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Influence of water use efficiency parameterizations on flux variance similarity-based partitioning of evapotranspiration

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ABSTRACT

Despite the high sensitivity of water use efficiency (WUE) estimates to intracellular carbon dioxide concentrations (c_i) in the Flux Variance Similarity (FVS)-based partitioning method, a systematic analysis of the sensitivity of WUE to c_i parameterizations has largely been lacking. Using high-frequency (10 Hz) eddy covariance data for two crop sites: wheat (*Triticum aestivum* L.) and canola (*Brassica napus* L.), we performed a sensitivity analysis of four c_i parameterizations (constant c_i value, constant c_i/c_a ratio, and c_i/c_a as square root and linear functions of vapor pressure deficit) and compared them with the optimized WUE approach with no adjustable parameter. The results illustrated the role of c_i parameterizations on the evapotranspiration (ET) partitioning results (*i.e.*, transpiration (T) to ET ratios). Notably, constant c_i value and constant c_i/c_a ratio parameterizations for the largest considered c_i values (commonly used default values in most previous studies) showed comparable T:ET with the optimized WUE approach. Additionally, all these three models produced reduced T:ET in wet periods and increased T:ET in dry periods. In contrast, square root and linear models were unable to accurately capture expected trends of T:ET for wet and dry periods, and also showed large discrepancies when compared with the optimal WUE approach. The results suggest that optimal parameterizations of c_i should be derived in constant c_i value and constant c_i/c_a ratio methods to accurately capture temporal variations of WUE and T:ET. The results also indicate the potential of the optimum model for inter-model comparison, especially in sensitivity analysis, for FVS partitioning in C_3 species. This study provides novel insights into the implications of the choice of parameterization on the WUE estimations and partitioning outcomes.

1. Introduction

Partitioned evaporation (E) and transpiration (T) are used for multiple purposes (e.g., input, calibration, and validation) in numerous land surface, satellite, and hydrological models (Dong et al., 2020; Kumar and Duffy, 2015; Stoy et al., 2019; Villegas et al., 2014). Additionally, partitioning of evapotranspiration (ET) is needed for assessing management strategies to reduce non-productive water loss in agricultural fields to conserve water (Wagle et al., 2020b; Zhou et al., 2018) as well as to improve our understanding of underlying biophysical processes that control E and T separately (Klosterhalfen et al., 2019; Kool et al., 2014).

Eddy covariance (EC), the most commonly used technique to directly measure ecosystem-level ET, cannot provide E and T separately. Flux Variance Similarity (FVS)-based partitioning technique was proposed in the past decade to separate stomatal and non-stomatal fluxes by examining the correlation structure using high-frequency (*i.e.*, 10 or 20 Hz) EC raw data (Scanlon and Kustas, 2010; Scanlon and Sahu, 2008). This method offers numerous unique advantages, including spatiotemporal representativeness, the potential for partitioning using past EC raw data, and no additional data requirement other than high-frequency EC data. However, the requirement of high-frequency (*i.e.*, 10 or 20 Hz) EC raw data and the computational complexity are some of the practical challenges of the FVS method. The method has shown good performance in diverse biomes, including grassland (Good et al., 2014; Wang et al., 2016), forest or woody plant covers (Sulman et al., 2016; Wang et al., 2010), various C_3 and C_4 grain crops (Rana et al., 2018; Scanlon and Kustas, 2010; Wagle et al., 2021b), sugarcane (*Saccharum officinarum* L.) (Anderson et al., 2017a), alfalfa (*Medicago sativa* L.) (Wagle et al., 2020b), and fruit plantations (Peddinti and Kambhammettu, 2019; Skaggs et al., 2018).

The FVS method uses estimated water use efficiency (WUE) at the

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leaf level as the only input for partitioning. Although it has been clear that WUE estimates greatly influence FVS partitioning outputs (Klosterhalfen et al., 2019; Sulman et al., 2016; Wagle et al., 2021b), leaf-level WUE estimates have been derived using a single method in most studies. The necessity of continuous estimates of WUE is a major potential source of uncertainty or error for FVS-based partitioning.

In Fluxpart – an open-source software for FVS partitioning (Skaggs et al., 2018), the default estimate of leaf-level WUE is computed as follows:

$$WUE = \left(\frac{1}{DR}\right)\left(\frac{c_a - c_i}{q_a - q_i}\right) \tag{1}$$

where c_a and q_a represent ambient concentrations of carbon dioxide (CO_2) and water vapor (H_2O), respectively, and c_i and q_i represent intercellular concentrations of CO_2 and H_2O, respectively. The molecular diffusivity (DR) ratio for H_2O and CO_2 fluxes through stomata is 1.6 (Massman, 1998). Above-canopy EC tower measurements can be used to derive c_a and q_a (Scanlon and Kustas, 2010). In Fluxpart, q_i is set to 100% relative humidity and the leaf temperature is assumed to be equal to the above-canopy air temperature (Skaggs et al., 2018). The c_i can be parametrized using different algorithms such as constant c_i value (Campbell and Norman, 2012), constant c_i/c_a ratio (Kim et al., 2006; Sinclair et al., 1984), linear function of vapor pressure deficit (VPD) (Morison and Gifford, 1983), square root function of VPD/c_a (Katul et al., 2009), and optimized approach (Scanlon et al., 2019). Out of these five WUE algorithms, four algorithms (constant c_i value, constant c_i/c_a ratio, linear, and square root) have adjustable parameters to estimate c_i (details are provided in the Methods). The optimum model does not have an adjustable parameter as WUE is derived solely based on EC statistics.

