A simple model of the Calvin cycle has only one physiologically feasible steady state under the same external conditions

Xin-Guang Zhu\textsuperscript{a,}\textsuperscript{*}, Rafael Alba\textsuperscript{b}, Eric de Sturler\textsuperscript{c}

\textsuperscript{a} University of Illinois at Urbana Champaign, Department of Plant Biology, 379 erml, 1201 W. Gregory Drive, Urbana, IL 61801, United States
\textsuperscript{b} University of Illinois at Urbana Champaign, Department of Computer Sciences, 201 N. Goodwin Avenue, Urbana, IL 61801, United States
\textsuperscript{c} Virginia Tech, Department of Mathematics, 544 McBryde Hall, Blacksburg, VA 24061, United States

Received 20 May 2007; accepted 16 January 2008

Abstract

Most current photosynthesis research implicitly assumes that the photosynthetic process occurs only at one steady state. However, since the rate of each reaction in photosynthesis depends nonlinearly on its substrates and products, in theory, photosynthesis can have multiple steady states under given external conditions (i.e., in a given environment). The number of steady states of photosynthesis under the same external conditions has not been studied previously. Using the root finding program POLSYS\textsubscript{PLP} [S.M. Wise, A.J. Sommese, L.T. Watson, Algorithm 801: POLSYS PLP: A partitioned linear product homotopy code for solving polynomial systems of equations, ACM Trans. Math. Software 26 (2000) 176–2000], we study the number of potential steady states of a simplified model of the Calvin cycle. Our results show that the simplified model of the Calvin cycle can reside in multiple steady states, but that only one of these is physiologically feasible. We discuss the results from an evolutionary perspective.

© 2008 Elsevier Ltd. All rights reserved.

Keywords: Nonlinear system; Photosynthesis; Steady state; Evolution

1. Introduction

Photosynthesis is inherently a complex system. It includes biophysical and biochemical reactions associated with light energy absorption, conversion of light energy into chemical energy in the form of ATP and NADPH, and complex biochemical reactions involved in the photosynthetic carbon metabolism. The rate of each reaction in photosynthesis depends nonlinearly on the concentrations of its substrates and products. Photosynthesis shows the typical characteristics of complex dynamical systems, such as oscillations, see, e.g., [1,29,30]. In fact, leaves show oscillations of CO\textsubscript{2} uptake, O\textsubscript{2} evolution, and chlorophyll fluorescence when either light or CO\textsubscript{2} varies, see e.g., [32]. Another important characteristic of most dynamical systems is that they have multiple steady states [29,30,38]. For example, in a recent numerical study [38], Zwolak et al. showed that the cell cycle can exist in four
different steady states if total cyclin is within a certain range. Even though photosynthesis is one of the most important plant physiological processes on earth, the number of potential steady states has not been well studied.

Although it is extremely difficult to study the number of steady states for the complete photosynthetic process, some previous studies suggested that the CO\textsubscript{2} fixation process in photosynthesis, i.e., the Calvin cycle, might be able to exist in two different steady states [24,25]. For example, Poolman et al. [25] showed that photosynthesis resided in two different steady states in leaves of different age when capacities to utilize the final carbohydrate product of photosynthesis were different. Pettersson and Ryde-Pettersson [24] suggested that the Calvin cycle showed two different steady states when the cytosolic phosphate concentration was below 1.9 mM. In contrast with this theoretical study [24], experiments only showed one steady state, e.g., [6,10,24]. These observations however lead to the important question, how many steady-states photosynthesis can potentially reside in under the same external conditions. Currently, no experimental protocol is available to screen the number of potential steady states of photosynthesis. However, building mathematical models of photosynthesis and then identifying all steady-state solutions of the model appears a feasible route to tackle this problem. Recently, robust numerical methods for solving polynomial systems of equations have become available. In particular, the globally convergent, probability-one homotopy method is guaranteed to find all isolated solutions to polynomial systems of equations; this method has been implemented in the numerical package POLSYS\_PLP [34]. The use of this package to analyze steady states of a biological problem is described in [5]. Following the approach in [5], we explore the number of steady states in a simplified model of the Calvin cycle derived from our photosynthesis model in [37]. Specifically, we first rewrite the differential equations into a system of polynomial equations and set (equate) the right-hand sides of the differential equations to zero. Next, we use the POLSYS\_PLP package to compute all isolated solutions of the polynomial system. Finally, we evaluate the physiological feasibility of the solutions found to identify biologically relevant steady states. Based on our results we discuss implications of the number of steady states from an evolutionary perspective and provide comparisons with previous studies [24,25]. Under rare conditions it is possible that a dynamical system has steady states that are not isolated (and hence POLSYS-PLP may not identify them); we assume that this is not the case for the Calvin cycle and we will not consider this here.

