

## MODELING HEAT TRANSFER IN BUILT-UP CURVILINEAR PLATE

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**Abstract.** A mathematical model of material deposition on a curvilinear surface is constructed. The model considers convective heat transfer, heat transfer by radiation, heat and mass transfer during the material attachment to the surface. The possibility of model modification is shown by considering diffusive transfer of a material and the linear change of curvature through the plate thickness. The numerical algorithm developed allows finding the temperature profile in a curvilinear plate.

**Keywords:** chemical vapor deposition, curvilinear surface, numerical modeling

### 1. Introduction

One of the important directions of modern industry is creation of new materials based on additive technologies, i.e. technologies of buildup of various solid bodies. Chemical vapor deposition (CVD) is one of such technologies that represents the deposition of a film or coating of a continuous layer, including a nanocrystalline material, on a cooled plate [1]. First, this method was only used for deposition of metals by transferring their vapor in vacuum. An important feature of such compositions is the qualitative change in the physical properties compared to the massive material [1, 2]. Chemical vapor deposition allows to create at relatively low temperatures, layers with thicknesses from hundredth fractions of a micrometer to several micrometers [3]. Modeling the deposition of silicon coatings and materials on aluminum plates is studied in Refs. [4 – 6].

The necessary stage in creation and using these compositions is development of mathematical models allowing to describe vapor deposition. But most works of this line neglect heat exchange between a gas and a surface. Besides, they consider only elementary surfaces (plane surface, cylindrical surface). The current work considers the most general case of a curvilinear surface and includes special boundary conditions.

### 2. Mathematical model

In Figure 1 curvilinear plate of thickness  $H$  with curvature  $\kappa_0$  is shown. We assume that chemical vapor deposition of a material is going on with the constant rate  $\nu$ ; the temperature of gas  $T_g$  and of cooling medium  $T_m$  being constant. Convective heat transfer occurs on the exterior and interior plate surfaces. Because of the gas high temperature, we take into account the gas radiation on the surface and the radiation of the deposition surface, the deposition being the attachment of heated gas particles to the surface.

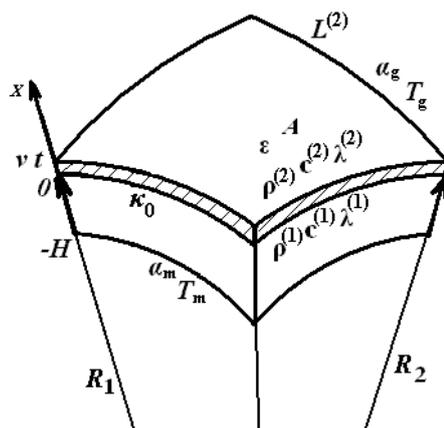


Fig. 1. Curvilinear plate

The temperature distribution in the curvilinear surface layer is described by the equation [7]

$$c^{(k)} \rho^{(k)} \frac{\partial T}{\partial t} = - \frac{\partial q^{(k)}}{\partial x} - 2\kappa(x) q^{(k)}. \quad (1)$$

Here the  $Ox$  axis is directed normally to the surface. The equation is correct for the plate ( $k=1$ ) and deposited material ( $k=2$ ) if the plate thickness is much less than the radius of curvature  $H \ll |1/\kappa(x)|$ . In the case of basic model we assume the mean curvature  $\kappa(x)$  be constant:

$$\kappa(x) \approx \kappa(0) = \kappa_0 = (1/R_1 + 1/R_2)/2. \quad (2)$$

The heat flux in the plate can be found as

$$q^{(k1)} = -\lambda^{(k1)} \nabla T. \quad (3)$$

From equations (1), (2) and (3) we can obtain the equation of heat conduction in a curvilinear orthogonal coordinate system for the plate and deposited material [8]:

$$c^{(k)} \rho^{(k)} \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( \lambda^{(k)} \frac{\partial T}{\partial x} \right) + 2\kappa_0 \left( \lambda^{(k)} \frac{\partial T}{\partial x} \right). \quad (4)$$

