Heat transfer from the heated by an electric current vertical rod in the regime of non-stationary natural convection

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Abstract. The heat transfer from a vertical silicon rod heated by passing an electric current, placed in a cylindrical container filled with gas, with isothermal cold side walls, in the regime of non-stationary conjugate natural convection heat exchange, is studied numerically by the finite element method in a three-dimensional formulation of the problem. On the surface of the rod, a control point is selected, at which a constant temperature is maintained by changing the voltage of the electric current. The equations of thermogravitational convection are solved in the Boussinesq approximation in the terms of temperature, vortex, and vector field potential. The spatial form of convective flows is investigated. Temperature fields in a gas and in a solid are investigated. The calculations were performed with the Prandtl number equal to 0.67 and the Rayleigh number range from $10^4$ to $5 \cdot 10^5$.

1. Introduction
Poly silicon produced by Siemens processes is mainly used as a feedstock to produce high-quality silicon single crystals all over the world [1-3]. The essence of the Siemens process is the hydrogen reduction of trichlorosilane or monosilane on electrically heated seed silicon rods. A free-convective boundary layer develops on a vertical rod heated to a high temperature at low speeds of gas purging through the reactor [4-7]. With an increase in the mass flow rate of the initial gases through the reactor, heat exchange occurs in mixed or forced convection modes [6]. Complete suppression of the influence of buoyancy forces in this technology is almost impossible to achieve. In the thermogravitational convection regime, the local heat transfer and mass transfer coefficients are inhomogeneous in the direction from the lower end of the rod downstream (up the rod) in laminar regimes and even more inhomogeneous (and non-stationary) in the laminar-turbulent transition regimes [5-7].

An actual problem is to determine the optimal thermal conditions of the technological process. Optimization of the thermal conditions of the process is reduced to the need to ensure a high degree of uniformity of the silicon rod heated by electric current. For geometry characteristics of hydrogen reduction reactors, the studies are either preliminary [2], or they are characterized by an extremely simplified approach [3]. In the class of problems under consideration, the processes of heat and mass transfer must be considered in the conjugate formulation. In the full formulation, they are practically cannot be solved, as it considers the properties of real gas mixtures with chemical reactions and radiative-convective heat transfer. This work is a development of works [8, 9], in which the conjugate convective heat exchange of a U-shaped rod with a square cross-section heated by passing an electric...
current is considered. The effect of non-stationary heat transfer from a silicon rod heated by an electric current on the temperature fields in the rod is studied. The studies were carried out in the regime of non-stationary conjugate natural convective heat exchange.

2. Model

The calculations are carried out in a three-dimensional formulation of the problem in Cartesian coordinates. The design area consists of a vertical cylindrical container (reactor vessel) with thermally insulated ends and isothermal cold walls with a radius-to-height ratio of 1:5. The origin is in the center of the rod. The container is filled with argon gas. The conditions of adhesion and non-flow of gas are set on all rigid surfaces of the system. On the side surface of the rod near the upper end there is a control point at which the set temperature is maintained by selecting the voltage of the electric current passing through the rod. At the ends of the rod, a different electric potential is set, and the distribution of the electric potential in the volume of the rod is calculated. Then, from the local drop in the electric potential (voltage), considering the dependence of the silicon resistance on temperature, the volume density of the heat generated during direct current transmission is calculated. Nonstationary conjugate convective heat transfer in the thermogravitational convection regime is described by a dimensionless system of Navier-Stokes equations in the Boussinesq approximation in terms of temperature, vector potential of velocity field and velocity vortex:

\[
\begin{align*}
\nabla \cdot \mathbf{v} &= 0, \\
\rho \frac{D\mathbf{v}}{Dt} &= -\nabla p + \nabla \cdot (\mu \nabla \mathbf{v}) + \mathbf{f}, \\
\nabla \cdot \mathbf{j} &= 0, \\
\rho \frac{D\mathbf{j}}{Dt} &= -\nabla \cdot (\mathbf{u} \mathbf{j}) + \mathbf{E} - \mathbf{v} \times \mathbf{B}.
\end{align*}
\]

