The role of energy potential in the mass transfer of moisture in the capillaries of woody plants

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Abstract. Theoretical and experimental studies of the growth and development of tree and shrub vegetation are determined by sorption characteristics, which depend on the moisture content in capillary-porous materials of phytomass stands. Thermodynamic parameters of mass transfer and their gradients are of fundamental importance. The purpose of this theoretical study was to solve a scientific problem on the development of theoretical foundations for mathematical modeling of mass transfer of moisture and nutrients in the vascular system of growing wood material, taking into account the energy potential. The research provides a theoretical justification and consideration of the thermodynamics of moisture mass transfer in the capillaries of wood materials. Based on the study of thermodynamic driving forces in capillary-porous growing wood bodies, it is established that the mass transfer potential is the chemical potential, which in the vascular system of wood and bast depends on free and chemically-bound moisture. The equations of filtration effect of moisture and moisture gradients on the mass transfer of moisture in capillary-growing wood materials, given the thermodynamic potential in non-isothermal conditions for wood phytomass, depending on the rate of change of thermodynamic potentials.

1. Introduction

Modern ideas about capillary-porous bodies, which primarily include bast-shaped tubes and wood vessels (xylem) of woody-shrub plants, include a complex of scientific knowledge in the field of molecular physics, thermodynamics, and the theory of heat and mass transfer.

Theoretical and experimental studies of the growth and development of tree and shrub vegetation are determined by sorption characteristics that are associated with the moisture content in capillary-porous materials of phytomass stands. Thermodynamic parameters of mass transfer and their gradients are of fundamental importance.

The basics of theoretical studies of mass transfer in wet materials are described in [1-3] and are reflected in studies [4-8]. However, theoretical studies of the role of energy potential in the growth of stands are not given due attention.

Accounting for mass transfer in growing wood materials, as a result of theoretical research, is the most important characteristic of the growth of wood-shrub plants in forest stands. Mass-exchange characteristics of growing tree species depend significantly on the ecological state of the environment. This process is particularly evident in the man-made impact of road transport on forest stands along roads and motorways. Therefore, the study of mass transfer and its mass-exchange characteristics in forest stands is an essential tool for monitoring changes in the ecological state.
In this regard, theoretical studies were conducted and mathematical models were obtained using operational calculus [9-12] on the influence of adverse factors of technogenic impact of road transport on the environmental condition of the environment. Numerous observations and experimental studies on the impact of technogenic effects of road transport on the state of the environment and vegetation along motorways are presented in [13-15].

Therefore, the purpose of the presented theoretical studies is to consider the physical and biological nature of the process of growth of phytomass suppression of forest stands due to the anthropogenic impact of vehicles as a result of mass transfer control, taking into account the energy potential and mass exchange characteristics.

2. Materials and methods

Mass transfer in capillary-porous wood materials is of special scientific interest. The process of filtration mass transfer in this case requires theoretical research and requires solving the scientific problem of developing the theoretical foundations of mathematical modeling of mass transfer taking into account energy materials.

When theoretically considering the process of moisture transfer in the phytomass of stands, it was assumed that the field of sorption forces in a capillary-porous body (sorbent) is the space in which the sorbate (moisture) molecules are held by sorption forces. The process of moistening wood material is its sorption, and its reduction is desorption.

The article uses a theoretical review of the processes of energy potentials that affect the mass transfer of moisture in the capillaries of woody plants. The conducted theoretical research uses functions and variable parameters of influence based on existing methods of both operational calculus and basic concepts from the theory of heat and mass transfer.

3. Results and discussion

Of special scientific interest is the task of determining the relationship between the amount of moisture in the soil and consequently in capillary-porous bodies of phytomass of forest stands and energy level that is important, for example, to determine the location of forest belts from highways, composition spaces and a class of bonitet. In this case, the total potential energy of the molecules of sorbate in the sorption field strength measured by the job $A$ that needs to be performed when moving into the field of sorption forces, i.e., to do some work $L$ against the forces of molecular interaction between sorbate and surface of sorbent. In such an ideal model, the total potential energy $E$ of all sorbate molecules will differ from their total potential energy in the field of sorption forces $U$ by the amount measured by work $L$, that is

$$E = U + L,$$  \(1\)

where $E = A$.

