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AB INITIO MODELING OF THERMODYNAMICS OF A FRUIT TREE FLOWER: THE FIRST STAGE OF THE MODEL

Abstract – A bionic model of thermodynamic processes in flowers of fruit trees is proposed. This model takes into account a number of physical and morphological properties of fruit tree flowers and some environmental factors. On the basis of the model the computer program "BioNA-1" was created. The program is able to calculate the flower pistil temperature vs. time under different lighting conditions (natural sunlight) accordingly to "ab initio" rules. The calculations made on the basis of the proposed model using the authors' program "BioNA-1" are in good agreement with experimental data.

Keywords: physics-based simulations, bionic model, floral thermogenesis, solar energy accumulator.

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АВ INITIO МОДЕЛИРОВАНИЕ ТЕРМОДИНАМИКИ ЦВЕТКА ПЛОДОВОГО ДЕРЕВА: БАЗОВАЯ БИОНИЧЕСКАЯ МОДЕЛЬ

<u>Аннотация</u>. Предложена базовая бионическая модель для описания энергетического баланса внутренней полости цветка плодового дерева. Эта модель по принципу "ab initio" учитывает ряд физических и морфологических свойств цветка и некоторых факторов внешней среды. На базе этой модели была создана авторская компьютерная программа"BioNA-1", которая состоит их двух модулей – расчетного и иллюстративного. Расчетный модуль программы вычисляет зависимость температуры цветочного пестика от времени экспозиции цветка на Солнце при различных параметрах внешней среды. Расчеты, проведенные на основе предложенной модели, хорошо согласуются с независимыми экспериментальными данными. Ключевые слова: бионическая модель, компьютерное моделирование, биофизика, термогенезис цветка.

Introduction

The floral diversity of the Earth impresses our imagination. Plants are been developing at least 475 million years, and flowering plants appeared about 130 million years ago. Flowers play an important physiological function: due to them plants are able to be reproduced over and over. But none of flowers itself does not generate energy for its existence in nature. For the necessities of life it uses an external source – and almost inexhaustible – the stream of sunlight that falls on the Earth. A flower consumes this radiant energy for its vital needs and even it can accumulate a suitable part of the energy for development of its own seeds (fruit). And does it very effectively.

Most of fruit tree flowers have the shape of a paraboloid of rotation. It is a successful form because it allows to collect solar radiation via the effective cross section of the paraboloid-like flower. And due to this form a certain part of the radiant solar energy that "is caught" by the flower petals will be transferred onto its pistil, which stands as the main recipient of the energy reflected from petals.

In this regard, the authors are interested to find the answer to the following question: how to simulate the energy balance of a biological object, which does not produce energy on their own?

Unfortunately, the authors couldn't find any research works on mathematical modeling of any biophysical or physiological processes concerning to thermodynamics of floral chamber: it seems the number of the works which are devoted to the item of modeling or simulation of thermodynamics of floral inner cavities is really very little. When working on the current problems some similar research works and reference content from different sources of different authors were considered and elaborated [1-5]. While searching we met a lot of works with similar topics, but almost all of them were "descriptive", but not "modeling" ones.

After a detailed study of available scientific literature and reviews with similar topics the authors of current work conclude that this topic was not disclosed, and therefore requires further research and development.

Thus, the **objective of the work** is to create a biophysical model of thermodynamic processes which take place in a flower of authentic parabolic form: this model is required as for carrying out of specific calculations about the heat balance of the flower ovary, as well for illustration the progress of the processes. So, the work consists of two parts which can be fulfilled by means of programming: solution of the corresponding physical problems and visualization of the obtained results.

The **object of study of the work** were thermodynamic processes which take place inside of the fruit plant flower of the paraboloidal form and their progress in time, as well as clarification of the dependence of these processes on the size of the flower, intensity of light and color of the petals.

The **subject of the study of the work** is temperature dependence of flower pistils on various factors (such as the size of the flower, colors of the flower petals, the light intensity, the outdoor temperature and others).

When compiling the mentioned above model the following working hypothesis were formulated:

1. both the very shape of flowers, and the physical properties of biological tissue of petals provide heating of internal cavity of flowers and thereby increased (relatively to the surrounding air) temperature of its pistil, and this eventually ensures the development of its fetus;

- 2. the heating temperature of pistil depends on the optical "albedo" of the flower petals;
- 3. the realistic energy balance for the mentioned flowers exists even in a calm (i.e. windless) weather.

This work consists of four sections. The Section 1 contains the theoretical foundation of physical processes that are the basis of thermodynamic balance of the biological object (a flower) as well description and analysis of some of the factors that affect these processes, namely: the sunlight intensity, a flower dimensions, features and details of light reflection caused by flower petals. The Section 2 describes the mentioned biophysical problem and algorithm of its solution by numerical techniques. The 3rd Section contains the results of calculations within the given model and their interpretation. The Section 4 of the work is devoted to discussion of obtained results and the authors' conclusion.