2. Method

This section is divided into three subsections. First, we describe a simplified kinetic model of the Calvin cycle; second, we describe the procedure to find the steady-state solutions of a dynamical system; and third, we describe the numerical experiments to identify all physiologically feasible solutions of the simplified model for the Calvin cycle.

2.1. A simplified model of the Calvin cycle

Our simplified model of the Calvin cycle has two sets of equations, namely, (a) rate equations and (b) differential equations.

(a) Rate equations

The reactions in the Calvin cycle are shown in Fig. 1. Although the diagram represents a simplified Calvin cycle, it includes the two major characteristics of the Calvin cycle: the autocatalytic cycle and photosynthate (including 3-Phosphoglycerate (PGA) and Glyceraldehyde 3-phosphate (GAP)) utilization. We assume that all reactions obey Michaelis–Menten kinetics. For a nonreversible reaction, \( A + B \rightarrow C + D \), the generalized rate equation is:

\[
v = \frac{V_m A \times B}{(A + K_{m_A})(B + K_{m_B})}
\]

after [27], where \( K_{m_A} \) and \( K_{m_B} \) are the Michaelis–Menten constants of substrate A and B respectively, and A and B represent the concentrations of the respective substrates. The complete set of rate equations is summarized in Appendix A. We obtained the relevant constants/parameters by surveying the peer-reviewed literature (see Appendix B for sources). The Michaelis–Menten constants for the PGA and GAP utilization were estimated to ensure realistic rates of PGA and GAP utilization.

(b) Differential equations

The rate of change of each metabolite concentration is given by the difference between the rate(s) of the reaction(s) generating the metabolite and the rate(s) of the reaction(s) consuming the metabolite. For example, RuBP is generated...
Fig. 1. The diagram showing reactions in the simplified model of the Calvin cycle. RuBP: Ribulose 1,5-bisphosphate; PGA: 3-Phosphoglycerate; DPGA: 1,3-Bisphoglycerate; GAP: Glyceraldehyde 3-phosphate; Ru5P: Ribulose 5-phosphate. The symbols such as $v_1, \ldots, v_{13}$ represent the rate of each reaction in the diagram. Arrow indicates the direction of a reaction. Sink represents utilization of PGA and GAP through sucrose synthesis or starch synthesis.

from the phosphorylation of Ru5P ($v_{13}$) via Ru5P kinase and consumed through RuBP carboxylation ($v_1$) via Rubisco (Fig. 1). Thus, the rate of RuBP concentration change is

$$\frac{d[RuBP]}{dt} = v_{13} - v_1.$$  \hspace{1cm} (2)

The differential equations describing the rate of change for each metabolite concentration form a system of coupled differential equations that represents a simplified model of the Calvin cycle (Appendix A). We use the routine ode15s from MATLAB® [19] to solve this system of differential equations, using the following initial concentrations: [RuBP] = 2 mM; [PGA] = 2.4 mM; [DPGA] = 1mM; [GAP] = 1 mM; and [Ru5P] = 1 mM cf. [9]. After 400 s (seconds), the system reaches a steady state. Subsequently, at 650 s, we perturb the system with a constant RuBP concentration for 50 s to check how the system responds to a perturbation in an individual metabolite concentration. The photosynthetic CO$_2$ uptake rate is calculated based on the rate of RuBP carboxylation. The photosynthetic CO$_2$ uptake rate calculated from the model has a unit of mmol l$^{-1}$ s$^{-1}$ on stroma volume basis (stroma is the space where the reactions in the Calvin cycle take place). This calculated rate is converted into leaf area basis by assuming that 1 mmol l$^{-1}$ s$^{-1}$ corresponds to 33.3 $\mu$mol m$^{-2}$ s$^{-1}$ on leaf area basis [9]. Furthermore, we assume 1 gram of chlorophyll in 1 m$^2$ leaf area and 30 ml stroma per gram chlorophyll [9].