For equations (4), the ideal thermal contact condition can be written in the following form:

$$\begin{cases} T(t, 0-0) = T(t, 0+0); \\ \lambda^{(1)} \frac{\partial T}{\partial x} \Big|_{x=0-0} = \lambda^{(2)} \frac{\partial T}{\partial x} \Big|_{x=0+0}. \end{cases} \quad (5)$$

The boundary conditions are:

$$\begin{cases} \lambda^{(1)} \frac{\partial T}{\partial x} \Big|_{x=-H} = \alpha_m (T(t, -H) - T_m); \\ \lambda^{(2)} \frac{\partial T(x)}{\partial x} \Big|_{x=vt} = \alpha_g (T_g - T(t, vt)) - \\ - \varepsilon \sigma_0 T^4(t, vt) + A q_1^g + c^{(2)} \rho^{(2)} v (T_g - T(t, vt)) + \rho^{(2)} v L^{(2)}. \end{cases} \quad (6)$$

The initial temperature distribution  $T_0(x)$  in the plate can be obtained from the steady-state heat-conduction equation for stationary boundaries in the absence of material deposition:

$$\begin{cases} \frac{d}{dx} \left( \lambda^{(1)} \frac{dT_0}{dx} \right) + 2\kappa_0 \lambda^{(1)} \frac{dT_0}{dx} = 0; \\ \lambda^{(1)} \frac{dT_0}{dx} \Big|_{x=-H} = \alpha_m (T_0(-H) - T_m); \\ \lambda^{(2)} \frac{dT_0}{dx} \Big|_{x=0} = \alpha_g (T_g - T_0(0)) - \varepsilon \sigma_0 T_0^4(0) + Aq_1^g. \end{cases} \quad (7)$$

### 3. Numerical solution

To solve the heat-conduction equation (4) with the boundary conditions (5, 6), we assume that at each time  $\tau$  a layer of thickness  $h_2 = \nu\tau$  adheres to the exterior plate surface. We introduce space-coordinate grid:

$$\omega_h = \{x_i = -H + i \cdot h_1, i = 0..N_1, h_1 = H / N_1; x_i = (i - N_1) \cdot h_2, i = N_1 + 1..N_1 + N_2, h_2 = \nu\tau\}. \quad (8)$$

To construct a difference scheme, we use the integro-interpolation method [9 – 11]. We integrate first Eq. (4) over the segments  $[x_{i-1/2}, x_{i+1/2}]$  with respect to space and  $[t_j, t_{j+1}]$  with respect to time. Passing from the continuous function  $T(t, x)$  to a grid function  $u_i^j$ , introduce the notation  $u = u_i^j$ ,  $\hat{u} = u_i^{j+1}$ ,  $\hat{u}_+ = u_{i+1}^{j+1}$ ,  $\hat{u}_- = u_{i-1}^{j+1}$ . Then, after the integration of (4), we obtain

$$c^{(k)} \rho^{(k)} \frac{\hat{u} - u}{\tau} h_k = \left( \lambda^{(k)} \frac{\hat{u}_+ - \hat{u}}{h_k} - \lambda^{(k)} \frac{\hat{u} - \hat{u}_-}{h_k} \right) + 2\kappa_0 \lambda^{(k)} \left( \frac{\hat{u}_+ - \hat{u}_-}{2} \right). \quad (9)$$

The ideal-contact condition can be approximated as follows [12]:

$$\begin{aligned} \left( c^{(1)} \rho^{(1)} \frac{h_1}{2} + c^{(2)} \rho^{(2)} \frac{h_2}{2} \right) \left( \frac{\hat{u} - u}{\tau} \right)_{N_1} = & \left( \lambda^{(2)} \left( \frac{\hat{u}_+ - \hat{u}}{h_2} \right)_{N_1} - \lambda^{(1)} \left( \frac{\hat{u} - \hat{u}_-}{h_1} \right)_{N_1} \right) + \\ & + 2\kappa_0 \left( \lambda^{(2)} \left( \frac{\hat{u}_+ - \hat{u}}{2} \right)_{N_1} + \lambda^{(1)} \left( \frac{\hat{u} - \hat{u}_-}{2} \right)_{N_1} \right). \end{aligned} \quad (10)$$