Our recent study showed substantially different performances of these five WUE algorithms owing to their inherent assumptions and necessities (Wagle et al., 2021b). Given that a detailed investigation of the sensitivity of WUE algorithms to partitioned fluxes is lacking (Klosterhalfen et al., 2019; Sulman et al., 2016), there is a need to assess the sensitivity of adjustable parameters of several WUE algorithms for FVS partitioning. In this study, we performed a sensitivity analysis using five coefficients in each of the four WUE algorithms and compared them with the outputs of the optimum model. We hypothesized that changing coefficients would greatly alter WUE estimates resulting in different partitioned outputs (*i.e.*, T:ET ratios) for all four WUE algorithms. The study provides novel insights into the role of c_i parameterizations on partitioned outputs from the FVS-based partitioning method.

2. Materials and methods

2.1. Study sites and EC measurements

This study was performed at two crop sites: wheat and canola. The sites are located at the United States Department of Agriculture (USDA), Agricultural Research Service, Grazinglands Research Laboratory near El Reno, Oklahoma, USA. The major soil types are the complex of Renfrow-Kirkland silt loams, Bethany silt loams, and Norge silt loams in both sites (USDA-NRCS, 1999).

These rainfed sites experience a temperate continental climate, with a long-term (1981-2010) annual rainfall of ~925 mm (Wagle et al., 2020a). Both wheat (*cv.* Gallagher) and canola crops were planted in rows (~19 cm apart) by mid-October 2016 and harvested in mid-June 2017. Both fields were conventionally tilled. The 2016-2017 growing season for wheat and canola was one of the most favorable growing seasons (*i.e.*, well-distributed seasonal rainfall of 517 mm and slightly warmer spring, with the absence of any severe drought periods). Both fields were managed for high yield potential using standard management (e.g., applications of fertilizer based on soil tests and applications of herbicide/pesticide as needed). Maximum dry biomass (aboveground) was approximately 1.3 kg m^{-2} for wheat and 0.82 kg m^{-2} for canola in April. Maximum LAI was approximately 7 m^2 m^{-2} for wheat and 4.75 m^2 m^{-2} for canola. Grain yield was approximately 4.86 t ha^{-1} for wheat and 1 t ha^{-1} for canola (roughly 50% of the grain yield was lost due to shattering because of delayed harvesting caused by rains).

Eddy covariance systems, comprised of a sonic anemometer (CSAT3 - Campbell Scientific Inc., Logan, UT, USA) and an open-path infrared gas analyzer (LI-7500 - LI-COR Inc., Lincoln, NE, USA), were deployed near the center of wheat (27.5 ha) and canola (17.2 ha) fields to collect EC measurements at 10 Hz frequency for the entire growing seasons. High-frequency (10 Hz) EC data were processed using the EddyPro software (LI–COR Inc., Lincoln, NE, USA) to compute 30 min values of ET. Fluxes with bad quality flags (*i.e.*, the quality flag of 2) and unreliable numbers or statistical outliers (beyond ±3.5 SD for 14 days) were removed (Sun et al., 2010; Wagle and Kakani, 2014; Zeeman et al., 2010). Gaps in fluxes were filled using the REddyProc package (Wutzler et al., 2018). Details on crop growth and development, EC measurements and data processing, and management practices in both fields for the study period can be found in a previous publication (Wagle et al., 2021a).

2.2. FVS partitioning of ET using multiple WUE algorithms, and sensitivity analysis

We used high-frequency (10 Hz) EC raw data to partition ET using Fluxpart (source code is accessible at https://github.com/usda-ars-ussl/fluxpart) (Skaggs et al., 2018). Leaf-level WUE is the only input for FVS partitioning. However, the following different models can be used to parametrize c_i for the estimates of leaf-level WUE in FVS partitioning:

i) Constant c_i value (Const_value): c_i (kg m^{-3}) is computed using a constant value. In Fluxpart, the default constant ppm value is 280 ppm for C_3 and 130 ppm for C_4 species (Campbell and Norman, 2012).

$$c_i = f(c_{i\_PPM}; temperature,\ pressure) \tag{2}$$

Measured c_i for four winter wheat cultivars under various meteorological conditions ranged from 120 to 300 ppm (Xue et al., 2004). Based on this finding, a range of 200 and 300 ppm was chosen for winter wheat for the sensitivity analysis in a previous study (Klosterhalfen et al., 2019). In this study, we chose 220, 240, 260, 280, and 300 ppm for c_i in both winter wheat and canola.

ii) Constant c_i/c_a ratio (Const_ratio): In Fluxpart, default constant c_i/c_a ratios (k) are 0.7 for C_3 (Sinclair et al., 1984) and 0.44 for C_4 species (Kim et al., 2006).

$$\frac{c_i}{c_a} = k \tag{3}$$

To match the same proportion of ranges from constant value (220 to 300 ppm), we computed c_i for five values of k ranging from 0.55 to 0.75 [e.g., k1 = 0.7(220/280) = 0.55 and k5 = 0.7(300/280) = 0.75].

iii) Linear: c_i/c_a is derived as a linear function of vapor pressure deficit (VPD)

$$\frac{c_i}{c_a} = b - m * VPD \tag{4}$$

where b is ~1 (unitless) and m is 1 (Pa^{-1}). In Fluxpart, default values for the (b, m) pair are (1, $1.6e^{-4}$) and (1, $2.7e^{-4}$) in C_3 and C_4 species, respectively (Morison and Gifford, 1983).

