Here, we present the model of the PPDK system with its dynamic equations.

PPDK has three forms: PPDK_0, PPDK_1 and PPDK_2. Only PPDK_1 is active in catalyzing the production of PEP. PPDK_1 is formed by auto-phosphorylation of PPDK_0 (with ATP and Pi as substrates) at a rate β_1(Pi,ATP) and by de-phosphorylation of PPDK_2 by RP (with Pi as a substrate and ADP and PPI as effectors of the catalytic rate) at a rate: V_p(Pi,ADP,PPI).

PPDK_1 is converted back to PPDK_0 by phosphotransfer to pyruvate to form PEP at a rate β_2(pyruvate), and by the phosphorylation of PPDK_1 by RP (which is dependent on ADP and Pi) at a rate V_k(ADP,Pi). RP can bind PPDK in either a binary complex (RP with one PPDK subunit) or a ternary complex (RP with two subunits on the same tetramer). Therefore, the rate of change of PPDK_1 concentration is

\[ \frac{d}{dt} \text{PPDK}_1 = \beta_1(Pi,ATP) \text{PPDK}_0 + V_p(Pi,ADP,PPI)([\text{PPDK}_1 \text{RP} \text{PPDK}_2] + [\text{RP} \text{PPDK}_2]) - \beta_2(\text{pyruvate}) \text{PPDK}_1 - V_k(ADP,Pi)([\text{PPDK}_1 \text{RP} \text{PPDK}_2] + [\text{RP} \text{PPDK}_1]) \]

The same considerations yield dynamic equations for PPDK_0 and PPDK_2

\[ \frac{d}{dt} \text{PPDK}_0 = \beta_2(\text{pyruvate}) \text{PPDK}_1 - \beta_1(Pi,ATP) \text{PPDK}_0 \]

\[ \frac{d}{dt} \text{PPDK}_2 = V_k(ADP,Pi) ([\text{PPDK}_1 \text{RP} \text{PPDK}_2] + [\text{RP} \text{PPDK}_1]) - V_p(Pi,ADP,PPI)([\text{PPDK}_1 \text{RP} \text{PPDK}_2] + [\text{RP} \text{PPDK}_2]) \]

There are two conservation laws, for total PPDK and RP protein levels:

\[ \text{PPDK}_T = \text{PPDK}_0 + \text{PPDK}_1 + \text{PPDK}_2 + [\text{PPDK}_1 \text{RP}] + [\text{PPDK}_2 \text{RP}] + [\text{PPDK}_1 \text{RP} \text{PPDK}_2] \]

\[ \text{RP}_T = [\text{PPDK}_1 \text{RP}] + [\text{PPDK}_2 \text{RP}] + [\text{PPDK}_1 \text{RP} \text{PPDK}_2] + \text{RP} \]

The feedback loop in the model involves PPI which is formed by PPDK_0 auto-phosphorylation at a rate β_1(Pi,ATP) and by dephosphorylation of PPDK_2 at a rate V_p(Pi,ADP,PPI). PPI is also formed by other processes in the chloroplast at an effective rate denoted β_{chl}. PPI is removed at a rate α, so that its dynamic equation reads

\[ \frac{d}{dt} \text{PPI} = \beta_1(Pi,ATP) \text{PPDK}_0 - V_p(Pi,ADP,PPI)([\text{PPDK}_1 \text{RP} \text{PPDK}_2] + [\text{RP} \text{PPDK}_2]) - \alpha \text{PPI} \]
As mentioned in the text, we neglect $\beta_{\text{chl}}$ assuming that the unusually high physiological concentration of PPDK makes it the most dominant producer of PPI (see Additional Information for more details). In addition, we neglect PPI production from the dephosphorylation of PPDK because RP is more than 100 times less abundant than PPDK.

Other metabolites, such as Pi and ADP are assumed not to be significantly affected by their reactions with the enzyme RP (due to its small amounts and slow catalytic rate). Thus, they are held as parameters in the model.

Finally, the model requires equations for the formation of the binary and ternary complexes which have the following equations (see Fig 2b and the Methods section for more details),

\begin{align*}
(6) \quad \frac{d\left[P\Pi\right]}{dt} &= \beta_{\text{chl}} + \beta_1\left(Pi,ATP\right) \text{PPDK}_0 + V_p\left(Pi,ADP,PPI\right) \left[\text{PPDK}_1 \text{ RP} \text{ PPDK}_2\right] - \alpha \left[P\Pi\right] \\

\text{where } p_1 \text{ is the probability for a PPDK}_2 \text{ site near a PPDK}_1 \text{ site, and } p_2 \text{ is the same for a PPDK}_1 \text{ site near a PPDK}_2 \text{ site. To calculate } p_1 \text{ and } p_2 \text{ we used two approaches. In a mean field approach, } p_1 &= \text{PPDK}_2/\text{PPDK}_T \text{ and } p_2 = \text{PPDK}_1/ \text{PPDK}_T. \\

\text{We also calculated } p_1 \text{ and } p_2 \text{ from a detailed model for the configurations on a PPDK tetramer. Both approaches yield qualitatively similar results. Avidity is important in the present context, since it makes } kon2 \text{ and } kon3 \text{ at least 100-fold larger than } kon1 \text{ and } kon4. \\

\text{We solve the model at steady-state, where all dynamic equations equal zero to find the steady-state solution for the output of the system: the PEP production rate by PPDK}_1. \]