Thus, the distribution energy is the sum of the potential energy of the sorbate molecules in the field of sorption forces and its change, measured by the work to be performed against the forces of interaction between themselves and the surface of the sorbent (capillary-porous medium of woody-shrub plants), in other words, to perform the work of pushing the sorbate.

The thermodynamic potential of mass transfer in capillary-porous bodies of wood material $\Theta_T$, is the free energy of the connection of moisture with the studied body. The value $\Theta_T$ can be defined from the expression [1]:

$$\Theta_T = -RT \ln \varphi,$$  \(2\)

where $R$ – universal gas constant, J/kg K; $T$ - absolute temperature, K; $\varphi$ - relative pressure of humidity and dissolved nutrients in capillary-porous bodies of wood material.

Based on the study of thermodynamic driving forces in capillary-porous bodies, it is established that the mass transfer potential is the chemical potential $\mu$, which in the vascular system of wood and bast depends on free and chemically-bound moisture [2]. The study of the dependence of the chemical
potential $\mu$, on the moisture content and temperature is devoted to the work [2, 6, 8]. In these works, it is shown that the chemical potential is a function of the moisture content of the $u$ capillary-porous body and the temperature $T$, that is,  

$$\mu = \varphi(u, T),$$  

where $u$ – moisture content of capillary-porous wood material; $\mu$ – chemical potential.

The authors [7, 8] found that in capillary-porous bodies, the thermodynamic potential $\Theta$ corresponds to the chemical potential $\mu$, so $\Theta = \mu$, from here  

$$\Theta = \varphi(u, T).$$  

Therefore, the energy potential of mass transfer in capillary-porous bodies of wood material corresponds to the thermodynamics of driving forces [2, 6].

Mass transfer in capillary-porous bodies of wood material, taking into account the energy potential, can be presented in the form of the following equation [1], proposed by academician A.V. Lykov, namely:  

$$j_m = -\lambda_m \nabla \Theta,$$  

where $j_m$ – mass transfer in capillary-porous bodies of wood material; $\lambda_m$ – mass conductivity of the capillary-porous body of wood material; $\nabla \Theta$ – changes in the thermodynamic potential of mass transfer; $\nabla$ – Laplace operator.

It follows from dependence (4) that according to the expression of the full differential, for $\nabla \Theta$ it is possible to write:  

$$\nabla \Theta = \left(\frac{\partial \Theta}{\partial u}\right)_T \nabla u + \left(\frac{\partial \Theta}{\partial T}\right)_u \nabla T,$$  

where $u$ – moisture content of the capillary-porous body of wood material.

Then, under isothermal conditions, at $\nabla T = 0$, the expression (6) for the change in the thermodynamic potential of mass transfer will take the form:  

$$\nabla \Theta = \left(\frac{\partial \Theta}{\partial u}\right)_T \nabla u.$$  

Therefore, for isothermal conditions $\nabla T = 0$, the moisture content gradient when substituting the value $\nabla T = 0$, the expression (7) in the expression (5) will have the form:  

$$j_m = -\lambda_m \left(\frac{\partial \Theta}{\partial u}\right)_T \nabla u,$$  

In non-isothermal conditions $\nabla T \neq 0$, the mass flow is caused by the simultaneous action of two thermodynamic forces $\Delta \Theta$ and $\Delta T$ [2]. In this case, the mass transfer equation in capillary-porous wood material will be written as follows:  

$$j_m = -\lambda_m \nabla \Theta - \lambda_m \delta_\Theta \nabla T,$$

where $\delta_\Theta$ – thermogradient coefficient related to the mass transfer potential difference.

