Petri net Modeling and Property Analysis of C3 plant Photosynthesis and Photorespiration

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Gajendra Pratap Singh
Jawaharlal Nehru University

Corresponding Author
ORCiD: https://orcid.org/0000-0002-7642-2715

gajendra@mail.jnu.ac.in

Madhuri Jha
Jawaharlal Nehru University

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Abstract

Metabolic pathway - Modeling and Analysis, is the emerging research area in Biochemistry over the past few years. C3 plants are the best carbohydrate producers and also are the most common plants found in the nature. These plants are very much efficient in photosynthesis in cool and wet climate while, in very hot climatic condition it undergoes photorespiration process. In this paper we model the process of making food by C3 plants to study the behavior in different climate conditions.

Background

In biochemistry a metabolic pathway is a combination of chemical reactions inside a cell. There are various chemical reactions which occurs in our body as well in the plants to release usable energy. These chemical reactions drive the processes that keep the living organism ‘alive’. There are two types of metabolic pathways found, anabolic and catabolic pathways depending on their ability to either combines the molecules with the use of energy or splitting/breakdown of complex molecules by producing some energy in the process. The reactant, product and the intermediates may or may not be same. Sometimes these compounds act as enzymes to perform the certain reactions. Somewhere the product of one reaction acts as enzyme for other one. Some of the major metabolic networks in our body are glycolysis, citric acid cycle, urea cycle etc. Some metabolic pathways are present in the nature too such as photosynthesis and photorespiration. The food making process by plants is the most basic metabolic pathways found in environment but still have a greater importance. Increase in demand of food especially Carbohydrate rich food in India always encourage researchers to develop strategies to increase in food production. So, we are focusing on the carbohydrate giving plants and that is C3 plants. There are three different type of plants occurs in nature namely C3, C4, and Crassulacean Acid Metabolism (CAM) plants, which named on the number of carbon present in the first stable compound formed during the photosynthesis process. Three photosynthesis pathways exist among terrestrial plants. Different plants have different networks depending on certain conditions [1,2]. Graph theory results are also available in several biological networks and in photosynthetic effect [3, 4]. Several other mathematical models are proposed in order to understand the network of plants photosynthesis and explain the stomatal behavior of leaf-level C3
photosynthesis but they all are analytical model [5,6]. In this paper we propose a Descriptive mathematical model which approaches through graphical representation and draws some better qualitative and quantitative properties of any biological model or any complex system network. In order to understand the dynamic property and behavior of $C_3$- plants Carboxylation process (Photosynthesis) and the Oxygenase process (Photorespiration), we propose a mathematical and graphical approach of modeling and that is Petri Net (PN). Due to its adaptability Petri net is very much efficient to model any biological system and can handle any concurrent and distributed complex system perfectly This model is Petri net (PN) which is a discrete event system first proposed by Carl Adam Petri in early sixties to model the concurrent, asynchronous, distributed system [7,8]. Petri net is also used in several other field of sciences determining binary vectors or can be used as a recommender system in several networks [9,14]. Petri net has also application in biological networks like in Cardiovascular disease or in tuberculosis [15,18]

In this paper we focus on $C_3$ plants metabolic network and will compare the networks with $C_4$ plants using Petri net model. There are several software available to trace Petri net model and validate the system modeled and provide several results to explain the behavior of network considered. In this paper we are using PIPE v4.3.0 to draw the network and uses the results to explain the $C_3$ plant network [19]