For sensitivity analysis in this study, we kept b =1 in all cases and changed the parameter m to match the ranges considered in constant value or constant ratio methods above. The value of m ranged from (m1) $2.4e^{-4}$ to (m5) $1.33e^{-4}$, with m4 is equal to default value of $1.6e^{-4}$.

iv) Square root (sqrt): c_i/c_a is determined as a function of the square root of (VPD/c_a) only in C_3 species (Katul et al., 2009), due to the lack of equivalent relationship between c_i/c_a and VPD in C_4 species (Leakey et al., 2019).

$$\frac{c_i}{c_a} = 1 - \left(DR*\lambda*\frac{VPD}{c_a}\right)^{0.5} \tag{5}$$

The default coefficient of λ (kg-CO_2 m^{-3} Pa^{-1}) in Fluxpart is $22e^{-9}$. For sensitivity analysis, we changed the parameter λ to match c_i ranges as considered in constant value or constant ratio methods above. The value of λ ranged from $49.5e^{-9}$ to $3.82e^{-9}$, with λ4 being equal to the default value of $22e^{-9}$.

v) Optimum (Opt): WUE is determined using the optimized approach (Scanlon et al., 2019) using only EC data (*i.e.*, no parameterized model is required to compute c_i).

$$WUE_{opt} = \frac{DR\cdot VPD\cdot m - \sqrt{DR\cdot VPD\cdot m(c_a + DR\cdot VPD\cdot m)}}{DR\cdot VPD} \tag{6}$$

where

$$m = -\frac{\sigma_c^2 F_q - R_{c,q}\sigma_q\sigma_c F_c}{\sigma_q^2 F_c - R_{c,q}\sigma_q\sigma_c F_q} \tag{7}$$

where R_{qc} represents the correlation coefficient for q and c. F_c and F_q represent c and q fluxes, respectively. σ_q and σ_c represent standard deviations of q and c, respectively. The Optimize approach may not be applicable in C_4 species due to the potential inconsistent formulation of $\overline{c_i}/\overline{c_a} \geq 0.5$ for C_4 physiology (Oren et al., 1999).

2.3. Gap filling of partitioned outputs and determining T:ET ratios

The FVS partitioning may not yield successful partitioned outputs for every 30 min time interval because high-frequency EC data for all times may not satisfy numerous theoretical and numerical constraints (e.g., incompatible EC data and WUE estimates) of FVS partitioning (Scanlon et al., 2019). Instead of gap-filling longer data gaps by interpolation, we created diurnal mean (half-hourly) values of T and ET, obtained from Fluxpart, for each week and then summed those half-hourly binned values to determine the weekly average T:ET (*i.e.*, a constant T:ET ratio for each week). These weekly average T:ET ratios were used to partition EC-measured daily ET to daily E and T.

3. Results and discussion

3.1. Seasonality of ET

The seasonality of ET was similar for wheat and canola due to their similar crop seasonality (Fig. 1). Both crops were planted by mid-October and harvested in mid-June. In both crops, the magnitudes of ET increased with increasing crop growth during the early growing season. Daily ET rates decreased to <1.0 mm around mid-December through mid-January due to cold temperatures and lower solar radiation. With increasing crop growth, rising temperature, and higher solar radiation, the magnitudes of ET began to increase after mid-January and peaked in early May for wheat and mid-May for canola, with 7-day average daily ET rates of approximately 5 and 4.7 mm for wheat and canola, respectively. The ET rates declined sharply during grain filling and senescence of crops.

3.2. Sensitivity of WUE estimates to c_i parameterizations

During the peak growth period, mean diurnal (monthly average) patterns of WUE estimates for the range of c_i parameters showed different magnitudes of variations for WUE algorithms (Fig. 2). For example, differences in WUE estimates using five c_i parameterizations for const_value and const_ratio were substantially larger during predawn hours, the periods of largest WUE (negative sign convention) due to smallest VPD values. However, WUE estimates using different c_i parameterizations for both const_value and const_ratio models were relatively similar from noon to the afternoon (*i.e.*, during periods of higher temperature, VPD, and solar irradiance). In both models, WUE estimates decreased (negative sign convention) with an increasing magnitude of

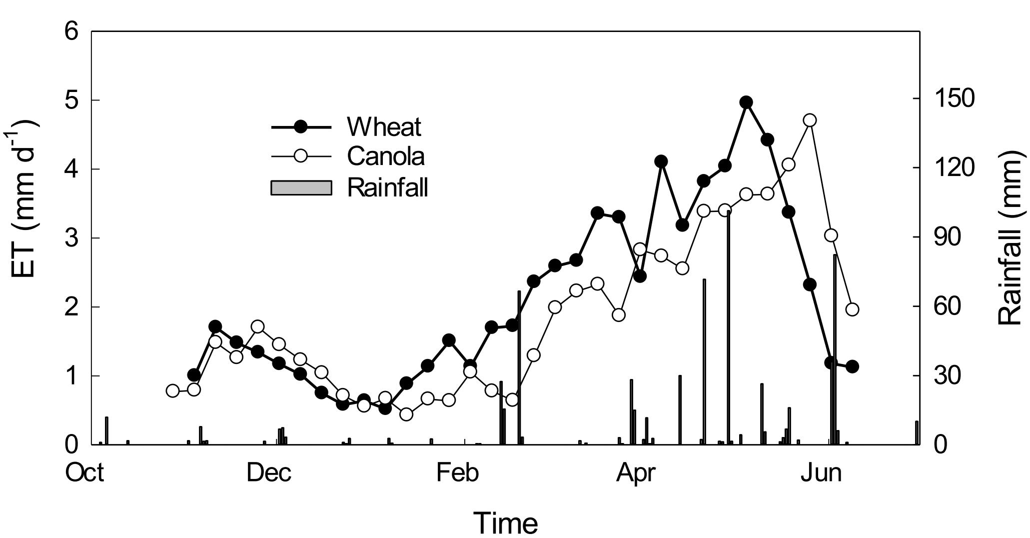

Fig. 1. Seasonal patterns of eddy covariance measured evapotranspiration (ET) in wheat and canola for the 2016-2017 growing season. Daily rainfall data are also shown.