where \(T, \mathbf{v}, \omega, \psi, V\) are respectively the temperature, electric potential, vortex, vector potential of the velocity field and the velocity field. The radius of the container filled with gas is \(R\), this is chosen as the geometric scale. For the velocity, the scale \(v/R\) is used, where \(v\) is the kinematic viscosity of the liquid. The temperature scale is \(\Delta T = T_{\text{max}} - T_{\text{min}}\), where \(T_{\text{max}}\) and \(T_{\text{min}}\) are the temperatures at the selected point on the heated rod and on the cold wall of the vessel, respectively. The time scale is \(R^2/\nu\). In dimensionless equations, \(Gr = (\beta g \nu^2) \Delta T R^3\) is the Grashof Number. Here \(\beta\) is the coefficient of volumetric expansion of the liquid, \(g\) is the acceleration of gravity, \(\nu\) is the kinematic viscosity of the liquid, and \(AT\) is the temperature drop. The Prandtl number \(Pr = v/\alpha\), where \(\alpha = \lambda/\rho C_p\) is the thermal diffusivity of the fluid \(\lambda\) – coefficient of thermal conductivity of the gas, \(\rho\) is the density, \(C_p\) is the heat capacity at constant pressure. \(Q = U^2/R(T)\) is the volume density of the heat generated when passing a
electric current, here \( U \) is the local voltage drop (calculated as the potential difference), \( R(T) \) is the electrical resistance of silicon, depending on the temperature. \( R(T) = \frac{1}{\sigma(T)} \), where \( \sigma(T) = \sigma_0 \exp\left[-\Delta E_g / (2kT)\right] \), where \( \Delta E_g = 1.13 \text{[eV]} - \) bandgap (is a function of temperature and above 250K is fairly linear approximation \( \Delta E_g = 1.205 - 2.84 \cdot 10^{-4}T \text{[eV]} \)), \( \sigma_0 \) is electrical conductivity inverse of its own electrical resistance (for high-purity silicon \( \rho = 2 \cdot 103 \text{[Ω·m]} \) at 20°C); \( k = 8.617343(15) \cdot 10^{-5} \text{[eV]} \) is the Boltzmann’s constant. In calculations, it is assumed that \( R(T) = e^{143(17.24 \cdot 10^{-5} T) / (1.027 \cdot 10^6)} \) is the local resistance of the silicon rod, depending on the temperature in the rod \([10]\).

The ends of the container and the rod are heat-insulated \( \partial T / \partial n \bigg|_{F_1} = 0 \). The side wall of the container is maintained at the minimum temperature in the system \( T_{\Gamma_0} = 0 \). The initial value of the electric potential at the lower end of the rod \( F_{\Gamma_1} = \phi_\Gamma \), at the upper end of the rod, the ends and the side wall of the container, the electric potential is zero \( F_{\Gamma_2} = 0 \). On the rod generatrix, the condition of ideal thermal contact is set

\[
-\frac{\lambda_s}{\lambda_f} \frac{\partial T}{\partial n} \bigg|_{F_1} = -\frac{\partial T}{\partial n} \bigg|_{\Gamma_1} = T_{\Gamma_1} - T_{\Gamma_2}.
\]

A similar condition is given for the electric potential

\[
-\sigma_s \frac{\partial F}{\partial n} \bigg|_{F_1} = -\sigma_f \frac{\partial F}{\partial n} \bigg|_{\Gamma_1} = F_{\Gamma_1} - F_{\Gamma_2}.
\]

At all rigid boundaries of the system, the condition of non-flow boundaries is set

\[
\psi_{\Gamma_1} = 0 \quad \text{and adhesion of gas is set} \quad \omega_{\Gamma_1} = \left(\partial V_y / \partial z - \partial V_z / \partial y\right) \bigg|_{F_1}, \quad \omega_{\Gamma_2} = \left(\partial V_z / \partial x - \partial V_x / \partial z\right) \bigg|_{F_1}.
\]

