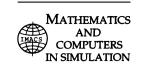


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Original article

In search for an accurate model of the photosynthetic carbon metabolism

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Abstract

The photosynthetic carbon metabolism, including the Calvin–Benson cycle, is the primary pathway in C₃-plants, producing starch and sucrose from CO₂. Understanding the interplay between regulation and efficiency of this pathway requires the development of mathematical models which would explain the observed dynamics of metabolic transformations. Here, we address this question by casting the existing models of Calvin–Benson cycle and the end-product processes into an analysis framework which not only facilitates the comparison of the different models, but also allows for their ranking with respect to chosen criteria, including stability, sensitivity, robustness and/or compliance with experimental data. The importance of the photosynthetic carbon metabolism for the increase of plant biomass has resulted in many models with various levels of detail. We provide the largest compendium of 15 existing, well-investigated models together with a comprehensive classification as well as a ranking framework to determine the best-performing models for metabolic engineering and planning of *in silico* experiments. The classification can be additionally used, based on the model structure, as a tool to identify the models which match best the experimental design. The provided ranking is just one alternative to score models and, by changing the weighting factor, this framework also could be applied for selection of other criteria of interest.

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Keywords: Calvin-Benson cycle; Carbon metabolism; Model ranking; Differential and algebraic equations

1. Introduction

One of the central challenges in plant physiology is the enhancement of plant growth and yield. Therefore, optimizing the Calvin–Benson cycle (CBC, for abbreviations see Table S23), as the initial pathway of carbon fixation in C_3 -plants, and the related end-product pathways, producing starch and sucrose, is of great importance. A powerful tool for *in silico* probing of such biological systems is mathematical modeling of the integrated processes [30]. It allows to place these important pathways in the context of their cellular milieu and the entire carbon cycle. Moreover, modeling provides the means for predicting systemic behavior on various levels of the system, rendering it valuable in planning laborious experiments aimed at confirming posited hypotheses.

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Here, we present a detailed description of an analysis and ranking framework for models of the photosynthetic carbon metabolism to determine those model candidates which provide accurate predictions for the levels of intermediates and show biologically plausible dynamics. These candidates, in turn, can be used in metabolic engineering [44] and in the design of synthetic metabolic pathways for improved carbon fixation, growth and yield [4].

2. Model compendium

By thoroughly reviewing the literature spanning the past three decades, we have assembled the largest compendium of models for the CBC. The compendium consists of 15 models, including the initial modeling attempts and some of their widely cited extensions [8,10,12,16,18,25,26,29,32,34–36,42–44]. The existing models cover various contexts of photosynthesis-related processes and, thus, they differ in size as well as in the complexity of the underlying mathematical formulation. They have been developed with several applications in mind, such as: describing carbon fixation [8,10,29,35,36], examining regulatory processes [12], applying systems biology methods [16] or investigating evolutionary development [44].

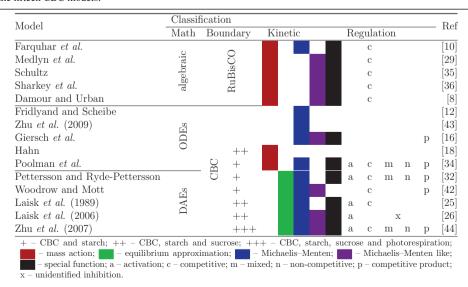
The main goal of the here proposed ranking framework is to determine the best-performing models with respect to their potential usage in metabolic engineering. Therefore, we would like to stress that a worse ranking implies only that the model may not be suitable for metabolic engineering.

3. Model classification

First, we provide a detailed classification of the models included in the compendium based on: (1) model boundaries, *i.e.*, the coverage of CBC together with the end-product pathways, (2) mathematical apparatus, *i.e.*, the type of equations by means of which the model is evaluated, (3) complexity of kinetics [17], translating the model structure into mathematical equations for analyzing spatiotemporal properties and (4) included regulatory processes, specifying the regulators, their types and the resulting formalization.

The considered models differ in their boundaries due to the covered aspects of photosynthesis. Five of the models focus on the initial step, whereby CO₂ enters the CBC. It is termed the ribulose-1,5-bisphosphate carboxylase/oxygenase (RuBisCO, EC 4.1.1.39) reaction. Within these models, the remaining steps of the CBC are merged into one regeneration step (Table 1, column 3). There are three models describing the CBC in detail but omit related processes. A group of three models investigate the processes taking place in the chloroplast, *i.e.*, the CBC and starch synthesis, and the

Table 1 Classification of the fifteen CBC models.



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