

Supporting Information

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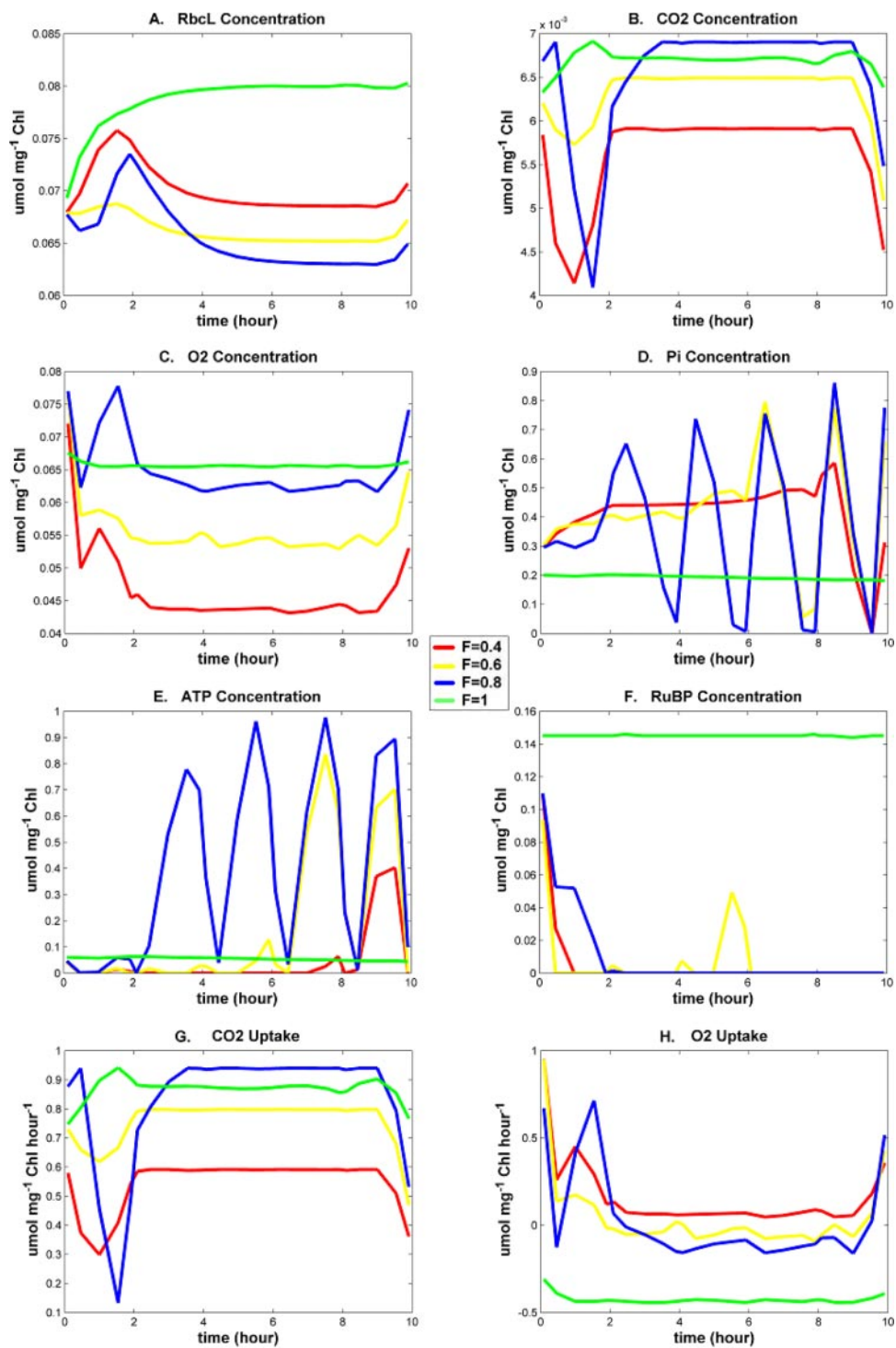


Fig. S1. Objective function is set as maximum PGA production rate of photosynthetic metabolism in the chloroplast of C_3 plants by the Dynamic Flux Balance Analysis (DFBA) method in the different levels of water stress. F represents water stress. Green represents the normal condition ($F = 1$), blue represents the mild ($F = 0.8$), yellow represents the moderate ($F = 0.6$), red represents the severe (0.4).

