Mathematical Models For Meso- And Nano-Domain Heat, Mass, Pulse Transfer Processes

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Abstract. The results for development of new physical and mathematical processes of heat, mass, pulse transfer processes based on the local non-equilibrium thermodynamics principles.

1. Introduction
The traditional theory of transfer processes is based on the local thermodynamic equilibrium principle and continuous medium theory, according to which a local equilibrium state is observed in every minor medium component irrespective of presence of gradients of temperatures, concentrations etc. in the system in general, which is possible only in the case, when the changing rate of the system microparameters is considerably lower than the local equilibrium setting rate. However, any transfer process is non-local since energy transfer from one point to another is not immediate, but it takes quite a finite amount of time instead. Consequently, when assuming the local equilibrium principle, finite transfer process velocity is neglected. Otherwise, transfer process will be non-local and local non-equilibrium transfer model has to be used to describe it [1 - 4].

2. Mathematical models of local non-equilibrium transfer processes
In this paper, local non-equilibrium transfer process equations are derived by using the summands in the formulas of phenomenological Fourier’s law, Newton’s law and Hooke’s law, which consider time acceleration of the driving forces (reasons - temperature, velocity, displacement gradients) and consequences caused by them (heat flow, shear stress, displacement). Their general formula has the form of

$$\eta + \sum_{i=1}^{n} \tau_i \frac{\partial \eta}{\partial t} = z \left( \frac{\partial R}{\partial x} + \sum_{i=1}^{n} \tau_i \frac{\partial R}{\partial x} \right),$$

where $\tau_i$ – relaxation factors; $\eta$ – heat flow; $q$ shear stress $\tau$ and normal stress $\sigma$ respectively in the formulas of the Fourier’s law, Newton’s law and Hooke’s law; $R$ – temperature $T$, velocity $\vartheta$ and displacement $U$ in the formulas of the above laws; $t$ – time; $x$ – coordinate (in the Newton’s law formula $x = y$); $z = -\lambda$ (Fourier’s law); $z = \mu$ (Newton’s law); $z = E$ (Hooke’s law); $\lambda$ – heat conductivity; $\mu$ – dynamic viscosity; $E$ – elasticity modulus.
For example, at $n = 2$ the formulas of the Fourier’s law, Newton’s law and Hooke’s laws take the form of
\[
q + \tau_1 \frac{\partial q}{\partial t} + \tau_2^2 \frac{\partial^2 q}{\partial t^2} = -\lambda \left( \frac{\partial T}{\partial x} + \tau_1 \frac{\partial^2 T}{\partial y^2} + \tau_2^2 \frac{\partial^2 T}{\partial y^2 \partial x^2} \right) ;
\]
\[
t + \tau_1 \frac{\partial t}{\partial t} + \tau_2^2 \frac{\partial^2 t}{\partial t^2} = \mu \left( \frac{\partial \varphi}{\partial y} + \tau_1 \frac{\partial^2 \varphi}{\partial y \partial t} + \tau_2^2 \frac{\partial^2 \varphi}{\partial y^2 \partial t^2} \right) ;
\]
\[
\sigma + \tau_1 \frac{\partial \sigma}{\partial t} + \tau_2^2 \frac{\partial^2 \sigma}{\partial t^2} = E \left( \frac{\partial U}{\partial x} + \tau_1 \frac{\partial^2 U}{\partial y^2} + \tau_2^2 \frac{\partial^2 U}{\partial y^2 \partial x^2} \right) .
\]

If we neglect the last summands of the right and left part of relations (2) – (4), they will coincide with the formulas obtained from the differential equation system by Onzager formulated by A.V. Lykov (based on the hypothesis of finite rate of change of potentials of the fields studied) [2]. In addition, the relation (4) will coincide with the viscoelastic solid sophisticated models known as the Maxwell and Kelvin-Voigt models.

