# Supporting Information

# Relationship between photosynthetic $CO_2$ assimilation and chlorophyll fluorescence for winter wheat under water stress

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**Notes S1. Calculation of $\Phi_P$, $\Phi_F$, $\Phi_N$, $\Phi_D$, NPQ, $\Phi_{Pmax}$ and $J_{a\_PAM}$**

Note that NPQ, $\Phi_P$ and $J_{a\_PAM}$ are defined as (obtained from the PAM measurement):

$$NPQ = \frac{(F_m - F_1) - (F_m' - F_1)}{(F_m' - F_1)}$$

$$\Phi_P = \frac{(F_m' - F_1) - (F_t - F_1)}{(F_m' - F_1)}$$

$$J_{a\_PAM} = PAR \times \Phi_P \times 0.84 \times 0.5$$

where $F_m$ is the maximal fluorescence in the dark; $F_m'$ is the maximal fluorescence chlorophyll yield from light-adapted state; $F_t$ is the steady-state fluorescence emission; $F_1$ is the PSI fluorescence yield; PAR is photochemically active radiation. The fluorescence yields ($F_o$, $F_m$, $F_m'$, $F_t$) were directly measured by the PAM fluorometer.

We have (van der Tol *et al.*, 2014):

$$K_N = \left(\frac{(F_m - F_1) - (F_m' - F_1)}{(F_m' - F_1)}\right) \times (K_F + K_D)$$

$$K_P = \left(\frac{(F_m' - F_1) - (F_t - F_1)}{(F_t - F_1)}\right) \times (K_N + K_F + K_D)$$

where $K_N$ and $K_P$ are the rate coefficients of energy-dependent heat dissipation and photochemistry, respectively (van der Tol *et al.*, 2014); $K_F$ and $K_D$ are the rate constant for constitutive heat loss and fluorescence emission (van der Tol *et al.*, 2014). In this study, $K_D$ and $K_F$ are assumed to be 0.9 and 0.1, respectively (Liu *et al.*, 2022). Note that NPQ should be equal to $K_N$ because NPQ = $K_N/(K_F + K_D)$, and $K_F + K_D = 1$.

Thus:

$$\Phi_P = \frac{K_P}{K_D + K_F + K_N + K_P}$$

$$\Phi_F = \frac{K_F}{K_D + K_F + K_N + K_P}$$

$$\Phi_N = \frac{K_N}{K_D + K_F + K_N + K_P}$$

$$\Phi_D = \frac{K_D}{K_D + K_F + K_N + K_P}$$

where the quantum yields ($\Phi$) for the four different pathways: fluorescence ($\Phi_F$), photosynthesis ($\Phi_P$), regulated heat dissipation ($\Phi_N$), and basal heat dissipation ($\Phi_D$) are obtained from the PAM measurement. It is noteworthy that $\Phi_P$, $\Phi_F$, $\Phi_N$ and $\Phi_D$ were also corrected for PSI fluorescence.

**Figure S1. Variations in $\beta_S$ and $\beta_B$ for the water stress (WS, diamonds) treatments under 12 days of progressive drought stress. The red diamonds represent $\beta_S$ in the WS treatment, and the black diamonds indicate $\beta_B$ in the WS treatment.** $\beta_S$ and $\beta_B$ are the normalized soil moisture dependent stress functions describing the effect of water stress in the modified Ball–Woodrow–Berry model.