2.2. The procedure to find all isolated steady-state solutions

The system of ordinary differential equations describing the simplified Calvin cycle can be succintly represented as:

$$\frac{dY}{dt} = f(Y, t, C),$$ \hspace{1cm} (3)

where $Y$ is a vector of metabolite concentrations, $t$ is time, and $C$ represents parameters or constants used in the model.

To obtain all steady-state solutions of this dynamical system (for a number of parameter sets), we consider the system of nonlinear equations obtained from setting the right-hand side of (3) to zero. The solutions to this system of nonlinear equations are the steady-state solutions of (3). For example, the differential equation for RuBP can be transformed as follows:

$$\frac{V_{13\text{max}} \times \text{Ru5P} \times \text{ATP}}{\text{(Ru5P} + K_{m131}) \times (\text{ATP} + K_{m132})} - \frac{V_{1\text{max}} \times \text{RuBP}}{\text{RuBP} + K_{m1}} = 0.$$ \hspace{1cm} (4)

Please cite this article in press as: X.-G. Zhu, et al., A simple model of the Calvin cycle has only one physiologically feasible steady state under the same external conditions, Nonlinear Analysis: Real World Applications (2008), doi:10.1016/j.nonrwa.2008.01.021
Table 1
The number of different types of roots when doubling maximal activities of enzymes in the simplified model of the Calvin cycle

<table>
<thead>
<tr>
<th>Category $V_{\text{max}}$</th>
<th>Total</th>
<th>Real solutions</th>
<th>Physiologically feasible real solutions</th>
<th>Physiologically nonfeasible real solutions</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_1_{\text{max}}$</td>
<td>40</td>
<td>5</td>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>$V_2_{\text{max}}$</td>
<td>40</td>
<td>4</td>
<td>0</td>
<td>4</td>
</tr>
<tr>
<td>$V_3_{\text{max}}$</td>
<td>40</td>
<td>4</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>$V_4_{\text{max}}$</td>
<td>40</td>
<td>5</td>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>$V_5_{\text{max}}$</td>
<td>40</td>
<td>4</td>
<td>0</td>
<td>4</td>
</tr>
<tr>
<td>$V_{13\text{max}}$</td>
<td>40</td>
<td>5</td>
<td>1</td>
<td>4</td>
</tr>
</tbody>
</table>

When doubling the maximal activity of one enzyme, the maximal activities of other enzymes are assumed to be at their default values. The concentration of ATP is assumed to be 0.5 mM [2,11,35]. The column Total indicates the total number of solutions; the column Real solutions indicates the number of real solutions. The real solutions were further differentiated as either physiologically feasible solutions or physiologically nonfeasible solutions.

Following the procedure of Zwolak et al. [38], we transform all the differential equations (Appendix A) into nonlinear polynomial equations, and then we use POLSYS_PLP to identify all the isolated roots. We develop a PERL script (RootFinder.pl) to generate the required input for POLSYS_PLP.

2.3. Identifying all isolated solutions of the simplified model of the Calvin cycle

We compute all the (isolated) solutions of the simplified model of the Calvin cycle for the default values of all parameters (the maximal enzyme activities, i.e., $V_{\text{max}}$, for each chemical reaction) and identify the physiologically feasible ones. In addition, we explore solutions of the model when the $V_{\text{max}}$ of each enzyme (governing a chemical reaction) involved in the model is varied between 50% and 300% of the default (Appendix B). When varying the $V_{\text{max}}$ of one enzyme (the $V_{\text{max}}$ for a specific reaction), we kept activities of all other enzymes at their default values.