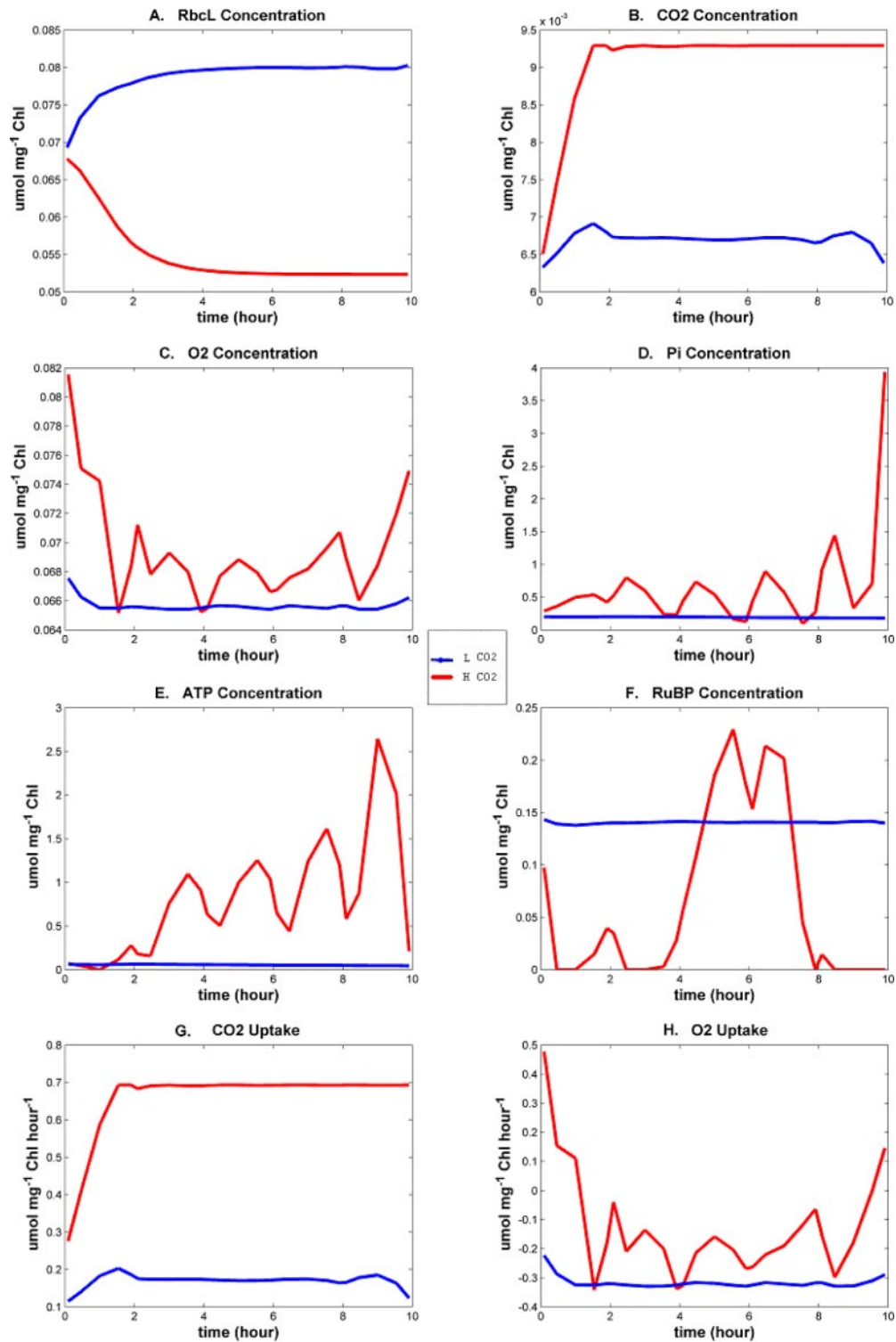


Fig. S2. Objective function is set as maximum PGA production rate of photosynthetic metabolism in the chloroplast of C_3 plants by the DFBA method in the normal (blue) and double concentration of CO_2 (red).

