Development of unsteady boundary layers on the generatrices of a vertical silicon rod heated by electric current in the mode of conjugate radiation-convective heat transfer

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Abstract. The nonstationary conjugate radiation-convective heat transfer of a single silicon rod heated by an electric current with the surrounding gas medium is studied numerically in the axisymmetric formulation by the finite element method. The calculations were carried out at the Prandtl number Pr = 0.68, and the range of the Grashof number, determined by the temperature difference and the radius of the rod 9 703 ≤ Gr ≤ 261 977. It is shown that after a short incubation period, a circulation flow is formed. As a result, a significantly inhomogeneous temperature field in the longitudinal direction is formed in a silicon rod heated by an electric current. As the Grashof number increases, the inhomogeneity of the longitudinal distribution of the temperature field increases.

1. Introduction

Many technological systems are characterized by the processes of non-stationary conjugate convective or radiation-convective heat transfer under non-stationary (transient) conditions or with access to steady-state boundary conditions. Under the action of buoyancy forces on the walls of various configurations under non-stationary temperature boundary conditions, non-stationary boundary layers develop, in which laminar-turbulent transitions can occur. These processes have been studied extremely poorly, especially in the conjugate formulation of problems. One example of such a system is a separate silicon rod in a silicon hydrogen reduction reactor using the Siemens method [1-3]. In the simplest version of the reactor, from a complex multi-core system, a single silicon rod remains heated by a constant electric current.

An important problem of the Siemens process is the need to ensure the uniformity of the temperature distribution on the surface of the silicon rod heated by an electric current. Depending on the temperature on the rod surface, the rate of hydrogen reduction of trichlorosilane and the rate of silicon deposition on the surface of the rod change. Studies of heat and mass transfer processes for hydrogen reduction reactors are preliminary in nature [1-2]. For the conditions, characteristic of real technology, the study of heat and mass transfer processes must be carried out in a complete and conjugate formulation. To understand the general laws of the heat transfer process in the reactor, which are necessary for designing growth plants and optimizing technological processes, it is advisable to use the partial modeling approach. Partial modeling allows determining at a qualitative level the main trends in the behavior of the systems under consideration when individual control parameters or a group of them change. This work is a development of the works [4-6]. In [4, 5], the conjugate freely convective heat exchange of a U-shaped rod with a square cross-section heated by
passing an electric current in a steady-state mode is numerically studied. It is shown that the temperature field in the rod is distributed essentially inhomogeneously. In [6], in the three-dimensional formulation of the problem, the heat transfer from a vertical silicon rod heated by an electric current, placed in a cylindrical container filled with argon, with isothermal cold sidewalls, is investigated in the modes of steady and non-stationary conjugate free-convective heat exchange. The calculations were performed with the Prandtl number equal to 0.67 and the Rayleigh number range from $10^4$ to $5\cdot10^5$. It is shown that in the considered range of Rayleigh numbers, the temperature fields remain close to axisymmetric. Thus, it becomes possible to perform a parametric study of the non-stationary conjugate radiation-convective heat transfer of a single silicon rod heated by an electric current with the surrounding gas medium in a two-dimensional axisymmetric formulation.

2. Model

The nonstationary conjugate radiation-convective heat transfer of a single silicon rod heated by an electric current with the surrounding gas medium is considered numerically in the axisymmetric formulation by the finite element method [7]. A control point is selected on the surface of the rod, where the temperature of 1100°C is maintained due to the selection of voltage. At the ends of the vertical rod, a different electric potential is applied, the distribution of the electric potential in 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 by a direct electric current is calculated. The temperature difference between the control point and the walls of the vessel is assumed in all calculations to be 100°C. When modeling conductive heat transfer, a non-stationary dimensionless heat conduction equation was used:

$$\frac{\partial T}{\partial t} - \frac{1}{\Pr} \frac{\lambda_s}{\lambda_f} \left( \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2} \right) = \frac{R_s^2}{\Pr \cdot (T_{\text{max}} - T_{\text{min}})} \frac{Q_s}{\lambda_s}$$

Here $t$ is the dimensionless time, $T$ is the dimensionless temperature, $R_s$ is the radius of the rod, $\lambda_s$ is the thermal conductivity of silicon, $\lambda_f$ is the thermal conductivity of argon, $r$ and $z$ are the radial and axial coordinates, respectively, $T_{\text{max}}$ and $T_{\text{min}}$ are the temperatures at the control point and on the cold walls of the housing, respectively. The Prandtl number $\Pr = \nu/\alpha_f$, where $\nu$ is the kinematic viscosity of argon, $\alpha_f$ is the thermal conductivity coefficient of argon. $Q_s = U^2/R(T)$ is the volume density of the heat generated by a direct electric current, here $U$ is the local voltage drops (calculated as a potential difference), $R(T)$ is the resistance of silicon, depending on temperature. $R(T) = 1/\sigma(T)$, where $\sigma(T) = \sigma_0 \exp[-\Delta E_s/(2kT)]$, where $\Delta E_s = 1.13$ [eV] is the band gap width (is a function of temperature; above 250K, it is approximated linearly $\Delta E_s = 1.205 - 2.84\cdot10^{-4}T$ [eV]) $\sigma_0$ is the intrinsic electrical conductivity, inverse to the intrinsic resistivity (for high-purity silicon, $\rho = 2\cdot10^3$ [Ohms-m] at a temperature of 20°C); $k = 8.617343(15)\cdot10^{-5}$ [eV] is the Boltzmann constant. In the calculations, it is assumed that the local resistance of the silicon rod depends on the temperature in the rod according to the relationship $R(T) = e^{1.13/(17.24\cdot10^{-5}\cdot T)}/(1.027\cdot10^6)$ [8].