Photosynthesis is the most common and most important biochemical reaction occurring in nature. Almost all types of plants undergo photosynthesis under different conditions. $C_3$ plants are the most common plants found in nature. Most of the carbohydrate producers are the $C_3$ plants for example Beans, Rice, Wheat, Potato etc, which are also called energy giving plants. The process in which these plants produce energy is Photosynthesis. This process has a network explained in Figure 1, as they are efficient at photosynthesis in cool and wet climates. $C_3$ plants do photosynthesis using NORMAL CALVIN CYCLE. Photosynthesis is the process where Reduced Nicotinamide Adenine Diphosphate (NADPH) and Adenosine Diphosphate (ATP) are created in CBB (Calvin Benson Bassham). In the suitable weather CO$_2$ enters through the tiny pores on leaves called stomata. This carbon dioxide
then combines with an enzyme called RuBisCO to produce Sugar. This process produces a molecule made up of three carbon atoms, and that is why C_3 plants named. For C_3 plants, this process takes place in a chloroplast layer, the green cells present in plants which helps in photosynthesis which makes any plant green. The cycle continues and with the help of energy in the form of light from the sun, sugar is made as well as RuBp is also produced for the future use [20]. Sometimes the C_3 plant consumes oxygen too, which can slow down the process of photosynthesis. This process is called Photorespiration also called oxidative photosynthetic carbon cycle, or C_2 cycle. C_2 cycle is named so as the first stable compound formed is a two carbon molecule. In Figure 2, one can observe the network involved in producing energy in C_3 plants during Photorespiration. It is the process of taking O_2 instead of CO_2 in the process of Photosynthesis. Instead of fixing carbon when Rubisco fixes oxygen under certain conditions results in Photorespiration (PR). Sometimes it is also called anti-photosynthesis process. Under hot conditions RuBisCo has more affinity towards oxygen, so under hot weather when stomata closed so CO_2 can’t diffuse in and O_2 can’t diffuse out. Earlier it was said that this process is harmful for plants but recent researches shows the importance of this process. The process PR converts 2-phosphoglycolate (2PGP) into 3-phosphoglycerate (3PGA) and is escorted by O_2 intake and CO_2 release. PR plays the role of salvage or metabolic repair process which convert the toxic compound produced i.e., PGP into a useful compound PGA which produced during CBB cycle. PR also leads to the loss of CO_2 and NH_3. Eventually, PR decreases the rate of photosynthesis by 30% in current atmospheric concentration of CO_2 and O_2 [21].

Results And Discussion

While modeling the process we are considering the stable intermediate products as places and the enzymes responsible for the reactions are taken as transitions. Tokens on the places are the number of molecules available of the corresponding compounds. The weight of the arc is according to the number of molecules required in the reactions. Flow of tokens implies the formation of one product to another product according to the firing rule of Petri net. In Figure 3, we have shown the Petri net modeling of metabolic network in producing energy by C_3 plants in both conditions either involving
light reaction or dark reaction. In Table 1, the description of places and transitions are shown according to the model.

Here we have modeled both the process of i.e., photosynthesis and photorespiration in a single model. When CO₂ is present in the stomata of the plant cell then the normal photosynthesis process will take place as \( t_1 \) will fire and further CO₂ combines with RuBp which is already present in the plant cells to form PGA then G3P followed by the formation of Glucose to produce energy for the plant.

Hence the path of firing of these transitions leads to normal photosynthesis \( t_0 \ t_{11} \ t_{12} \ t_{13} \ t_{14} \ t_{15} \ t_{16} \). This cycle of model is validated from PIPE v4.3.0 software and some results follows which can be explained by the properties of Petri net.

The model is bounded, signifies the compounds formed during photosynthesis is in limited number of molecules. There is no accumulation of any product formed during the process either the product has been used for the further process or being used by the plants growth. The number of molecules formed is different for different compound, so this model is not Safe. In this model we are not concerning after the formation of glucose so this model must have a deadlock. But the product RuBp is produced again during the process so the process is also Live.

In other case when there is no CO₂ enters through stomata then tokens on \( p_0 \) will be zero. Then \( t_1 \) attached by the inhibitor arc will fire to extract O₂ which is already present there in the cells of the plants and the tokens shifts to place \( (O_2) \) according to the weight associated with the preceding arcs to process the further reactions for photorespiration. The compound RuBp is already present in the plant, So to start the process we are taking the six molecules of RuBP i.e., \( \mu^0(RuBp) = 6 \), and for all other places in \( P, \mu^0(p_i) = 0 \).

Here, only transition \( t_1 \) will fire due to inhibitor arc property and consume O₂ to start the process. Now, O₂ combines with RuBp in the presence of RuBisCo enzyme to form two compounds PGA and PGP. PGA will again start normal Calvin cycle and PGP goes through a certain number of steps to form
PGA back to follow Calvin cycle to produce Glucose.