1. What we know on Thermodynamic balance of fruit tree Flowers

1.1 A Flower as a natural Accumulator of Solar energy

Any natural process requires energy. Since flower of fruit plants is not a generator of energy for own life, then it should "borrow" the energy from outside, in this case from the Sun. To do this plants during over millions of years of evolution "have learned to successfully use" simple and effective way for getting and accumulating of solar radiation: as a result they had created their significant physique – the flower in the shape of a paraboloid of revolution (Figure 1).

It is well known that such a parabolic surface is capable to focus radiation. So it makes sense to assume that fruit plant flower has its own structure of a parabolic antenna: the Sun rays reflected from the flower petals are then concentrated in the central part of the flower – exactly where fertilization occurs.

By the laws of physics, the bodies which are heated must give back a portion of the acquired energy to the environment through certain channels – by radiation of heat and through convection [6]. Thus, there is competition of two thermodynamic processes within the flower – heating of the flower pistil due to supplying of heat energy and cooling of the pistil at the same time, i.e. heat dissipation by convection and by radiation of energy to outdoors. As a result the flower pistil which receives a portion of heat energy that is needed to its successful functioning, and which is required for proper development and maturation of its seeds (fruit). It seems accordingly to the laws of thermodynamics, that in the middle of the "paraboloidal" flower the temperature of its pistil should be considerably higher than the temperature of ambient air.



(author: Marianna Ruiz, the source: Wikipedia, Public Domain) Fig. 1: The cross section of typical fruit plant Flower (Credit: www.wikipedia.org)

1.2 On the flux of Solar radiation on the Earth

According to the well established value of the solar constant S_{const} ($S_{const} = (1370\pm10)^{\text{W}/\text{m}^2}$ [7]) every square meter of the Earth's atmosphere can catch about 82 kJ of solar energy per 1 minute. But the Earth's atmosphere is not perfectly transparent: when passing through it the flux of solar radiation weakens due to absorption, scattering, and even reflection: i.e. a part of the solar energy is absorbed by the atmosphere and/or is reflected back into outer space.

For quite accurate calculations of quantity of radiant energy, that can reach the Earth's surface, one

commonly uses the coefficient of the atmosphere transparency Tr_A . According to the reference data [7], $Tr_A = (0,8...0,3)$ – this range is made by the rule "*clearly* \rightarrow *foggy* \rightarrow *cloudy*" (see Table 1). For any degree of transparency of the sky, the power of the solar radiation P_{Sun} that reaches the ground can be obtained as follows:

Table 1

$$P_{Sun} = S_{const} \cdot Tr_A.$$

Degrees of transparency of the Earth's atmosphere [7]					
the weather symbol	interpretation of the symbol	coefficient of transparency of atmosphere Tr_A			
*	Clear	$Tr_A = 0,8$			
0	Sunny intervals	$Tr_A = 0,7$			
0	Light clouds	$Tr_A = 0,6$			
MIST	Mist	$Tr_A = 0,5$			
ද	Thick clouds	$Tr_A = 0,4$			
С С	Drizzle	$Tr_A = 0,3$			

1.3 Calculation of the Solar Energy absorbed by Flower

To solve this problem – creating of a basic bionic model for thermodynamic processes occurring within the flower of paraboloid form, we used several simplifications and certain initial conditions like it follows:

- a fruit tree flower is schematically seen as a "paraboloid-like" unit;

- the flower is aimed at zenith: it means that the symmetry axis of the paraboloidal unit is oriented vertically in the space;

- we believe that the value of the solar constant of S_{const} (solar radiation intensity) is equal to 1370 $^{\rm W}/{\rm m}^2$:

- we believe that the temperature of ambient air T_{air} is a constant value for at least several minutes, and we supposed absence of wind;

- in order of simplifying the model it is accepted that the flower pistil is a combination of two cylinders like it shown in Figure 2;

- additional simplification: the flower petals are tightly connected or overlapped – the fact is the reason to believe that *all* descending radiant energy can reach the surface of its petals;

- we believe that flower petals are able to reflect a certain amount of radiant energy that reaches the surface of the petals: i.e. the model takes into account the mirror-like features of biological tissue of petals, which one can characterize by a certain coefficient of reflection of R_{petal} ;

let us assume one more simplification that the color of the flower petals is white.



Fig. 2: The structure of flower pistil [8] and its simplified geometric model

2. The biophysical Problem formulation and computational Methodology

The authors of current research work have proposed the following basic bionic model of thermodynamic processes taking place in a flower of fruit plants during the effect of solar radiation.