3. Results

Fig. 2 shows that the system of coupled differential equations quickly moves to a steady state (at about 400 s), where the steady-state concentration of each metabolite is within its physiologically relevant concentration range, cf. [9]. Moreover, the photosynthetic CO$_2$ uptake rate is also within the range of field-measured rates [36]. This suggests that the system of coupled differential equations (Appendix A) effectively simulates the CO$_2$ uptake rate. At 650 s, the system is perturbed from its steady state by enforcing a constant RuBP concentration for 50 s. This external perturbation effectively drives the concentrations of all metabolites in the system away from their steady-state concentrations. Upon removal of this perturbation, the system returns to its (original) physiologically feasible steady state in about 200 s, suggesting that our simple model is consistent with photosynthesis performance of actual plants in the lab, cf. [22]. For the default values of the model parameters (see Appendix B), POLSYS_PLP finds 40 solutions. A solution is considered to be physiologically feasible only if the concentration of each metabolite falls within its physiologically relevant range (0.0001–5 mM) [9]. Out of 40 solutions, 39 solutions have concentrations with values that are too close to zero or negative or complex. Only one solution is physiologically feasible (see Appendix C for a sample solution). Under variation of the $V_{\text{max}}$ (parameter) for each reaction the total number of solutions does not change; more importantly, the system still has only one solution that is physiologically feasible. This demonstrates the relevance of our study to a wide variety of plant species, which may have different enzyme concentrations and hence different maximal reaction rates. Table 1 shows the total number of solutions, the number of real solutions, the number of physiologically feasible real solutions, and the number of physiologically nonfeasible solutions when $V_{\text{max}}$ of one enzyme is doubled (Table 1).

The physiologically feasible solutions and solutions with values close to zero are shown in Figs. 3 and 4. The substrate or product of the reaction for which $V_{\text{max}}$ is modified (shown at top left corner) shows the greatest steady-state concentration change (Fig. 3). For example, when $V_3_{\text{max}}$, the maximal rate of the GAP dehydrogenase, is modified, the concentration of DPGA shows the greatest change in its steady-state concentration. For low GAP dehydrogenase activity, the DPGA concentration is higher than for high GAP dehydrogenase activity (Fig. 3B), because with a higher enzyme activity a lower substrate concentration is needed to maintain the same flux rate through the reaction. On
the other hand, metabolites that are ‘far’ from the reaction with modified enzyme activity show little or no change in concentration, where ‘far’ refers to the minimum number of reactions that link a metabolite to the reaction with modified activity. For example, when $V_{\text{max}}$, the maximal activity of the enzyme Rubisco, is modified, the steady-state concentration of Ru5P shows a negligible change (Fig. 3A).

We observe that the Calvin cycle has a physiologically feasible steady state for a wide range of maximal activities of Rubisco, GAP dehydrogenase, Phosphoribulose kinase, and the enzyme converting GAP to Ru5P (Fig. 3). However, when the maximal activities of either PGA kinase or PGA utilization are altered, the simplified model of the Calvin cycle loses its physiologically feasible solution and switches to a steady state where the concentrations of all metabolites are (too) close to zero (Fig. 4).

4. Discussion

As photosynthesis, including both the light reactions and the carbon metabolism, is a complex dynamical system governed by coupled nonlinear differential equations, one might expect photosynthesis to have multiple steady states under the same light, CO$_2$ and O$_2$ conditions (the external conditions considered). So far, there has been no analysis to characterize the number of steady states of the entire photosynthesis system, partly due to the lack of appropriate tools for such an analysis. As the first step, this study uses the package POLSYS.PL to identify steady-state solutions corresponding to isolated solutions of the associated polynomial system of equations representing a simplified model...
Fig. 3. The physiologically feasible and the close-to-zero steady-state concentrations of four metabolites in the simplified model of the Calvin cycle under different maximal enzyme activities. In each panel, the maximal enzyme activity of one enzyme varies from 50% to 300% of its default value while the maximal enzyme activities of all other enzymes are set to be at their default values. This figure shows that there is only one physiologically feasible steady-state solution under the same external conditions.

