
Simulation of non-linear heat conduction by means of thermodynamics-based algorithm

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conduction

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Introduction

Heat conduction is a well investigated phenomenon. Its mathematical description is based on Fourier's law[1]

$$\vec{q} = -\lambda \nabla T, \quad (1)$$

which couples heat flux, \vec{q} , with temperature gradient, ∇T , (λ is heat conductivity). This law leads to a parabolic field equation for the temperature (if λ is constant)

$$\frac{\partial T}{\partial t} = \frac{\lambda}{\rho c} \nabla^2 T. \quad (2)$$

Here t is time, ρ is density, c is heat capacity per unit mass. Fourier's law holds for many media in the sufficiently small temperature gradient range.

Heat conduction is the simplest example both for transport processes and for thermal phenomena. Above we have had a mechanical description of the transport process in terms of fields and fluxes. At the same time, thermal properties of the medium are given by certain equations of state.

It is not evident which way the thermal properties correspond to the mechanical description (1), (2) even in the simple cases, to say nothing of such equation of state as the following one given by Sato[2] for water

$$\left(\frac{p + B}{p_{cr}} \right)^A = \frac{\rho}{\rho_{cr}} \frac{C}{\rho_{cr}}, \quad (3)$$

where

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$$\begin{aligned}
 A &= 3.6817T_r - 14.8512T_r^{1.5} + 22.6257T_r^2 - 11.7554T_r^{2.5} , \\
 \frac{B + p_{cr}}{p_{cr}} &= 19.5298T_r + 335.393T_r^4 - 1687.22T_r^7 + 3049.27T_r^{12} , \\
 \frac{C - \rho_{cr}}{\rho_{cr}} &= -3.6572159T_r^{0.4} + 16.035045T_r^{0.8} - 93.910446T_r^{1.2} + \\
 &+ 240.02105T_r^{1.5} - 552.30101T_r^2 + 966.10801T_r^{2.5} - 849.10947T_r^3 + \\
 &+ 497.86697T_r^4 - 327.45300T_r^5 + 105.61822T_r^6 , \\
 T_r &= 1 - \frac{T}{T_{cr}} , T_{cr} = 647.1K , p_{cr} = 218 atm ,
 \end{aligned}$$

where subscript *cr* denotes values corresponding to critical point.

The motivation for the paper comes from the desire to give a thermodynamic description of heat conduction process to perform calculations for real substances.

As it is known, thermodynamic concepts are usually introduced into mechanical problems by means of the hypothesis of local equilibrium[3]. Such a hypothesis is needed to assign to a non-equilibrium state of an element of a continuum, the entropy and thermodynamic temperature of an accompanying equilibrium state[4]. Thermodynamic parameters of the element are considered to be identical to its physical parameters, as it takes place for mass and volume. However, some properties of the thermodynamic parameters expose themselves only in the Gibbsian state space. In particular, each thermodynamic parameter should have the property of being a function of state. Such a feature is often lost by pure mechanical description. Namely, as it was shown by Chen and Eu[5], there is no possibility that entropy will become a function of state in the physical space.

The interaction between elements of a continuum leads finally to certain relationships between the parameters of neighbouring elements. At the same time, this should affect their thermodynamic states. Consequently, accompanying equilibrium states of interacting elements should be also coupled. Therefore, we try to establish the relations between thermodynamic parameters of interacting elements and to apply them for heat conduction problems.

The difficulty here is that, as was noted by Truesdell and Bharatha[6], "the formal structure of classical thermodynamics describes the effects of changes undergone by some single body. While it allows these effects for one body to be compared with corresponding effects for another body, it does not represent the effects associated with two bodies simultaneously or in any way conjointly". Therefore the "marriage between thermodynamics and continuum mechanics is neither simple nor straightforward"[4,7].

