot.* 66, 2253–2269. doi: 10.1093/jxb/erv034

Farquhar, G. V., von Caemmerer, S. V., and Berry, J. A. (1980). A biochemical model of photosynthetic CO₂ assimilation in leaves of C3 species. *Planta* 149, 78–90. doi: 10.1007/BF00386231

Gimeno, T. E., Crous, K. Y., Cooke, J., O'Grady, A. P., Ósvaldsson, A., and Medlyn, B. E., Ellsworth, D. S. (2016). Conserved stomatal behaviour under elevated CO₂ and varying water availability in a mature woodland. *Funct. Ecol.* 30, 700–709. doi: 10.1111/1365-2435.12532

Gutschick, V. P., and Simonneau, T. (2002). Modelling stomatal conductance of field grown sunflower under varying soil water content and leaf environment: comparison of three models of stomatal response to leaf env ironment and coupling with an abscisic acid. based model of stomatal response to soil drying. *Plant Cell Environ.* 25, 1423–1434. doi: 10.1046/j.1365-3040.2002.00937.x

Héroult, A., Lin, Y. S., Bourne, A., Medlyn, B. E., and Ellsworth, D. S. (2013). Optimal stomatal conductance in relation to photosynthesis in climatically contrasting Eucalyptus species under drought. *Plant Cell Environ.* 36, 262–274. doi: 10.1111/j.1365-3040.2012.02570.x

Kaminski, K. P., Kørup, K., Nielsen, K. L., Liu, F. L., Topbjerg, H. B., Kirk, H. G., et al. (2014). Gas exchange, water use efficiency and yield responses of elite potato (*Solanum tuberosum* L.) cultivars to changes in atmospheric carbon dioxide concentration, temperature and relative humidity. *Agric. For. Meteorol.* 187, 36–45. doi: 10.1016/j.agrformet.2013.12.001

Kang, S. Z., and Zhang, J. H. (2004). Controlled alternate partial root zone irrigation: its physiological consequences and impact on water use efficiency. *J. Exp. Bot.* 55, 2437–2446. doi: 10.1093/jxb/erh249

Leakey, A. D., Bernacchi, C. J., Ort, D. R., and Long, S. P. (2006). Long-term growth of soybean at elevated [CO₂] does not cause acclimation of stomatal conductance under fully open-air conditions. *Plant Cell Environ.* 29, 1794–1800. doi: 10.1111/j.1365-3040.2006.01556.x

Liu, F. L., Andersen, M. N., and Jensen, C. R. (2009). Capability of the 'Ball-Berry'model for predicting stomatal conductance and water use efficiency of potato leaves under different irrigation regimes. *Sci. Hortic.* 122, 346–354. doi: 10.1016/j.scienta.2009.05.026

Liu, F. L., Jensen, C. R., Shahanzari, A., Andersen, M. N., and Jacobsen, S. E. (2005). ABA regulated stomatal control and photosynthetic water use efficiency of potato (*Solanum tuberosum* L.) during progressive soil drying. *Plant Sci.* 168, 831–836. doi: 10.1016/j.plantsci.2004.10.016

Liu, F. L., Shahnazari, A., Andersen, M. N., Jacobsen, S. E., and Jensen, C. R. (2006). Physiological responses of potato (*Solanum tuberosum* L.) to partial root-zone drying: ABA signalling, leaf gas exchange, and water use efficiency. *J. Exp. Bot.* 57, 3727–3735. doi: 10.1093/jxb/erl131

Liu, F. L., Song, R., Zhang, X. Y., Shahnazari, A., Andersen, M. N., Plauborg, F., et al. (2008). Measurement and modelling of ABA signalling in potato (*Solanum tuberosum* L.) during partial root-zone drying. *Environ. Exp. Bot.* 63, 385–391. doi: 10.1016/j.envexpbot.2007.11.015

Medlyn, B. E., Barton, C. V. M., Broadmeadow, M. S. J., Ceulemans, R., De Angelis, P., Forstreuter, M., et al. (2001). Stomatal conductance of forest species after long-term exposure to elevated CO₂ concentration: a synthesis. *New Phytol.* 149, 247–264. doi: 10.1046/j.1469-8137.2001.00028.x

Miner, G. L., Bauerle, W. L., and Baldocchi, D. D. (2017). Estimating the sensitivity of stomatal conductance to photosynthesis: a review. *Plant Cell Environ.* 40, 1214–1238. doi: 10.1111/pce.12871

Misson, L., Panek, J. A., and Goldstein, A. H. (2004). A comparison of three approaches to modeling leaf gas exchange in annually drought-stressed ponderosa pine forests. *Tree Physiol.* 24, 529–541. doi: 10.1093/treephys/24.5.529

Pazzagli, P. T., Weiner, J., and Liu, F. L. (2016). Effects of CO₂ elevation and irrigation regimes on leaf gas exchange, plant water relations, and water use efficiency of two tomato cultivars. *Agric. Water Manage.* 169, 26–33. doi: 10.1016/j.agwat.2016.02.015

Sala, A., and Tenhunen, J. D. (1996). Simulations of canopy net photosynthesis and transpiration in *Quercus ilex* L. under the influence of seasonal drought. *Agric For Meteorol.* 78, 203–222.

Speirs, J., Binney, A., Collins, M., Edwards, E., and Loveys, B. (2013). Expression of ABA synthesis and metabolism genes under different irrigation strategies and atmospheric VPDs is associated with stomatal conductance in grapevine (*Vitis vinifera* L. cv Cabernet Sauvignon). *J. Exp. Bot.* 64, 1907–1916. doi: 10.1093/jxb/ert052

Tausz-Posch, S., Norton, R. M., Seneweera, S., Fitzgerald, G. J., and Tausz, M. (2013). Will intra-specific differences in transpiration efficiency in wheat be maintained in a high CO₂ world? A FACE study. *Physiol. Plant.* 148, 232–245. doi: 10.1111/j.1399-3054.2012.01701.x

Wei, Z. H., Du, T. S., Li, X. N., Fang, L., and Liu, F. L. (2018). Interactive effects of CO₂ concentration elevation and nitrogen fertilization on water and nitrogen use efficiency of tomato grown under reduced irrigation regimes. *Agric. Water Manage.* 202, 174–182. doi: 10.1016/j.agwat.2018.02.027

Wei, Z. H., Du, T. S., Zhang, J., Xu, S. J., Cambre, P. J., and Davies, W. J. (2016). Carbon isotope discrimination shows a higher water use efficiency under alternate partial root-zone irrigation of field-grown tomato. *Agric. Water Manage.* 165, 33–43. doi: 10.1016/j.agwat.2015.11.009

Wilkinson, S., and Davies, W. J. (2002). ABA-based chemical signalling: the co-ordination of responses to stress in plants. *Plant Cell Environ.* 25, 195–210. doi: 10.1046/j.0016-8025.2001.00824.x

Xu, L., and Baldocchi, D. D. (2003). Seasonal trends in photosynthetic parameters and stomatal conductance of blue oak (*Quercus douglasii*) under prolonged summer drought and high temperature. *Tree Physiol.* 23, 865–877. doi: 10.1093/treephys/23.13.865

Yan, F., Li, X. N., and Liu, F. L. (2017). ABA signaling and stomatal control in tomato plants exposure to progressive soil drying under ambient and elevated atmospheric CO₂ concentration. *Environ. Exp. Bot.* 139, 99–104. doi: 10.1016/j.envexpbot.2017.04.008