

# Simulation Of Microalgae Photosynthesis Electron Transfer With Magnetic Energy Influencing

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**Abstract-** A mathematical modelling is applied to illuminate and predict the mechanism of electron transfer in microalgae photosynthesis. A magnetic field can accelerate its reaction by decreasing the frequency of reverse reactions in the radical pair mechanism. The effect of magnetic field (MF) changes  $K_{ISC}$  and give significant effect tot internal energy, the simulation result indicates that the external energy that affects the process of electron transfer often leads to an increase in temperature energy which causes the induction effect to be overcome by the presence of heat energy. The highest value of  $\Delta G_2^*$  occur at 8 miltesla magnetic exposure with internal energy of 1.08 eV.

**Index Terms-** magnetic field; microalgae; internal energy.

## I. INTRODUCTION

In most biological systems are believed to have effects and influences on exposure to Electro-magnetic-field (EMF). This is explained by Faraday concepts and theories that state that current flow through certain mediums is capable of induced magnetic force (MF) [1]. Biological systems generally based on fluid, and chemical reactions involving enzymatic processes involving ionic induced (i.e. ions flowing through cell membranes, ionic transfer in chemical reactions, etc.) affect EMF induction, altering the original electromagnetic behavior [2]. The effect of MF affect the energy distribution in biological systems and have the potential to alter cell physiological function, catalyze the reactions, accelerate cell's functions, and activation of the systems involved [3].

The investigation discovers how MF extremely affects microalgae growth. A weak value of MF below than 10 $\mu$ T [4] does not agitate cellular processes because there is no physical mechanism to interact . Lot of literature claimed that the weak magnetic fields (less than 1 Tesla) does not give any significant influences and effects on chemical or photochemical reactions because it was believed he required reaction time are lower than reaction time contribute by activation energy and thermal energy.

There are few assumptions and hypotheses made on the effects MF on biological system. Considering the overall biological systems cannot being consider as a linear system, one particular species may experience different effects on magnetic exposure [5]. The sensitivity of magnetic effect responds into sympathetically or Para sympathetically effect, providing an insight to inhomogeneous effect of MF across different biological systems.

## II. Transition State Theory (TST)

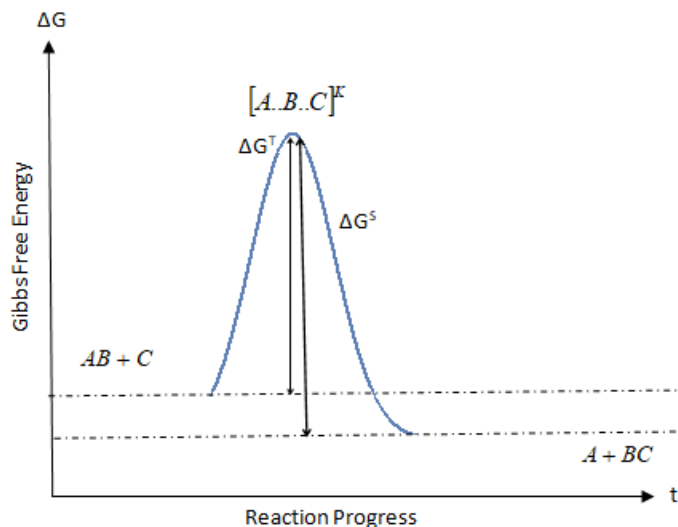
The transition state theory (TST), which is also known as theory of absolute reaction rates and the theory of activated state (Enzyme), is essentially a fundamental of enzymatic reaction theory, which treats the reacting enzyme molecules as the active site that being filled by substrate in reaction process. The theory explains the rate of chemical reaction assuming a special type of chemical equilibrium (quasi-equilibrium) between the reactants and activated state (transition state complex). This special molecule decomposes to form the products of reaction. The rate of this reaction is then equal to the rate of decomposition of activated complex.

Magnetic influences in photosynthesis is predicted to speed-up the reaction in enzyme activity in algae photosystem, magnetic effect have an ability to enhance the catalyst of enzyme reaction in biological of photosynthesis. Magnetic effect speed-up the rate of chemical reaction as decreasing the time that is needed for reaction to took place until its reach equilibrium [6]. Consider a simple reaction as represent below:



Note that  $[A \bullet B \bullet C]$  represent the partially broken and formed bond as  $K$  represent the rate at transition state took place. The reaction of enzyme activity without any catalyst or external force as an influence in the system can be simply described as energy diagram as shown in figure 1. As presented in **figure 1**, the Y axis represents the Gibbs free energy level and the X axis is the reaction progress based on time. From the diagram we can conclude that the free energy at the enzyme product  $\Delta G^s$  is slightly lower than the substance  $AB + C$ , which note as  $\Delta G^T$  give a basic understanding that free energy will release within a product in enzyme reaction. These give a spontaneous reaction in enzyme activity as long as the reactions at the substance have enough energy to overcome the Gibb free energy for reaction activation  $\Delta G^T$ .