If we take $j_m = 0$, then we get the following expression from equation (9) when determining $\delta_\Theta$:  

$$\delta_\Theta = \left(\frac{\nabla \Theta}{\nabla T}\right)_{j_m = 0} \text{ or } \delta_\Theta \approx -\left(\frac{\Delta \Theta}{\Delta T}\right)_{j_m = 0}.$$  

The first term of the right side of the mass transfer equation (9) characterizes the filtration process caused by the gradient of the thermodynamic potential of the mass transfer, and the second term – filtration due to the temperature gradient.

After the transformation of equation (9), the mass transfer in a capillary-porous wood material will have the form:  

$$j_m = -\lambda_m \left(\nabla \Theta + \delta_\Theta \nabla T\right),$$  

The total gradient of the thermodynamic mass transfer potential from dependence (11) can be represented as:
\[ \nabla \Theta_1 = \nabla \Theta + \delta_\Theta \nabla T, \]  

then the mass transfer for isothermal and non-isothermal conditions will have the form:

\[ j_m = -\lambda_m \nabla \Theta_1, \]  

(13)

Mass transfer in non-isothermal conditions relative to the moisture content gradient in capillary-porous wood material is obtained by substituting the value of the thermodynamic potential of mass transfer \( \nabla \Theta \) according to (6) in the dependence (9), that is

\[ j_{m,T} = -\lambda_m \left( \frac{\partial \Theta}{\partial u} \right)_T \nabla u - \lambda_m \left( \frac{\partial \Theta}{\partial T} \right)_u \nabla T - \lambda_m \delta_\Theta \nabla T \]

(14)

or, after the conversion, equation (14) will take the form:

\[ j_{m,T} = -\lambda_m \left( \frac{\partial \Theta}{\partial u} \right)_T \nabla u - \lambda_m \left[ \left( \frac{\partial \Theta}{\partial T} \right)_u - \delta_\Theta \right] \nabla T \]

(15)

Thus, the mass transfer depending on (15) will be characterized by gradients of the thermodynamic potential of the mass transfer \( \frac{\partial \Theta}{\partial u} \), that is, its change depending on the humidity \( u \) at a constant temperature \( T \), and also \( \left( \frac{\partial \Theta}{\partial T} \right)_u \) – change \( \partial \Theta \) depending on temperature \( T \) at constant humidity \( u \).

It follows from expressions (11) and (15) that the mass transfer in a capillary-porous wood material will be due to the simultaneous action of \( \nabla \Theta \) and \( \nabla T \), and their gradient values.

The rate of change of the thermodynamic mass transfer potential \( \Theta \) over time \( t \) is described by the following differential equation [1, 2]:

\[ C_m \gamma_0 \frac{\partial \Theta}{\partial t} = -\text{div}(j_m), \]

(16)

where \( C_m \) – specific isothermal mass capacity determined from the expression \( C_m = \left( \frac{\partial u}{\partial \Theta} \right)_T \) [1]; \( \gamma_0 \) – bulk mass of dry material (for example, wood).

Hence, according to (13), we obtain the energy potential of mass transfer in the General form for isothermal and non-isothermal conditions in the following form:

\[ C_m \gamma_0 \frac{\partial \Theta}{\partial t} = -\text{div}(\lambda_m \nabla \Theta_1). \]

(17)

Equation (17) can be represented as follows:

\[ C_m \gamma_0 \frac{\partial \Theta}{\partial t} = \lambda_m \nabla^2 \Theta_1, \]

(18)

where \( \nabla^2 \Theta = \left( \frac{\partial^2 \Theta}{\partial x^2} + \frac{\partial^2 \Theta}{\partial y^2} + \frac{\partial^2 \Theta}{\partial z^2} \right) \) – Fourier-Kirchhoff differential equation.

If you enter parameter \( a_m \) in equation (18), it will take the form:

\[ \frac{\partial \Theta}{\partial t} = a_m \nabla^2 \Theta_1, \]

(19)

where \( a_m = \frac{\lambda_m}{\gamma_0 C_m} \) – potential conductivity of mass transfer.