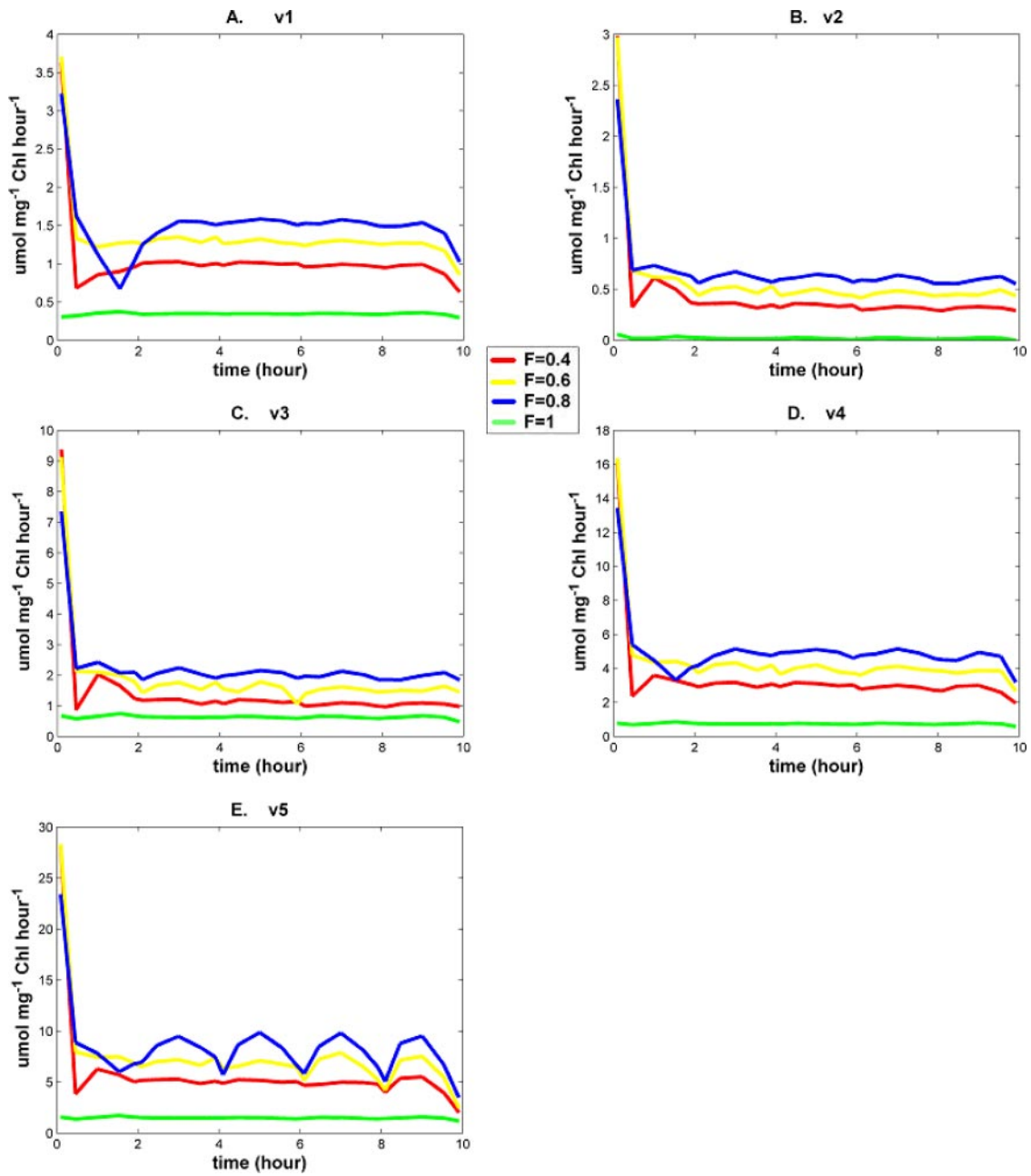


Fig. S3. Velocity of five fluxes under water deficit conditions. Objective function is set as maximum PGA production rate of photosynthetic metabolism in the chloroplast of C_3 plants by the DFBA method. F represents water stress. Green represents the normal condition ($F = 1$), blue represents the mild ($F = 0.8$), yellow represents the moderate ($F = 0.6$); red represents the severe (0.4).

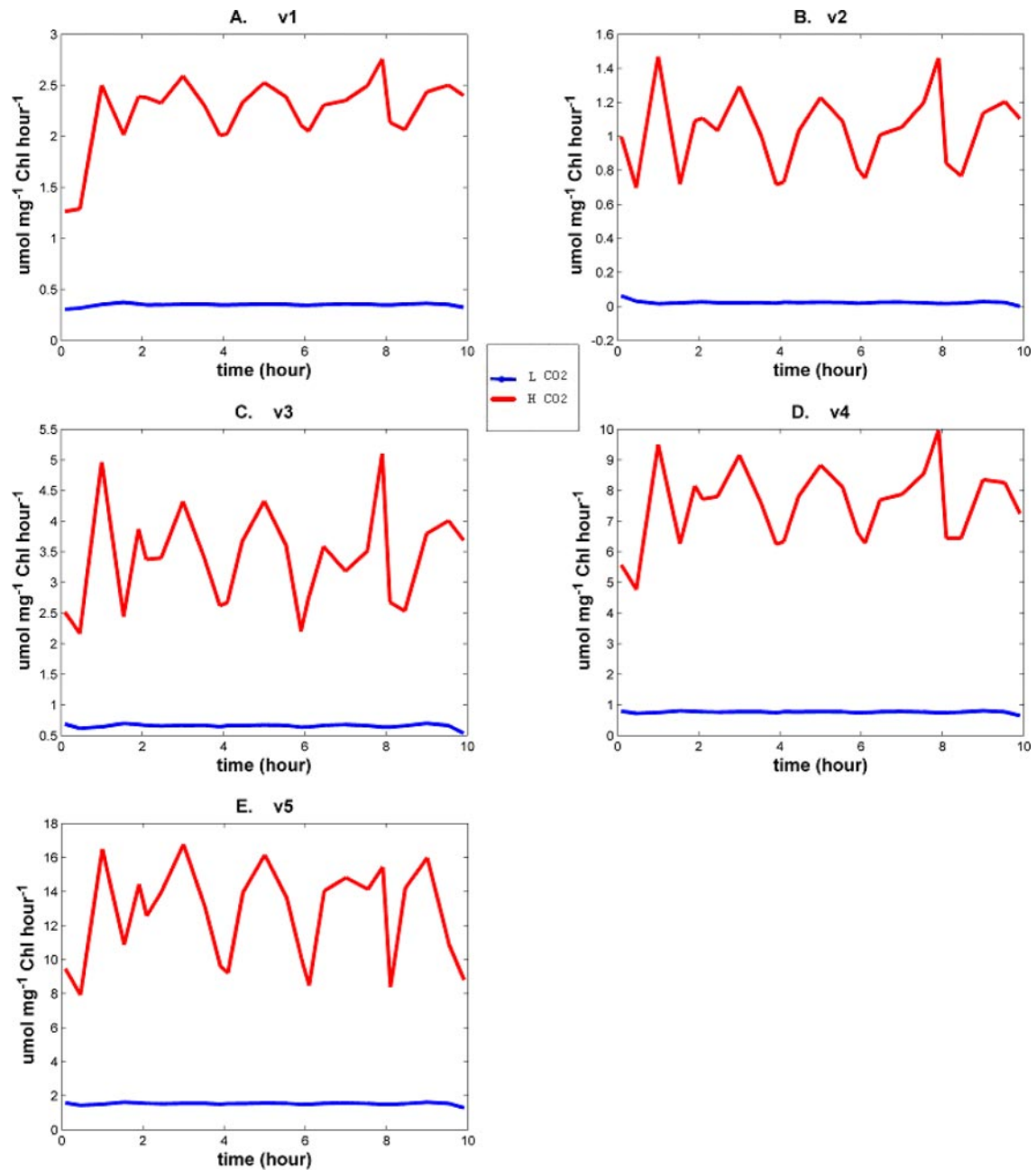


Fig. S4. Velocity of five fluxes under the double concentration of CO₂ condition. Objective function is set as maximum PGA production rate of photosynthetic metabolism in the chloroplast of C₃ plants by the DFBA method. Blue represents the normal condition, red represents double concentration of CO₂.