In enzyme terminologies the reaction in enzymatic processes does not affect the free energy value of the product and reactant as well as if the system are exposed to the external MF, the value of free energies from both reactant and product are no affected[7]. The main effect of external forces such as heat and MF in enzymatic activity is the kinetic speed and of the motion at the transition state with label as  $[A \bullet B \bullet C]$  in **figure 1**.



**Figure 1:** Gibb Free Energy Diagram of the Enzyme Reaction with No-external Forces.  $AB + C$  represent substance,  $[A \bullet B \bullet C]^K$ , transition state,  $A + BC$ , end product,  $\Delta G^T$ ,  $\Delta G^S$  represent the activation energy.

The transition state  $[A \bullet B \bullet C]$  is at a state in enzyme activity where the  $AB$  bond will be break at the same as the  $BC$  bond will form. The state of  $[A \bullet B \bullet C]$ , or the transition state is determining by the highest peak of Gibbs free energy diagram as shown in figure 1. In the particular state, enzyme-substrate complexes are formed by utilizing the energy in reaction processes as the substrate will bind in enzyme active site, leads to the breakage of  $AB$  bond and formulation of  $BC$  until equilibrium point reach at  $\Delta G^S$ . Since speed is determined by the energy of activation one can observed a decreasing of free energy value of both reactant and product in enzyme activity as being influence by external forces [8].

The enzymes-kinetic formulation in the reaction was represented by Eyring model as the rate of collisions depends on temperature from the original reaction kinetic in (2).



The linear reaction equation is;

$$\frac{dAB}{dt} = -K_{-1}[AB][C] + K_1[A \bullet B \bullet C] \quad (3)$$

$$\frac{dC}{dt} = -K_{-1}[AB][C] + K_1[A \bullet B \bullet C] - K_2[BC] \quad (4)$$

$$\frac{d[A \bullet B \bullet C]}{dt} = K_1[AB][C] - K_{-1}[A \bullet B \bullet C] - K_2[A \bullet B \bullet C] \quad (5)$$

The  $[A \bullet B \bullet C]$  is the intermediate state as known as activated complex which at equilibrium rate and can be represent

$$K^{TH} = \frac{[A \bullet B \bullet C]}{\{[AB][C]\}} \quad (6)$$

Where  $K^{TH}$  is the thermodynamic equilibrium constant.

The rate of a reaction is equal to the number of activated complexes decomposing to form products. Hence, it is the concentration of the high-energy complex multiplied by the mean velocity of an ideal gas  $\nu$  [9].

As the rate of reaction may be expresses as follow:

$$Rate = \nu[A \bullet B \bullet C] = AK^{TH} \{[AB][C]\} \quad (7)$$

Where  $\nu$  is determine as the frequency of crossing of activation energy of activation state complex  $[A \bullet B \bullet C]$ ,

$$A = \frac{K_B T}{h} \quad (8)$$

Where  $K_B$  is the Boltzmann constant ( $1.3806568 \times 10^{-23} \text{ J K}^{-1}$ ): and  $h$  is Planck's constant ( $6.6260755 \times 10^{-34} \text{ Js}$ ), since the rate  $K = \nu K^{TH}$  expression of the reaction rate for the system be simplify as follow

$$K^{TH} = \frac{[A \bullet B \bullet C]}{[A \bullet B][C]} = \frac{\exp\left(\frac{-G_0}{k_B T}\right)}{\exp\left(\frac{-G_{AB}}{k_B T}\right) \exp\left(\frac{-G_C}{k_B T}\right)} = \exp\left(\frac{(G_{AB} + G_C) - G_0}{k_B T}\right) \quad (9)$$

$$K^{TH} = \exp\left(\frac{-\Delta G}{k_B T}\right) \quad (10)$$

$$K = \frac{K_B T}{h} \exp\left(\frac{-\Delta G}{k_B T}\right) \quad (11)$$

In **Figure 1**,  $\Delta G^T$  embeds free energies associated with the formation of the activated complex and with the subsequent steps to the electron transfer. The rate  $K$  expressed in an Arrhenius form as