For isothermal conditions, the regularity (12) follows:

\[ \nabla \Theta_1 = \nabla \Theta, \]

(20)

as a result of substituting (12) into (19), we get:

\[ \frac{\partial \Theta}{\partial t} = a_m \nabla^2 \Theta, \]

(21)
In non-isothermal conditions, according to equations (11) and (17), we obtain:

$$C_m \gamma_0 \frac{\partial \Theta}{\partial t} = div[\lambda_m (\nabla \Theta + \delta_\Theta \nabla T)].$$  

(22)

If we ignore the changes $\lambda_m$ and $\delta_\Theta$ in the coordinates [3], then we have:

$$C_m \gamma_0 \frac{\partial \Theta}{\partial t} = \lambda_m V^2 \Theta + \lambda_m \delta_\Theta V^2 T,$$  

(23)

After the transformation of formula (23), which consists of the introduction of $a_m$, as it followed in the dependence (19), we get:

$$\frac{\partial \Theta}{\partial t} = a_m V^2 \Theta + a_m \delta_\Theta V^2 T,$$  

(24)

Equation (21) and (24) reflect the rate of change in the thermodynamic mass transfer potential for isothermal conditions (21) and for non-isothermal conditions (24). Along with this, the speed of measuring the moisture content of $t$ in capillary-porous wood materials under both isothermal and non-isothermal conditions is of particular research interest.

According to [1], the rate of change in moisture content over time can be described by the following equation:

$$\gamma_m \frac{\partial u}{\partial t} = -div(j_m).$$  

(25)

Since $j_m$ can be represented as [2]

$$j_m = -a_m \gamma_0 \nabla u,$$  

(26)

then equation (25) can be represented as:

$$\gamma_0 \frac{\partial u}{\partial t} = -div(a_m \gamma_0 \nabla u).$$  

(27)

From equation (27), the rate of change in moisture content over time $t$ for isothermal conditions will take the form:

$$\frac{\partial u}{\partial t} = a_m V^2 u.$$  

(28)

Since mass transfer in non-isothermal conditions relative to the moisture content gradient in capillary-porous bodies can be represented as [1]:

$$j_m = -a_m \gamma_0 \nabla u - a_m \gamma_0 \nabla \nabla T,$$  

(29)

If $j_m = 0$, then from (29) we get:

$$\delta = \left(\frac{\nabla u}{\nabla T}\right)_{j_m=0} \approx \left(\frac{\Delta u}{\Delta T}\right)_{j_m=0}.$$  

(30)

where $\delta$ – thermogradient coefficient that characterizes the rate of change in moisture content by temperature at a constant relative pressure of moisture and nutrients.

For non-isothermal conditions in (25), when substituting $j_m$ values from (29), we get:

$$\gamma_0 \frac{\partial u}{\partial t} = div(a_m \gamma_0 \nabla u + a_m \gamma_0 \nabla \nabla T).$$  

(31)

Finally, the rate of change in moisture content over time in capillary-porous wood materials under non-isothermal conditions will be:

$$\frac{\partial u}{\partial t} = a_m \gamma_0 V^2 u + a_m \gamma_0 \nabla \nabla^2 T.$$  

(32)

Equation (32) characterizes the effect of the moisture content gradient in capillary-porous wood materials, taking into account the thermodynamic potential, on mass transfer under non-isothermal conditions.
4. Conclusion
Thus, mass transfer (filtration of moisture with nutrients dissolved in it) in capillary-porous bodies of phytomass of wood-shrub plants depends on the rate of change in the thermodynamic potential over time (21) and (24), as well as changes in time and moisture content (28) and (32).

The obtained differential equations allow us to consider the mass transfer process in both isothermal (equations (21) and (28)) and non-isothermal (equations (24) and (32)) conditions. However, the values of the parameters \( a_m, \lambda_m, \gamma_0, C_m, \delta_h, \delta \) are still poorly understood, which makes it difficult to conduct numerical studies (calculations). Therefore, the article presents only theoretical studies on the influence of thermodynamic energy on the filtration mass transfer of moisture and nutrients in the vascular system of woody and shrub plants.

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