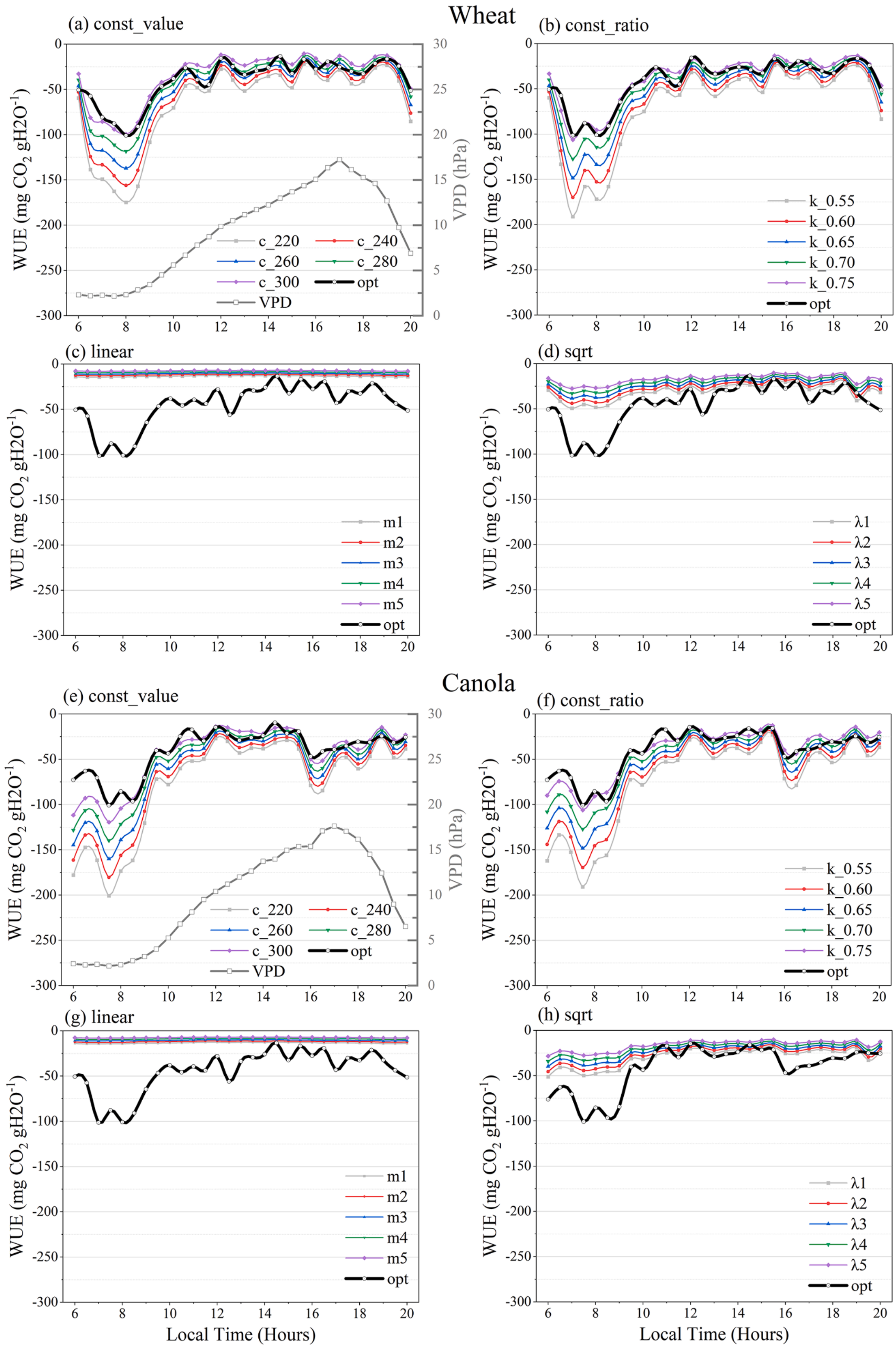

Fig. 2. Half-hourly binned (monthly mean) daytime patterns of water use efficiency (WUE) for different parameterizations of intercellular carbon dioxide concentrations in WUE algorithms for wheat and canola during peak growth (from March 15 to April 14 for both crops).

c_i. The WUE estimates from the opt model showed similar diurnal patterns as those from the const_value and const_ratio models in both wheat and canola. During predawn hours, the magnitudes of WUE for the opt model were similar to those for the largest c_i parameters for const_value (300 ppm) and const_ratio (0.75) models. The linear model produced estimated WUE with no clear diurnal patterns and negligible variations for custom input parameters. The sqrt model yielded WUE estimates with a smaller diurnal pattern [*i.e.*, slightly larger (negative sign convention) values during predawn hours] and smaller variations for the custom c_i parameters as compared to const_value and const_ratio. The results were consistent for both wheat and canola. These results support the hypothesis that the selection of an appropriate coefficient in WUE algorithms is required to accurately partition stomatal and non-stomatal fluxes.