$$K = (A) \exp\left[\frac{\Delta G^T}{K_B T}\right] \quad (12)$$

Where  $K(s^{-1})$ ,  $K_B$  is the Boltzmann constant ( $1.3806568 \times 10^{-23} \text{ J K}^{-1}$ ) or  $8.617333262145 \times 10^{-5} \text{ eV/K}$  and  $T$  is the temperature in Kelvin.  $\Delta G^T$  is the standard molar Gibbs energy of activation as represented as

$$\Delta G^T = G^0(\text{Activation}) - G^0(\text{Reactants}) \quad (13)$$

### III. Enthalpy and Entropy of Cyanobacteria Photosystem

Referring to **Figure 2**, pigment  $P680(P)$  is located within a thylakoid membrane. Absorption of light promotes  $P680(P)$  to the excited state  $P680(P^*)$  as the photocell is illuminated by sunlight, the rate of absorptions is measured by the integration the product of incident solar spectrum by the absorption spectrum chlorophyll” [10]. The total energy  $\Delta G$  is the summation of  $\Delta H^0$  and  $\Delta S^0$  correspond to temperature (kelvin) thus if one treats the excited state of chlorophyll in microalgae was the main part of radical pair mechanism took place, the overall Gibbs free energy equation for the chlorophyll system are given as

$$\Delta G = \Delta H - T\Delta S = hv_0 - T\Delta S \quad (14)$$

The term  $\Delta S^0$  concern the free energy due to the negative contribution of the entropic term and normally represent as

$$K_B T \ln \left[ \frac{P680(P^*)}{P680(P)} \right] \text{ with } K_B, \text{ Boltzmann constant } (1.3086568 \times 10^{-23} \text{Js or } 8.617333263145 \times 10^{-5} \text{ eV. K}^{-1}) \text{ which lead to Eq.}$$

(15) as

$$\Delta G_0 = \Delta H_0 - T\Delta S_0 = hv_0 - K_B T \ln \left[ \frac{P680(P^*)}{P680(P)} \right] \quad (15)$$

Assumption of “one photon absorbed per chlorophyll per second for full sunlight”[11]. Taking ~20ns for natural lifetime of chlorophyll excited state  $P680(P^*)$  with means the reaction rate of  $P680(P^*) / P680(P) \approx 2 \times 10^{-8}$ ,

$$\Delta G_0 = \Delta H_0 - T\Delta S_0 = 1.8 \text{ eV} - K_B T \ln [2 \times 10^{-8}] \approx 1.36 \text{ eV} \quad (16)$$

The electron flow in photosystem II will proceed to the singlet formation of  $(P^+ Pheo^-)$  as the recombination process took place

to  $((P^*) \bullet Pheo) \xrightleftharpoons[k_{-2}]{k_2} (P^+ Pheo^-)$  with a reversible radical pair rate of  $k_2$  and  $k_{-2}$  (ground state). For positive net flux, at

temperature 25°C (T, 298K) one can write

$$\left[ \frac{(P^*) \square Pheo}{P^+ \square Pheo^-} \right] \geq \frac{K_1}{K_{-1}} = \exp \left( \frac{\Delta G_0 - \Delta G_1}{K_B T} \right) \quad (17)$$

Utilizing the Literature constant value of exciton radical pair model [12], with rate constant  $K_1$  and  $K_{-1}$ , ( $1.59 \text{ ns}^{-1}, 0.3 \text{ ns}^{-1}$ ),  $\Delta G_1$  value calculated as follows

$$\left[ \frac{(P^*) \square Pheo}{P^+ \square Pheo^-} \right] \geq 5.3 = \exp \left( \frac{1.36 - \Delta G_1}{K_B T} \right) \quad (18)$$

Resulting the value of  $\Delta G_1$ , (1.32 eV).

