The Use of Cellular Automata in the Study of Heat and Mass Transfer Processes in Particular During Wood Drying

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Abstract. This paper demonstrates the use of cellular automata in the study of heat and mass transfer processes, in particular during wood drying. For study, we developed a three-dimensional mathematical model. This model is described by a system of interconnected differential equations. These equations are described in partial time derivatives and coordinates in space. The peculiarity of this work is the possibility of combining a three-dimensional mathematical model and the theory of cellular automata in solving the problem. Usage of the theory of cellular automata requires the presence of a certain number of identical elements of the system. In this case, we propose to present the studied CAD model in the form of cubes of the same size. The paper also describes the relationships between the created cubes. In addition, we give the algorithm of calculations. Based on the described algorithm, we carried out the number of experiments, which prove the possibility of using the theory of cellular automata in solving the problem.

1. Introduction
As practice shows, when we drying wood, the various physical processes and phase transitions occur. These processes directly affect the change of mechanical and physical properties of the material, its geometric shape, presence of cracks and the possibility of collapse. In this regard, the task of creating new and increasingly effective methods of wood drying control remains very important [1].

When we are modeling such systems, we often encountered complex initial and boundary conditions. This makes it difficult to obtain reliable analytical solutions when we solve such problems. Because of this, we often use a various numerical methods, which are often not stable. In turn, if we use differential equations in the modeling of physical processes it does not always allow us to obtain an acceptable result. In this regard, there is an important need to develop effective software and mathematics with the possibility of their implementation with algorithmic tools [2].

In performing this work, we use the finite element method for the existing three-dimensional mathematical model. However, the use of this method requires significant time, especially at very high densities. In this regard, we propose to use the theory of cellular automata, which should significantly speed up the calculation process even at very high densities.

One of the most important contributions to the development of the theory of cellular automata made by S. Wolfram, who in his work [3] gives their detailed description and possibilities of application for almost all branches of science. At the same time, in [4] we can see the rules of transitions when using cellular automata, taking into account their internal variables. This paper also presents the possibilities of using cellular automata in modeling various heat transfer processes and spatial dynamics.

In works [5-9] we can see the features of the use of composite materials by using effective mechanical properties based on micro level cellular structural models. In this regard, we can assume that we can use cellular automata in modeling different dynamic systems that have a characteristic similarity between the basic elements. All this allows us to outline the prospects of this area.
2. Description of the studied model and its presentation

In this work, we have 3D model of wood. To determine the value of temperature and humidity in the middle of this model, we use a three-dimensional mathematical model of heat and mass transfer and the theory of cellular automata [10].

First, we need to present 3D model of wood in the form of a set of cubes. We can do that by considering the physical size of the 3D model of wood and the density of its separation. This representation allows us to use the theory of cellular automata [11, 12].

Next, we need to define the boundary cubes. We consider a boundary cube if the number of his adjacent cubes is less than six. To determine the number of adjacent cubes it is necessary to know their location. To do this, we used the neighborhoods of von Neumann of the first order (see Figure 1).

![Figure 1. Location of cubes in space according to the neighborhood of von Neumann.](image)

Cubes that have six adjacent cubes are internal. Each cube in our system has eight main points, which are located at the corners of the cube. One of these points is the target. The coordinates of this point correspond to the location of the cube according to the grid. Knowing the coordinates of the target point, we can determine the coordinates of the other seven main points [13].

Having the coordinates of the eight main points of the cube, we can determine the coordinates of the tangents of adjacent cubes by using the binary code, which you can see in table 1.

| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|
| 0 | 1 | 0 | 1 | 0 | 1 | 0 | 1 |
| 0 | 0 | 0 | 0 | 1 | 1 | 1 | 1 |
| 0 | 0 | 1 | 1 | 0 | 0 | 1 | 1 |

Table 1. The coordinates of the tangents of adjacent cubes in the binary code.