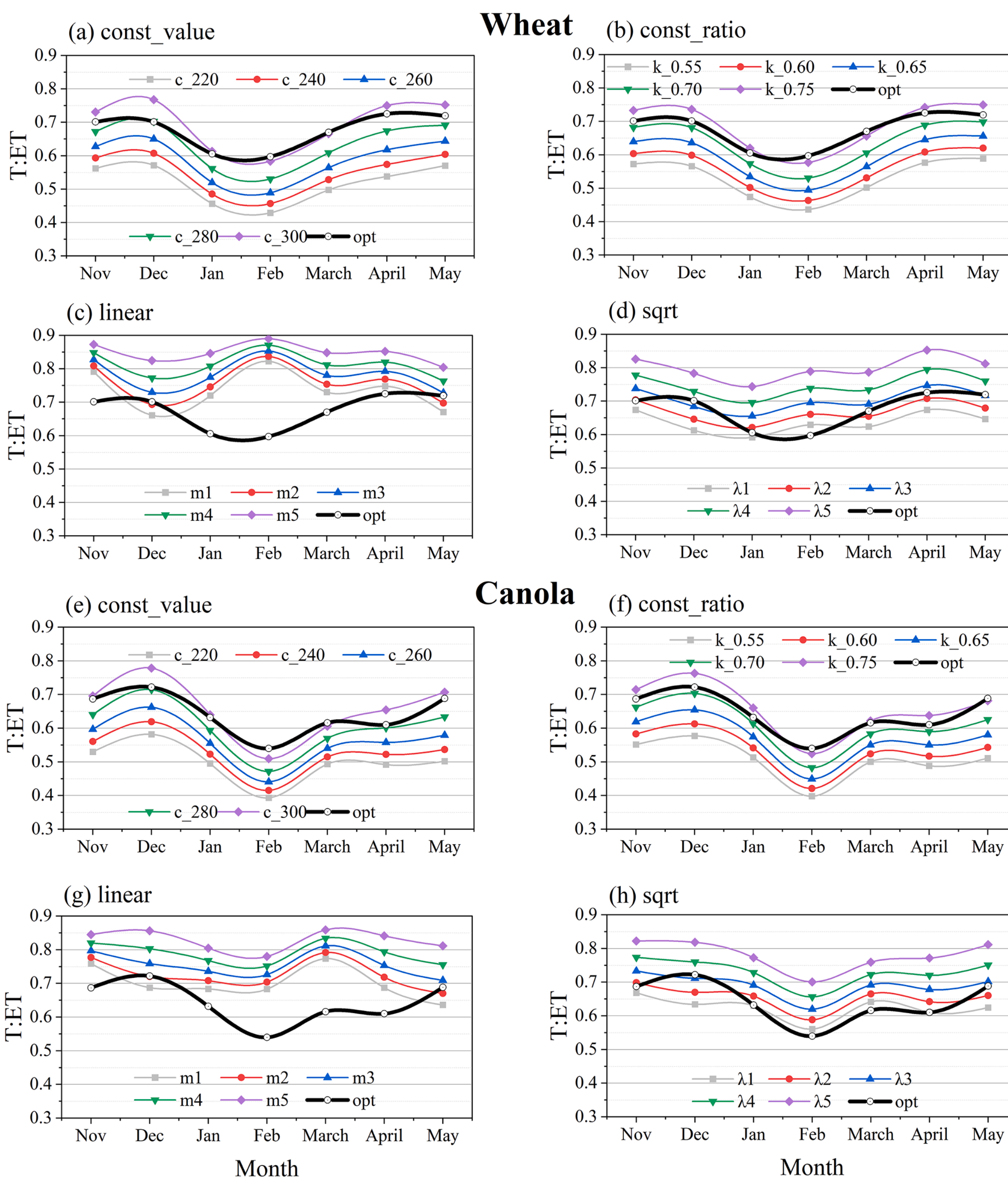

Fig. 3. Seasonal dynamics of transpiration (T) to evapotranspiration (ET) ratios for different parameterizations of intercellular carbon dioxide concentrations in leaf-level water use efficiency (WUE) algorithms for wheat and canola. The T:ET ratios were derived from sums of diurnal mean values (half-hourly binned) of T and ET for a month.

Large differences in diurnal patterns of WUE estimates by different WUE algorithms (Fig. 2) can be attributed to differences in their sensitivity to VPD. For both const_value and const_ratio, WUE is proportional to VPDˆ-1. For linear, WUE is insensitive to VPD. For sqrt, WUE is moderately sensitive to VPD as it is proportional to VPDˆ-0.5. For opt, WUE is not directly proportional to VPD, but it is closest to varying with VPDˆ-1 (similar to const_value and const_ratio). As a result, const_value, const_ratio, and opt models yielded similar diurnal patterns of WUE estimates.

In four winter wheat cultivars, measured c_i ranged from 120 to 300 ppm under various soil water potential and VPD conditions (Xue et al., 2004). Given that c_i is greatly influenced by soil water status and VPD (Monteith and Greenwood, 1986; Turner, 1986; Xue et al., 2004), our results highlight that errors in temporal variations of c_i estimates can lead to significant errors in WUE at a range of time scales. Notably, soil water status and VPD fluctuate over time during the growing season, resulting in significant impacts on gas exchange parameters. Additionally, VPD fluctuates even during the same day as it increases with increasing air temperature during the daytime and peaks in the late afternoon (around 4-5 pm local time as shown in Fig. 2a, e). Greater stomatal limitation (*i.e.*, partial or full stomatal closure) at higher VPD reduces c_i, resulting in decreased stomatal conductance (g_s) and net CO_2 assimilation rate (A_n). In addition, soil water stress may modulate WUE, g_s, and T simultaneously (Liu et al., 2020; Turner, 1986). Thus, using direct measurements of leaf-level WUE could be an option for improving the performance of FVS partitioning (Anderson et al., 2017b; Sulman et al., 2016). However, upscaling of non-continuous (e.g., only a few days in a season) leaf-level WUE measurements to canopies and ecosystems is a complicated process as underlying mechanisms and processes vary at those spatial scales (Medlyn et al., 2017).

As FVS partitioning requires continuous estimates of WUE at 30 min intervals, large differences in diurnal patterns of WUE for custom input c_i within the same WUE algorithm and among WUE algorithms, as shown in Fig. 2, can induce large discrepancies in partitioned outputs. Thus, we explore this next by comparing the sensitivity of T:ET ratios.

3.3. Differences in the seasonality of T:ET with WUE algorithms and c_i parameterizations

Seasonal patterns of T:ET for all WUE algorithms were consistent in both crops (Fig. 3). Seasonal patterns of T:ET were similar for const_value, const_ratio, opt, and sqrt models. The linear model produced a different seasonal pattern of T:ET ratios. The T:ET ratios for const_value, const_ratio, opt, and sqrt models decreased in the winter months (lowest in February) and increased with increasing temperature and crop growth in spring. The T:ET ratios for the linear model increased in January and February and decreased from March to May for wheat, but they slightly decreased in January and February, increased in March, and decreased during April-May for canola.