Fig. 4. The physiologically feasible and the close-to-zero steady-state metabolite concentrations in the simplified Calvin cycle under different $V_{2\text{max}}$ and $V_{5\text{max}}$ (see Fig. 3 for detailed legend).

of the Calvin cycle. It is surprising that even though 40 solutions are identified for the simplified Calvin cycle, only one of them is physiologically feasible.

Although the model of the Calvin cycle we use in this study is relatively simple, it possesses the two key characteristics of the Calvin cycle: (1) the autocatalytic cycle and (2) the utilization of photosynthate (i.e., GAP and PGA) (Fig. 1). It is intriguing that only one physiologically feasible steady state is found under the given external conditions (CO$_2$, O$_2$, light intensity). Studies in the past have suggested multiple steady states. In [25] Poolman et al. demonstrated that the Calvin cycle can potentially exist in different steady states for leaves at different ages and at different external conditions. However, whether photosynthesis can reside in two different states for the same leaf age under the same external conditions was not studied [25]. Pettersson and Ryde-Pettersson [24] showed that the Calvin cycle had two feasible steady states, one with high flux rate and another with low flux rate. The Calvin cycle model used in this study is simpler than that of Pettersson and Ryde-Pettersson [24], which might explain the differences in the number of steady states identified. On the other hand, all previous experiments on real plants

Please cite this article in press as: X.-G. Zhu, et al., A simple model of the Calvin cycle has only one physiologically feasible steady state under the same external conditions, Nonlinear Analysis: Real World Applications (2008), doi:10.1016/j.nonwa.2008.01.021
showed that photosynthesis only exists in one steady state under a fixed set of external conditions [16,31], while dramatic changes in the external conditions (for example, from very low light to very high light) may lead to long transient phases marked by significant oscillations [8,32]. The accuracy of the Farquhar et al. [4] model to predict the photosynthetic CO$_2$ uptake rate under a wide variety of external conditions also suggests that photosynthesis exists only in one steady state under fixed conditions. Given these partially contradictory results, a detailed analysis of the number of potential steady states for a complete model of the photosynthetic carbon metabolism [37] will be required to ultimately determine whether photosynthesis has the potential to exist in multiple steady states in a leaf and if so what mechanisms prevent it from switching freely between different steady states.

Existing experimental evidence suggests that in the field photosynthesis stays predominantly if not always in one steady state under given external conditions [4,10,24]. If this is true, then what is the advantage of staying in only one steady state? If photosynthesis has multiple steady states with each having different photosynthetic CO$_2$ uptake rate, it would be advantageous for photosynthetic cells to stay in the steady state with a higher photosynthetic CO$_2$ uptake rate. It is possible that during evolution mechanisms evolved to keep photosynthesis operating only in the state with high photosynthetic CO$_2$ uptake rate. In line with this idea, the structure of the Calvin cycle has been conserved from cyanobacteria all the way through high plants [20,33], possibly for the purpose of staying in the steady state with the higher photosynthetic CO$_2$ uptake rate. It is possible that various mechanisms of enzyme activity regulation, e.g., modification of the redox state of Ferrodoxin–Thioredoxin system, or pH of stroma, or Mg$^{2+}$ concentration [18,26] might be involved in keeping photosynthesis operating in a state with high photosynthetic CO$_2$ uptake rate.

In summary, this theoretical study explored a number of potential steady states of a simplified model of the Calvin cycle. Results from this and the previous studies suggest that, although the Calvin cycle has the potential to stay in multiple steady states, it seems to stay only in one steady state. This property of the Calvin cycle might be a result of the natural selection for a higher CO$_2$ uptake rate. A detailed study of the number of steady states for a complete model of photosynthesis is needed to identify the total potential number of steady states of photosynthesis in the field.

Acknowledgements

This research was supported by the National Center for Supercomputing Applications, the National Science Foundation, IBN 04-17126, and the McNair Scholars Program of the University of Illinois.