3. Mathematical models of local non-equilibrium heat conductivity

By substituting (2) in the heat balance equation $c_p \partial^2 T / \partial x^2 = -\partial q / \partial x$, we will find
\[
\frac{\partial \Theta}{\partial F_0} + F_{01} \frac{\partial^2 \Theta}{\partial F_0^2} + F_{02} \frac{\partial^4 \Theta}{\partial z^4} + F_{03} \frac{\partial^3 \Theta}{\partial z^3 F_0} + F_{04} \frac{\partial^2 \Theta}{\partial z^2 F_0^2} + F_{05} \frac{\partial^3 \Theta}{\partial z^3 F_0^2} ,
\]
where $\Theta = (T - T_{cr})/(T_0 - T_{cr})$; $\xi = x / \delta$; $F_0 = at / \delta^2$; $F_{01} = a t v / \delta^2$; $F_{02} = a t^2 v^2 / \delta^4$.

When assuming $F_{01} = F_{02} = 0$, the equation (5) is reduced to the traditional parabolic heat conductivity equation.

A precise analytical solution to the equation (5) for the infinite plate at the first-class boundary conditions takes the form
\[
\Theta(\xi, F_0) = \sum_{k=1}^{\infty} \left[ D_{1k} \exp(z_1 F_0) + D_{2k} \exp(z_2 F_0) + D_{3k} \exp(z_3 F_0) \right] \cos((r \pi / 2)(1 - 2\xi)) ,
\]
where $z_1$, $z_2$, $z_3$ – the roots of characteristic equation $D_{1k}$, $D_{2k}$, $D_{3k}$ – integration constants determined based on the initial conditions of the boundary problem; $r = 2k - 1$.

Calculations made by the formula (6) allowed determining the fact of time delay in taking the first-class boundary condition, which evidences that the immediate heating of the body at the boundary is impossible under any conditions of heat exchange with the ambient medium.

![Fig. 1 Temperature distribution by the formula (6) at n = 100000, Fo1 = Fo2 = 10^{-6}; (n – number terms of series (6))](fig.png)

4. Pressure oscillations in liquid considering relaxation properties

By using formulas (3), (4) and the equilibrium (displacement) equation, a differential equation was obtained describing oscillations of the pressure in the elastic fluid under the hydraulic impact conditions. The mathematical task setting in this case takes the form
\[
F_{01} \frac{\partial^2 \Theta(\xi, F_0)}{\partial F_0^2} + F_{02} \frac{\partial^3 \Theta(\xi, F_0)}{\partial F_0^3} + F_{03} \frac{\partial^3 \Theta(\xi, F_0)}{\partial F_0 \partial F_0^2} = \frac{\partial^3 \Theta(\xi, F_0)}{\partial \xi^2 F_0} + F_{04} \frac{\partial^3 \Theta(\xi, F_0)}{\partial \xi^2 F_0^2} .
\]
\[ \Theta(\xi,0) = 1; \quad \frac{\partial \Theta(\xi,0)}{\partial F_0} = 0; \quad \frac{\partial^2 \Theta(\xi,0)}{\partial F_0^2} = 0; \quad (8) \quad \frac{\partial \Theta(0,F_0)}{\partial \xi} = 0; \quad \Theta(1,F_0) = 0, \quad (9) \]

where \( \Theta = (p - p_1)/\Delta p \); \( F_0 = ct/l \); \( \xi = x/l \); \( F_0 = ct_1/c \); \( \Theta, F_0, \xi \) – timeless pressure, time, coordinate \( F_0 \), \( F_0 \) – non-dimensional relaxation and resistance factor; \( p \) – pressure; \( p_0 \) – initial pressure; \( p_0 \) – pipe inlet pressure; \( x \) – coordinate; \( l \) – pipe length; \( c \) – sound velocity in fluid; \( 2a = 3d^2/v \); \( v \) – viscosity; \( d \) – pipe diameter; \( \Delta p = (p_0 - p_1) \).