The proposed algorithm of calculations uses cellular automata technique. Cellular automata can be viewed as prototypical models for spatially distributed systems consisting of a large number of simple, identical, and locally connected components. Cellular automata techniques yield models that differ from, but are consistent with, those obtained from a continuous approach, and the simulations based on cellular automata often provide an enormous increase in computational efficiency[8,9]. The offered algorithm is an extension of cellular automation because states of cells are identified with thermodynamic states of elements and the rules of updating of cells' states applied are not artificial but follow from thermodynamic laws. Thermodynamic foundation of these rules is given in the second part of the paper. First, the conditions for the thermodynamic descriptivity are established. Further, these conditions are applied to the interaction between three neighbouring elements or cells. As a result, a relationship is obtained coupling the non-equilibrium state of an element with the states of its neighbours. This condition is used in the rule for updating of cells' states in the simulation of a one-dimensional heat conduction problem. It is shown that this algorithm can be reduced to the classical finite-difference approximation in the case of homogeneous solids. The results of calculations for the temperature distributions in a stationary layer are presented in the third part for various temperature gradients. In the case of solids, steady-state temperature profiles are strongly linear in full correspondence with the classical theory. They become significantly non-linear in water, especially in regions of phase transitions and under sufficiently strong gravitation. Some conclusions are given in part four of the paper.

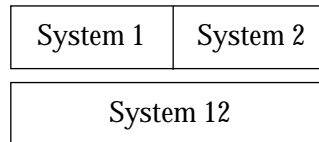
Thermodynamic background

We shall be restricted to the one-dimensional heat conduction problem. It is quite natural to begin from the most simple case in the elaboration of a new method because of easy and clear presentation of results. Thus, the problem under consideration can be formulated as follows: what kind of temperature distribution has an infinite layer placed between parallel surfaces each of which has its own specified course of temperature variation? We apply the cellular automata technique for the solution of the formulated problem. As it is known[8,9], a cellular automation is spatial lattice of N cells, each of which is in a certain state at time t . Each cell follows the same rule of updating its state. The cell's state at time $t + 1$ depends on its own state and the state of neighbouring cells at time t . The cellular automation starts with some initial configuration of cell states, and at each time step the states of all cells in the lattice are updated simultaneously.

Turning to the heat conduction problem, we divide the layer into N sublayers, each of which corresponds to a cell. Each sublayer has the same size h so that full thickness is $H = Nh$. The state of each cell we determine as the thermodynamic state of the corresponding sublayer.

The essential feature of cellular automation is the rule of updating of cells' states. Usually such a rule is expressed as a reference table connecting the state of a cell with its local neighbourhood.

To formulate the rules of updating of cells' states, we shall consider previous local interaction between these cells. For the description of interaction we shall be guided by a general principle, according to which of the thermodynamic laws should be enforced in each separate cell, and in any of their set. Accordingly, the interaction between any two neighbouring cells should satisfy the conditions of coexistence of these cells in the structure of an extended system, including both considered cells.



We shall show the general expression for the variation of internal energy in the extended system as follows:

$$dU_{12} = dU_1 + dU_2 - dE_{1-2}, \tag{4}$$

where E_{1-2} is the energy of interaction between subsystems 1 and 2, which is considered as a function of state.

Owing to the additivity of energy, we can expand the interaction energy into two parts, which correspond to each subsystem

$$dE_{1-2} = dE_1 + dE_2, \tag{5}$$

and rewrite the expression of energy variation in the form

$$dU_{12} = dU_1 + dU_2 + dE_1 + dE_2. \tag{6}$$

Using property of internal energy as being a function of state, we shall present its total differential in the form

$$dU = \left(\frac{\partial U}{\partial T}\right)_{V,M} dT + \left(\frac{\partial U}{\partial V}\right)_{T,M} dV + \left(\frac{\partial U}{\partial M}\right)_{T,V} dM, \tag{7}$$

where variables T, V, M are considered as independent.

Applying this procedure to each system, we have

$$\begin{aligned} & \left(\frac{\partial U_{12}}{\partial T_{12}}\right)_{V,M} dT_{12} - \left(\frac{\partial(U_1 + E_1)}{\partial T_1}\right)_{V,M} dT_1 - \left(\frac{\partial(U_2 + E_2)}{\partial T_2}\right)_{V,M} dT_2 + \\ & + \left(\frac{\partial U_{12}}{\partial V_{12}}\right)_{T,M} dV_{12} - \left(\frac{\partial(U_1 + E_1)}{\partial V_1}\right)_{T,M} dV_1 - \left(\frac{\partial(U_2 + E_2)}{\partial V_2}\right)_{T,M} dV_2 + \\ & + \left(\frac{\partial U_{12}}{\partial M_{12}}\right)_{T,V} dM_{12} - \left(\frac{\partial(U_1 + E_1)}{\partial M_1}\right)_{T,V} dM_1 - \left(\frac{\partial(U_2 + E_2)}{\partial M_2}\right)_{T,V} dM_2 = 0. \end{aligned} \tag{8}$$