Appendix A. Equations used in the simplified model of the Calvin cycle

The differential equations:

$$\frac{d\text{RuBP}}{dt} = v_1 - v_1$$
$$\frac{d\text{PGA}}{dt} = 2 \times v_1 - v_2 - v_5$$
$$\frac{d\text{DPGA}}{dt} = v_2 - v_3$$
$$\frac{d\text{GAP}}{dt} = v_3 - v_4 - v_6$$
$$\frac{d\text{Ru5P}}{dt} = 0.6 \times v_4 - v_13.$$  

The rate equations:

$$v_1 = \frac{V_{1\text{max}} \times \text{RuBP}}{\text{RuBP} + K_{m1}}$$
$$v_2 = \frac{V_{2\text{max}} \times \text{PGA} \times \text{ATP}}{(\text{PGA} + K_{m21}) \times (\text{ATP} + K_{m22})}$$
$$v_3 = \frac{V_{3\text{max}} \times \text{DPGA}}{\text{DPGA} + K_{m3}}$$
Appendix B. Parameters used in the simplified model of the Calvin cycle

See Tables B.1 and B.2.

Table B.1
The maximal activities \( (V_m) \) of each enzyme in the simplified model of the Calvin cycle

<table>
<thead>
<tr>
<th>Maximal activity</th>
<th>Enzyme name</th>
<th>Reaction</th>
<th>( aV_m ) (mmol l(^{-1})s(^{-1}))</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>( V_1 )</td>
<td>Rubisco</td>
<td>RuBP + CO(_2) → 2PGA</td>
<td>3.78</td>
<td>[15,23,35]</td>
</tr>
<tr>
<td>( V_2 )</td>
<td>PGA Kinase</td>
<td>PGA + ATP → ADP + DPGA</td>
<td>11.75</td>
<td>[15,23,35]</td>
</tr>
<tr>
<td>( V_3 )</td>
<td>GAP dehydragenase</td>
<td>DPGA + NADPH → GAP + OP + NADP</td>
<td>5.04</td>
<td>[15,23,35]</td>
</tr>
<tr>
<td>( V_4 )</td>
<td>Conversion of GAP into Ru5P</td>
<td>GAP → 0.6Ru5P</td>
<td>3.05</td>
<td>Model estimate</td>
</tr>
<tr>
<td>( V_{13} )</td>
<td>Ribulose biphosphate kinase</td>
<td>Ru5P + ATP → RuBP + ADP</td>
<td>8</td>
<td>[15,23,35]</td>
</tr>
<tr>
<td>( V_5 )</td>
<td>Sink capacity</td>
<td>PGA → Sink</td>
<td>3</td>
<td>[15,23,35]</td>
</tr>
<tr>
<td>( V_6 )</td>
<td>Sink capacity</td>
<td>GAP → Sink</td>
<td>0.1</td>
<td>Model estimate</td>
</tr>
</tbody>
</table>

Table B.2
The Michaelis–Menten constants of enzymes used in the simplified model of the Calvin cycle

<table>
<thead>
<tr>
<th>RN(^a)</th>
<th>Reaction</th>
<th>Parameter(^b)</th>
<th>Value (mM)</th>
<th>Description(^c)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>RuBP + CO(_2) → 2PGA</td>
<td>( K_{m13} )</td>
<td>1</td>
<td>RuBP</td>
<td>Model estimate, cf. [31]</td>
</tr>
<tr>
<td>2</td>
<td>PGA + ATP → ADP + DPGA</td>
<td>( K_{m21} )</td>
<td>0.240</td>
<td>PGA</td>
<td>[12,14]</td>
</tr>
<tr>
<td>2</td>
<td>PGA + ATP → ADP + DPGA</td>
<td>( K_{m22} )</td>
<td>0.390</td>
<td>ATP</td>
<td>[12,14]</td>
</tr>
<tr>
<td>3</td>
<td>DPGA + NADPH → GAP + OP + NADP</td>
<td>( K_{m3} )</td>
<td>0.5</td>
<td>DPGA</td>
<td>Model estimate, cf. [3,5,17,28]</td>
</tr>
<tr>
<td>4</td>
<td>GAP → 0.6Ru5P</td>
<td>( K_{m4} )</td>
<td>0.84</td>
<td>GAP</td>
<td>Model estimate</td>
</tr>
<tr>
<td>5</td>
<td>PGA → Sink</td>
<td>( K_{m5} )</td>
<td>0.75</td>
<td>PGA</td>
<td>Model estimate</td>
</tr>
<tr>
<td>6</td>
<td>GAP → Sink</td>
<td>( K_{m6} )</td>
<td>5</td>
<td>GAP</td>
<td>Model estimate</td>
</tr>
<tr>
<td>13</td>
<td>Ru5P + ATP → RuBP + ADP</td>
<td>( K_{m131} )</td>
<td>0.15</td>
<td>Ru5P</td>
<td>[7,21]</td>
</tr>
<tr>
<td>13</td>
<td>Ru5P + ATP → RuBP + ADP</td>
<td>( K_{m132} )</td>
<td>0.059</td>
<td>ATP</td>
<td>[7,13,21]</td>
</tr>
</tbody>
</table>

