The effects of the CO2 database on a localized AquaCrop model construction based on a field experiment

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Abstract
To examine whether the use of the default CO2 database affected the simulation, this paper built AquaCrop models of winter wheat based on the measured CO2 database and the default CO2 database. The results showed that the maximum relative error (RE) of the simulated values of biomass and yield under both databases was below 4%, and the residual coefficient method (CRM) and normalized root mean square error (NRMSE) were within ±2%. Compared with the default database, the accuracy under the measured database was higher. To further verify the model, the simulated values of evapotranspiration and soil water content were analysed. The results showed that the RE of evapotranspiration was between 2% and 6% compared with the measured value in the seedling, overwintering and mature periods. In general, the simulated values of evapotranspiration were consistent with the measured values at different irrigation levels. The simulated values of the soil water content were all higher than the measured values, but the simulated results basically reflected the dynamic changes in the soil water content. The results showed that in the absence of measured CO2 data, the default CO2 database can be used and the accuracy of the model meets the actual demand.

KEYWORDS
AquaCrop model, CO2, evapotranspiration, soil water content, winter wheat

Résumé
Afin d’examiner si l’utilisation de la base de données de CO2 par défaut a affecté la simulation, cet article a construit des modèles AquaCrop de blé d’hiver basés sur la base de données de CO2 mesurée et la base de données de CO2 par défaut. Les résultats ont montré que l’erreur relative maximale (RE) des valeurs simulées de la biomasse et du rendement dans le cadre de deux bases de données était inférieure à 4%, et que la méthode du coefficient résiduel (CRM) et l’erreur quadratique moyenne normalisée (NRMSE) se situaient à ±2%. Par rapport à la base de données par défaut, la précision de la base de données mesurée était plus élevée. Pour vérifier davantage le modèle, les valeurs simulées de l’évapotranspiration et de la teneur en eau du sol ont

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1 | INTRODUCTION

The water on Earth is approximately 1.4 billion km$^3$; however, the amount of available water is less than 45,000 km$^3$ (approximately 0.003% of the total), and only 9,000–14,000 km$^3$ (approximately 0.001% of the total) of this water is suitable for human use. At present, approximately 1.5 billion people are facing a shortage of fresh water in more than 80 countries around the world, of which 300 million people in 26 countries are living in a state of water shortage. It is estimated that 3 billion people in the world will lack the needed amount of water, which will involve more than 40 countries and regions by 2025. During the twenty-first century, water resources have become a precious and scarce resource. The problem of water resource scarcity is not only a matter of resource scarcity but also a major strategic issue that relates to the sustainable development of a country’s economy, society and long-term security. China, the world’s most populous developing country, feeds 22% of the world’s population with 7% of the world’s land and 8% of its freshwater. However, as the population continues to grow, the climate becomes more arid, pollution continues to worsen and water and arable land resources continue to decrease, China will face significant pressures and challenges in terms of water resources and food security (Zhang et al., 2005). The North China Plain (NCP) covers an area of $0.44 \times 10^6$ km$^2$ and has a population of over 200 million. It is one of the most productive and intensive agricultural areas in China (Iqbal et al., 2014). The main crops are wheat and corn. Wheat and corn production account for 20% of the country’s total output, of which wheat accounts for 11% and corn accounts for 9%. Due to the growth cycle of winter wheat from October to June of the second year, the water supply during this time is insufficient in North China, resulting in a large amount of groundwater being overexploited for irrigation. There is a more prominent contradiction between water resources and food security issues in North China. To solve water resources and food security issues, it is necessary to build a water-driven crop growth model to simulate and formulate reasonable future adjustment schemes for food crop patterns (Xia, Liu, & Jia, 2004).

At present, a series of crop growth models have been developed, such as CERES-Maize (Kisekka et al., 2016), WOFOST (Diepen et al., 2007), CropSyst (Stockle, Donatelli, & Nelson, 2003), DSSAT-CSM (Jones et al., 2003) and the Hybrid-Maize model (Yang et al., 2004). However, due to the complexity of these models and the large number of input parameters, it is difficult to use such models for popularization and application (Malik et al., 2017). The Food and Agriculture Organization (FAO) of the United Nations developed the AquaCrop model in 2009. Compared with the above models, AquaCrop is a user-friendly and practitioner-oriented software (Ahmadi & Mosallaeepour, 2015). The AquaCrop model has been extensively tested and applied in different regions (Bird et al., 2016; Li, Yu, & Zhao, 2019; Raes et al., 2009). The main problem of the AquaCrop model is its applicability. Hsiao et al. (2009) concluded that the applicability of the AquaCrop model should be further verified for different soil properties, crop characteristics and climatic conditions around the world. Yin (2013) studied the applicability of the AquaCrop model in semiarid regions and applied the AquaCrop model to the management of deficient irrigation of spring wheat and obtained irrigation regimes in different years. Iqbal et al. (2014) studied the applicability of the
AquaCrop model in the NCP and simulated winter wheat biomass, yield, actual evapotranspiration and total soil water content (0 ~ 120 cm). Mhizha et al. (2014) calibrated the AquaCrop model using measured corn data and simulated yield through an optimized program. Linker and Sylaios (2016) used 9 years of climate data from northern Greece and a locally calibrated AquaCrop model to test an efficient model-based procedure for computing seasonal suboptimal irrigation schedules. Sandhu and Irmak (2019) evaluated the AquaCrop model relative to maize growth, yield and water use parameters/variables under different water stress conditions over 6 years (2005 ~ 2010) in Nebraska, USA. Li, Yu, & Zhao (2019) studied the applicability of the model in the NCP and applied the AquaCrop model to optimize irrigation strategies.