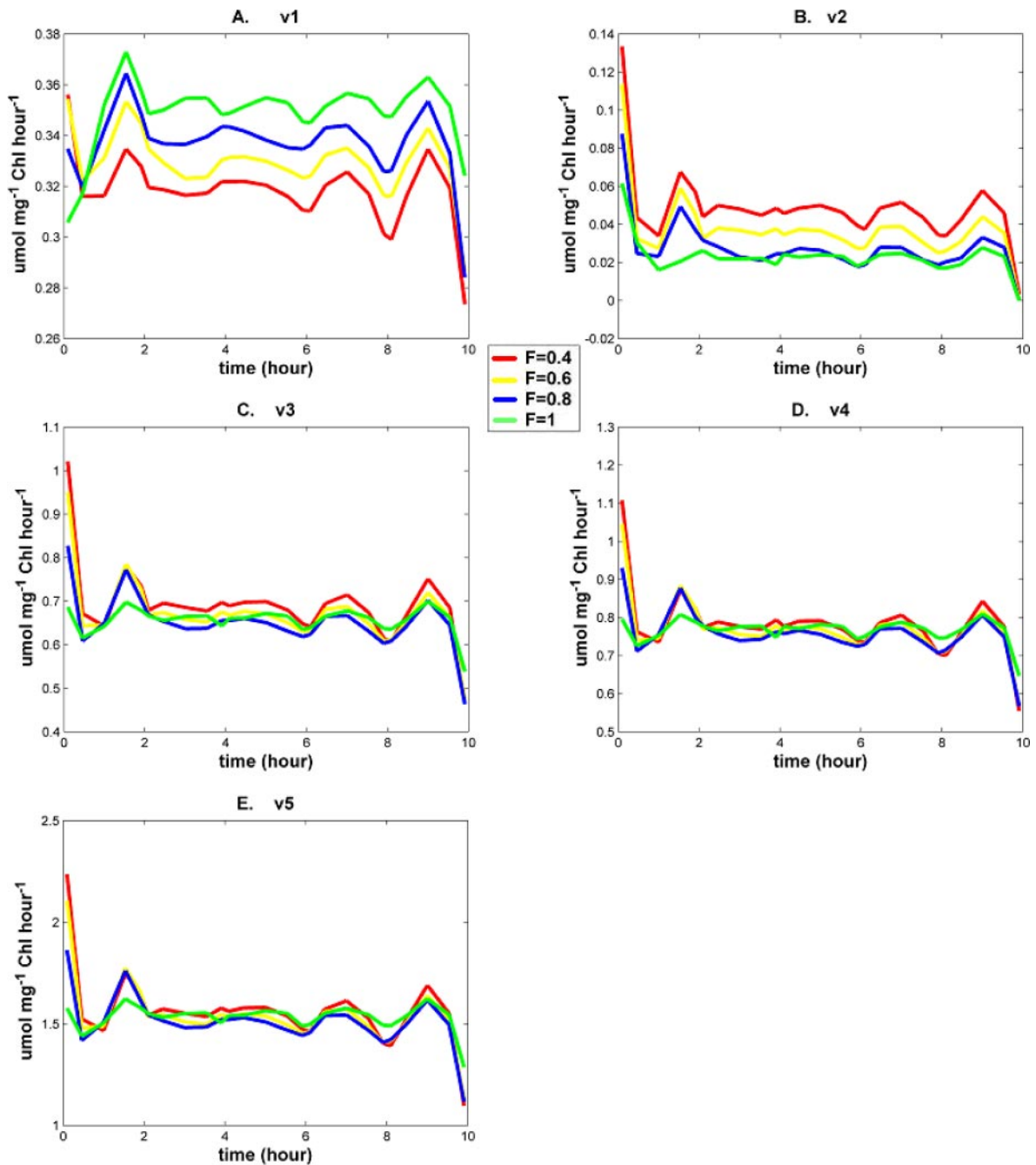


Fig. S5. Velocity of five fluxes under water deficit conditions. Objective function is set as minimum fluctuation of the profile of metabolites concentration of photosynthetic metabolism in the chloroplast of C_3 plants by the M.DFBFA method. F represents water stress. Green represents the normal condition ($F = 1$), blue represents the mild ($F = 0.8$), yellow represents the moderate ($F = 0.6$), red represents the severe ($F = 0.4$).