Since T , V and M variables are independent, all three parts are equal to zero separately, i.e.

$$\left(\frac{\partial U_{12}}{\partial T_{12}}\right)_{V,M} dT_{12} - \left(\frac{\partial(U_1 + E_1)}{\partial T_1}\right)_{V,M} dT_1 - \left(\frac{\partial(U_2 + E_2)}{\partial T_2}\right)_{V,M} dT_2 = 0, \quad (9)$$

$$\left(\frac{\partial U_{12}}{\partial V_{12}}\right)_{T,M} = \left(\frac{\partial(U_1 + E_1)}{\partial V_1}\right)_{T,M} = \left(\frac{\partial(U_2 + E_2)}{\partial V_2}\right)_{T,M}, \quad (10)$$

$$\left(\frac{\partial U_{12}}{\partial M_{12}}\right)_{T,V} = \left(\frac{\partial(U_1 + E_1)}{\partial M_1}\right)_{T,V} = \left(\frac{\partial(U_2 + E_2)}{\partial M_2}\right)_{T,V}. \quad (11)$$

The first of the obtained conditions depends on temperature variations and determines the heat capacity of the integral system. The third one is used for entropy calculations. The second condition is most useful for our goals. It connects not only parameters of systems 1 and 2 with those of the integral system 12, but also parameters of systems 1 and 2 themselves. Consequently, it is a necessary condition for the consistency of thermodynamic states in interacting systems. Together, these conditions ensure the equivalence between the thermodynamic description on the level of subsystems and that on the level of the integral system. To emphasize this fact, in what follows we refer to them as the thermodynamic descriptivity conditions.

If we apply the thermodynamic descriptivity conditions to the interaction between three systems contacting each other as shown below:

System 1	System 2	System 3
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it should be done both for systems 1 and 2 and for systems 2 and 3

$$\left(\frac{\partial u_1}{\partial v_1}\right)_T + \left(\frac{\partial e_{12}}{\partial v_1}\right)_T = \left(\frac{\partial u_2}{\partial v_2}\right)_T + \left(\frac{\partial e_{21}}{\partial v_2}\right)_T, \quad (12)$$

$$\left(\frac{\partial u_3}{\partial v_3}\right)_T + \left(\frac{\partial e_{32}}{\partial v_3}\right)_T = \left(\frac{\partial u_2}{\partial v_2}\right)_T + \left(\frac{\partial e_{23}}{\partial v_2}\right)_T, \quad (13)$$

where e_{ij} is the interaction energy per unit mass for the system i with respect to the system j . Thus, to different interactions there should correspond various energy dependencies.

The process of heat conduction can be characterized by the symmetry of interactions with respect to neighbouring elements. Owing to the symmetry of the problem, we have no preferences between systems 1 and 3 with respect to system 2, because heat diffusion is independent of a direction. Consequently, their actions relative to system 2 should be equal

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$$\left(\frac{\partial e_{21}}{\partial v_2}\right)_T - \left(\frac{\partial e_{12}}{\partial v_1}\right)_T = -\left(\frac{\partial e_{23}}{\partial v_2}\right)_T + \left(\frac{\partial e_{32}}{\partial v_3}\right)_T = D. \quad (14)$$

Then we can subtract the second thermodynamic descriptivity condition from the first one

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$$\left(\frac{\partial u_1}{\partial v_1}\right)_T - \left(\frac{\partial u_3}{\partial v_3}\right)_T = 2D. \quad (15)$$

The subtraction can be interpreted as the total external action relative to system 2, which results in the influence of systems 1 and 3 simultaneously. Therefore, we can represent the thermodynamic descriptivity conditions in terms of the states of neighbouring systems only

$$\begin{aligned} \left(\frac{\partial u_2}{\partial v_2}\right)_T &= \left(\frac{\partial u_1}{\partial v_1}\right)_T - \frac{1}{2} \left[\left(\frac{\partial u_1}{\partial v_1}\right)_T - \left(\frac{\partial u_3}{\partial v_3}\right)_T \right] = \\ &= \left(\frac{\partial u_3}{\partial v_3}\right)_T + \frac{1}{2} \left[\left(\frac{\partial u_1}{\partial v_1}\right)_T - \left(\frac{\partial u_3}{\partial v_3}\right)_T \right]. \end{aligned} \quad (16)$$

Thus, now we have the method for the calculation of the state of a system if states of its neighbouring systems are known. It is the basis of the algorithm for heat conduction simulations similar to cellular automata.