The above researchers run the AquaCrop model with the default CO2 database (MaunaLoa. CO2). When the measured CO2 database is missing, AquaCrop will automatically apply the default CO2 database. The CO2 concentration varies by place, which has certain effects on crop growth, and the local CO2 concentration can be more useful for modelling (Li et al., 2020; Ma et al., 2005; Meng et al., 2015; Xiao et al., 2005). In this study, a local AquaCrop model was established to simulate the biomass and yield of winter wheat based on the measured and default CO2 database and to analyse how much influence the default database can have on the simulation results of the model in the NCP.

2 | MATERIALS AND METHODS

2.1 | Study area

The NCP is one of the most productive agricultural regions in China. Seventy per cent of the water used in the wheat-growing seasons comes from groundwater pumped from wells with a depth of over 40 m, resulting in a rapid decline in the groundwater table in the NCP (Yuan & Shen, 2013). As the global climate changes, the disparity between groundwater resources and the water consumption of agricultural production will further intensify (Falloon & Betts, 2010).

The study area (Scientific Irrigation Experimental Station of Jinzhou City) is located in the NCP, with the coordinates 37°30′ ~ 38°18′ N, 114°19′ ~ 116°30′ E, and an average altitude of 42 m (Figure 1). The annual rainfall is 455.8 mm, which is concentrated from June to September, and the mean annual evaporation is approximately 1,000 ~ 1,200 mm, which is characterized by a semiarid subhumid monsoon climate with an average annual temperature of 13.3 °C, an average number of sunshine hours of 2,397.2 h and an annual frost-free period of 236 days.

The selected cultivar of winter wheat was Guan-35, and the seeding rate was 187.5 kg·ha⁻¹. The sowing time was during mid-late October of each year, and the harvest time was in early June of the next year. The winter wheat planting times for the 2017 ~ 2018 season and...
2018 ~ 2019 season were 28 October and 17 October, respectively. There were nine test plots, each with an area of 8 m × 15 m. The irrigation mode was border irrigation, which was conducted in the wintering, jointing and grouting periods. Before sowing, 750 kg ha⁻¹ of a compound fertilizer was applied as the base. The tillage mode was rotary tillage. The irrigation schedule of winter wheat for 2017 ~ 2019 is shown in Table 1. T1 is 100% of the local irrigation level, T2 is 80% of the local irrigation level, and T3 is 60% of the local irrigation level in Table 1.

### 2.2 Description of AquaCrop model

The principle of the AquaCrop model is the crop yield–water effect relationship proposed by Doorenbos and Kassam (1979), which is expressed as follows:

\[
\frac{Y_m - Y_a}{Y_m} = K_y \left( \frac{ET_m - ET_a}{ET_m} \right),
\]

where \(Y_m\) and \(Y_a\) are the maximum output (kg m⁻²) and actual output (kg m⁻²), respectively; \(ET_m\) is the maximum evapotranspiration (mm); \(ET_a\) is the actual evapotranspiration (mm); and \(K_y\) is the crop yield response factor (dimensionless).

In AquaCrop, \(ET\) is decomposed into evaporation (\(E\)) and transpiration (\(T_c\)), which can avoid the interference of soil evaporation on crop yield, especially when the canopy coverage reaches the maximum (CCmax). The core formula of AquaCrop is as follows (Steduto et al., 2009):

\[
B = WP^* \cdot \sum \frac{T_c}{ET_0},
\]

and

\[
Y = B \cdot HI,
\]

where \(WP^*\) is the normalized crop water productivity (kg m⁻²), and its value varies with the annual average CO₂ concentration and the difference in crop species; \(B\) is the cumulative aboveground biomass production (kg m⁻²); \(T_c\) is the daily crop transpiration (mm day⁻¹); \(ET_0\) is the daily reference evapotranspiration (mm day⁻¹); \(Y\) is the yield production (kg m⁻²); and \(HI\) is the harvest index (%).

In the AquaCrop model, the aboveground biomass is simulated by the normalized water productivity (\(WP^*\)) (Equation (2)). The \(WP^*\) is normalized for atmospheric CO₂ concentration, using the annual mean CO₂ concentration measured at Mauna Loa Observatory, Hawaii, for the individual years. The year 2000, with a mean CO₂ concentration of 369.41 ppm, is chosen as the reference year for CO₂. The actual concentration of CO₂ will affect \(WP^*\). Rising CO₂ concentrations are a novel environmental aspect that should be considered when projections for future agricultural productivity are made. In addition to a reducing effect on stomatal conductance and crop transpiration, elevated CO₂ concentrations can stimulate crop production. AquaCrop will adjust \(WP^*\) when running a simulation for a year at which the atmospheric CO₂ concentration differs from its reference value (369.41 ppm). The adjustment is obtained by multiplying \(WP^*\) with the correction coefficient \(f_{CO2}\) (Vanuytrecht, Raes, & Willems, 2011). The coefficient considers the difference between the reference value and the atmospheric composition for that year:

\[
WP^*_{adj} = f_{CO2} WP^*,
\]

and

\[
0 \leq w = \left( 1 - \frac{550 - [CO_2]_i}{550 - [CO_2]_0} \right) \leq 1,
\]

| Irrigation date (month/day) | Net irrigation amount (mm) | Irrigation date (month/day) |
|-----------------------------|----------------------------|-----------------------------|
| 12/11 (10/25)               | 60 50 40                   | 11/27 (10/23)               |
| 4/2                         | 60 50 40                   | 4/16                        |
| 5/13                        | 60 50 40                   | 5/17                        |