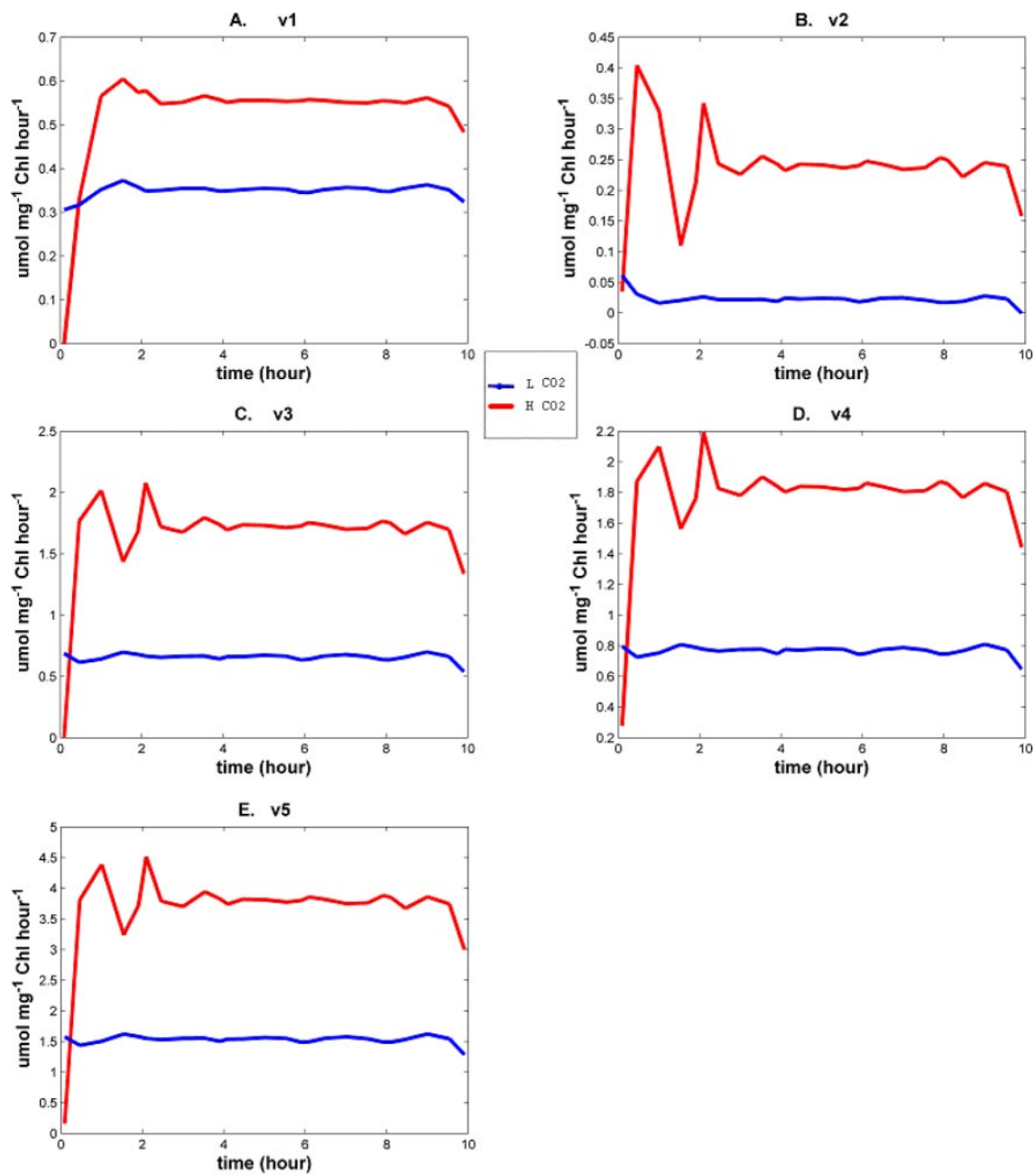


Fig. S6. Velocity of five fluxes under the double concentration of CO_2 condition. Objective function is set as minimum fluctuation of the profile of metabolites concentration of photosynthetic metabolism in the chloroplast of C_3 plants by the M.DFBA method. Blue represents the normal condition, red represents double concentration of CO_2 .