An exact analytical solution of the task (7) – (9) is in the form

\[ \Theta(\xi,F_0) = \sum_{\ell=1}^{\infty} \left[ c_{1\ell} \exp(z_{1\ell} F_0) + c_{2\ell} \exp(z_{2\ell} F_0) + c_{3\ell} \exp(z_{3\ell} F_0) \right] \cos(\pi \xi/2), \quad (10) \]

where \( c_{1\ell}, c_{2\ell}, c_{3\ell} \) are integration constants determined by the initial conditions (8); \( z_{1\ell}, z_{2\ell}, z_{3\ell} \) – roots of the characteristic equation; \( r = 2k - 1 \).

The calculation results of by the formula (10) are given in fig. 2 (for \( \xi = 0 \)). Their analysis allows concluding that solution of the task (7) – (9) in the quasi-static setting (at \( F_0 = 0 \)) is slightly different from that one obtained in [5] with the employment of the Bernoulli-Fourier method. However, the results of the two theoretical methods are considerably different from the experimental data [6]. Consideration of non-stationary of the velocity gradient and shear stress results in a considerable approximation of the calculation data to the experiment results. Based on the experimental data, by using the relation (10) the relaxation factor \( \tau_1 = 0,0108 \) was found in solving the reverse task.

5. Heat exchange in the moving fluid considering its relaxation properties

In the above model (7) - (9) pressure change is studied under the hydraulic impact conditions. Let’s consider the equation derivation applicable to the non-stationary heat exchange at laminar flow in the two-dimensional duct (energy equation). Formulas for heat flow by axes \( x \) and \( y \) have the form [7]

\[ q_x = -\frac{\lambda}{v} \frac{\partial T}{\partial x} - \tau_1 \frac{\partial^2 q_x}{\partial v^2} - \lambda \tau_1 \frac{\partial^2 T}{\partial v^2}, \quad (11) \]
\[ q_y = -\frac{\lambda}{v} \frac{\partial T}{\partial y} - \tau_1 \frac{\partial^2 q_y}{\partial v^2} - \lambda \tau_1 \frac{\partial^2 T}{\partial v^2}, \quad (12) \]

where \( q_x, q_y \) – heat flows; \( \omega_x, \omega_y \) – velocities; \( i \) – heat content; \( x, y \) – lateral and transverse coordinates; \( \tau_1 \) – relaxation factor.

By substituting (11), (12), in the heat balance equation \( \rho c_p \frac{\partial T}{\partial t} = (\partial q_x/\partial x + \partial q_y/\partial y) \) with neglecting the lateral heat conductivity direction, we find

\[ \frac{\partial \Theta}{\partial F_0} + F_0 \frac{\partial^2 \Theta}{\partial F_0^2} + (1 - \eta) \frac{\partial \Theta}{\partial \eta^2} = \frac{\partial^2 \Theta}{\partial \xi^2} + F_0 \frac{\partial}{\partial F_0} \left( \frac{\partial^2 \Theta}{\partial \xi^2} + \frac{\partial^2 \Theta}{\partial \eta^2} \right), \quad (13) \]

where \( \Theta = (T - T_0)/(T_0 - T_m) \); \( \eta = y/\delta \); \( F_0 = at/\delta^2 \); \( F_0 = at_1/\delta_1^2 \); \( \xi = (2ax/(3\delta^2 \omega_{cp})) \); \( \Delta = (2a/(3\omega_{cp} \delta)^2) \); \( T_m \) – initial temperature; \( T_0 \) – duct inlet temperature; \( T_{cr} \) – fluid temperature at wall; \( \delta \) – duct width; \( \omega_{cp} = 3 \omega_{cp}(1 - y^2/\delta^2)/2 \); \( \omega_{cp} \) – average velocity.
Initial and boundary conditions to the equation (13) take the form
\[ \Theta(\xi, \eta, 0) = \Theta_u ; \quad \partial \Theta(\xi, \eta, 0) / \partial \xi = 0 ; \quad \Theta(0, \eta, \text{Fo}) = 1 ; \]
\[ \partial \Theta(\xi, \eta, \text{Fo}) / \partial \xi = 0 ; \quad \partial \Theta(0, \text{Fo}) / \partial \eta = 0 ; \quad \Theta(\xi, \text{Fo}) = 0 , \]  
where \( \Theta_u = (T_u - T_{cr}) / (T_0 - T_{cr}) \) — non-dimensional initial temperature.