**Table 1** The 2017 ~ 2019 winter wheat irrigation scheme
where WP*adj is WP* adjusted for CO2; \( f_{\text{CO2}} \) is the correction coefficient for CO2; \([\text{CO2}]_f\) is the reference atmospheric CO2 concentration (369.41 ppm); \([\text{CO2}]_i\) is the actual atmospheric CO2 concentration for year \( i \) (ppm); the value of \( b_{\text{stead}} \) is 0.000138 (Steduto et al., 2007); \( b_{\text{FACE}} \) is 0.001165 (derived from FACE experiments); \( w \) is the weighing factor, for which the threshold of 550 ppm is selected as the representing value for the elevated CO2 maintained in the FACE experiments; and \( f_{\text{sink}} \) is the crop sink strength coefficient. The value of \( f_{\text{sink}} \) is used as zero in this study (based on an analysis of crop responses in FACE environments by Vanuytrecht, Raes, & Willems, 2011).

\[
f_{\text{CO2}} = \frac{([\text{CO2}]_f/[\text{CO2}]_i)}{1 + ([\text{CO2}]_i- [\text{CO2}]_a) [(1 - w)b_{\text{stead}} + w(f_{\text{sink}}b_{\text{stead}} + (1 - f_{\text{sink}})b_{\text{FACE}})]},
\]

where \( M \) is the model output, with winter wheat biomass and yield as the output result; \( e_i \) is different model parameters; \( \Delta e_i \) is the slight disturbance of the \( e_i \) parameter; the \( S \) value is the size of the sensitivity and dimensionless value; and the sensitivity index is divided into four grades (Table 2). A higher \( S \) value indicates that the parameter has a higher impact on the results of the model output (Table 3).

The extremely sensitive to both biomass and yield was crop water productivity WP*; the extremely sensitive to yield was the harvest index establishment time; the parameter sensitive to biomass and yield was the maximum canopy cover; and the sensitive to yield was the reference harvest index HI0; the generally sensitive to biomass and yield was the duration of canopy senescence; the generally sensitive to biomass was the initial soil moisture content; and the effects of other parameters on biomass and yield were insensitive. In summary, it is recommended that the parameters with higher sensitivity should be considered and appropriately adjusted.

Depending on the calculated parameter sensitivity \( S \), some parameters have a greater impact on the simulation results of the model, such as WP*, HI0 and the maximum canopy coverage. To improve the simulation accuracy, the parameter calibration was reasonably adjusted for parameters such as WP*, HI0 and the maximum canopy coverage.

### 2.3 Construction of AquaCrop model

#### 2.3.1 Sensitivity analysis of AquaCrop model parameters

The most important parameters of crops included initial canopy coverage, threshold for extreme growth temperature, maximum effective root depth and planting density. The soil parameters in the model included: saturated moisture content, permanent wilting point content and initial value of field capacity, which need to be set according to the soil characteristics of the experimental fields.

The value of the input parameters of the AquaCrop crop model has a certain impact on the output of the model, and it is necessary to determine the impact of each parameter on the output through an appropriate test method. Sensitivity analysis of the main parameters (soil parameters and crop parameters) in the model was performed using the local analysis method (Tian et al., 2010). The local analysis method was a parameter sensitivity analysis of a certain point in the multidimensional parameter space, and the parameter sensitivity \( S \) was calculated by default value or assignment at this point. The sensitive value \( S \) was worth changing \( \Delta e \) while keeping the other parameters unchanged:

\[
S = \left| \frac{M(e_1, \ldots, e_i+\Delta e_i, \ldots, e_n) - M(e_1, \ldots, e_i, \ldots, e_n)}{\Delta e_i} \right| \times 100\% , \quad (7)
\]

### Table 2: Sensitivity index \( S \) grading table

| Grade | \( |S| \)  | Sensitivity      |
|-------|--------|-----------------|
| I     | 0 ≤ |S| < 5 | Insensitive     |
| II    | 5 ≤ |S| < 20 | Generally sensitive |
| III   | 20 ≤ |S| < 100 | Sensitive       |
| IV    | |S| ≥ 100 | Extremely sensitive |

The soil texture in the experimental fields is loam. The depth of the soil in the experimental fields is 0 ~ 120 cm, which is divided into six layers, each with a thickness of 20 cm. The soil characteristics of each layer are shown in Table 4.
During the two-season winter wheat growth period of 2017–2019 (the seeding time was 25 October 2017 and 23 October 2018, respectively), soil samples of 0–60 cm depth were collected every 5–10 days, and the soil water content was measured by sampling every 10 cm. The soil water content was measured 1 day before irrigation and 1, 2 and 3 days after irrigation in the key growth stages of winter wheat (seeding period, overwintering period, jointing period, filling period and maturity period).