Depending on the selected direction of displacement (x + 1, x – 1, y + 1, y – 1, z + 1, z – 1), the values of 0 and 1 will be represented by certain coordinates, which are given in table 2, and the values x, y, z will correspond to the coordinates of the target point of the main cube.
3. Description of the mathematical model

In this work, we use a three-dimensional mathematical model of heat transfer of wood during its drying [14]. The description of this mathematical model by means of system of differential equations in partial derivatives on spatial coordinates and time has the following form:

\[
\begin{align*}
&c\rho \frac{\partial T^{(i)}}{\partial t} = \sum_{j=1}^{3} \lambda_j \frac{\partial^2 T^{(i)}}{\partial x_j^2} + \epsilon \rho_0 r \frac{\partial U^{(i)}}{\partial t} \\
&\frac{\partial U^{(i)}}{\partial t} = \sum_{j=1}^{3} a_j \frac{\partial^2 U^{(i)}}{\partial x_j^2} + \delta \sum_{j=1}^{3} a_j \frac{\partial^2 T^{(i)}}{\partial x_j^2}
\end{align*}
\]  

(1)

where \( \rho \) is density, \( x, y, z \) represent the coordinates, \( i \) is serial number of cube, \( T^{(i)}(t, x_j, x_2, x_3) \) is the temperature of the \( i \)-th cube, \( t \) is simulation time and \( c \) is specific heat. In turn, \( \rho_0 \) is basic density, \( a_j \) are humidity coefficients, \( \lambda_j \) are the coefficients of thermal conductivity, \( U^{(i)}(t, x_j, x_2, x_3) \) is the moisture content of the \( i \)-th cube, \( r \) is specific heat of vaporization, \( \delta \) is the thermo gradient coefficient and \( \epsilon \) is phase transition coefficient. After that, we introduce a time-space grid in area \( G = \{(t, x_1, x_2, x_3): 0 \leq t \leq t, 0 \leq x_1, x_2, x_3 \leq l\}:

\[
\Omega_{\Delta t, \Delta x(j-1)} = \{(t^k, x_{1(n)}, x_{2(m)}, x_{3(p)}): t^k = k\Delta t, k = 0, K, \\
\Delta t = \frac{r}{K}; x_{1(n)} = (n - 1)h_1, n = 1, N, h_1 = \frac{l}{N - 1}; x_{2(m)} = (m - 1)h_2, \\
m = 1, M, h_2 = \frac{l}{M - 1}; x_{3(p)} = (p - 1)h_3, p = 1, P, h_3 = \frac{l}{P - 1}\}
\]

(2)

The initial conditions for a constant rate of wood drying has the following form:

\[
T^{(i)} \bigg| t = 0 = T_0^{(i)} \quad U^{(i)} \bigg| t = 0 = U_0^{(i)}
\]

(3)

For the period of falling speed of the drying process of capillary-porous materials, the initial moisture content can be describe by the following quadratic function:

\[
U^{(i)} \bigg| t = 0 = U_c^{(i)} - \left[1 - \left(\frac{x_1 - l_1/2}{l_1/2}\right)^2\right] \times \left[1 - \left(\frac{x_2 - l_2/2}{l_2/2}\right)^2\right] \times \\
\left[1 - \left(\frac{x_3 - l_3/2}{l_3/2}\right)^2\right] \times (U_c - U_s)
\]

(4)

where \( U_c \) is the moisture content in the center and \( U_s \) is the moisture content on the surface.
For a three-dimensional mathematical model, we used boundary conditions of the third kind \([15]\), each of which corresponds to one coordinate. The boundary conditions for the X coordinate have the following form:

\[
\begin{align*}
\lambda_i T_{N,m,p}^{k(i)} - T_{N-1,m,p}^{k(i)} &+ \rho_0 (1 - \varepsilon) \beta (U_{N,m,p}^{k(i)} - U_p) = \alpha (T_{N,m,p}^{k(i)} - T_c) \\
\frac{a_i}{h_i} T_{N,m,p}^{k(i)} - T_{N-1,m,p}^{k(i)} &+ a_1 U_{N,m,p}^{k(i)} - U_{N-1,m,p}^{k(i)} = \beta (U_p - U_{N,m,p}^{k(i)})
\end{align*}
\]