The left-hand boundary condition is:

$$c^{(1)} \rho^{(1)} \frac{\hat{u}_0 - u_0}{\tau} \cdot \frac{h_1}{2} = \left( \lambda^{(1)} \frac{\hat{u}_1 - \hat{u}_0}{h_1} - \alpha_m (\hat{u}_0 - T_m) \right) + 2\kappa_0 \lambda^{(1)} \frac{\hat{u}_1 - \hat{u}_0}{2}. \quad (11)$$

An approximation of the right-hand boundary condition involves two problems: the fourth power of temperature in the boundary condition and the absence of a point on the previous time layer (in connection with the growing grid):

$$\begin{aligned} c^{(2)} \rho^{(2)} \frac{\hat{u}_{N_1+N_2} - \tilde{u}}{\tau} \cdot \frac{h_2}{2} = & \alpha_r (T_r - \hat{u}_{N_1+N_2}) - \varepsilon \sigma_0 \tilde{u}^4 + Aq_{\text{fl}}^r + c^{(2)} \rho^{(2)} \nu (T_r - \hat{u}_{N_1+N_2}) + \\ & + \rho^{(2)} \nu L^{(2)} - \lambda^{(2)} \left( \frac{\hat{u} - \hat{u}_-}{h_2} \right)_{N_1+N_2} + 2\kappa_0 \lambda^{(2)} \left( \frac{\hat{u} - \hat{u}_-}{2} \right)_{N_1+N_2}. \end{aligned} \quad (12)$$

It is desirable to implement the internal iterative process and take, as  $\tilde{u}^4$ , the approximation

$$\hat{u}_{N_1+N_2}^4 \approx u_{N_1+N_2-1}^4 + 4(\hat{u}_{N_1+N_2} - u_{N_1+N_2-1}) = u_{N_1+N_2-1}^3 (4\hat{u}_{N_1+N_2} - 3u_{N_1+N_2-1}) = \tilde{u}^4. \quad (13)$$

If  $\tilde{u}^4$  is not equal to  $\hat{u}_{N_1+N_2}^4$  with an acceptable error, the obtained value of  $\hat{u}_{N_1+N_2}^4$  is used in approximation (13) instead of  $u_{N_1+N_2-1}$  until a necessary degree of accuracy is obtained. Once the temperature ceases to change substantially, we can write in the difference scheme, from formula (13),  $\tilde{u}^4 = u_{N_1+N_2-1}^3 (4\hat{u}_{N_1+N_2} - 3u_{N_1+N_2-1})$  without constructing the iterative process.

In the growing grid there is no point  $u_{N_1+N_2}$  on the previous time layer, so any variant of selection of  $\tilde{u}$  will give rise to a conditional approximation in scheme (12). Thus, the selection of  $\tilde{u} = u_{N_1+N_2-1}$  will give rise to a term of the form  $O(h_2/\tau) = O(v)$  in the approximation order. If we select as  $\tilde{u}$ ,  $2u_{N_1+N_2-1} - u_{N_1+N_2-2}$  or  $3u_{N_1+N_2-1} - 3u_{N_1+N_2-2} + u_{N_1+N_2-3}$ , in the approximation order, the terms  $O(h_2^2/\tau) = O(h_2v)$  or  $O(h_2^3/\tau) = O(h_2^2v)$  will be added. However, in this case the condition of positiveness of the coefficients is violated that can result in stability loss. Practice shows that these formulas can be used once the temperature ceases to change substantially.