According to the model, a flower of fruit plants, which in its structure looks like a paraboloid of revolution, exposed to radiant energy of the Sun, and absorbs a proper share of this energy, but it can also reflect a certain portion of the energy from its petals towards the flower pistil. Because the flower was formed as a paraboloid, its petals are able to reflect the Sun rays and concentrate them in the focus of the figure, in which – and this is no simple coincidence – is placed the flower pistil. The radiant energy from the Sun is the energy of electromagnetic waves with different frequencies, and this radiation after absorbing by certain biological substance (by the plant tissue) on the Earth is transformed into the heat energy of the body.

The solar energy of E_{1sec} , that every second passes through the atmosphere with certain status of transparency of Tr_A , reaches the surface of a flower petals (the petals are *white* according to the model above), then reflects from them and by the laws of geometrical optics concentrates in the focus of the paraboloid. Its quantity can be calculated by the formula: $E_{1sec} = P_{Sun} \cdot R_{petal}$ (where R_{petal} is the reflection coefficient of biological tissue of the petals).

For the calculation regarding thermodynamic processes in the flower one should compose the appropriate energy balance with all the factors taken into consideration: the energy balance is based on the law of conservation of energy.

As we know, the energy balance for any body can be represented as the following equation: $Q_{absorb} = Q_{exit}$. Concerning to our model, we have: Q_{absorb} – the value of the solar radiation which can be absorbed after reflection from the flower petals; Q_{exit} – the total heat lost by the flower pistil as sum of natural (or *free*) convection and effective radiation. In terms of the proposed model, the total energy from the Sun, which can be absorbed by the pistil, has to be calculated by the formula: $Q_{absorb} = t \cdot P_{Sun} \cdot R_{petal}$ (here *t* is the exposure time of the flower under the Sun rays). But the pistil can not endlessly accumulate the heat that comes to it from outside: first, accordingly to the Stefan-Boltzmann law, it loses some of its energy for re-radiation; and second, the flower pistil begins to lose its own heat by natural air convection [6]. It means the heat Q_{exit} (which is lost) consists of two parts – the convectional one Q_{conv} and the radiative one Q_{S-B} : $Q_{exit} = Q_{conv} + Q_{S-B} = (P_{conv} + P_{S-B}) \cdot t$ (here: P_{conv} , P_{S-B} – the respective power, t – time).

As to convection, then, according to Newton-Richman law, capacity of heat flux at heat transfer is proportional to the surface area of heat exchange S_{pistil} and the temperature difference $\Delta T = T - T_{air}$ between the heated surface and environments [6]: $P_{conv} = h_{conv}(T - T_{air}) \cdot S_{pistil}$, where the heat transfer coefficient h_{conv} can be calculated as follows (see [6], pp. 3-4, Eq. (3.1.6)): $h_{conv} = \frac{2\pi L}{S_{pistil} \ln(r_2/r_1)}k$ (here k is the

thermal conductivity of the material).

As for the generating of radiant energy from the heated body by Stefan-Boltzmann law: the power of radiation P_{S-B} of heated body can be calculated by the formula: $P_{S-B} = \sigma \cdot \varepsilon \cdot S \cdot (T^4 - T_{air}^4)$, where σ is the Stefan-Boltzmann constant ($\sigma \approx 5,67 \times 10^{-8} W \cdot m^{-2} \cdot K^{-4}$), ε – the emissivity of the surface of a flower pistil ($\varepsilon = 0...1$), S – the surface area of the body that emits.

If rewrite the equation for the energy of Q_{absorb} , which is oncoming to the pistil, then in terms of the proposed model it will be as follows: $t \cdot P_{Sun} \cdot R_{petal} = c_{plant} \cdot m_{plant} \cdot (T - T_{air}) = c_{plant} \cdot m_{plant} \cdot \Delta T$, where c_{plant} is the specific heat capacity of the plant tissue, $m_{plant} = \rho_{tissue} \cdot V_{pistil}$ (the density of the substance ρ_{tissue}).

The same equation, but submitted in the differential form, will be like this: $dT = \frac{P_{Sun} \cdot R_{petal}}{c_{plant} \cdot m_{plant}} \cdot dt$.

Now the energy balance equation in terms of the components of the proposed model can be rewritten like this:

$$\frac{dT}{dt} = \frac{P_{Sun} \cdot R_{petal} - P_{conv} - P_{S-B}}{c_{plant} \cdot m_{plant}}.$$
(1)

3. Obtained results and their interpretation

For the necessary calculations by the principle of *ab initio* within the given model we used appropriate initial data set related to the physical properties of a plant tissue (e.g. tissues of flower pistil, of petals): actual dimensions (so-called geometric parameters) both of typical flowers of plants that are selected for consideration, and of their structural parts according to the reference books [9]; the specific density of the substance ρ_{tissue} [10] and the specific heat capacity of certain plant tissues c_{plant} [11]; the reflection coefficient of biological tissues (flower petals) R_{petal} [12]; the emissivity of the body (i.e. pistil) ε [6], etc. When calculating the convection heat loss we used the appropriate data and methodology specified in [6].