To solve the task (13), (14), the finite difference method was employed. It follows from the calculation results analysis (for \( \Theta_u = 0.5 \)) that when setting the boundary conditions of the temperature impact at the wall in case when the relaxation properties of the medium are considered, the wall temperature does not take the temperature \( \Theta(\xi, \text{Fo}) = 0 \) immediately. The results obtained are in the complete agreement with the solution of the form (6) [7].

6. Oscillations of elastic solids

By using the modified formula of the Hooke’s law in the form (4) and equilibrium equation \( \rho \partial^2 U / \partial t^2 = \partial \sigma / \partial x - \rho \partial^2 U / \partial t \), the following elastic solid oscillation equation was obtained
\[ F_2 \frac{\partial \Theta(\xi, \text{Fo})}{\partial \text{Fo}} + F_1 \frac{\partial^3 \Theta(\xi, \text{Fo})}{\partial \xi^3} + \frac{\partial^2 \Theta(\xi, \text{Fo})}{\partial \xi^2} = \frac{\partial^2 \Theta(\xi, \text{Fo})}{\partial \xi^2} + F_1 \frac{\partial^3 \Theta(\xi, \text{Fo})}{\partial \xi^3} , \]  
where \( \Theta = U/U_0 ; \quad \xi = x / \delta ; \quad \text{Fo} = et / \delta ; \quad F_1 = \epsilon \gamma / e ; \quad F_2 = \delta \gamma / e ; \quad \Theta, \ \xi, \ \text{Fo} \) — non-dimensional displacement, coordinate, time; \( U_0 = b \delta ; \quad F_1, F_2 \) — non-dimensional relaxation and resistance factors; \( \tau \) — relaxation factor; \( \delta \) — rod length; \( b, r \) — factors; \( \rho \) — density; \( \gamma = r / \rho \) — resistance factor; \( e = \sqrt{E/\rho} \) — wave velocity.

The boundary conditions for the rod deformed in the initial time moment, whose one end is rigidly fixed with applying load to another end, which is changing according to the harmonic law, have the form
\[ \Theta(\xi, 0) = 1 - \xi ; \quad \partial \Theta(\xi, 0) / \partial \xi = 0 ; \quad \partial^2 \Theta(\xi, 0) / \partial \xi^2 = 0 ; \quad \partial \Theta(0, \text{Fo}) / \partial \xi = 0 ; \quad \Theta(1, \text{Fo}) = 0 , \]  
where \( F_2 = \delta U_0 \) and \( F_1 = \omega \delta / e \) are non-dimensional amplitude and external load oscillation frequency.

The analysis of results obtained by the finite difference method allows concluding that in the coincidence of own oscillation frequencies of \( (\omega_0) \) the road and external load \( (\text{Fo}) \) resonance oscillations are observed, whose amplitude, while increasing in the initial time period, then becomes stabilized at some constant value.

At frequencies, which are close to resonance, ones, bifurcational flutter fluctuations (beats) occur, at which the rod oscillation frequency increases periodically from zero to some maximum value in the undamped oscillation process (fig. 3). At frequencies, which are far from resonance ones, each road point participates in two oscillating processes with high-frequency and low-amplitude oscillations taking place in the first process and low-frequency and high-amplitude oscillations in the second one.

Fig. 3 Bifurcational flutter oscillations \( (\omega_0 = 1.57) \)
\[ F_1 = 10 ; \quad F_2 = 0.3 ; \quad F_3 = 0.1 ; \quad F_4 = 1.66 ; \quad B = 0 \]

Fig. 4 Double-amplitude fluctuations \( (\omega_0 = 1.57) \)
\[ F_1 = 10 ; \quad F_2 = 0.3 ; \quad F_3 = 0.1 ; \quad F_4 = 0.2 ; \quad B = 0 \]
At the forced oscillation frequencies, which are considerably higher than own ones, the rod oscillation frequency remains constant and equal to the forced oscillation amplitude. Consequently, maintaining such load fluctuations allows avoiding conditions predetermining the structure breakdown. 