\(a\) RN: Reaction number corresponding to the number in Fig. 1.

\(b\) Parameters beginning \( K_M \) represent the apparent Michaelis–Menten constant of the metabolite listed in the description column.

\(c\) The description column lists the compounds to which the kinetic constant applies.

Appendix C. Sample real solutions of the simplified model of the Calvin cycle

Given a set of \( V_{\text{max}} \) values, the system of nonlinear polynomials derived from the differential equations representing the simplified model of the Calvin cycle has 40 roots. Among them 4–5 were real definite roots. A set of sample real solutions for the model is shown below. In this sample, the \( V_{1\text{max}} \) is set to be 200\% of the default \( V_{1\text{max}} \) and the \( V_{\text{max}} \) values of all other enzymes are set to be at their default values. X(1): RuBP, X(2): PGA, X(3): DPGA, X(4): GAP, X(5): Ru5P. We can see that only the first real solution is a physiologically feasible solution.

Real solution 1
\[
\begin{align*}
X(1) &= 2.56097627171181E-01 \\
X(2) &= 1.3809652799639E-01
\end{align*}
\]
\[
\begin{align*}
X(3) &= 5.39698924750138 \times 10^{-1} \\
X(4) &= 4.48565670978998 \\
X(5) &= 4.1119859296765 \times 10^{-2}.
\end{align*}
\]

Real solution 2
\[
\begin{align*}
X(1) &= -3.57848262985460 \times 10^{-17} \\
X(2) &= 8.75644031437841 \times 10^{-18} \\
X(3) &= 2.61129825157095 \times 10^{-18} \\
X(4) &= 1.75408016482927 \times 10^{-16} \\
X(5) &= 7.04135520029619 \times 10^{-18}.
\end{align*}
\]

Real solution 3
\[
\begin{align*}
X(1) &= 4.09031898442628 \times 10^{-1} \\
X(2) &= -5.50930499218444 \times 10^{-1} \\
X(3) &= -8.2933703387913 \times 10^{-1} \\
X(4) &= -5.05596520084859 \times 10^{-1} \\
X(5) &= 6.62434472205359 \times 10^{-2}.
\end{align*}
\]

Real solution 4
\[
\begin{align*}
X(1) &= -1.00000000089146 \times 10^{0} \\
X(2) &= -2.40000000104034 \times 10^{-1} \\
X(3) &= -5.0000000015637 \times 10^{-1} \\
X(4) &= -8.40000000158337 \times 10^{-1} \\
X(5) &= -1.5000000012672 \times 10^{-1}.
\end{align*}
\]

Real solution 5
\[
\begin{align*}
X(1) &= 5.55406405928947 \times 10^{-1} \\
X(2) &= 3.80006541425408 \times 10^{-1} \\
X(3) &= 3.37815725345562 \times 10^{0} \\
X(4) &= -2.60784352798313 \times 10^{0} \\
X(5) &= 9.06998056463301 \times 10^{-2}.
\end{align*}
\]

References