The largest discrepancy in T:ET ratios, obtained from different WUE algorithms, was found during the winter months. For example, monthly T:ET ratios from the opt model were ~0.6 compared to 0.7-0.9 found with the linear model for different c_i parameterizations during January-February in wheat. Similarly, for canola in January and February, T:ET ratios from the opt model were 0.63 and 0.54 compared to 0.7-0.8 (for different c_i parameterizations) obtained using the linear model. Notably, T:ET ratios of 0.8-0.9 for the linear model during winter months, when crop growth slows down and canopy coverage decreases due to physical damages, might be considered beyond the reasonable range. Even for the dry period during peak crop growth (*i.e.*, full canopy cover), T:ET ratios were only around ~0.8 in canola (Wagle et al., 2021a) and maize (*Zea mays* L.) (Zhou et al., 2016). These results illustrate that the choice of appropriate WUE algorithms can result in large discrepancies in seasonal patterns of T:ET ratios.

Additionally, differences in c_i parameterizations within the same WUE algorithm caused large differences in monthly T:ET ratios (Fig. 3). Monthly T:ET ratios generally differed by approximately 10-20% for the smallest and largest c_i parameters for all WUE algorithms in both crops. Monthly T:ET ratios obtained from the opt model were similar to T:ET ratios found with the largest c_i coefficients (which were usually used as default values in most previous studies) for const_value or const_ratio models in both crops. As compared to monthly T:ET ratios obtained using the opt model, T:ET ratios from linear and sqrt models were larger for most of the c_i parameters in both crops. Due to large variations in monthly T:ET ratios in response to input parameters throughout the growing season, we explore the impact of c_i parameterizations in WUE algorithms on seasonal T:ET ratios in the next section.

3.4. Sensitivity of seasonal T:ET ratios to c_i parameterizations

Overall, seasonal T:ET ratios in both wheat and canola increased (by 10-15% for the range of considered c_i values) with an increasing magnitude of c_i parameterization in all four WUE algorithms (Table 1). Smaller input of c_i yielded larger (negative sign convention) WUE values (Fig. 2), resulting from relatively smaller T losses, which leads to smaller T:ET ratios. In general, seasonal T:ET ratios were higher for sqrt and linear models than for const_value, const_ratio, and opt models. Lower WUE estimates by the sqrt and linear models (Fig. 2) resulted in higher T:ET ratios (*i.e.*, higher loss of T) for those models. In comparison, the seasonal T:ET ratio for the opt model was 0.71 in wheat (similar to the T:ET ratio for c_240 ppm and k_0.65) and 0.72 in canola (similar to the T:ET ratio of c_300 ppm and k_0.75).

Overall, seasonal T:ET ratios were smaller when T:ET ratios were determined only for the periods when partitioned fluxes were available for all five WUE algorithms (see T:ET ratios in parentheses in Table 1). However, variability in T:ET ratios with parameters still showed a similar variation (*i.e.*, 13-18% for the range of considered c_i values) as described above.

Additionally, successful fractions of partitioned outputs declined with the increasing magnitude of c_i in each WUE algorithm (Table 2). On average, the number of successful partitioned outputs decreased by ~10% for the range of considered coefficients in both crops. This reduction is related to the declining magnitude of WUE to the point that it is less than the magnitude of Fc/Fq (see Eq. (8) in Scanlon et al., 2019) with increasing c_i values (Fig. 2), which is theoretically not possible. Although the performance of different WUE algorithms may not be

Table 1
Seasonal average ratios of transpiration (T) to evapotranspiration (ET) for different parameterizations of water use efficiency (WUE) in wheat and canola. The T:ET ratios computed only for the periods when partitioning solutions were available for all algorithms are presented in parentheses.

WUE algorithms		Wheat	Canola
Const_value	c_220 ppm	0.66 (0.53)	0.61 (0.51)
	c_240 ppm	0.70 (0.56)	0.61 (0.54)
	c_260 ppm	0.75 (0.60)	0.64 (0.58)
	c_280 ppm	0.77 (0.65)	0.68 (0.62)
	c_300 ppm	0.80 (0.71)	0.71 (0.67)
Const_ratio	k_0.55	0.64 (0.55)	0.59 (0.52)
	k_0.60	0.67 (0.58)	0.62 (0.55)
	k_0.65	0.71 (0.61)	0.64 (0.59)
	k_0.70	0.75 (0.65)	0.66 (0.63)
	k_0.75	0.80 (0.70)	0.70 (0.68)
Linear	m1	0.81 (0.70)	0.80 (0.70)
	m2	0.83 (0.73)	0.81 (0.73)
	m3	0.84 (0.76)	0.82 (0.76)
	m4	0.86 (0.80)	0.83 (0.79)
	m5	0.89 (0.84)	0.85 (0.83)
Sqrt	λ1	0.75 (0.63)	0.71 (0.63)
	λ2	0.77 (0.67)	0.74 (0.67)
	λ3	0.80 (0.70)	0.76 (0.70)
	λ4	0.83 (0.75)	0.79 (0.74)
	λ5	0.85 (0.80)	0.82 (0.79)
Opt		0.71 (0.66)	0.72 (0.66)

Table 2
Successful fractions of half-hourly partitioned solutions for different parameterizations of intercellular carbon dioxide concentrations (c_i) in different water use efficiency (WUE) algorithms during a growing season for wheat and canola. Total partition attempts for the opt model were 10,073 and 9,697, while they were 18,876 and 17,380 for the other four WUE models in wheat and canola, respectively.

WUE algorithms		Successful fractions	
		Wheat	Canola
Const_value	c_220 ppm	0.65	0.66
	c_240 ppm	0.64	0.64
	c_260 ppm	0.61	0.62
	c_280 ppm	0.59	0.58
	c_300 ppm	0.54	0.54
Const_ratio	k_0.55	0.65	0.66
	k_0.60	0.64	0.64
	k_0.65	0.62	0.62
	k_0.70	0.60	0.60
	k_0.75	0.57	0.56
Linear	m1	0.50	0.51
	m2	0.48	0.48
	m3	0.46	0.45
	m4	0.43	0.43
	m5	0.41	0.40
Sqrt	λ1	0.61	0.62
	λ2	0.58	0.59
	λ3	0.56	0.56
	λ4	0.52	0.52
	λ5	0.48	0.48
Opt		0.66	0.65

judged solely based on the number of successful partitioned outputs, a large number of partitioned outputs are needed to accurately determine T:ET ratios.