Availability of sufficient amount of CO₂ results in Photosynthesis and insufficient amount of CO₂ results in photorespiration with availability of O₂. In either case the Petri net is non-terminating. Also, the process is **Live** always. We can infer that the formation of glucose which is very essential for plants will never stop and the production of food given by C₃ plants can be increased by maintaining a suitable atmospheric composition. During modeling of metabolic pathways in photosynthesis and photorespiration, as the starting molecule is produced back to start the reactions again so the process is always reversible[25].

**Conclusions And Scope**

We have discussed the modeling of metabolic pathways as discrete-event systems. The benefit of modeling the bio-chemical process in Petri net graph is to analyze in a better way about the different stable compounds formed and the inter-conversion of one compound to another compound. The reachability graph makes a clear concept of formation of glucose from a certain available gases from air. C₃ plants like beans, rice, wheat, potatoes etc are the major plants for the survival of human being. One can model the Rice plant system or any other carbohydrate giving plants network. This will help to check how nitrogen can improve the productivity just by placing one more place in the model without affecting the basic properties of the model [26,27].

For any specific C₃ plant like Soya bean (a high source of Protein) which is a very important C₃ plant in nature, one can model the photosynthesis process for the plant in such a way to know the exact way in order to increase the production. Certain nanoparticles are also available by the addition which the productivity of soyabean plant or certain other C₃ plants can be increased. For examples Cerium Oxide (CeO₂NP₅) has the average size 19mm is a useful nanoparticles for C₃ plants. One can also model the other type of photosynthesis like C₃ and CAM plants photosynthesis network and can compare that by C₃ plants network. These plants are capable of resisting the photorespiration process.
by storing \( \text{CO}_2 \) in different layer. One can model for these plants that in the absence of \( \text{CO}_2 \) how these plants process the further reactions to produce Glucose. These days the modeling of \( \text{C}_4 \) pathways in the existing \( \text{C}_3 \) crops is very important by observing in these plants how RuBisCo not combines with \( \text{O}_2 \) can be modeled using Petri Net graph.

With modeling of all these networks, validation and simulation is also very important with Petri net software like PIPE or in MATLAB with Petri Net tool box.

**Methods**

**Petri Net (PN)**

Petri net is a special kind of directed graph where two kinds of nodes are present, one is place and another is transition. While drawing the graphical representation of any model, places are draw as a circle, and transitions as rectangle. It describes the complex system in graphical manner and gives an easy visualization of the system. Peterson describes further advantages of Petri net as a model of concurrent and conflict systems. The power of Petri net means the properties of the net can help to describe the modeled system in a better way. An advance Petri net analysis of techniques provides systematic and qualitative results of the modeled system. Petri net model analysis is drawing attention because of its simple graphical approach and certain high level Petri nets like timed Petri net, stochastic Petri net and colored Petri nets are proved very useful to study about any complex system. Petri net is 5-tuple set, consisting of a finite set of places, a finite set of transitions, a positive incidence function that denotes the number of arc from any transition to place, a negative incidence function that denotes the number of arc from any place to transition and an initial marking which represents the number of tokens on each place initially.

Mathematically represented as \( \text{PN} = (P, T, I^-, I^+, \mu_0) \). Any transition fires at the given marking if and only if the outgoing arcs from all the places is less than and equal to the present marking of that place. After firing the tokens are moved from the input places and deposited on the output places accordingly.
The Reachability Graph of a Petri net is denoted by $R(PN, \mu)$ where, all the markings $\mu$ are taken as the vertices and the transition responsible for the corresponding marking is taken as edges. It helps in drawing the results of reachability of one state to another state. One state is reachable from another state if there is a directed connected path found between them [22,23].

Properties of Petri Net

Reachability Graph/ Coverability Graph: The graphical representation of the firing sequences and all possible marking states is called Reachability Graph of the Petri net. Here, nodes are the marking states and the arcs show the corresponding transition which fires to attain that state. In biological system the reachability graphs help to find the possible ways in the formation of the required product.

Boundedness: A Petri net is Bounded if the number of tokens on any of the places involved never exceeds a finite or a fixed amount. In biological system it helps to implies that the number of molecules formed in the product compound is limited. Accumulation of any compound is not taking place. Hence it shows the property of conservation of mass.