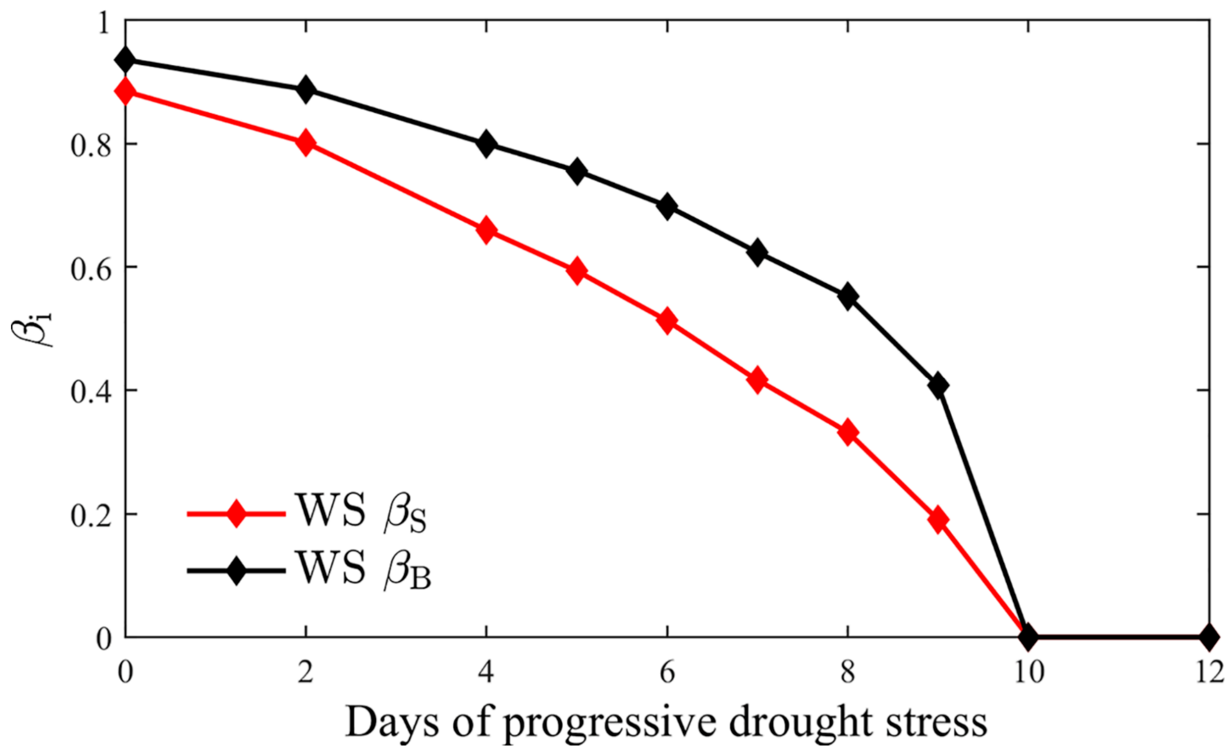

**Figure S2. Average absorbed photosynthetically active radiation (APAR, µmol m$^{-2}$ s$^{-1}$) under changing light intensity over the duration of the drought.** The numbers in the upper right corner of each plot are the number of days after withholding water. The soil water content (SWC, %) is also indicated in each panel. The solid lines represent the mean, and the shaded areas ± one standard deviation.

