Application of Method of Continuous Asynchronous Cellular Automata for Simulation of Heat Conduction with First Order Phase Transitions

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Abstract. *The main object of this work is to construct a cellular automaton (CA) model of heat conductivity processes with first order phase transitions. The paper discusses main approaches and general methodology for development of cellular automata models. The studies were conducted on the example of cellular automata to model moving phase boundary problems for freezing of moist soil, the process of band Bi_2Te_3 growing and changing forms of solidification front. It is shown that the CA models can be an alternative to the use of classical differential equations. It is proven that the model as a system of cellular automata is quite a convenient tool for the study of nonlinear heat transfer problems, despite the simplicity of its description, and may describe very complex system behaviour.*

Keywords

First order phase transition, cellular automata, thermal conductivity.

1 Introduction

The matter of solving heat conductivity problems is quite important, especially for cases with non-linear parameters of materials. For the majority of these problems, a numerical solution is a common approach. But when it comes to systems with complex boundary conditions or phase transitions of the substance, the computational complexity makes us look for alternative methods. Cellular automata algorithm easily describes such complex systems.

2 Related works

In recent years, alternative approaches to numerical methods for problems of heat conductivity and diffusion are widely used. Cellular automata algorithms are quite successfully used [1, 2] for this purpose. It should be noted that discrete models are used in most cases for calculation of diffusion processes [3], and continuous models of cellular automata [4, 5] are used to approximate heat transfer processes.

A lot of attention of researchers in the field of solid state physics is directed towards the study of problem of structural parameters of real materials with different physical nature and different spatial dimensions. In such cases, it makes sense to use modelling techniques that easily describe complexity of system geometry [1]. Cellular automata simulation has this property. The purpose of this paper is to develop a model of continuous cellular automata and use it to describe the processes of heat conductivity complicated by a first order phase transition.

3 Cellular Automata Model Description and Analysis of Calculation Results

The description of systems with complex boundary conditions or phase transition is in many cases difficult. This is due to the fact that a numerical solution of this problem is quite difficult to obtain because of the large number of calculations.

An example is the problem of describing such complex phenomena as evolution and self-organization, diffusion and thermal conductivity. Let us consider the last process, complicating it by first order phase transition. This task belongs to the class of so-called Stefan problems.

Mathematical formulation of Stefan problem for a three-dimensional case is:

$$\frac{\partial T_S(x,y,z,t)}{\partial t} = a_S \Delta T_S(x,y,z,t),\ a_S = \frac{k_S}{c_S \rho_S}, \tag{1}$$

$$\frac{\partial T_L(x,y,z,t)}{\partial t} = a_L \Delta T_L(x,y,z,t),\ a_L = \frac{k_L}{c_L \rho_L}, \tag{2}$$

$$\left| k_S \nabla T_S(x,y,z,t) - k_L \nabla T_L(x,y,z,t) \right| = \left| H_f \rho_{(L/S)} \frac{d\xi}{dt} \right|, \tag{3}$$

where $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$;– the Laplace operator; $\nabla = \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}$– the Hamiltonian operator; T_S and T_L, a_S and a_L, k_S and k_L, c_S and c_L, ρ_S and ρ_L – accordingly: temperature, thermal diffusivity, thermal conductivity, specific heat capacity, specific density of the solid and liquid phases; H_f – latent heat of fusion; ξ – coordinate of the interface of two phases. Specific density symbol $\rho_{(L/S)}$ on the right side of equation (3) means that the corresponding value of liquid /solid phase is selected depending on the direction of the phase transition – crystallisation /melting.

The essence of simulation of processes of thermal conductivity by cellular automata is to present a model as a set (array) of the same cells connected to each other the same way. All cells form a so-called lattice cellular automaton. In turn, the contents of cells-automatic field may be a single linear array of certain characteristics. This can be illustrated as follows:

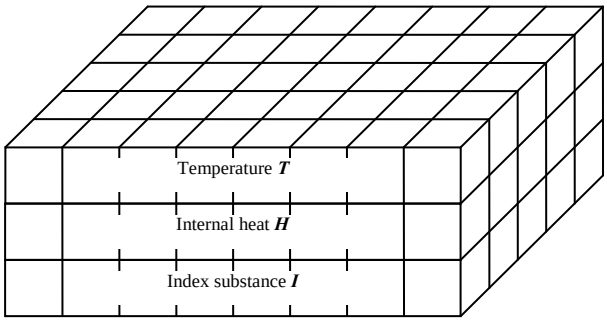

Fig. 1. Structure of the cellular automaton field for a two-dimensional model

In this paper we use asynchronous scheme of interactions of cellular automata, providing cyclic execution of three typical steps:

1. Some cell $i = 1$ with integer coordinates x_1, y_1 is selected randomly on a cellular automata field.
2. A neighbouring cell $i = 2$ with integer coordinates x_2, y_2 is selected in an equiprobable way. The Neumann neighbourhood is accepted as a neighbourhood scheme in this case, i.e. a cell has only four neighbours.
3. A cellular automata interaction between the two cells takes place.

The essence of cellular automata interactions is to modify the values of corresponding continuous layers of cells according to the following system of equations:

$$\begin{cases} T^i{}' = T^i + (T_m - T^i) a_m / a_{max}; \\ \text{if } (T^i{}' > T_f) \text{ and } (H^i < H_f), \\ \quad \text{then } \{H^i{}' = H^i + c_S^i (T^i{}' - T_f); T^i{}' = T_f;\} \\ \text{if } (H^i{}' > H_f), \\ \quad \text{then } \{T^i{}' = T^i{}' + (H^i{}' - H_f)/c_L^i; H^i{}' = H_f;\} \\ \text{if } (T^i{}' < T_f) \text{ and } (H^i > 0), \\ \quad \text{then } \{H^i{}' = H^i + c_L^i (T^i{}' - T_f); T^i{}' = T_f;\} \\ \text{if } (H^i{}' < 0), \text{ then } \{T^i{}' = T^i{}' + H^i{}'/c_S^i;\ H^i{}' = 0;\} \end{cases} \tag{4}$$

$$a_m = (a^1 + a^2)/2;\ a^i = k^i/\rho^i c^i; \qquad T_m = \frac{w^1 T^1 + w^2 T^2}{w^1 + w^2};\ w^i = \rho^i c^i,$$

where i = 1, 2 – index value that corresponds to the selected cell and the adjacent cell with coordinates (x_1, y_1) and (x_2, y_2) respectively. Values at the next moment are stroke-marked.

It turned out that the computation time depends on the number of cellular automata. And the accuracy is directly dependent on the dimension of a CA field. The paper shows that the time of one CA interaction is defined as follows (for a three-dimensional model with the dimensions $N_x \times N_y \times N_z$):

$$t_{1CA} = \frac{d_x^2}{a_{\max}} \frac{1}{6N_x^3 N_y N_z} = \frac{d_y^2}{a_{\max}} \frac{1}{6N_y^3 N_x N_z} = \frac{d_z^2}{a_{\max}} \frac{1}{6N_z^3 N_y N_x}, \quad (5)$$

where a – thermal diffusivity, d_x, d_y and d_z – size of the sample along the coordinates x, y and z, respectively.

By drawing an analogy between the CA method and Monte Carlo simulation, it is easy to notice a similar relationship – the longer the computation time, the more accurate the result. Herewith, as in the case of proposed probabilistic scheme of asynchronous sampling of cellular automata, use of probabilistic mechanisms also takes place in the Monte Carlo method. But unlike the Monte Carlo method for solving equations, cellular automata method is a method of simulation and it can be used to model systems that can not be described in terms of theory of differential equations [1].

Let's proceed to consider a non-stationary task of the process of thermal conductivity with first order phase transition – freezing of moist soil. Calculations of temperature distributions in the depth of the soil were performed at various time points (t = 4316 s, t = 19464 s, t = 90875 s, t = 266246 s), using the cellular automata approach. The results of calculations for one-dimensional (N_x = 500), two-dimensional ($N_x \times N_y$ = 500×100) and three-dimensional ($N_x \times N_y \times N_z$ = 500×10×10) CA models along the x axis are shown in Fig.2. Models of different dimensions agree with one another and with the corresponding results of numerical solutions of equations (1) – (3) for a given problem of freezing of moist soil[6].