The meteorological data came from the data monitored by the automatic meteorological station, with a multifactor automatic weather station produced by the domestic manufacturer in China, according to the observation standards of the World Meteorological Organization. It was installed in the experimental fields, whose data were recorded at intervals of 30 min, including temperature, relative humidity, wind speed at 2 m altitude, duration of sunshine, atmospheric pressure, rainfall, heat flux, net radiation, etc. The bias of the recording data from this climate station was calibrated by the manufacturer. The extremums in the observed data were first excluded, and then the remaining data were processed evenly to obtain the sample mean. Reference evapotranspiration (ET0) can be estimated by the Penman–Monteith equation, and the ET0 calculation software recommended by the Land and Water Division of the FAO was applied to calculate the reference crop evapotranspiration.

\[
ET_0 = \frac{0.408\Delta(R_n - G) + \frac{900}{R_n + 0.37T}U_2(e_s - e_a)}{\Delta + \gamma(1 + 0.34U_2)},
\]

where \(R_n\) is the net radiation on the crop surface (MJ m\(^{-2}\) day\(^{-1}\)); \(G\) is the soil heat flux (MJ m\(^{-2}\) day\(^{-1}\)); \(T\) is the average temperature (°C); \(U_2\) is the average wind speed at a height of 2 m (m s\(^{-1}\)); \(e_s\) is the saturated water pressure (kPa); \(e_a\) is the actual water pressure (kPa); \(\Delta\) is the slope of the saturated water vapour pressure and temperature curve (kPa °C\(^{-1}\)); and \(\gamma\) is the dry and wet surface constant (kPa °C\(^{-1}\)).

The concentration of CO\(_2\) gas was measured using Agilent 5890 Series II gas chromatographs in the winter wheat experimental field. The conditions for analysing and detecting atmospheric CO\(_2\) with the 5890 SERIES II gas chromatograph were as follows: silica gel column

| Table 3 | Parameter sensitivity analysis of the AquaCrop model |
|---|---|---|---|
| Parameters | Sensitive value S (%) | Parameters | Sensitive value S (%) |
| Biomass | Yield | Biomass | Yield |
| Planting density | 1.038 | 0.959 | Maximum effective root depth \(Z_{\text{max}}\) | 1.189 | 0.728 |
| Maximum canopy coverage | 61.621 | 61.546 | Crop water productivity WP* | 100.007 | 100.052 |
| Maximum canopy cover time reached | 1.989 | 1.533 | Reference harvest index \(H_0\) | 0.000 | 98.867 |
| The duration of canopy senescence | 8.304 | 8.419 | The harvest index establishing | 0.000 | 110.628 |
| Flowering time | 0.836 | 1.579 | Crop growth temperature threshold | 2.054 | 2.158 |
| Initial soil water content | 7.564 | 4.794 | Wilting water content | 4.209 | 2.426 |
| Field capacity | 2.281 | 2.636 | Saturated water content | 0.000 | 0.000 |
| Soil thickness | 2.465 | 3.202 | Runoff curve value | 0.912 | 1.095 |

| Table 4 | Soil parameters of study area |
|---|---|---|---|---|---|---|---|---|
| Soil parameters | Thickness (cm) | 0 ~ 20 | 20 ~ 40 | 40 ~ 60 | 60 ~ 80 | 80 ~ 100 | 100 ~ 120 |
| Silt content (%) | 92.04 | 88.37 | 90.66 | 60.32 | 58.60 | 57.36 |
| Clay content (%) | 3.30 | 4.73 | 4.46 | 30.88 | 31.45 | 31.88 |
| Sand content (%) | 4.65 | 6.90 | 4.88 | 8.80 | 9.95 | 10.76 |
| Permanent wilting point (m\(^3\)·m\(^{-3}\)) | 10.6 | 10.8 | 11.3 | 13.6 | 13.6 | 14.3 |
| Soil bulk density (g·cm\(^{-3}\)) | 1.21 | 1.23 | 1.29 | 1.38 | 1.47 | 1.45 |
| Water content at saturation (weight) (%) | 42.14 | 42.63 | 42.56 | 46.05 | 47.17 | 47.25 |
| Field capacity (weight) (%) | 23.27 | 23.78 | 26.93 | 30.27 | 25.17 | 28.74 |
(aged at 150°C for 24 h before measurement), injection temperature was 130°C, oven temperature was 120°C and detector temperature was 150°C. The carrier gas of thermal conductivity detection (TCD) was high-purity N₂ (mol/mol, ≥99.999%) with a flow velocity of 40 ml/min; the sample volume of the gas was 1.0 ml, and the retention time of the CO₂ peak area on the chromatogram was 1.5 min.

The CO₂ concentration of atmospheric samples was determined within 2 days after being sampled by using a gas chromatograph. When CO₂ samples were collected, the atmospheric temperature was recorded at the same time each time. The gas samples were collected by using professional gas pump equipment, a hand-held gas sampling pump with a gas flow of 1.5 L/min and a standard air pressure of 0.03 MPa, starting from 10 o’clock in the morning for a total of four times every 20 min. The gas sample was collected every 5 ~ 7 days, and the sample gas was added 2 ~ 3 times in the case of irrigation, fertilization, etc.

For the CO₂ concentration detection method, a standard gas with a known CO₂ concentration was injected into the gas chromatograph to obtain the stable peak area values of the standard gas (the bias of two consecutive peak areas was within 0.1%). The CO₂ concentration of the sample gas was detected based on the peak area and the known CO₂ concentration of the standard gas.