Simulations of one-dimensional heat conduction

Remember that we have N cells of identical size, each of which corresponds to a sublayer. The initial situation is given by values of temperatures and pressures in each cell. We suppose that in the initial situation all sublayers have the same temperatures, $T_i = T_0 \forall i, 1 \leq i \leq N$. In a moment, one of the boundaries receives another value of temperature and holds it in time.

To obtain the values of temperatures in the next time step, we apply a recurrent relation as the leading part of the rule of updating of cells' states

$$\left(\frac{\partial u_{i,k+1}}{\partial v_{i,k+1}}\right)_T = \frac{1}{2} \left[\left(\frac{\partial u_{i-1,k}}{\partial v_{i-1,k}}\right)_T + \left(\frac{\partial u_{i+1,k}}{\partial v_{i+1,k}}\right)_T \right], \quad (17)$$

which follows from the condition of local interaction between thermodynamic systems. Supplementary conditions needed to completely determine the thermodynamic state of a cell are equations of state and usual thermodynamic relations.

We start with the case of solids. In this case, mechanical properties are determined usually by means of the Young's modulus, G , and the Poisson's ratio, ν . Thermal properties are taken into account by the thermal expansion coefficient, α . Generally speaking, all properties of solids depend on

temperature. However, in the first approximation, we can consider them as uniform, as it is treated in a lot of applications.

From the thermodynamic point of view, it is more convenient to use the bulk modulus, K ,

$$K = \frac{G}{3(1 - 2\nu)}, \quad (18)$$

because it has the clear thermodynamic meaning, namely,

$$K = -v \left(\frac{\partial p}{\partial v} \right)_T, \quad (19)$$

where v is the specific volume, p is pressure, T is temperature. The thermal expansion coefficient is expressed in thermodynamic terms as well

$$\alpha = \frac{1}{v} \left(\frac{\partial v}{\partial T} \right)_p. \quad (20)$$

The product of the bulk modulus and the thermal expansion coefficient determines one more thermodynamic derivative

$$\alpha K = -v \left(\frac{\partial p}{\partial v} \right)_T \frac{1}{v} \left(\frac{\partial v}{\partial T} \right)_p = \left(\frac{\partial p}{\partial T} \right)_v, \quad (21)$$

which is immediately contained in the thermodynamic descriptivity conditions, because owing to the differential equations of thermodynamics,

$$\left(\frac{\partial u}{\partial v} \right)_T = T \left(\frac{\partial s}{\partial v} \right)_T - p = T \left(\frac{\partial p}{\partial T} \right)_v - p. \quad (22)$$

Our assumption about the uniformity of thermal properties simplifies the rule of cells' states updating (17)

$$\alpha_i K_i T_{i,k+1} - p_{i,k+1} = \frac{1}{2} (\alpha_{i-1} K_{i-1} T_{i-1,k} - p_{i-1,k} + \alpha_{i+1} K_{i+1} T_{i+1,k} - p_{i+1,k}). \quad (23)$$

In the case of a homogeneous medium with uniform pressure, all sublayers have the same thermomechanical properties, and the temperature in each sublayer is determined as the arithmetical mean of its neighbour's temperatures at the previous time step

$$T_{i,k+1} = \frac{1}{2} (T_{i-1,k} + T_{i+1,k}), \quad (24)$$

and it is fully independent of the kind of material. It must be noted that the latter relation is identical to that for the random walk of particles on the straight line. It is easy to see that such a rule is equivalent to the finite-difference

algorithm for heat conduction equation. In fact, we can rewrite this relation in the form

$$T'_{i,k+1} - T_{i,k} = \frac{1}{2} (T'_{i-1,k} - 2T'_{i,k} + T'_{i+1,k}). \quad (25)$$

If we introduce the usual dependence between space and time steps

$$\frac{\lambda}{\rho c} = \frac{h^2}{2\tau}, \quad (26)$$

we obtain after dividing both parts of the relation (25) by the same value of time step τ

$$\frac{T'_{i,k+1} - T_{i,k}}{\tau} = \frac{\lambda}{\rho c} \frac{T'_{i-1,k} - 2T'_{i,k} + T'_{i+1,k}}{h^2}. \quad (27)$$

The latter equation is nothing more than the well known finite-difference approximation of heat conduction equation [10]. Thus, the proposed algorithm can be reduced to the usual one in this simple case. As a result, we come to strong linear steady-state temperature distribution across the solid layer in full correspondence with the classical theory (Figure 1).