Liveness: A Petri net is live for $\mu$ (initial marking), if there exists a firing sequence to reach to one marking from any other marking by a suitable firing sequence. In biological network it implies that the involved reactions will occurs repeatedly which contributes to the development depending on time.

Reversible: A Petri Net is reversible if the initial marking is reachable from all the other reachable markings. In biological system it implies that the compound which starts the reaction is formed or produced again within the process.

Extended Petri-net: The extended Petri net is somehow an extension of standard Petri net where it has a form of arc called an inhibitor arc. An inhibitor arc is from a place $p$ to a transition $t$ which enables only when there are no tokens on $p$. This makes the concurrent phenomena much easier to model [24].

Abbreviations
RuBp: Ribulose 1,5-bisphosphate, RB: Ribulose 5-phosphate, RuBisCO: Ribulose-1,5-bisphosphate carboxylase Oxygenase, CO$_2$: Carbon dioxide, O$_2$: Oxygen, PGA: Phosphoglyceric acid,
PGP:Phosphoglycolate phosphatase, G3P: Glyceraldehyde 3- Phosphate, H$_2$O$_2$:Hydogen peroxide,
H$_2$O: Water, NH$_3$: Amonia Gas, NH$_2$: Amino radical, HPR:Hydroxypyruvate reductase, ATP: Adenosine
triphosphate, ADP: Adenosine diphosphate, NADPH: Reduced Nicotinamide Adenine Diphosphate, PR: pyruvate.

Declarations

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Authors’ Contributions

GPS has modeled the process with helping in manuscript writing while MJ validated the model with its properties and wrote the paper. Final manuscript approval has been done by both the authors after reading the paper.

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Availability of data and material

The software PIPE v4.3.0 used in the paper is easily available on the link http://pipe.allapp.biz/downloaded.html.

Ethics approval and consent to participate

Not applicable
Consent for Publication

Not applicable

Competing interests

The authors declare that they have no competing interests.

Author details

1,2Mathematical Sciences and Interdisciplinary Research Lab, School of Computational and Integrative Sciences, Jawaharlal Nehru University, New Delhi-110067, India, E-mail: gajendra@mail.jnu.ac.in, jhamadhuri81@gmail.com

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Tables
Table 1: Name and Description of Places and Transitions taken in the model in Figure 3

| Places | Description | Transitions | Description |
|--------|-------------|-------------|-------------|
| p0     | CO₂ entering from stomata | t₀         | Extract CO₂ |
| p₁     | CO₂         | t₁         | Extract O₂ |
| p₂     | O₂          | t₂         | RuBisCo performing Carboxylation |
| p₃     | RuBP        | t₃         | RuBisCo as Oxygenase |
| p₄     | PGA         | t₄         | Phosphoglycollate phosphatase enzyme |
| p₅     | PGP         | t₅         | Carboxylation with NADPH to release NADP⁺ |
| p₆     | Glycolate   | t₆         | Catalysis |
| p₇     | H₂O₂        | t₇         | Deamination |
| p₈     | Glyoxylate  | t₉         | Decarboxylase and methyltransferase |
| p₉     | H₂O         | t₁₀        | Catalysis in presence of ATP |
| p₁₀    | NH₂         | t₁₁        | Reduction in presence of phosphatase |
| p₁₁    | Glycine     | t₁₂        | Reduction in the presence of triosephosphate dehydrogenase |
| p₁₂    | NH₃         | t₁₃        | Reduction and rearrangement in the presence of some metabolic enzymes |
| p₁₃    | Serine      | t₁₄        | Reduction and isomerization in the presence of phosphatase |
| p₁₄    | HPR         | t₁₅        | ATP + Phosphate pentose Kinase |
| p₁₅    | Glycerate   | t₁₆        | Reduction and isomerization |
| p₁₆    | G3P         |            |             |
| p₁₇    | Fructose    |            |             |
| p₁₈    | RB          |            |             |
| p₁₉    | Glucose     |            |             |
Figure 1

C3 photosynthesis
Figure 2

C3 photorespiration

Figure 3

PN modeling of C3 Photosynthesis and Photorespiration