Overall, seasonal T:ET ratios varied greatly (*i.e.*, up to >15%) when they were derived using all successful partitioned outputs for individual WUE algorithms or they were determined only for the periods when all WUE algorithms produced successful partitioned outputs (Table 1). Most studies use a single method to estimate leaf-level WUE in FVS partitioning. Our results demonstrate that the use of a single WUE algorithm or multiple WUE algorithms to determine T:ET ratios for FVS partitioning can lead to large differences in seasonal T:ET ratios for water balance interpretations.

Seasonal T:ET ratios found with the opt model were comparable to the T:ET ratios found with const_value and const_ratio models in both wheat and canola (Fig. S1). When compared to the opt model, the ranges of mean absolute percent error (MAPE) for different c_i parameterizations in const_value and const_ratio models were 13-19% in wheat and 14-22% in canola (Fig. S1). In comparison, the MAPE range for different c_i parameterizations in the linear model was 47-59% in wheat and 49-65% in canola. Similarly, the MAPE range for the sqrt model was 20-37% in wheat and 21-40% in canola. Since const_value and const_ratio models produce nearly identical seasonal T:ET ratios for identical c_i, either of these models can be selected for FVS partitioning. Additionally, const_value and const_ratio models yield a higher frequency of T:ET estimates than does the opt model. Despite a substantially lower number of successful partitioning solutions, the opt model also showed its potential for inter-model comparison, especially in sensitivity analysis, for FVS partitioning in C_3 species. However, the formulation constraint of $\overline{c_i} / \overline{c_a} \geq 0.5$ limits the applicability of the opt model in C_4 species (Scanlon et al., 2019; Wagle et al., 2021b).

3.5. Sensitivity of weekly T:ET ratios in response to rainfall and dry periods

Since large ranges in seasonal patterns of T:ET ratios were found for different WUE algorithms, we further investigated weekly T:ET ratios for variable input parameters in WUE algorithms for wet and dry periods during peak growth (Fig. 4). Week to week T:ET variations were different for different WUE algorithms (Fig. 4). The T:ET ratios are larger during dry periods due to reduced E and smaller during wet (rain or irrigation) periods due to higher E loss from wet surfaces (soil, plant canopy, and litter). In the first week of peak growth with no rainfall and higher VPD (diurnal peak VPD of ~23 hPa), we observed comparable T:ET ratios for all five WUE algorithms in both crops. In both crops, T:ET ratios differed only slightly for five WUE algorithms in the second week that received 47 mm rainfall towards the end. Additional rainfall in the third week caused large discrepancies in T:ET for WUE algorithms as T:ET ratios decreased for const_value and const_ratio, but T:ET ratios did not decrease for linear and sqrt in both crops. In the fourth week of peak growth (no rainfall at all), T:ET ratios in wheat increased by ~10% from the third to the fourth week for const_value, const_ratio, and opt, but remained constant for linear and only increased by 2-3% for sqrt. Similarly, T:ET ratios in canola increased by ~30% for const_value and const_ratio, and 23% for opt, but only increased by ~5% for linear and ~15% for sqrt. Similar temporal variations in T:ET ratios for const_value, const_ratio, and opt models, and their ability to capture reduced T:ET in wet and increased T:ET in dry conditions indicate their greater potential to accurately partition ET into E and T in wheat and canola.

As mentioned above, the opt model showed great potential to be used for inter-model comparison and sensitivity analysis for FVS partitioning. However, it is important to mention that the total number of partitioning attempts and successful fractions of partitioned outputs for the opt model was substantially lower in both wheat and canola, indicating the need for careful consideration of bypassing some filtering constraints for retrieving a large number of successful partitioning solutions. Additionally, previous studies have shown inapplicability of the opt model in C_4 species (Scanlon et al., 2019; Wagle et al., 2021b). Particularly, the opt model could be more useful for mixed vegetation as upscaling of leaf-level measurements of WUE is challenging for mixed vegetation due to dissimilarities in stomatal strategies among species (Scanlon et al., 2019). Results illustrated the poor performance of linear and sqrt models to accurately capture expected trends of T:ET in wet and dry periods as they were unable to capture reduced T:ET ratios under wet conditions, most probably due to estimation errors in WUE. Linear and sqrt models are solely based on VPD to compute c_i, but variations in other drivers such as soil moisture can alter the performance of these models by influencing plant gas exchange parameters and stomatal conductance (Monteith and Greenwood, 1986; Turner, 1986; Xue et al., 2004).

4. Conclusions

A constant defined value has been usually used for parameterizing intercellular CO_2 concentrations (c_i) in four WUE algorithms (const c_i value, const c_i/c_a ratio, and c_i/c_a as linear and square root functions of VPD) for FVS partitioning. In this study, we performed a sensitivity analysis of chosen inputs (a range of five values) for parametrizing c_i on ET partitioning for four WUE algorithms (const_value, const_ratio, linear, and square root) and compared them with the outputs of the optimum model for inter-model comparison. Notably, the optimum model (*i.e.*, optimized WUE approach based on eddy covariance statistics only) has the advantage of not having an adjustable parameter for c_i parameterization. As we hypothesized, changing c_i parameters resulted in varied partitioned outputs (*i.e.*, T:ET ratios), due to the direct impact on WUE estimates and T, for all four WUE algorithms. Seasonal T:ET ratios differed by 10-15% for different c_i coefficients for the same WUE algorithm in both crops. In general, the optimum model produced mid to upper-range estimates of WUE and T:ET ratios as compared to const_value and const_ratio. Three models (const_value, const_ratio, and optimum) were able to produce expected T:ET patterns during dry and wet periods in both wheat and canola. These results indicated the potential for using const_value and const_ratio models for FVS partitioning by continuing to use the commonly used c_i, especially as these methods provide more number of T:ET estimates as compared to the optimum