where \(\beta\) is the moisture exchange coefficient, \(\alpha\) is the coefficient of heat exchange, \(l\) is the length of one face of one of cube. \(U_p = F(T_c, \varphi)\), where \(T_c\) is a temperature and \(\varphi\) is a relative humidity of the drying agent. The three-dimensional mathematical model has the following finite-difference form:

\[
cp \frac{T_{n,m,p}^{k+1(i)} - T_{n,m,p}^{k(i)}}{\Delta t} = \sum_{j=1}^{3} \frac{\lambda_j}{h_j} \left(T_{n,m,p}^{k(i)} - 2T_{n,j-1}^{k(i)} + T_{n,j+1}^{k(i)}\right) + \varepsilon \rho_0 T \frac{U_{n,m,p}^{k+1(i)} - U_{n,m,p}^{k(i)}}{\Delta t}
\]

\[
+ \delta \sum_{j=1}^{3} a_j \left(T_{n,j-1}^{k(i)} - 2T_{n,j}^{k(i)} + T_{n,j+1}^{k(i)}\right)
\]

where \(\omega_1 = n, \, \gamma_1 = m, \, \rho; \, \omega_2 = m, \, \gamma_2 = n, \, \rho; \, \omega_3 = p, \, \gamma_3 = n, m;\)

4. Description of cell-automatic interaction

When we use cellular automata, we often use the coefficients of moisture and thermal conductivity. These coefficients used when we transmitting numerical values of temperature and humidity within one cube and provided that it has other points in addition to the main 8 points. Other points will exist if our step on the coordinates \(h\) has a value that is less than one. Therefore, we have dependences by which we can transfer numerical values between different points of one cube according to the scheme of relations within the selected edge \([16]\).

\[
H^{(i)}[1,3] = \frac{K, H^{(i)}[1,3] + C^{(i)}}{K_1 + C_1} \quad H^{(i)}[5,6] = \frac{K, H^{(i)}[5,6] + C^{(i)}}{K_2 + C_2} \quad H^{(i)}[2,4] = \frac{K, H^{(i)}[2,4] + C^{(i)}}{K_3 + C_3}
\]

where if \(H^{(i)} = T^{(i)}\) then \(K = \lambda\) and if \(H^{(i)} = U^{(i)}\) then \(K = \alpha\). In addition:

\[
C^{(i)} = \left\{\begin{array}{l}
K, H^{(i)}[5,6], C_1 = K_1 \\
K, H^{(i)}[2,4], C_1 = K_3 \\
K, H^{(i)}[1,3], C_1 = K_3 \\
K, H^{(i)}[2,4], C_2 = K_2 \\
K, H^{(i)}[1,3], C_2 = K_2 \\
K, H^{(i)}[5,6], C_3 = K_1 \\
K, H^{(i)}[2,4], C_3 = K_1 \\
K, H^{(i)}[1,3], C_3 = K_2
\end{array}\right.
\]

We also use cell-automatic interaction between two points of adjacent cubes. Each of these points has the values of temperature \((T_1, T_2)\) and humidity \((U_1, U_2)\). Therefore, if there is a temperature interaction between two points, then we follow the following rules:

\[
T_k = T_1 + (T_2 - 0.5 \cdot (T_1 + T_2))
\]

if \(T_k > T_1\) then \(T_k = T_1\)

if \(T_k < T_2\) then \(T_k = T_2\)

if \(T_k \geq T_2\) then \(T_k = T_k\)

If there is a moisture interaction between the two points, then follow the following rules:

\[
U_k = U_1 + (U_2 - 0.5 \cdot (U_1 + U_2))
\]

if \(U_k < U_1\) then \(U_k = U_1\)

if \(U_k > U_2\) then \(U_k = U_2\)

if \(U_k \geq U_2\) then \(U_k = U_k\)

if \(U_k < U_2\) then \(U_k = U_k\)
5. Description of the calculation algorithm

Therefore, in order to determine the values of temperature and humidity in the studied 3D model of wood, we can use the algorithm that you can see in Figure 2.