The change curve of atmospheric CO₂ concentration in the two seasons of winter wheat (2017 ~ 2018 and 2018 ~ 2019) is shown in Figure 2. The two average atmospheric CO₂ concentrations during the growth period of winter wheat were 462.6 and 478.0 ppm, respectively. Based on the measured CO₂ concentrations, a CO₂ database suitable for the local climatic conditions in the experimental fields was established instead of the default CO₂ database (Maunaloa. CO₂) provided by the model itself.

AquaCrop provided physiological parameters for 14 crops, including cotton, corn, wheat, potato and rice. Some parameters were conservative in the AquaCrop winter wheat crop model (Table 5). Other winter wheat parameters need to be calibrated by the AquaCrop model (the specific parameter types are described in the Winter Wheat section of the AquaCrop Crop Model Reference Manual).

2.3.3 | Model evaluation

The performance of the model was evaluated using the following indicators: the relative error (RE), the root mean square error (RMSE), residual coefficient method (CRM), normalized root mean square error (NRMSE) and determination coefficient ($R^2$).

$$RE = \left| \frac{O_i - P_i}{O_i} \right|,$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (P_i - O_i)^2}{n}}.$$

| Table 5  | Conservative parameters of the AquaCrop model |
|----------|-----------------------------------------------|
| Description | Value | Unit |
| Soil surface covered by an individual seedling at 90% emergence | 1.5 | cm² |
| Base temperature | 0.0 | °C |
| Upper temperature | 26.0 | °C |
| Crop determinacy linked with flowering | YES | – |
| Effect of canopy cover in reducing soil evaporation during the late season stage | 1.5 | – |
| Effect of canopy cover in reducing soil evaporation during the late season stage | 50 | – |
| Allowable maximum increase (%) of specified HI | 15 | % |
| Minimum air temperature below which pollination starts to fail (cold stress) | 5 | °C |
| Maximum air temperature above which pollination starts to fail (heat stress) | 35 | °C |
| Water productivity normalized for ET₀ and CO₂ | 15.0 | g·m⁻² |

Abbreviations: ET₀, reference evapotranspiration; HI, harvest index.
where \( n \) is the total number of observations of the sample and \( O_i \) and \( P_i \) are the observations and simulation values, respectively. \( O \) and \( P \) are the average of all observation and simulation values, respectively. RE describes the accuracy of the simulation value, and when the RE is within \( \pm 20\% \), the model can simulate the growth of crops well. RMSE indicates the deviation between the observed value and the simulation value. The smaller the value, the higher the accuracy of the model. The smaller the CRM value of the coefficient, the better the simulation effect. When the value of NRMSE is less than 10%, the simulation result is good, while a value between 10% and 20% indicates that the simulation effect is high. A value between 10% and 20% indicates that the simulation effect is good, while a value between 20% and 30% indicates that the simulation effect is average. The value of \( R^2 \) ranges from 0 to 1, with values close to 1 indicating good agreement, and typically values greater than 0.5 are considered acceptable in watershed simulations (Moriasi et al., 2007).

### 2.3.4 Determination of actual evapotranspiration

The \( \text{ET}_a \), called measured evapotranspiration, can be calculated according to the water balance method by using the rainfall and soil water content data. The water balance equation is as follows:

\[
\text{ET}_a = W_0 - W_t + P + I + K - R - D,
\]

where \( \text{ET}_a \) is the actual evapotranspiration (mm); \( W_0 \) and \( W_t \) are the soil water storage at the beginning and the end of the calculation period (mm); \( P \) is the total precipitation (mm); \( I \) is the amount of irrigation water (mm); \( K \) is the amount of groundwater recharge to the upper layer, and because the average buried depth of groundwater is approximately 15 m in the study area, the amount of groundwater recharge can be ignored (mm); \( R \) is the surface runoff (mm); and \( D \) is the deep leakage (mm). Due to the relatively small amount of rainfall (or irrigation) and barrier effect of the ridge of the field, the actual amount of surface runoff is relatively small and kept in fields; in addition, the amount of deep leakage loss is also quite small, so surface runoff and deep leakage can be ignored (Barros, Isidoro, & Aragüés, 2011; Mu & Wang, 2017).

### 3 RESULTS AND DISCUSSION

#### 3.1 Impact analysis of parameters under different CO2 databases

The calibration parameters of the AquaCrop under two different CO2 databases are shown in Table 6. The calibration parameters included harvest index HI, the maximum root depth, water productivity, crop growth temperature etc. According to Equations (4)–(6), the values in parentheses are the adjusted values of WP*. When the default CO2 database was used in the model, there was little influence on the calibration parameters of the model. When the value of \( f_{\text{CO2}} \) is calculated using the measured CO2 concentration value, the calculated WP* value will increase. In this study, the results will be 8% larger than the values calculated with the default CO2 data values.

| Model parameters                                      | Default CO2 | Measured CO2 |
|-------------------------------------------------------|-------------|--------------|
| Planting to maturity (days)                           | 230         | 230          |
| Maximum rooting depth (m)                            | 1.40        | 1.40         |
| Harvest index (HI) (%)                                | 46          | 46           |
| Plant density (plants m\(^{-2}\))                     | 318.75      | 318.75       |
| Water productivity normalized for ET\(_0\) and CO2 (g·m\(^{-2}\)) | 15 (15.9)   | 15 (17.2)    |
| Length to build up HI (days)                          | 34          | 34           |
| Planting to flowering (days)                          | 191         | 191          |
| Planting to maximum canopy cover (days)               | 196         | 196          |
| Maximum canopy cover (%)                              | 96          | 96           |
| Base temperature (°C)                                 | 0           | 0            |
| Upper temperature (°C)                                | 26          | 26           |

**Table 6** Calibration of some parameters of AquaCrop model under two CO2 databases

Abbreviation: ET\(_0\), reference evapotranspiration.
3.2 Analysis of biomass and yield simulation results under two CO₂ databases

To analyse the differences in simulation results using the various CO₂ databases, the default CO₂ database (Maunaloa. CO₂) and the measured CO₂ database were used. The results of the winter wheat biomass under different CO₂ databases are shown in Tables 7 and 9, respectively, and the results of the yield are shown in Tables 8 and 10, respectively.