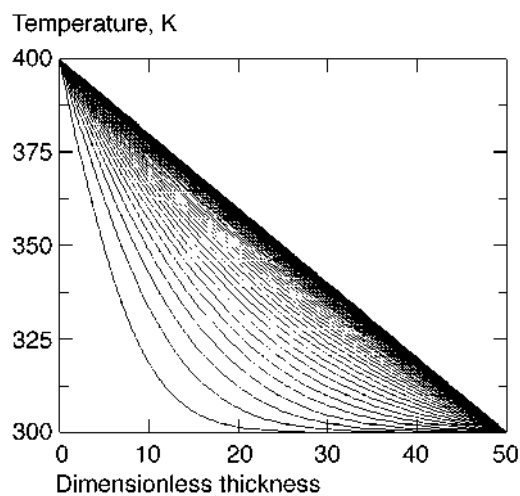
In the case of water, the situation becomes more complicated. The rule of cell's states updating

$$T_{i,k+1} \left(\frac{\partial p_{i,k+1}}{\partial T_{i,k+1}} \right), \quad p_{i,k+1} = \frac{1}{2} \left[T_{i-1,k} \left(\frac{\partial p_{i-1,k}}{\partial T_{i-1,k}} \right) - p_{i-1,k} + T_{i+1,k} \left(\frac{\partial p_{i+1,k}}{\partial T_{i+1,k}} \right) - p_{i+1,k} \right]. \quad (28)$$

is applied together with the equation of state (3)

$$\left(\frac{p_i + B(T_i)}{p_{cr}} \right)^{A(T_i)} = \frac{\rho}{\rho_{cr}} \frac{C(T_i)}{\rho_{cr}}, \quad (29)$$

Figure 1.
Evolution of temperature distributions in a homogeneous solid layer (copper), $\Delta T = 100^\circ\text{K}$, $\rho = 1\text{atm}$



to perform calculations. The pressure in each cell is prescribed as homogeneous or hydrostatic. Again, we start from the uniform initial temperatures, when one of the boundaries suddenly receives another temperature value and holds it in time. A steady-state temperature distribution is reached after heat flux goes to constant. The typical number of cells in our automation was 25.

The results of calculations of temperature distributions in stationary homogeneous water layer with sufficiently large temperature gradients ($\Delta T = 90^\circ$) are presented in Figure 2. The temperature profiles are given at every next 50 dimensionless time steps. In this case, the obtained final steady-state distribution of temperature is essentially non-linear.

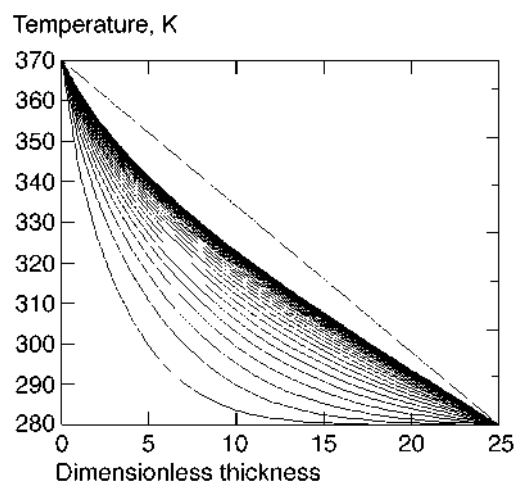


Figure 2.
Evolution of
temperature
distributions in a
stationary water layer
with large temperature
gradient, $\Delta T = 90^\circ\text{K}$,
 $\rho = 1\text{atm}$

The influence of gravitational force is taken into account by prescribing of the hydrostatic values for cell's pressures

$$p_i \equiv p_{i-1} + \rho g h_i, \quad \forall k. \quad (30)$$

This influence displays itself in the non-linearity of the steady-state temperature profile (Figure 3) even for small temperature gradients but under sufficiently strong gravitational force ($h = 0.5\text{m}$). It must be noted that the form of the latter distribution is significantly different from that in the homogeneous case. In the region of liquid-vapour phase transition we obtain one more example of the non-linear steady-state temperature distribution for small temperature gradient (Figure 4). Finally, in the region of solid-liquid phase transition the form of the steady-state temperature profile is rather similar to those under the influence of gravitation, as it can see in Figure 5.