And,

$$\left[ \frac{(P^+) \square Pheo^- Q_A}{(P^+) \square Pheo Q_A^-} \right] \geq \frac{k_2}{k_{-2}} = \exp \left( \frac{\Delta G_1 - \Delta G_2^*}{K_B T} \right) \quad (19)$$

Utilizing the Literature constant value of exciton radical pair model from chapter 2, (**Table 2.1**), with rate constant  $K_2$  and  $K_{-2}$ , ( $4 \text{ ns}^{-1}, 0.01 \text{ ns}^{-1}$ ),  $\Delta G_1$  value calculated as follows

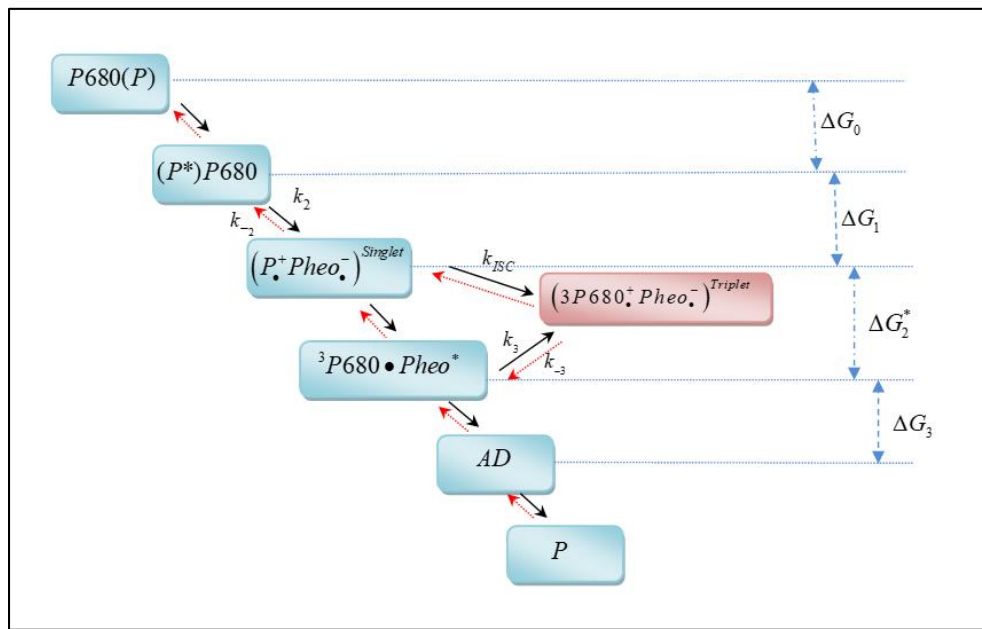
$$\left[ \frac{(P^*) \square Pheo}{P^+ \square Pheo^-} \right] \geq 400 = \exp\left(\frac{1.32 - \Delta G_1}{K_B T}\right) \quad (20)$$

Resulting the value of  $\Delta G_1$ , (1.17eV).

Applying the same concept, the electron transfers at the radical pair mechanism with the influences of (MF),

$(P^+ \cdot Pheo^-) \xleftrightarrow{k_{ISC}} 3(P680^+ Pheo^-)^{Triplet}$  can represent as,

$$\left[ \frac{(P^+) \square Pheo^- Q_A}{(P^+) \square Pheo Q_A^-} \right] \geq \frac{k_{ISC}}{k_{-2}} = \exp\left(\frac{\Delta G_1 - \Delta G_2^*}{K_B T}\right) \quad (21)$$