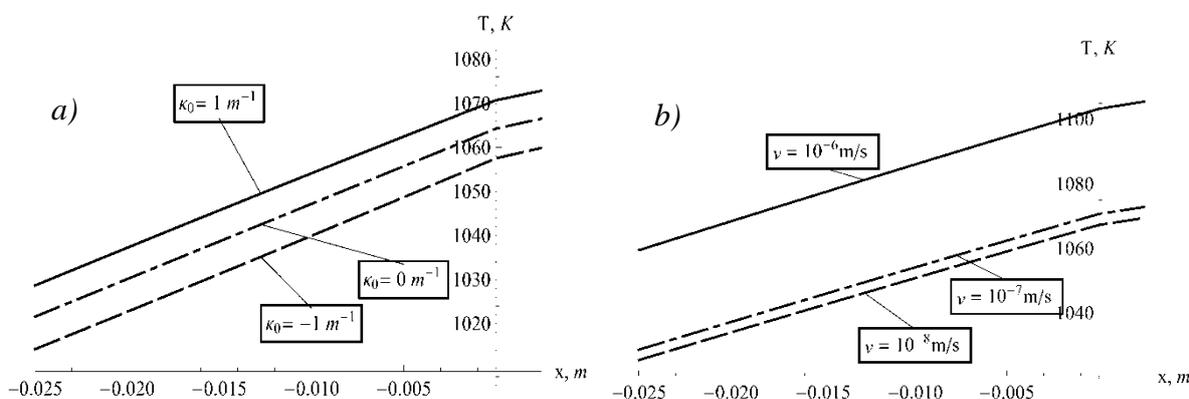
#### 4. Calculation results and possible modifications

Consider the deposition of titanium nitride on a steel plate. We use the following data [13]:

$$\rho^{(1)} = 7800 \text{ kg/m}^3; \rho^{(2)} = 5400 \text{ kg/m}^3; c^{(1)} = 460 \text{ J/(kg} \cdot \text{K)}; c^{(2)} = 600 \text{ J/(kg} \cdot \text{K)}; \lambda^{(1)} = 22,4 \text{ W/(m} \cdot \text{K)}; \\ \lambda^{(2)} = 41,8 \text{ W/(m} \cdot \text{K)}; \kappa_0 = 1 \text{ m}^{-1}; \alpha_m = 53 \text{ W/(m}^2 \cdot \text{K)}; \alpha_g = 72 \text{ W/(m}^2 \cdot \text{K)}; H = 0,025 \text{ m}; v = 10^{-7} \text{ m/s}; \\ \varepsilon = 0,7; A = 0,7; L^{(2)} = 2 \cdot 10^6 \text{ J/kg}; q_1^g = 9,2 \cdot 10^4 \text{ W/m}^2; T_m = 300 \text{ K}; T_g = 1400 \text{ K}.$$

Calculations are done for different curvature  $\kappa_0$  and different deposition rate  $v$ . In Fig. 2a the temperature profile dependence on the mean curvature  $\kappa_0$  is shown. In the plate of large positive curvature, the temperature in each section is higher than that of for small negative curvature. Note that for large values of curvature the one-dimensional equation (1) is incorrect. The rate of chemical vapor deposition also exerts substantial influence on the temperature field. (Fig. 2b): growth of the sputtering rate produces a substantial increase of the temperature.

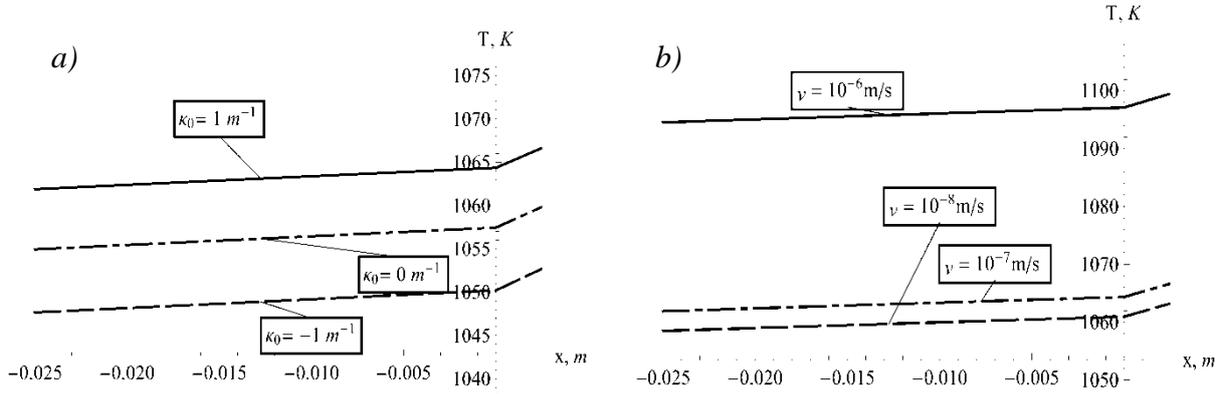
In Figure 3 the temperature field for other materials is illustrated. One can see that the high thermal conductivity of copper contributes to low thermal gradient in the plate because of the fast heat removal from the plate surface.