The RE value range of the winter wheat biomass simulation in the 2017~2018 season was 1%~2% under the default CO₂ database (Maunaloa. CO₂) in Table 7, and the values in the 2018~2019 season were 0%~1%. The CRM value of the winter wheat biomass simulation values in the 2017~2018 season was −0.6% under the default CO₂ database (Maunaloa. CO₂), and the value in the 2018~2019 season was −0.5%. The RMSE value was 0.182 t·ha⁻¹ in the 2017~2018 season, and the value in the 2018~2019 season was 0.093 t·ha⁻¹. The value of NRMSE in the 2017~2018 season was 1.4%, and the value in the 2018~2019 season was 0.6%. The biases of the RE, absolute CRM and NRMSE between the simulated and measured values of winter wheat biomass were acceptable and within 1.5%.

The RE value range of the winter wheat yield simulation in the 2017~2018 season was 0.07%~0.6% under the default CO₂ database (Maunaloa. CO₂) in Table 8, and the values in the 2018~2019 season were 0.06%~3%. The CRM value in the 2017~2018 season was 0.2%, and the CRM value in the 2018~2019 season was −1.2%. The RMSE value for winter wheat in the 2017~2018 season was 0.018 t·ha⁻¹, and the value in the 2018~2019 season was 0.126 t·ha⁻¹. The value of NRMSE in the 2017~2018 season was 0.3%, and the value in the 2018~2019 season was 1.9%. Similarly, the biases of the RE, absolute CRM and NRMSE between the simulated and measured values of winter wheat yield were within 3.5%.

### Table 7 Biomass of winter wheat at different irrigation levels (Maunaloa. CO₂)

| Planting season | Irrigation level | Simulated (t·ha⁻¹) | Measured (t·ha⁻¹) | RE (%) | CRM (%) | RMSE (t·ha⁻¹) | NRMSE (%) |
|-----------------|-----------------|--------------------|-------------------|--------|---------|---------------|-----------|
| 2017~2018       | T1              | 13.372             | 13.214            | 1.196  | −0.554  | 0.182         | 1.423     |
|                 | T2              | 12.790             | 13.030            | 1.842  | −0.527  | 0.182         | 1.423     |
|                 | T3              | 12.259             | 12.390            | 1.057  | 0.093   | 0.182         | 1.423     |
| 2018~2019       | T1              | 15.028             | 15.028            | 0      | 0       | 0             | 0.653     |
|                 | T2              | 14.284             | 14.418            | 0.29   | −0.527  | 0.093         | 0.653     |
|                 | T3              | 13.357             | 13.268            | 0.671  | 0.093   | 0.182         | 1.423     |

Abbreviations: CRM, residual coefficient method; NRMSE, normalized root mean square error; RE, relative error; RMSE, root mean square error.

### Table 8 Yield of winter wheat at different irrigation levels (Maunaloa. CO₂)

| Planting season | Irrigation level | Simulated (t·ha⁻¹) | Measured (t·ha⁻¹) | RE (%) | CRM (%) | RMSE (t·ha⁻¹) | NRMSE (%) |
|-----------------|-----------------|--------------------|-------------------|--------|---------|---------------|-----------|
| 2017~2018       | T1              | 6.126              | 6.119             | 0.114  | 0.237   | 0.018         | 0.313     |
|                 | T2              | 5.974              | 5.970             | 0.067  | 0.552   | 0.018         | 0.313     |
|                 | T3              | 5.641              | 5.610             | 0.552  | 0.018   | 0.093         | 0.653     |
| 2018~2019       | T1              | 6.921              | 7.139             | 3.054  | −1.180  | 0.126         | 1.920     |
|                 | T2              | 6.733              | 6.729             | 0.059  | 0.126   | 0.093         | 0.653     |
|                 | T3              | 6.087              | 6.106             | 0.311  | 0.126   | 0.093         | 0.653     |

Abbreviations: CRM, residual coefficient method; NRMSE, normalized root mean square error; RE, relative error; RMSE, root mean square error.
The RE value range of the winter wheat biomass simulation in the 2017/2018 season was 0.5% – 1.2% under the measured CO2 database in Table 9, and the values in the 2018/2019 season were 0.02% – 0.3%. The CRM of winter wheat in the 2017/2018 season was –0.3%, and the CRM in the 2018/2019 season was 0.06%. The RMSE value was 0.105 t·ha⁻¹, and the value in the 2018/2019 season was 0.0247 t·ha⁻¹. The value of NRMSE in the 2017/2018 season was 0.8%, and the value in the 2018/2019 season was 0.2%. The biases of the RE, absolute CRM and NRMSE between the simulated and measured values of winter wheat biomass were acceptable and within 1.5%.