According to the chosen model of thermodynamic processes that are basic for fruit tree flowers, it was created the differential equation (1) of the energy balance as a first order ODE that satisfies this initial condition: $T(0) = T_{air}$.

This equation was solved by using the authors' program named "BioNA-1", which consists of two modules – the computational one as well the illustrative one. In Figure 3 it is shown a schematic phase of coming of radiant energy onto a flower with subsequent transformation of this energy into thermal one.

The function $T_{pistil} = f(t)$, that is presented graphically in Figure 4, is the solution of the basic Diff. Eq. of the model: Figure 4 shows the time dependence of the apple flower pistil temperature, i.e. it is the plot of the function of $T_{pistil} = f(t)$, where T_{pistil} is the flower pistil temperature, t is the exposure time of the flower in the sunlight. From this graph you can see how the apple flower pistil is heated up with varying degrees of insolation at the air temperature of $T_{air} = 16^{\circ}$ C: after about 2 minutes of exposure in the Sun the pistil temperature can reach certain constant levels.

By means of program "BioNA-1" the authors received the calculated temperature values of flower pistils for several fruit plants, such as apple, plum, almond, pear and quince. These temperatures T_{pistil} in accordance with the model for thermodynamic balance of a flower are shown in Table 2.

How to appreciate obtained results. The performed calculations aimed to find the mentioned temperature for the given flower pistils, which is set during exposure to Sun (see Table 2), allow us to say that for similar plants (similar to the structure of the flower and its dimensions) the simulated values fall into the interval of $(25,9\pm1,1)$ °C. It means that the "paraboloid-like" flower for the millions of years of evolution has got all of its own qualities (the structure itself, geometry of organs, material and color of the petals) which permit to raise the temperature of its pistils about 10°C due to an external source of energy.



Fig. 3: Illustration of the process of solar energy accumulation by a flower



for different degrees of transparency of the Earth atmosphere (T_{air} = 16 °C)

Table 2

The calculated values of the temperature of pistils of different fruit plants at provided sunny weather and at ambient air temperature of 16°C

i	the Plant	by Binomial nomenclature	T_{pistil} , °C	$T_{pistil} - T_{air}$, °C
1	Almond	Prunus dulcis	25,1	9,1
2	Apple	Malus domestica	26,7	10,7
3	Pear	Pyrus communis	25,7	9,7
4	Plum	Prunus domestica	24,9	8,9
5	Quince	Cydonia oblōnga	27,1	11,1
		Average values :	25,9	9,9

4. Discussion and Conclusion

Thus, the authors of the work have proposed a bionic model to describe the energy balance of the inner cavity of a fruit tree flower during the specific phase of a flower life – from blooming stage up to petal fall stage. To simplify the model the authors certainly did not take into account several important facts. For example, it was not considered such external agent like a wind, and it was not taken into account the detailed optical properties of a flower petals. Nevertheless, the obtained results are well correlated with the results of the work of other researchers [13, 14, 15, 16]. For example, in [13] it was studied in detail the formation of the flower of saffron (*Crocus sativus*), namely the stage of maturation of egg cells in its embryonic bag (inside of its pistil): it was found that the optimal temperature for flower formation was in the range from 23 to 27°C, at that the temperature of 23°C is better. Next, when investigating nectar secretion in cherry laurel (Prunus Laurocerasus) it was recognized the optimal temperature for the pistil of the plant by measuring of the invert sugar concentration in the flowers [14]: it is 23°C. In [15] it was reported that the temperature inside a flower of the South American plant Prosopanche americana is up to 6°C above ambient at afternoon. In the work [16] it was informed about the study of long-term respirometry (CO₂ production) and thermometric measurements, which were carried out on intact flowers of African plants Hydnora Africana, Hydnora abyssinica, Hydnora esculenta in the field: the maximum value of metabolism was registered when the temperature inside the flower was within the range of (20-24)°C. It is clearly, the results of these studies confirm the good agreement between the calculated data and experimental ones.

So, the *ab initio* designed model of the basic thermodynamic processes in fruit tree flowers with certain simplifications does really "work": it provides the reliable results and it is sensitive to individual physical characteristics of flower pistils and to certain external factors. Based on the presented model it was developed appropriate algorithm for calculating the flower pistil temperature, which is implemented in the program "BioNA-1". The results of the computer program activity are in good agreement with many empirical data of field botany.

The authors believe that similar and more detailed modeling of the energy balance would undoubtedly be useful for searching and finding of optimal solutions to the problem of survival of certain plant species, as well in development of strategies of maximum yield of fruit plants under conditions of the global warming.

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