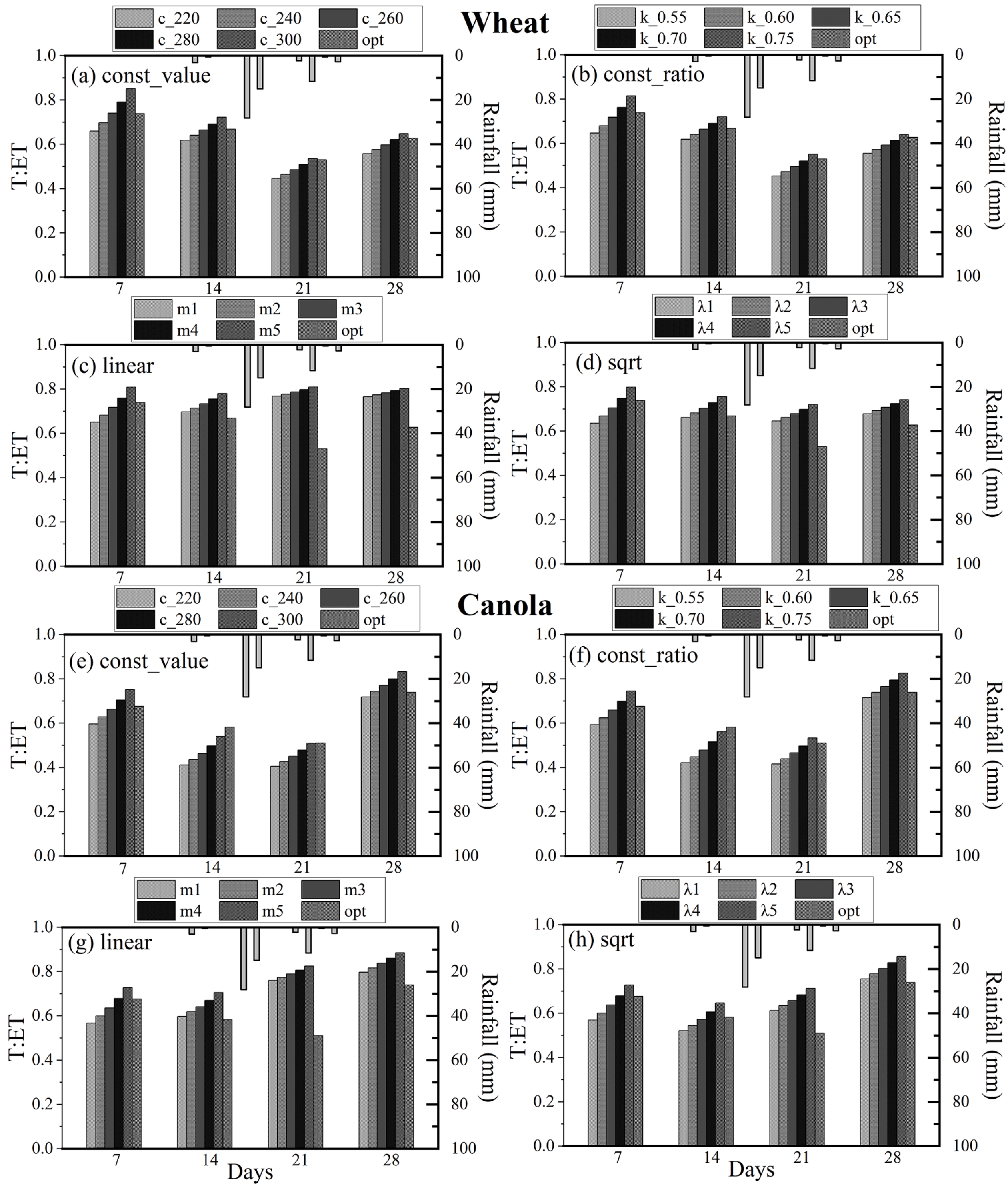

Fig. 4. Weekly ratios of transpiration (T) to evapotranspiration (ET) for different parameterizations of intercellular carbon dioxide concentrations in water use efficiency (WUE) algorithms for wheat and canola during the peak growth (from March 15 to April 14 for both crops). Rainfall data are also shown. Diurnal (weekly average) peak VPD (hPa) values for wheat and canola, respectively, were 22.81 and 22.65, 17.02 and 16.2, 13.66 and 13.45, and 14.68 and 18.6 during the first, second, third, and fourth weeks, respectively.

model in both crops. Despite a substantially lower number of successful partitioned outputs, the optimum model also showed its potential for inter-model comparison, especially in sensitivity analysis, for FVS partitioning in C_3 species. Linear and square root models showed poor performances (*i.e.*, inability to produce variable T:ET trends in wet and dry periods) in both crops. Additionally, the lower success rates of linear and square root models due to producing more physically impossible values (WUE > Fc/Fq) are also further evidence of their poor performance. Results illustrate that the choice of WUE algorithm and input value for c_i parameterization in WUE algorithms for FVS partitioning can lead to large biases in partitioned fluxes. Thus, more accurate estimates of c_i rather than assuming a constant value in WUE algorithms to account for a wide range of meteorological and water stress conditions are needed for further improvement of the performance of the FVS partitioning method. Techniques allowing temporally complete coverage of c_i could be immensely useful in reducing uncertainty in c_i parameterizations.

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CRediT authorship contribution statement

Pradeep Wagle: Formal analysis, Writing – original draft, Writing – review & editing. **Pushpendra Raghav:** Formal analysis, Writing – original draft, Writing – review & editing. **Mukesh Kumar:** Writing – review & editing. **Stacey A. Gunter:** Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.agrformet.2022.109254.

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