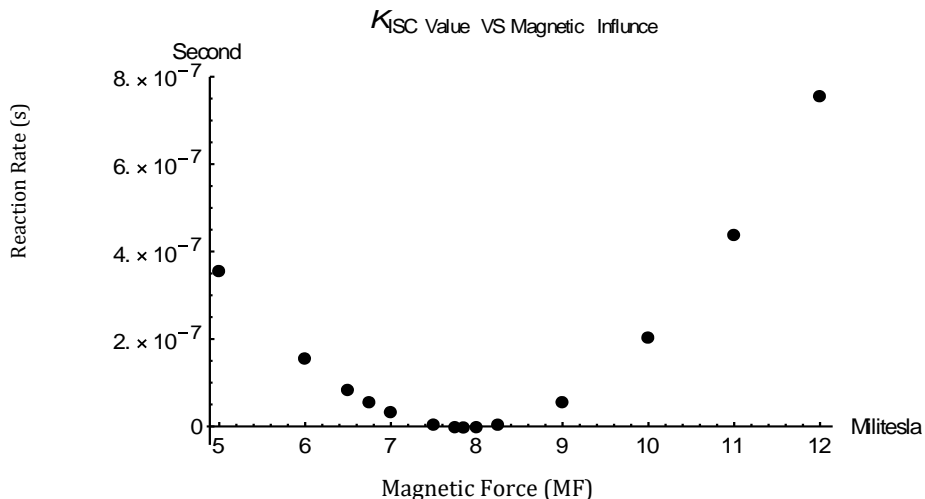


**Figure 2:** Energetic and kinetics of radical pair states in PSII.

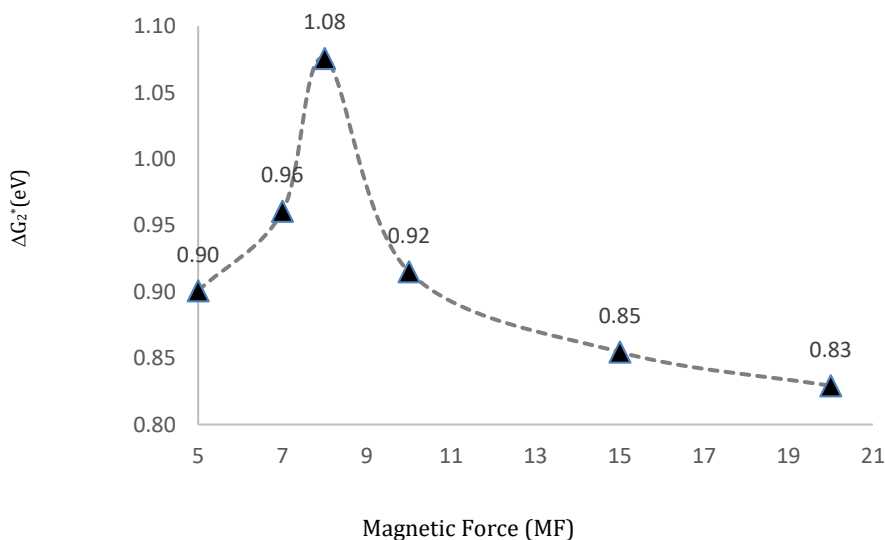
In the typical photosynthesis process, the energy of excited state in PSU I and II is obtained from photons and converted to free energy in the chlorophyll structure. In this thesis framework we simplying the internal energy of the photosystem is to be concluded as enthalpy  $H^0$  which is defined as  $\Delta H^0 = h\nu_0$  [11] since we took account the smallest possible unit of energy represent the relative population of the excited state. For instead we take (P) represented chlorophyll with a determine value of 1.8ev for  $h\nu$  [13]. The parameter  $\nu$  stands for frequency (in reciprocal seconds – written  $s^{-1}$  or Hertz (Hz)-  $1\text{Hz} = 1\text{ s}^{-1}$ ),  $h$  is Planck's constant (  $6.626 \times 10^{-34}$  J.s). Photon may have multiples of  $h\nu$ . The excited state of electron is defined as electron in an atom absorbs energy in the form of  $h\nu$ , moves it to a higher energy orbit and moves down to the lower orbit when the electron releases the same amount of energy in term of  $h\nu$ .

#### IV. Result and Discussion

Using the simulation value  $K_{ISC}$  the calibration of rate of  $\Delta G_2^*$  as shown in **Figure 3**



**Figure 3: Simulation of  $K_{ISC}$  value**



**Figure 4: The value of Internal Energy  $\Delta G_2^*$  with Rate of Radical Pair  $K_{ISC}$  with magnetic Effect**

The reaction rate per second show the influences of applied MF at range 5mT to 10mT, the reaction rate indicated a decreasing of reaction time from range of  $1 \times 10^{-6}$ second to  $1 \times 10^{-10}$ second with the increasing applied MF. effect (Mf) is also seen to increase internal energy G especially in areas where radical pair mechanism occurs. This can be explained by the presence of MF at a certain level affecting the process of electron transfer at a faster rate than usual leading to the formation of triplet magnetic state [14]. However, the presence of MF as an external energy that affects the process of electron transfer often leads to an increase in temperature energy which causes the induction effect to be overcome by the presence of heat energy. The highest value of  $\Delta G_2^*$  occur at 8 militesla magnetic exposure with internal energy of 1.08 eV, compare to the other magnetic exposure for examples 0.83ev for 20miliesla and 0.90eV at 5militesla exposure.

## V. Conclusion

In the present study, a simulation was conducted by combining rate of electron transfer KISC and internal energy at radical pair mechanism in algae photosynthesis. It describes the relationship of photosynthesis rate with exposure of MF. This model was used to predict distribution of internal energy at different magnetic. As the result show the significant effect at a certain range of MF exposure (5-10 militesla). However, to get a perfect prediction of photosynthesis by the simulation, it is important to develop a comprehensive model considering all possible factors such as culture temperature, nutrient (nitrate and phosphate), light intensity, initial inoculum size, Ph. and others factor contributing microalgae growth.

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