**Fig. 2.** Temperature change through a steel plate with titanium nitride coating:

a) Plate mean curvature  $\kappa_0 = 1, 0, -1 \text{ m}^{-1}$ , time  $t = 2.5 \cdot 10^4 \text{ s}$  ;

b) Deposition rates  $v = 10^{-6}, 10^{-7}, 10^{-8} \text{ m/s}$  at times  $t = 2.5 \cdot 10^3, 2.5 \cdot 10^4, 2.5 \cdot 10^5 \text{ s}$ .



**Fig. 3.** Temperature change through a copper plate with titanium nitride coating:

a) Plate mean curvature  $\kappa_0 = 1, 0, -1 \text{ m}^{-1}$ , time  $t = 2.5 \cdot 10^4 \text{ s}$  ;

b) Deposition rates  $v = 10^{-6}, 10^{-7}, 10^{-8} \text{ m/s}$  at times  $t = 2.5 \cdot 10^3, 2.5 \cdot 10^4, 2.5 \cdot 10^5 \text{ s}$ .

**Diffusive transfer.** Let us consider a modification of the mathematical model. If we accept a hypothesis of intensive heat transfer between the plate and gas particles, we can find the heat flux in the plate [14] as

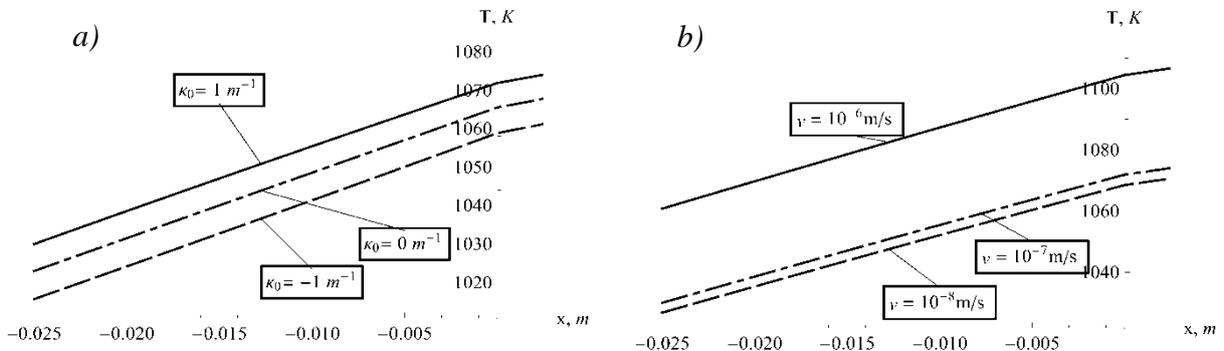
$$\mathbf{q}^{(k)} = -\lambda^{(k)} \nabla T - c^{(2)} T D^{(k)} \nabla Q \tag{14}$$

and equation (4) must be transformed into the system

$$\begin{cases} c^{(k)} \rho^{(k)} \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( \lambda^{(k)} \frac{\partial T}{\partial x} + c^{(2)} D^{(k)} T \frac{\partial Q}{\partial x} \right) + 2\kappa_0 \left( \lambda^{(k)} \frac{\partial T}{\partial x} + c^{(2)} D^{(k)} T \frac{\partial Q}{\partial x} \right), \\ \frac{\partial Q}{\partial t} = \frac{\partial}{\partial x} \left( D^{(k)} \frac{\partial Q}{\partial x} \right) + 2\kappa_0 D^{(k)} \frac{\partial Q}{\partial x}. \end{cases} \tag{15}$$

Addition of the boundary condition, contact condition [15] and initial distribution to these equations allows including the diffusive heat transfer in the mathematical model. However, as we can see in practice, the influence of the diffusive heat flux is less than the influence of the plate geometry (Fig. 4). From the figure it follows that the calculation results are close to those of Fig. 2.