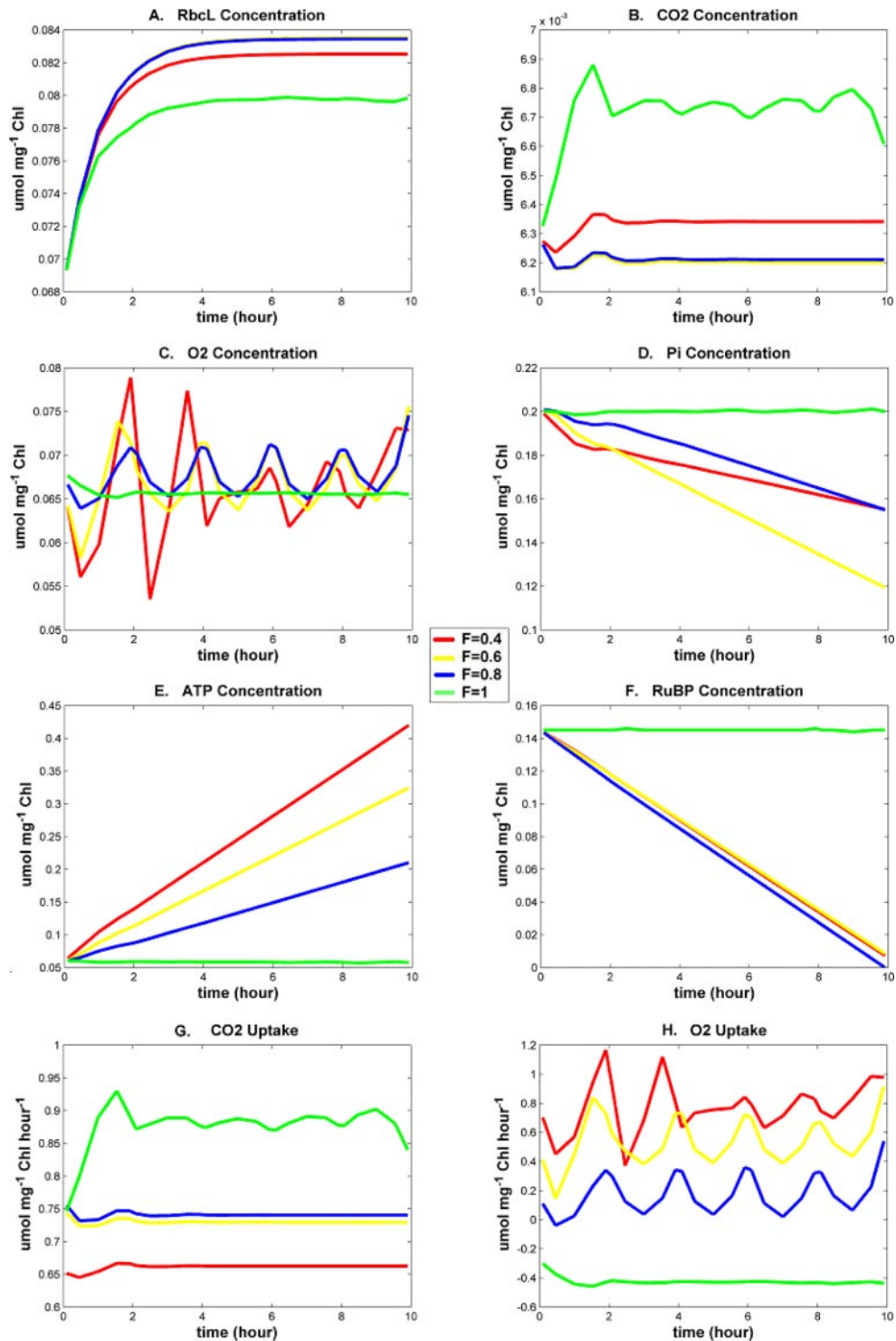


Fig. S7. Objective function is set as minimum fluctuation of the profile of the fluxes of photosynthetic metabolism in the chloroplast of C_3 plants by the M.DFBA method in the different levels of water stress. F represents water stress. Green represents the normal condition ($F = 1$), blue represents the mild ($F = 0.8$), yellow represents the moderate ($F = 0.6$); red represents the severe (0.4).

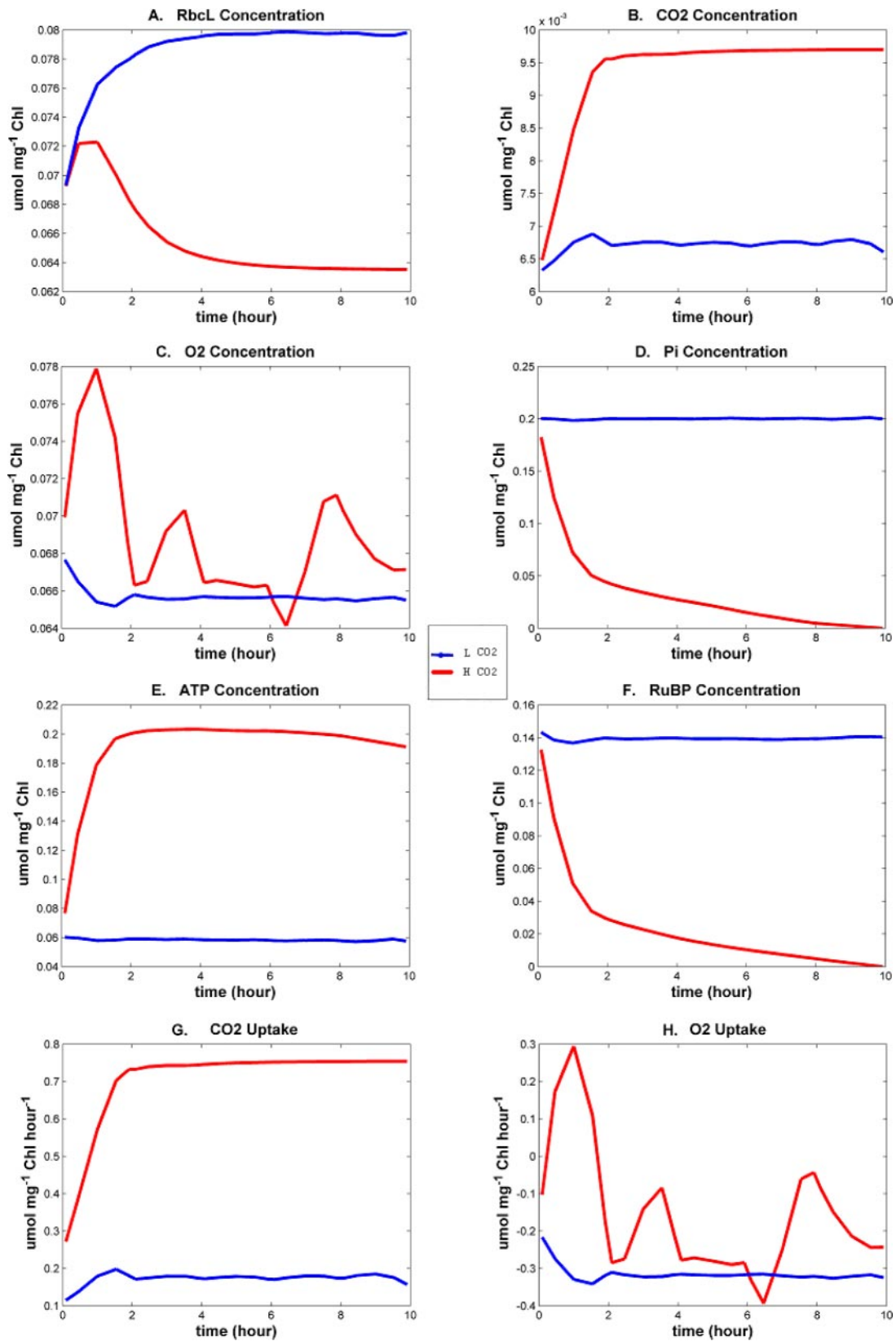


Fig. S8. Objective function is set as minimum fluctuation of the profile of the fluxes of photosynthetic metabolism in the chloroplast of C_3 plants by the M_DFBA method in the normal (blue) and double concentration of CO_2 (red).