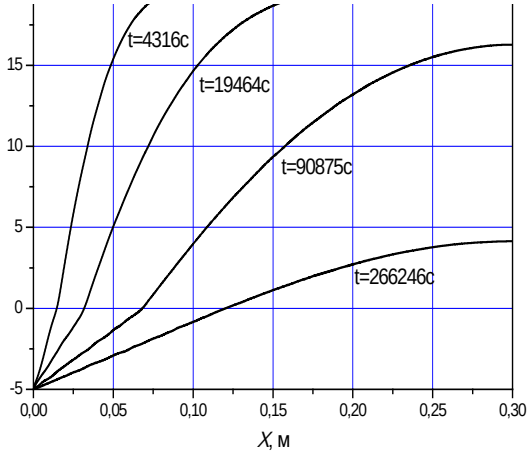

Fig. 2 Temperature distribution over the depth of the soil

Another example of the Stefan problem was examined in this paper. The process of zone growing of materials was modelled on the example of bismuth telluride (Bi_2Te_3). In practice, zone growing of materials often occurs in cylindrical quartz ampoules. For realization of cellular automaton model of the growth process, the cylindrical symmetry of the system (by including the multiplier $(1+\pi R)$ in (4) for weight coefficient) was taken into account, which made it possible to reduce a three-dimensional model to a two-dimensional one and by that reduce the computing time with other parameters of the model being constant. So the expression becomes: $w^i = \rho^i c^i (1+\pi R^i)$ where R^i – the distance from the axis of the cylinder to the i-th cell. Please note that the parameters a_m, $a_{\max}$, t_{1CA}, H_f does not depend on the multiplier, since the thermal parameters of the material does not change.To test our hypothesis, execute the computational experiments to cool square-section bar D × D and cylinder of diameter D. Significant discrepancies for the distribution of temperature of the bar and the cylinder in different times are shown at Fig. 3. But solutions completely coincide if we consider the multiplier.

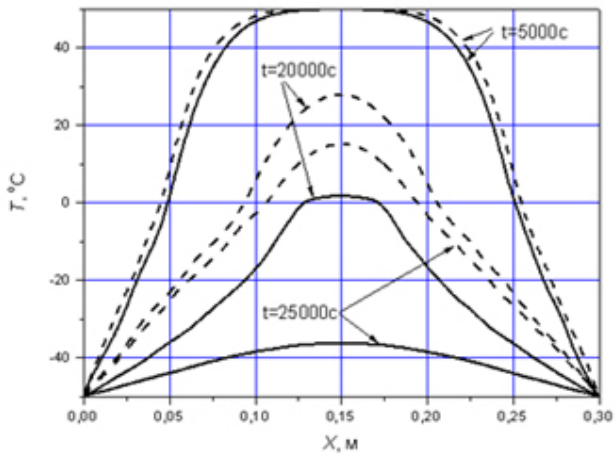

Fig. 3 Temperature distribution along the diagonal section of the cylinder (solid line) and along the cross section of the square bar (dotted lines)

Thus it is possible to realize a two-dimensional cellular automata model of zone growing materials in cylindrically symmetric quartz ampoules. An example of modelling the process of growing zone Bi_2Te_3 is shown at Fig. 4. The process parameters are: heater temperature – 840 °C, refrigerator temperature – 30 °C, the growth rate (speed of the heaters) – 0.2 m/h, the height of the ampoule fragment – 0.15 m, thickness of the inner ampoule – 0.03 m, height of the heater – 0.05 m , direction of movement of the heater – from bottom to top. Monocrystal is formed at the bottom of the ampoule and molten zone is fuelled from above polycrystal. Field size CA $N_x \times N_y = 120 \times 600$ cells.

Parameters that provide a flat crystallization front have also been obtained and empirically confirmed [7]. Their receipt ensured uniformity of physical parameters along the cross-section of the ingots. Equality of real and model growth parameters, in which there is a flat crystallization front [7] demonstrates the adequacy of the described cellular automata approach.

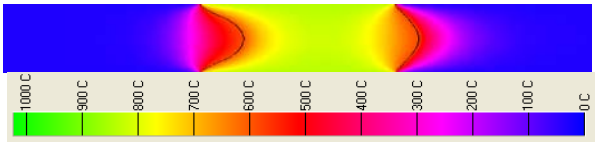

Fig. 4 Example of simulation of a zone growing Bi_2Te_3

4 Conclusion

As a conclusion, we note that the proposed method can be a worthy alternative to the previously known classical methods of Stefan problems solving and has prospects due to its versatility and simplicity. It implies that the method of continuous cellular automata can be used for description of dependence of the phase transition temperature on composition and modelling of instability of crystallization front.

References

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