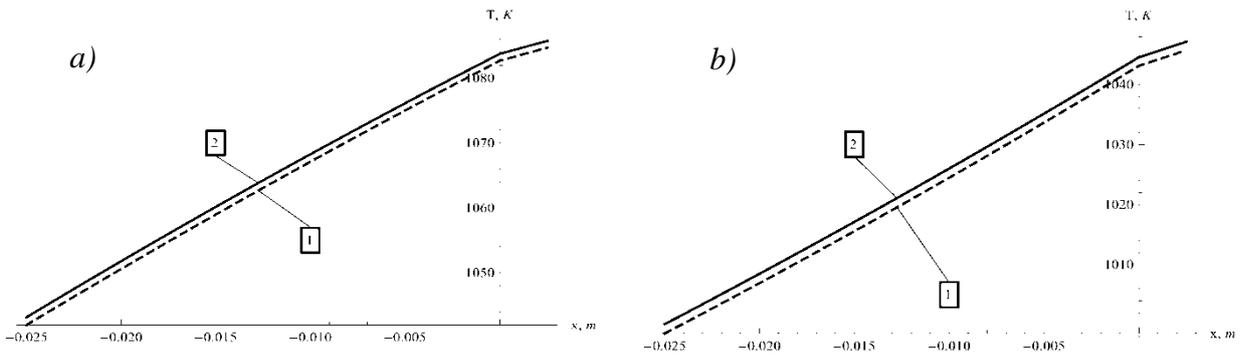
Let us compare both mathematical models. Figure 5 shows up that diffusive transfer influences more on a plate with negative mean curvature. The analogical calculations for various materials manifest that the diffusive process exerts greater influence on the temperature of materials with low thermal conductivity.



**Fig. 4.** Temperature change through a steel plate with titanium nitride coating (diffusive heat transfer is incorporated into the model):

a) Plate mean curvature  $\kappa_0 = 1, 0, -1 \text{ m}^{-1}$ , time  $t = 2.5 \cdot 10^4 \text{ s}$  ;

b) Deposition rates  $v = 10^{-6}, 10^{-7}, 10^{-8} \text{ m/s}$  at times  $t = 2.5 \cdot 10^3, 2.5 \cdot 10^4, 2.5 \cdot 10^5 \text{ s}$ .

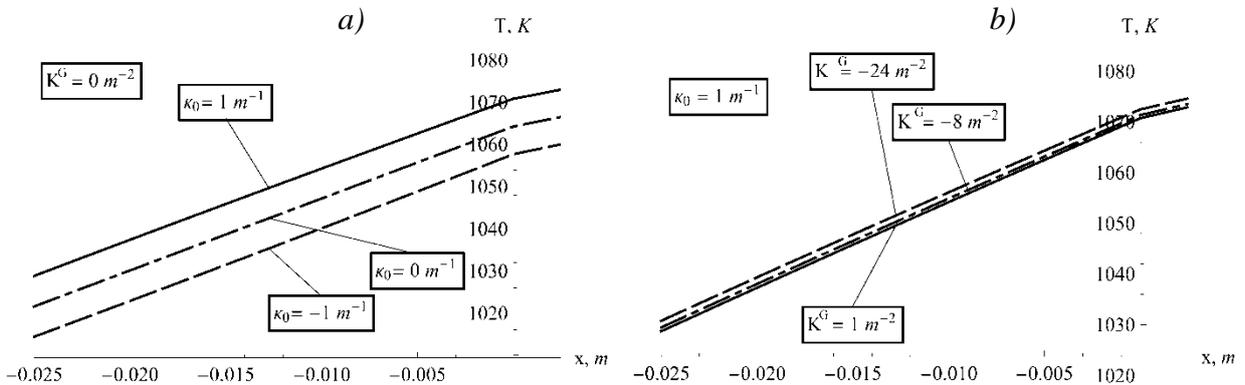


**Fig. 5.** Temperature change through a steel plate with titanium nitride coating according to basic model 1 (a) and model 2 with diffusion (b): Plate mean curvature  $\kappa_0 = 3 \text{ m}^{-1}$  (a) and  $\kappa_0 = -3 \text{ m}^{-1}$  (b), time  $t = 2.5 \cdot 10^4 \text{ s}$