Numerical simulation was carried out by the finite element method on a tetrahedral grid with 127 thousand nodes. Linear basis functions were used in the calculations. The grid fragment in the height section is shown in figure 1. The calculations were performed for the Prandtl number \( \text{Pr} = 0.67 \) and the set of Rayleigh numbers \( 10^4, 10^5, 2 \cdot 10^5, 3 \cdot 10^5, 5 \cdot 10^5 \) and the ratio of the thermal conductivity of the rod to the thermal conductivity of the gas \( \lambda_S / \lambda_f = 446 \).

### 3. Results and discussion

Calculations of heat transfer from a silicon rod heated by an electric current in the regime of natural convective conjugate heat exchange for a discrete set of Rayleigh numbers are carried out. Figure 2 shows the evolution of the temperature field over the entire computational domain with an increase in the Rayleigh number in steady-state heat exchange regimes in the range of Rayleigh numbers from \( 10^4 \) to \( 5 \cdot 10^5 \). In steady-state conditions, an upward flow of hot gas is formed at the surface of the heated silicon rod. The gas floats up to the upper heat-insulated end of the container, unfolds and flows onto the cold walls of the container, where the gas is cooled. The gas cooled on the side walls sinks to the bottom of the container, where it unfolds and flows onto the base of the heated silicon rod.
Temperature fields in steady-state regimes in the cross-section $y = 0$ at: a – $Ra = 10^4$; b – $10^5$; c – $2 \cdot 10^5$; d – $3 \cdot 10^5$; e - $5 \cdot 10^5$. The step of the isotherms is 0.05.

Temperature distributions and temperature gradients on the surface and in the volume of the silicon rod depend on this feature of gas circulation in the annular region (figures 2, 3). As a result, cooled gas flows onto the base of the heated silicon rod, local temperature gradients normal to the rod generators and the cooling efficiency of the rod increase (figure. 3b). Figures 2 and 3a show that for all the Rayleigh numbers considered, the rod heats up unevenly. The upper part of the rod is noticeably overheated relative to the lower part. In all regimes, the radial distribution of the temperature field inside the rod is inhomogeneous, the core is more heated than the outer surface of the rod. Since the upper part of the rod is heated more strongly, the gas rising along the rod generatrix will always be colder than the surface of the rod. That is, the gas cools the surface of the rod along its entire height, and the axial temperature gradient in the rod and on its surface will always be negative (figure 3c). Thus, the situation when the upward gas flow would be superheated relative to the surface of the rod and would begin to heat this surface is excluded. As a result, the core of the rod will always be heated to a higher temperature than the surface of the rod.

Distribution of temperature along the height of the rod generatrix (a) and temperature gradients along the normal to the rod generatrix (b), distribution of temperature gradients along the rod surface (c) at: 1 – $Ra = 10^4$; 2 – $10^5$; 3 – $2 \cdot 10^5$; 4 – $3 \cdot 10^5$; 5 - $5 \cdot 10^5$. 

Figure 2. Temperature fields in steady-state regimes in the cross-section $y = 0$ at: a – $Ra = 10^4$; b – $10^5$; c – $2 \cdot 10^5$; d – $3 \cdot 10^5$; e - $5 \cdot 10^5$. The step of the isotherms is 0.05.

Figure 3. Distribution of temperature along the height of the rod generatrix (a) and temperature gradients along the normal to the rod generatrix (b), distribution of temperature gradients along the rod surface (c) at: 1 – $Ra = 10^4$; 2 – $10^5$; 3 – $2 \cdot 10^5$; 4 – $3 \cdot 10^5$; 5 - $5 \cdot 10^5$. 

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Figure 4. Temperature field at $Ra = 5 \cdot 10^5$ in the cross-section $y = 0$ at time layers: a – $t = 40$; b – 80; c – 120; d – 160; e – 200. The step of the isotherms is 0.05.