The RE value range of the winter wheat yield simulation in the 2017/2018 season was 0.5% – 1.2% under the measured CO2 database in Table 9, and the values in the 2018/2019 season were 0.02% – 0.3%. The CRM of winter wheat in the 2017/2018 season was –0.3%, and the CRM in the 2018/2019 season was 0.06%. The RMSE value was 0.105 t·ha⁻¹, and the value in the 2018/2019 season was 0.0247 t·ha⁻¹. The value of NRMSE in the 2017/2018 season was 0.8%, and the value in the 2018/2019 season was 0.2%. The biases of the RE, absolute CRM and NRMSE between the simulated and measured values of winter wheat biomass were acceptable and within 1.5%.

### TABLE 9  Biomass of winter wheat at different irrigation levels (measured CO2)

| Planting season | Irrigation level | Simulated (t·ha⁻¹) | Measured (t·ha⁻¹) | RE (%) | CRM (%) | RMSE (t·ha⁻¹) | NRMSE (%) |
|-----------------|-----------------|-------------------|-------------------|--------|---------|---------------|-----------|
| 2017 ~ 2018     | T1              | 13.310            | 13.214            | 0.721  |         | 0.105         | 0.819     |
|                 | T2              | 12.968            | 13.030            | 0.478  | −0.280  |               |           |
|                 | T3              | 12.248            | 12.390            | 1.159  |         |               |           |
| 2018 ~ 2019     | T1              | 15.013            | 15.028            | 0.099  |         |               |           |
|                 | T2              | 14.458            | 14.418            | 0.277  | 0.063   | 0.0247        | 0.173     |
|                 | T3              | 13.270            | 13.268            | 0.015  |         |               |           |

Abbreviations: CRM, residual coefficient method; NRMSE, normalized root mean square error; RE, relative error; RMSE, root mean square error.

### TABLE 10  Winter wheat yield at different irrigation levels (measured CO2)

| Planting season | Irrigation level | Simulated (t·ha⁻¹) | Measured (t·ha⁻¹) | RE (%) | CRM (%) | RMSE (t·ha⁻¹) | NRMSE (%) |
|-----------------|-----------------|-------------------|-------------------|--------|---------|---------------|-----------|
| 2017 ~ 2018     | T1              | 6.193             | 6.119             | 1.195  |         | 0.047         | 0.792     |
|                 | T2              | 5.988             | 5.970             | 0.301  | 0.679   |               |           |
|                 | T3              | 5.639             | 5.610             | 0.280  | 0.105   |               |           |
| 2018 ~ 2019     | T1              | 7.113             | 7.139             | 0.366  |         |               |           |
|                 | T2              | 6.800             | 6.729             | 1.044  | 0.458   | 0.051         | 0.768     |
|                 | T3              | 6.153             | 6.106             | 0.764  |         |               |           |

Abbreviations: CRM, residual coefficient method; NRMSE, normalized root mean square error; RE, relative error; RMSE, root mean square error.

![FIGURE 3](image-url)  
Linear fitted relationship between measured and simulated values of biomass

The RE value range of the winter wheat yield simulation in the 2017 ~ 2018 season was 0.5% ~ 1.2% under the measured CO2 database in Table 9, and the values in the 2018 ~ 2019 season were 0.02% ~ 0.3%. The CRM of winter wheat in the 2017 ~ 2018 season was –0.3%, and the CRM in the 2018 ~ 2019 season was 0.06%. The RMSE value was 0.105 t·ha⁻¹, and the value in the 2018 ~ 2019 season was 0.0247 t·ha⁻¹. The value of NRMSE in the 2017 ~ 2018 season was 0.8%, and the value in the 2018 ~ 2019 season was 0.2%. The biases of the RE, absolute CRM and NRMSE between the simulated and measured values of winter wheat biomass were acceptable and within 1.5%.
As shown in Figure 3 and Figure 4, the $R^2$ values of biomass under different CO$_2$ databases for different irrigation levels of winter wheat were 0.992 and 0.967, respectively, and the $R^2$ values of the yield were 0.974 and 0.857, respectively. The accuracy of the biomass and yield simulations under the default and measured CO$_2$ database were both good. Compared with the default CO$_2$ database, the simulation accuracy of winter wheat yield and biomass under the measured CO$_2$ database was higher. Therefore, the measured CO$_2$ database can improve the model simulation accuracy. Although the measured data can effectively improve the accuracy of the model, the requirements on the data are high, which often does not meet the requirements in many research areas. Some researchers (Fu et al., 2012; Li, Yu, & Zhao, 2019; Li et al., 2020; Xing et al., 2016) used the default CO$_2$ database to construct the AquaCrop model in the study area, which indicated that the model had good accuracy. The water use efficiency of winter wheat in the 2018 ~ 2019 season under the measured CO$_2$ database was 1.63, 1.72 and 1.56 kg/m$^3$, respectively, under the three irrigation levels. The water use efficiency under the default CO$_2$ database was 1.66, 1.71 and 1.54 kg/m$^3$, respectively. The water use efficiency under the two CO$_2$ databases was the highest when the irrigation level was T2, which is consistent with the conclusion of Xing et al. (2016). The results showed that the higher and lower irrigation water reduced the water use efficiency of winter wheat. The quantity of the appropriate irrigation water was conducive to maintaining the highest water use efficiency of winter wheat, according to the growth status of winter wheat.