When we start calculations, we check the stability conditions for an explicit difference scheme [17].

\[
\Delta t \left( \frac{\lambda_1 + \lambda_2}{h_1} + \frac{\lambda_3}{h_3} \right) \leq \frac{c \rho - \epsilon \rho_0 \rho}{2}
\]

\[
\Delta t \left( \frac{a_1 + a_2}{h_1} + \frac{a_3}{h_3} \right) \leq \left(1 + \delta \right)^{-1} \frac{1}{2}
\]

If stability conditions fulfilled, then we can start the calculation, if not, then we need to change the values of the input parameters. In calculation, process we randomly select coordinates of certain number of internal cubes, where the values of temperature and humidity at the main points will be, calculate according to a three-dimensional mathematical model (1). The values of temperature and
humidity of the tangents of adjacent cubes will be determined by using the cell-automatic interaction, which described in the previous section.

In turn, the values of temperature and humidity for the points of the boundary cubes will be determined according to the boundary conditions of the third kind (4). Since we don’t use cellular automata when calculating boundary conditions, we need to use all boundary cubes to calculate.

6. Conducting a test experiment

Therefore, to verify the adequacy of the developed algorithm, we conducted a series of test experiments [18]. The main input parameters have the following values: \( T_0 = 30^\circ C, \ T_c = 100^\circ C \), \( U_0 = 0.35, \ \varphi = 0.75, \ \Delta t = 60 \text{ sec.}, \ \tau = 864000 \text{ sec.} \). In total, the studied model is represented by 9375 cubes, 6877 of which are internal cubes. By using a mathematical model, we will calculate the temperature and humidity of the points for 20% of the inner cubes. The values of temperature and humidity for the points of other inner cubes will be determined by using cellular automata.

Below you can see the results of calculations the temperature and humidity (see Figure 3) for the target point of the cube, which is in the center of the studied model. The figure on the left shows the graph of temperature distribution, and the figure on the right shows the graph of humidity distribution. The left axis is responsible for the numerical values of T or U, and the lower axis is responsible for the iteration number.

![Figure 3. The results of calculations the temperature and humidity for the target point of the cube.](image)

As a result of calculations, the target point located in the center of the studied model received the value of equilibrium humidity at 3046 iterations. That is, we need to spend 3046 * 60 sec. = 182,760 sec. (2,115 days) in order to dry the 3D model of wood of a given size. We also conducted another experiment, but without using the cellular automata. The result was found in 3019 iterations. It is worth noting that to perform the second experiment we needed about 7 minutes, while the implementation of the first experiment took us about 1.5 minutes. This proves that a cellular automata in the simulation of thermal conductivity problems of this type significantly speeds up the time of obtaining results. It is also worth noting that the use of cellular automata allows us to maintain the adequacy of calculations if more than 10% of internal cubes calculated according to a three-dimensional mathematical model (1).

Conclusions

In this work, we demonstrated the use of cellular automata in the study of heat and mass transfer processes, in particular during wood drying. During the calculations, we used a three-dimensional mathematical model, which described by a system of interconnected differential equations in partial derivatives by spatial coordinates and time. We also used cell automata during the study. To use them, we presented the studied model in the form of a set of cubes.

As a result of this work, we performed a number of experiments. Their conduction showed the possibility of using cellular automata in solving thermal conductivity problems. In addition to solving the problem of thermal conductivity, it was possible to achieve stability and accuracy of results, even with a significant increase in density and time step. In addition, the use of cellular automata allows us to significantly speed up the calculation process. This acceleration was achieved due to the ability to change the number of cubes in which the numerical values of temperature and humidity for points are determined according to a three-dimensional mathematical model. Numerical values of temperature
and humidity for the points of other cubes directed to the state of equilibrium according to the total simulation time by using developed cellular-automatic interactions between the internal points of one cube and between the tangents of different cubes.

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