**Non-constant curvature.** The other way of model modification is to introduce the linear change of curvature through the plate thickness:

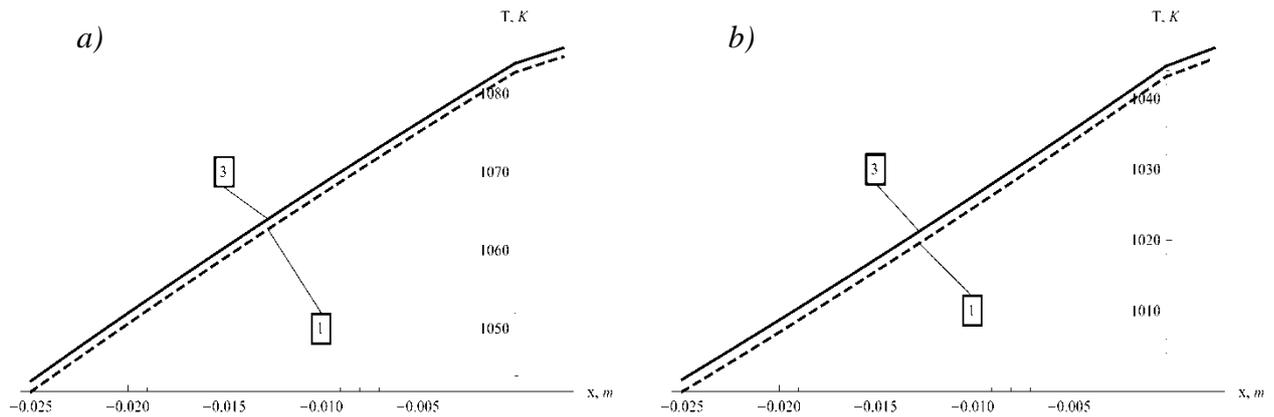
$$\kappa(x) = \left( \frac{1}{R_1 + x} + \frac{1}{R_2 + x} \right) / 2 \approx \kappa_0 - x \cdot \kappa_x. \tag{16}$$

Using formula (16) instead of (2) in equation (1), we can consider the plates of different mean and Gauss curvatures (Fig. 6). Gauss curvature has a maximum if both main curvature radii are equal. In this case we have the lowest temperature in each section (Fig. 6b). The reduction of Gauss curvature leads to increasing the temperature in each plate section.



**Fig. 6.** Temperature change through a steel plate with titanium nitride coating  
 a) Plate mean curvature  $\kappa_0 = 1, 0, -1 \text{ m}^{-1}$ , Gauss curvature  $K^G = 0 \text{ m}^{-2}$ ;  
 b) Gauss curvature  $K^G = 1, -8, -24 \text{ m}^{-2}$ , plate mean curvature  $\kappa_0 = 1 \text{ m}^{-1}$

Let us compare results of the basic mathematical model and the model with linear change of curvature. For a flat plate there is equivalence of the mathematical models. However for a curvilinear plate the results are different (Fig. 7). The basic model gives a lower temperature in plate section, especially for larger curvature values.



**Fig. 7.** Temperature change through a steel plate with titanium nitride coating according to basic model 1 (a) and model 3 with linear change of curvature (b):

Plate mean curvature  $\kappa_0 = 3 \text{ m}^{-1}$  (a) and  $\kappa_0 = -3 \text{ m}^{-1}$  (b), time  $t = 2.5 \cdot 10^4 \text{ s}$

## 5. Conclusions

The temperature distribution depends on materials of a plate and coating. The larger is the mean curvature, the larger is the temperature in a plate section. The temperature depends also on the deposition rate. The dependence of the temperature on geometry and deposition rate for the basic model are also valid for model modifications. The diffusive heat transfer influence more on a plate with a negative mean curvature. The linear change of curvature enlarges a field of application of the basic mathematical model and allows considering Gauss curvature of a plate.

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