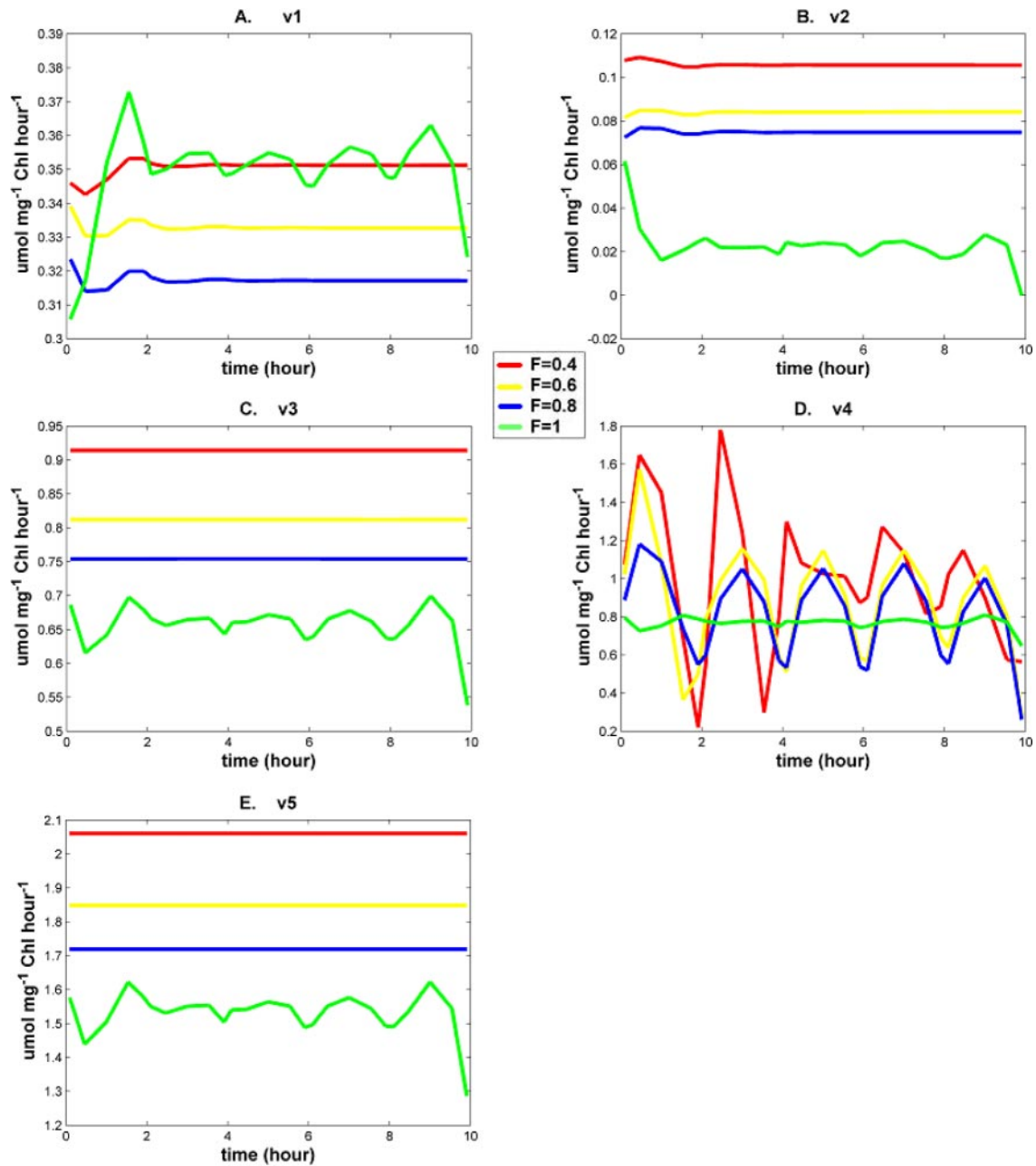


Fig. S9. Velocity of five fluxes under water deficit conditions. Objective function is set as minimum fluctuation of the profile of the fluxes of photosynthetic metabolism in the chloroplast of C_3 plants by the M.DFBA method. F represents water stress. Green represents the normal condition ($F = 1$), blue represents the mild ($F = 0.8$), yellow represents the moderate ($F = 0.6$), red represents the severe (0.4).