Certainly, the features of the temperature distributions in water are mainly determined by the equation of state (3). The method of simulation only provides its complete application.

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Figure 3.
Evolution of temperature
distributions in a
stationary water layer
under influence of
gravitational field,
 $\Delta T = 20^\circ\text{K}$, $\rho = 1\text{atm}$

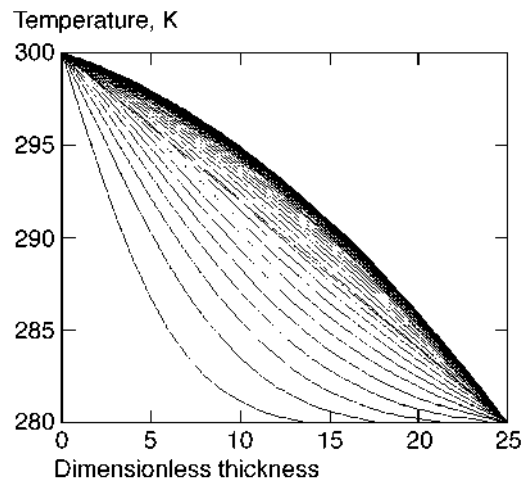
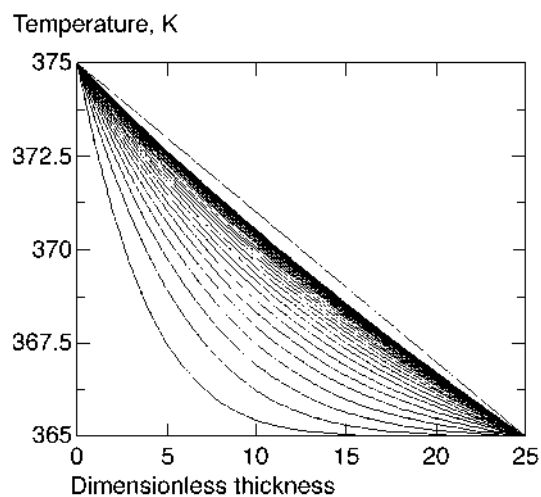


Figure 4.
Evolution of
temperature
distributions in a
stationary water layer
in the region of liquid-
vapour phase transition,
 $\Delta T = 10^\circ\text{K}$, $\rho = 1\text{atm}$



Conclusions

The offered method is rather a tool for the direct simulation of heat conduction process than for the solution of partial differential equations. In this method, the correspondence is used between points in the Gibbsian phase space and states of elements in a continuum. Therefore, the continuum elements are considered as cells, which states are changed according to thermodynamic laws. The appropriate choice is needed for the interaction energy expression in every particular case. Thermophysical properties of a substance are taken into account immediately by equations of state. The cellular automata technique is very convenient because every thermodynamic system must be homogeneous, and thermodynamic parameters have the property of being functions of state. The testing of this method showed that its predictions agree with those of the

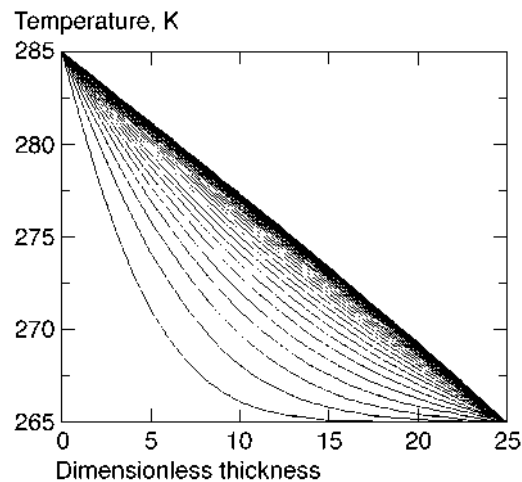


Figure 5.
Evolution of temperature
distributions in a
stationary water layer in
the region of solid-liquid
phase transition, $\Delta T =$
 20°K , $p = 1\text{atm}$

classical theory of heat conduction in the case of solids. At the same time, non-linear temperature distributions for large temperature gradients in water are different from classical ones, especially under the influence of gravitational forces and in the regions of phase transitions.

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