Figure 4 shows the evolution of the temperature field over time at $Ra = 5 \cdot 10^5$ in the cross-section $y = 0$. At the initial moment, under the influence of an electric current, the silicon rod begins to warm up. During a short incubation period, the gas near the forming rods is heated by conductive heat exchange. Then, the gas heated on the rod generatrix begins to rise and an upward convective flow is formed. As a result, cold gas from the bottom region begins to contract almost immediately to the base of the heated rod. This contributes to the fact that almost immediately the base of the rod begins to cool more efficiently than the upper part of the rod, and the rod initially begins to warm up unevenly. Rising along the forming convective gas flow reaches the thermally insulated end of the container, on which it unfolds and flows onto the cold side wall of the container. Then the gas is cooled and lowered along the side surface of the container to the bottom region, where it unfolds on the lower thermally insulated end of the container and flows onto the base of the silicon rod heated by electric current. A circulation flow is established in the entire area.

Figure 5 shows the time evolution of the temperature field in the rod. It can be seen that the heating of the rod initially occurs inhomogeneously, the temperature of the upper part of the rod is constantly
higher than the temperature of the lower part, the core of the rod is always more heated than the surface of the rod.

Figure 6. Temperature field (a, b, c) and velocity vector field (d, e, f) at $Ra = 5 \cdot 10^5$ in steady-state regime at levels a, d – $z = 1$; b, e – 2.5; c, f – 4.

An important feature, noticeable in figures 4 and 5, is that during the entire process of heating the rod and entering the steady state, a temperature field close to axisymmetric is formed. It can be seen that in steady-state regimes in the Rayleigh number range from $10^4$ to $5 \cdot 10^5$, the temperature fields near the rod generatrix remain close to axisymmetric. This means that in the considered range of Rayleigh numbers, it is possible to proceed to an axisymmetric formulation of the problem and, by reducing the requirements for computing resources, perform more detailed parametric studies of the influence of the Rayleigh number, and therefore of temperature differences on the laws of conjugate heat exchange. However, figure 6 shows that despite the conditional axial symmetry of the temperature field, asymmetric convective flows develop throughout the annular region. With increasing Rayleigh numbers, the influence of three-dimensional effects can begin to have a significant influence on the temperature field, both in the entire region and inside the rod, despite the significant difference in the thermal conductivity coefficients of silicon and argon.

4. Conclusion
The heat transfer from a vertical silicon rod heated by passing an electric current, placed in a cylindrical container filled with argon, with isothermal cold side walls, in the regimes of steady-state and non-stationary conjugate natural convective heat exchange is studied numerically by the finite element method in a three-dimensional formulation of the problem. The characteristic temperature difference between the cold walls of the reactor vessel and the heated silicon rod was maintained by setting the temperature at a control point on the surface of the rod. The calculations were performed with the Prandtl number equal to 0.67 and the Rayleigh number range from $10^4$ to $5 \cdot 10^5$. The
temperature fields in a gas and in a solid are studied in the processes of entering the steady-state heat exchange regimes and in steady-state regimes.

It is shown that in the considered range of Rayleigh numbers, the temperature fields remain close to axisymmetric. At the Rayleigh number $5 \cdot 10^5$, a non-axisymmetric velocity field is formed, and the influence of three-dimensional effects begins to increase, but their influence on the loss of symmetry by the temperature field is still insignificant.

It is shown that for all the considered Rayleigh numbers, a circulation flow is formed in the region after a short incubation period. The gas is heated on the forming silicon rod, rises to the upper end of the area, unfolds, reaches the cold walls of the container, where it cools and sinks into the bottom area. Then the flow of cooled gas unfolds and flows onto the base of the rod, as a result of which radial temperature gradients grow and the base of the rod begins to cool more efficiently. As a result, a substantially inhomogeneous temperature field in the longitudinal direction is formed in a silicon rod heated by passing an electric current. As the Rayleigh number increases, the inhomogeneity of the longitudinal distribution of the temperature field in the rod increases.

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