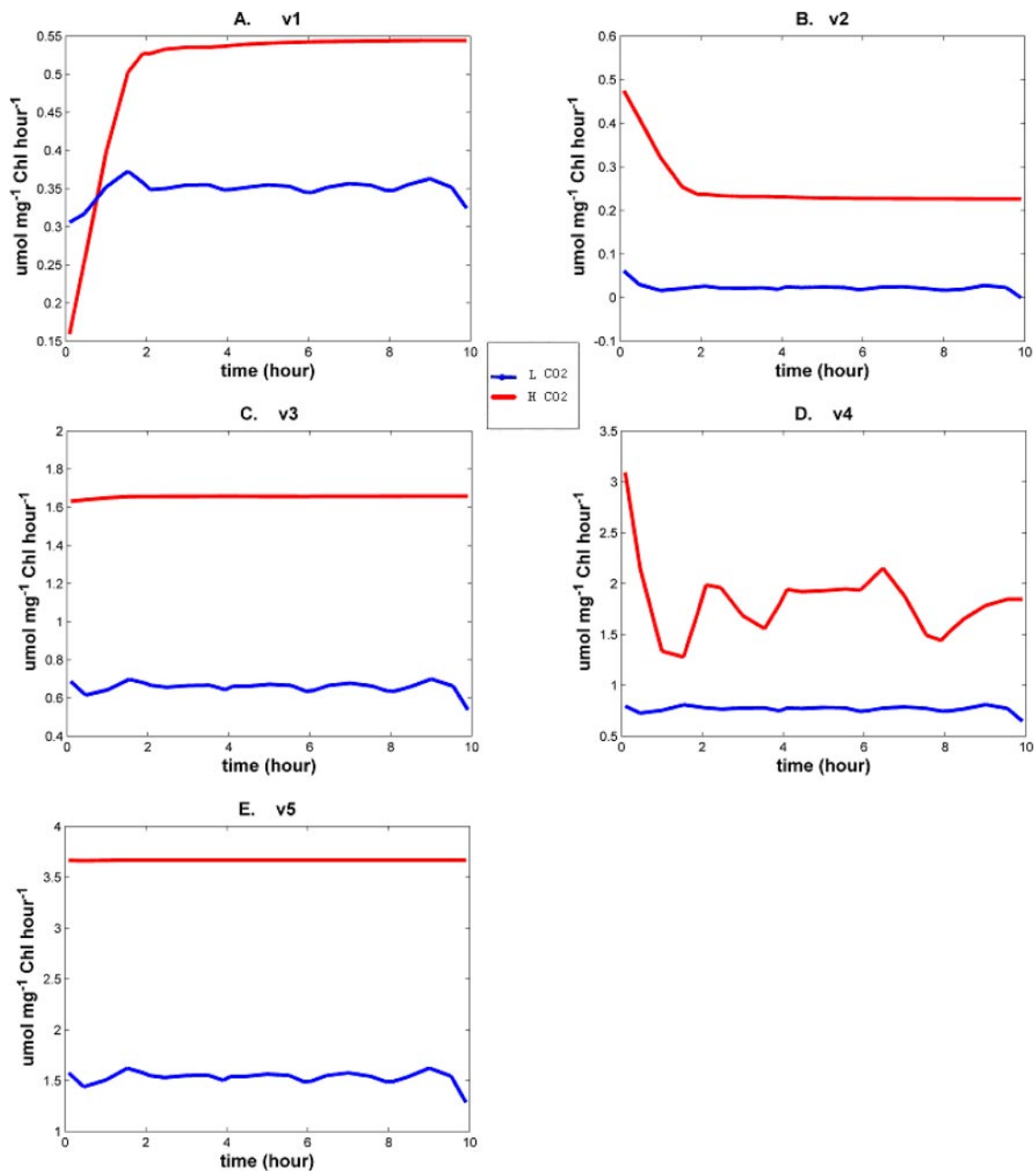


Fig. S10. Velocity of five fluxes under the double concentration of CO₂ condition. Objective function is set as minimum fluctuation of the profile of the fluxes of photosynthetic metabolism in the chloroplast of C₃ plants by the M_DFBA method. Blue represents the normal condition, red represents double concentration of CO₂.

Table S1. Parameters for equations

| Variable | Note | Value | Reference |
|----------------|--|---|-----------|
| x^{CO_2} | CO ₂ concentration in chloroplast | $6.3 \cdot 10^{-3} \mu\text{mol} \cdot \text{mg}^{-1} \text{Chl}$ | (1) |
| ζ_{CO_2} | CO ₂ diffusion coefficient | $150 \mu\text{mol} \cdot \text{mg}^{-1} \text{Chl} \cdot \text{h}^{-1}$ | (1) |
| Out_{CO_2} | CO ₂ concentration in cytoplasm | $4.45 \cdot 10^{-3} \mu\text{mol} \cdot \text{mg}^{-1} \text{Chl}$ | (2) |
| x^{O_2} | O ₂ concentration in chloroplast | $6.8 \cdot 10^{-2} \mu\text{mol} \cdot \text{mg}^{-1} \text{Chl}$ | (2) |
| ζ_{O_2} | O ₂ diffusion coefficient | $50 \mu\text{mol} \cdot \text{mg}^{-1} \text{Chl} \cdot \text{h}^{-1}$ | (3) |
| Out_{O_2} | O ₂ concentration in cytoplasm | $7.2 \cdot 10^{-2} \mu\text{mol} \cdot \text{mg}^{-1} \text{Chl}$ | (2) |
| x^{P_i} | P _i concentration in chloroplast | $0.2 \mu\text{mol} \cdot \text{mg}^{-1} \text{Chl}$ | (4) |
| ζ_{P_i} | P _i diffusion coefficient | $2.4 \cdot 10^{-3} \mu\text{mol} \cdot \text{mg}^{-1} \text{Chl} \cdot \text{h}^{-1}$ | (5) |
| Out_{P_i} | P _i concentration in cytoplasm | $0.28 \mu\text{mol} \cdot \text{mg}^{-1} \text{Chl}$ | (4) |
| x^{ATP} | ATP concentration in chloroplast | $6 \cdot 10^{-2} \mu\text{mol} \cdot \text{mg}^{-1} \text{Chl}$ | (4) |
| x^{RuBP} | RuBP concentration in chloroplast | $0.145 \mu\text{mol} \cdot \text{mg}^{-1} \text{Chl}$ | (4) |
| x^{NADPH} | NADPH concentration in chloroplast | $0.02 \mu\text{mol} \cdot \text{mg}^{-1} \text{Chl}$ | (6) |
| x^{PGA} | PGA concentration in chloroplast | $0.2 \mu\text{mol} \cdot \text{mg}^{-1} \text{Chl}$ | (4) |
| x^{rbCL} | rbCL concentration in chloroplast | $0.068 \mu\text{mol} \cdot \text{mg}^{-1} \text{Chl}$ | (7) |
| n | Constant | 1.2 | |
| K | Synthesis rate of rbCL protein | $0.12 \mu\text{mol} \cdot \text{mg}^{-1} \text{Chl} \cdot \text{h}^{-1}$ | (8) |
| R | Degradation rate of rbCL protein | $1 \mu\text{mol} \cdot \text{mg}^{-1} \text{Chl} \cdot \text{h}^{-1}$ | (8) |
| K_{L1} | Kinetic parameter of Rubisco | 80 | |
| K_{L2} | Kinetic parameter of Rubisco | 40 | |

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