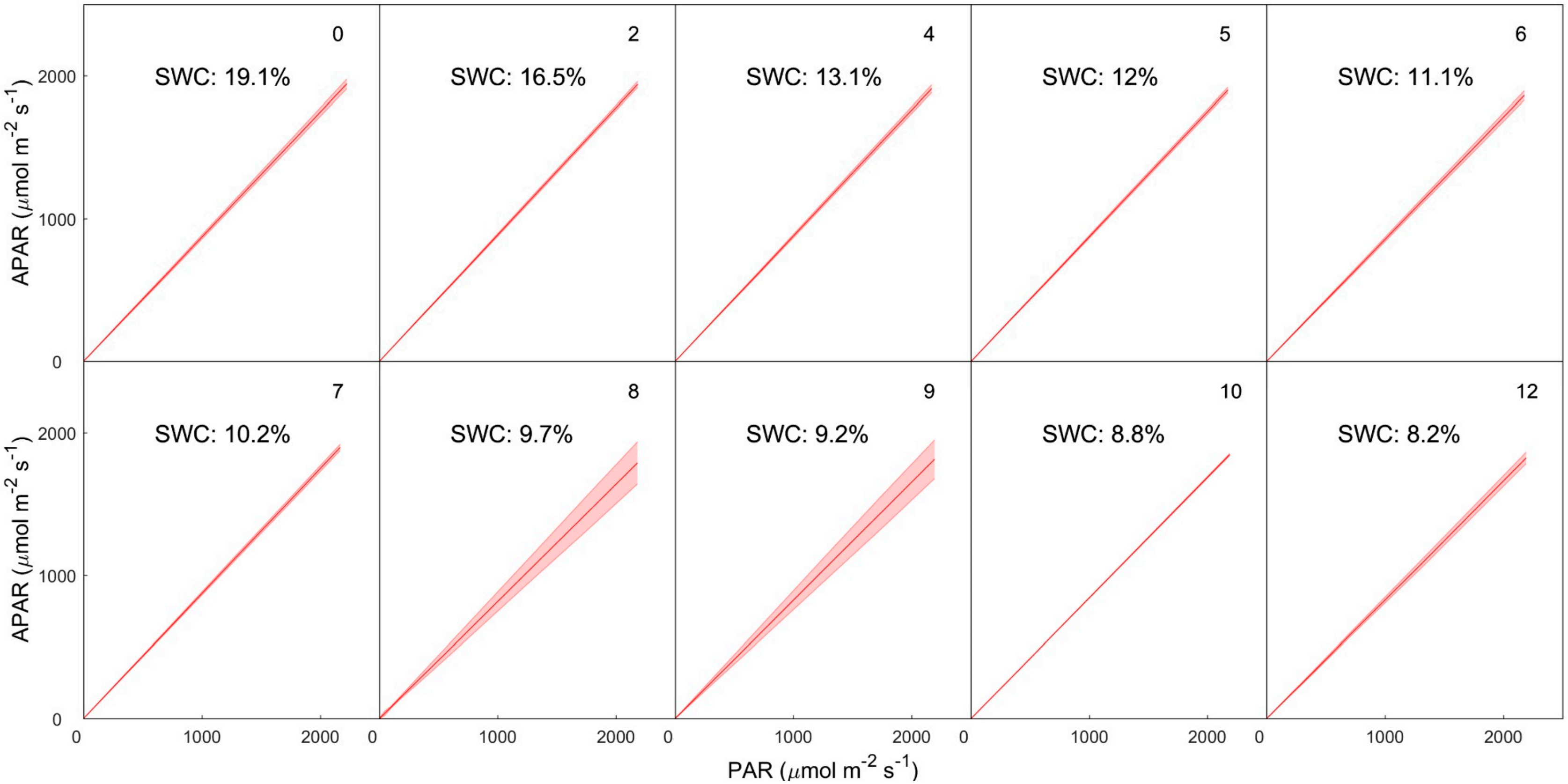

**Figure S3. The responses of full-band chlorophyll fluorescence emission at the photosystem level ($ChlF_{P\_F}$, µmol $m^{-2}$ $s^{-1}$) to changing light intensity during the period between 14 and 28 days (WS14 to WS28) after withholding water.** Numbers in the upper right corner represent days of progressive drought stress. The soil water content (SWC, %) is also given in each panel. The solid lines represent the mean, and the shaded areas ± one standard deviation, of four replicates.

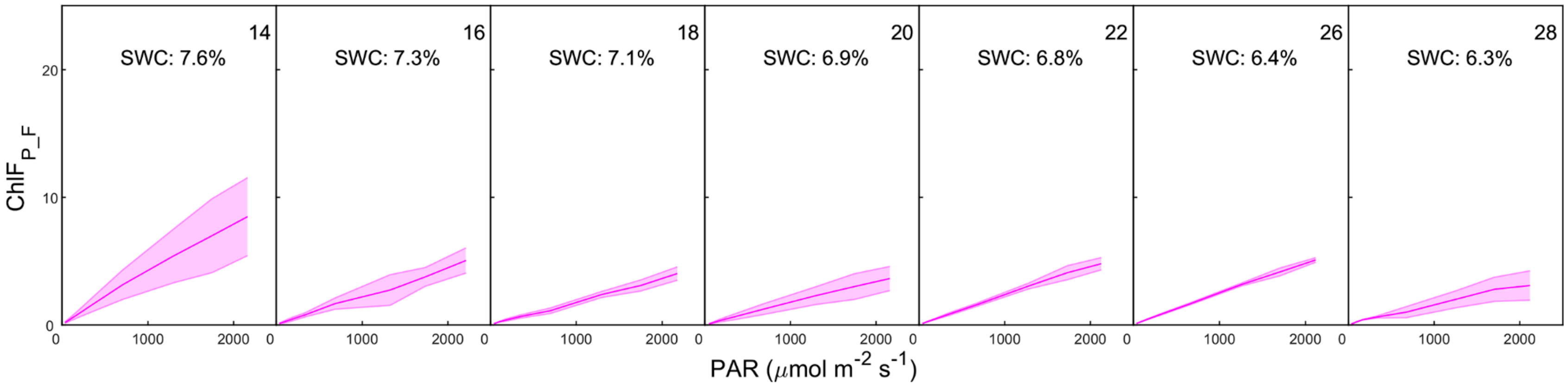

**Table S1. List of retrieved parameters, their initial values, lower boundaries (LB), upper boundaries (UB) and constraints.**

| | Initial values | LB | UB | Constraints |
|---|---|---|---|---|
| g | -22030 | -500000 | 0 | NPQ |
| h | 1.142 | 0 | 5 | NPQ |
| j | 2.539 | 0 | 5 | NPQ |
| k | -88.11 | -100 | 0 | $\Phi_P$ |
| l | 1.027 | 0 | 5 | $\Phi_P$ |
| m | 0.489 | 0 | 5 | $\Phi_P$ |
| $q_B$ | 0.5 | 0 | 3 | $V_{cmax}$ |
| $q_S$ | 0.5 | 0 | 3 | $G_S$ |

## Supplemental reference:

**Liu ZQ, Zhao F, Liu XJ, Yu Q, Wang YF, Peng XB, Cai HJ, Lu XL.** 2022. Direct estimation of photosynthetic $CO_2$ assimilation from solar-induced chlorophyll fluorescence (SIF). Remote Sensing of Environment 271, 112893.

**van der Tol C, Berry J, Campbell P, Rascher U.** 2014. Models of fluorescence and photosynthesis for interpreting measurements of solar-induced chlorophyll fluorescence. Journal of Geophysical Research: Biogeosciences 119, 2312-2327.