4 | VALIDATION OF AQUACROP MODEL UNDER MEASURED CO$_2$ DATABASE

4.1 | Validation analysis of field evapotranspiration

The evapotranspiration calculated by the AquaCrop model was compared with the actual evapotranspiration. Figure 5 shows that the change process of measured and simulated evapotranspiration was consistent under different irrigation levels. The field evapotranspiration was close to the measured value in the seedling, overwintering and mature periods, and the RE was between 2% and 6%. Due to the combined effect of rainfall and irrigation, there was some bias between the measured values and the simulated values during the filling and waxing period of winter wheat. The maximum bias value between the measured values and simulated values of ET was close to 1 mm, and the RE was approximately 10%. In general, the simulated values of field evapotranspiration were consistent with the measured values of winter wheat in the 2018 ~ 2019 season under different irrigation levels.

The evapotranspiration of winter wheat was dominated by field soil evaporation before and after the seedling stage, and soil transpiration accounted for approximately 90%. The main reason was that the crop plants were small, and the bare soil was dominant in the field. Therefore, the transpiration of the crop was smaller than the soil evaporation. With the development of seedlings and the decrease in air temperature, the evaporation capacity of field soil weakened. Field evapotranspiration, soil evaporation and crop transpiration of winter wheat in the overwintering period were very small, with average values of 0.58, 0.43 and 0.11 mm, respectively. When winter wheat was in the jointing stage, the plants grew and developed rapidly as the temperature increased, and the canopy of winter wheat also expanded rapidly. The transpiration of crops started to increase, while the evaporation of soil started to decrease. The transpiration of winter wheat gradually reached the maximum value from the filling stage to the waxing stage. Field evapotranspiration and crop transpiration began to decrease; concurrently, soil evaporation began to increase during the mature period of winter wheat.

4.2 | Validation analysis of soil water content

The main factors affecting soil water storage were precipitation, ambient temperature, field irrigation and crop water consumption during the growth and development
of winter wheat. The AquaCrop model is a water-driven model, so the crop water consumption during the crop growth period determined the simulation precision of crop biomass and yield. The crop water consumption was mainly provided by the soil water content. Therefore, the performance of the AquaCrop model was determined by the dynamic change in soil water content (Ahmadi & Mosallaeepour, 2015). The process of soil water content change (within the effective root depth of 0 ~ 140 cm) in the test plots during the growth period of winter wheat in the 2018 ~ 2019 season is shown in Figure 6.

The bias between the simulated and measured values of the soil water content at irrigation amounts T1 and T3 was large, with a maximum bias value of up to 50 mm, and the RE was 16%. While the bias under the appropriate irrigation amount (T2) was small, as shown in Figure 6, with a maximum bias of close to 20 mm, the RE was 9%. The reason might be that the smaller irrigation amount (T3) had a more severe effect on the growth of winter wheat by water stress, which led to an increased demand for soil moisture during the growth of winter wheat, resulting in a large deviation between the actual measured soil water content and the simulated value. The larger irrigation amount (T1) may lead to deep leakage of soil water, resulting in a large deviation between the simulated value and the measured value. In addition, the simulation accuracy of the larger irrigation amount (T1) was higher than that of the lower irrigation amount (T3). The reason might be that when the soil was replenished with a large amount of irrigation, the soil could store redundant water to meet the growth of the crop. When the amount of irrigation was small, soil moisture could not be replenished, and the impact of water stress on crop growth increased. The simulated values of the AquaCrop model for soil water content at the three levels of irrigation were all higher than the measured values. The deviation of the simulation results might be caused by the differences in the soil structure and texture in the test plots. At the same time, the failure of the AquaCrop model to consider the variability of soil texture and
structure in the soil module was also the reason for the deviation of the simulated values from the actual measured values. Overall, the simulated values for soil water storage were larger than the measured values, but the simulated results largely reflected the dynamic changes in soil water content throughout the growth period of winter wheat.

5 | CONCLUSIONS

1. To examine whether the use of the default CO$_2$ database affected the simulation results, this paper built AquaCrop models based on the measured CO$_2$ database and the default CO$_2$ database. The results showed that the accuracy of the model simulation under both CO$_2$ databases was acceptable, the maximum RE of the simulated values of biomass and yield was below 4%, and the CRM and NRMSE values were within ±2%; the latter had higher simulation accuracy.

2. The difference between crop transpiration and soil evaporation under the two CO$_2$ databases was not obvious. The RE of the field evapotranspiration was between 2% and 6% compared with the measured value in the seedling, overwintering and mature periods. The maximum RE of the ET value between the measured values and simulated values was approximately 10%. In general, the simulated values of field evapotranspiration were consistent with the measured values of winter wheat at different irrigation levels. The maximum RE between the simulated and measured values of the soil water content at irrigation amounts T1 and T3 was 16%, while the RE under the appropriate irrigation amount (T2) was 9%.

3. The results of this study are regional but have a certain reference significance in areas where there are no measured data. The AquaCrop model uses 369.47 ppm
as the reference value of CO₂ concentration. The model assumes a future increase rate of CO₂ concentration of 2.0 ppm. If the predicted value differs greatly from the actual value, the accuracy of the model may be affected. However, how much bias can be caused by differences in CO₂ concentration is also a problem worthy of further study in the future.

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CONFLICT OF INTEREST
The authors declare that they have no competing interests.

DATA AVAILABILITY STATEMENT
The datasets used during the current study are available from the corresponding author on reasonable request.

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