The following voltage selection mechanism is used. If the temperature at the control point is lower than 95% of the control point, the voltage increases by 5%. Otherwise, if the temperature at the control point is higher than 10% of the set value, the voltage is reduced by 5%. Otherwise, if the temperature at the control point is lower than the set value, the voltage increases proportionally to the ratio of the set temperature to the current one. Otherwise, if the temperature at the control point is higher than the set one, the voltage decreases proportionally to the ratio of the current temperature to the set one.

To simulate natural convection, a dimensionless system of Navier-Stokes equations, energy, and continuity in the Boussinesq approximation, written in the terms vortex, stream function, and temperature, is used:
The condition of an ideal thermal contact is set on the rod and the thermal conductivity of argon \( \lambda_s = 26 \text{ Wm}^{-1}\text{K}^{-1} \) and the thermal conductivity of argon \( \lambda_f = 5.43 \times 10^2 \text{ Wm}^{-1}\text{K}^{-1} \) and a set of rod radii \( R_s = 0.1 \text{ m}, 0.2 \text{ m}, 0.3 \text{ m} \). The thermal diffusivity of argon \( a = 3.74 \times 10^4 \text{ m}^2\text{s}^{-1} \), the volume expansion coefficient of gas \( \beta = 6.4 \times 10^4 \text{ K}^{-1} \), the kinematic viscosity of the gas \( \nu = 2.54 \times 10^{-4} \text{ m}^2\text{s}^{-1} \) \[10\].

The calculation of radiation fluxes was carried out based on the zonal method \[9\] under the following assumptions: the calculated area is limited by a closed system of surfaces; all surfaces of the system are gray, diffusely emitting, and diffusely reflecting; the surfaces are divided into zones within which the radiation properties and temperature can be considered constant; the medium filling the growth chamber is diathermic.

At the control point, due to the dynamic selection of voltage, a constant temperature is maintained equal: \( T_{\mid r_v} = 1 \). The sidewall of the container is maintained at the minimum temperature in the system:

\( T_{\mid r_v} = 0 \). The ends of the container and the rod are thermally insulated: \( \partial T/\partial n_{\mid r_v,4,5} = 0 \). The initial value of the electric potential at the lower end of the rod \( \phi_{\mid r_v} = \phi_n \), at the upper end of the rod, the ends, and the sidewall of the container, the electric potential is zero \( \phi_{\mid r_v,3} = 0 \). The condition of an ideal thermal contact is set on the rod generatrix, considering radiation fluxes (Qr)

\[-\frac{\lambda_s}{\lambda_f} \frac{\partial T}{\partial n_{\mid r_v}} = -\frac{\partial T}{\partial n_{\mid r_v}} + Q, \quad T_{\mid r_v} = T_{\mid r_v} \; \text{.} \]

A similar condition is given for the electric potential

\[-\sigma_i \frac{\partial \phi}{\partial n_{\mid r_v}} = -\sigma_i \frac{\partial \phi}{\partial n_{\mid r_v}}, \quad \phi_{\mid r_v} = \phi_{\mid r_v} \; \text{.} \]

At all rigid boundaries of the system, the condition of non-flow \( \psi_{\mid r_v,3,6} = 0 \) and adhesion of gas is set \( \omega_{\mid r_v,3,4} = \frac{\partial V_r}{\partial c} \bigg|_{r_v,3,4} - \frac{\partial V_r}{\partial r} \bigg|_{r_v,3,4} \).

Numerical simulation was carried out by the finite element method on an uneven grid of 151x301 nodes with a dimensionless height of rod 6 and 151x601 with a height of rod 12, consisting of triangular finite elements with linear functions specified on them. The calculations were carried out with the thermal conductivity of the rod \( \lambda_s = 26 \text{ Wm}^{-1}\text{K}^{-1} \) and the thermal conductivity of argon \( \lambda_f = 5.43 \times 10^2 \text{ Wm}^{-1}\text{K}^{-1} \) and a set of rod radii \( R_s = 0.1 \text{ m}, 0.2 \text{ m}, 0.3 \text{ m} \). The thermal diffusivity of argon \( a = 3.74 \times 10^4 \text{ m}^2\text{s}^{-1} \), the volume expansion coefficient of gas \( \beta = 6.4 \times 10^4 \text{ K}^{-1} \), the kinematic viscosity of the gas \( \nu = 2.54 \times 10^{-4} \text{ m}^2\text{s}^{-1} \) \[10\]. The emissivity factor of all surfaces of the system is 0.5.
3. Results and discussion
The calculations were carried out at the Prandtl number Pr = 0.68, in the dimensionless formulation of the problem, the radius of the rod R = 1, the radius of the reactor vessel Rs = 3. The problems were solved at two heights of the region H/Rs = 6 and 12, the Grashof numbers determined by the temperature difference and the radius of the rod were Gr = 9 703, 77622, and 261 977.