The results obtained were compared with the results of experimental studies made by JSC SRC Progress (Samara). Their analysis allows concluding about the satisfactory coincidence. Thus, with \( F_1 = 2 \); \( F_2 = 0.3 \) the theoretical oscillation frequency is 2380 \( 1/c \) (fig. 5), and the experimental one is 2400 \( 1/c \) (fig. 6). The average theoretical and experimental oscillation amplitudes are 0.0033 \( MM \) and 0.0028 \( MM \) (within the range \( 0 \leq \tau \leq 0.01 \)).

7. Dynamic thermoelasticity considering relaxation phenomena

Below given are the results of studying the exact analytical solution of the dynamic thermoelasticity equation obtained considering the relaxation properties of the material and medium resistance. The mathematical task setting for a free infinite plate under the temperature impact at its outer surfaces takes the form

\[
\frac{\partial^2 \sigma}{\partial \xi^2} + \frac{\partial^3 \sigma}{\partial \xi^2 \partial \Theta} = \frac{\partial^2 \sigma}{\partial \xi^2 \partial \Theta} - \frac{\partial^3 \sigma}{\partial \xi^2 \partial \Theta} = \frac{\partial^3 \Theta}{\partial \xi^2 \partial \Theta} + \frac{\partial^3 \Theta}{\partial \xi^2 \partial \Theta} - \frac{\partial \Theta}{\partial \Theta} ;
\]

\[
\sigma(\xi,0) = 0; \quad \partial \sigma(\xi,0)/\partial \Theta = 0; \quad \sigma(0,\Theta) = 0; \quad \sigma(1,\Theta) = 0,
\]

where \( \Theta = (T - T_{CT})/(T_0 - T_{CT}) \); \( \xi = x/(2\delta) \); \( F_1 = c(t_2 - t_1)E/(\delta \rho) \); \( F_2 = 0.5 t_1 E/(\delta \rho) \); \( F_3 = 2 t_1 \delta /V \); \( t - time; \delta - plate thickness; T_0 - initial temperature; T_{CT} - wall temperature; E - elasticity modulus; F_1, F_2 - non-dimensional relaxation factors; F_3 - resistance factor; \alpha - linear expansion factor; V - volume unit; t_1, t_2 - relaxation factors; \beta, A - constants. 

An exact analytical solution of the task (17), (18) is in the form

\[
\sigma(\xi,\Theta) = \sum_{k=1}^{\infty} \left[ C_{1k} e^{-v_{1k} F_0} + C_{2k} e^{-v_{2k} F_0} - (H_1 e^{z_{1k} m F_0} + H_2 e^{z_{2k} m F_0})/(H_3) \right] \cos((\pi/2)(1 - 2\xi)) ,
\]

where \( v_{1k}, v_{2k} = 0.5(F_0 + \sqrt{F_0^2 - 4\mu_k}) \); \( C_{1k}, C_{2k}, H_1, H_2, H_3 - constants; m = 2a/c(\delta) \); \( a - thermal conductivity factor; F_0 = \mu_k F_0 F_2; \mu_k = r^2 \pi^2; r = 2k - 1 \).

It follows from the stress calculations by the formula (19) that with \( F_0 = F_0 = F_0 = 0 \) stresses in each point of the road change abruptly with periodically reversing their sign. The oscillation process is undamped, which is explained by the non-consideration of relaxation properties and resistance of the medium (fig. 7). When considering relaxation properties and resistance of the medium, abrupt stress variation transforms into the harmonic one under the damped oscillation process (fig. 8). Further-
more, stress and displacement oscillation are identical in their form to the fluctuations of the unbalanced spring.

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