![Figure 1](https://example.com/figure1.png)

Figure 1. Isolines of the stream function (left) and isotherms (right) at the Grashof number a, b, c – Gr = 9 703; d, e, f – 261 977, at the time points: a, d – t = 10; b, e – 60; c, f - 400.

At the initial moment, the rod and its surrounding environment are evenly heated to 1000°C. After an electric current is applied to the rod, the rod begins to warm up due to internal heat sources. During a short incubation period, due to conductive heat transfer, the gas layer near the vertical forming rod warms up. Then the heated gas begins to float to the heat-insulated upper end of the area. Having reached the end, the heated gas flow unfolds and flows onto the cold walls of the vessel, on which it cools and descends to the heat-insulated lower end of the area. In the bottom region, the gas already cooled on the walls of the housing unfolds and flows onto the base of the crystal. Figure 1 shows that under the impact of a cold convective gas flow flowing onto the base of the rod and rising along the generatrix of an ascending hot gas flow, the rod heats up inhomogeneously. In the conditions of real technology, this is an important point, since the speed of silicon deposition depends on the temperature distribution over the surface of the rod. That is, the rate of growth of the silicon crystal will not be the same in the height of the rod.

With the growth of the Grashof number, the inhomogeneity of the distribution of the temperature field inside the rod increases. Due to the presence of internal heat sources and radiation-convective heat removal from the surface of the rod, the core of the rod is heated to a higher temperature than the surface of the rod, where the control point is located. This point must also be considered in real technology since thermal stresses will increase with increasing temperature.

At high Rayleigh numbers, the boundary layer on the rod generatrix loses stability, secondary vortices begin to form and float up along the generatrix (Figure 2). The motion of the liquid in the secondary vortices is directed clockwise. In the head part of the floating vortex, the heated liquid unfolds towards the core of the annular layer, reaches it, having cooled down, returns as a cold stream...
in the aft part of the vortex. Thus, heat transfer locally increases on the surface of the rod and a heatwave can begin to run along the rod generator.

Figure 2. Isolines of the stream function (left) and isotherm (right) at the Grashof number \(Gr = 261,977\) at time points: a – \(t = 652\); b – 653; c – 654; d – 655; e – 656; f - 657.

Figure 3a shows the dependence of the temperature at the control point at different Grashof numbers. It is noticeable that the voltage selection algorithm works suboptimal, as a result, the temperature at the control point fluctuates in the range of ±10% of the set temperature. First of all, this is due to the pronounced nonlinear dependence of the temperature at the control point on the voltage of the electric current associated with the nonlinearity of the process of conjugated radiation-convective heat transfer.

Figure 3b shows the temperature-time dependences for the Grashof number \(Gr = 261,977\) at points at the level \(z = 4.5\) located in the depth of the rod, on the surface of the rod, and the boundary layer of the gas. It is clearly noticeable that the core heats up more strongly in the depth. Temperature
fluctuations in the boundary layer caused by the appearance of secondary vortices are noticeable. It can be seen that the oscillations in the boundary layer do not have a significant effect on the temperature at the rod surface.

Figure 4. The isolines of the stream function (left) and the isotherm (right) at the Grashof number $Gr = 261\, 977$ at the time points: $a – t = 260; b – 265; c – 270; d – 275$.

Figure 4 shows the isolines of the stream function and the isotherm at the height of the rod $H/R_s = 12$. Noticeably, with an increase in the height of the rod, a local feature appears, i.e. the zone of separation of the boundary layer. In such a zone, the local efficiency of heat transfer will increase.

4. Conclusion
The nonstationary conjugate radiation-convective heat transfer of a single silicon rod heated by an electric current with the surrounding gas medium is studied numerically in the axisymmetric formulation by the finite element method. The calculations were carried out at the Prandtl number $Pr = 0.68$, in the dimensionless formulation of the problem, the radius of the rod $R_s = 1$, the radius of the reactor vessel $R_v = 3$. The problems were solved at two heights of the region $H/R_s = 6$ and 12, the Grashof numbers, determined by the temperature difference and the radius of the rod, were $Gr = 9\, 703, 77\, 622,$ and $261\, 977$.

It is shown that after a short incubation period, a circulation flow is formed. The gas is heated on the generatrix of the 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 an electric current. Due to the presence of internal heat sources, the rod warms up inhomogeneously in the radial direction, the core of the rod warms up noticeably more than the surface of the rod, from which radiation-convective heat removal is carried out. As the Grashof number increases, the inhomogeneity of the longitudinal distribution of the temperature field increases. The boundary layer loses its stability, secondary vortices pop up. As a result, the temperature field in the boundary layer begins to oscillate. However, this does not have a noticeable effect on the temperature field on the surface of the silicon rod.

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