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On approach for homogeneity increasing of films grown from the gas phase with account natural convection and changes in the rate of chemical interaction between materials

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Article Info	ABSTRACT
	We analyzed growth of films by gas phase epitaxy. Based on the analysis we formulate conditions to increase of homogeneity of properties of obtained films. We also present an analytical approach for analysis processes framework gas phase epitaxy with account natural convection and the possibility of changing the rate of chemical interaction between reagents.

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1. INTRODUCTION

At present large number of electronics devices based on heterostructures. Heterostructures could be grown by using different well-known approaches [1-12]. At the same time at large number of experimental studies on growth of heterostructures [1-12] we find small quantity of theoretical works with prognosis of processes [12]. Main aim of this paper is to analysis changing of properties of epitaxial layers with a changing of the values of different parameters of the epitaxy process with account chemical interaction natural convection.

We consider a vertical reactor for gas phase epitaxy (see Figure 1). The reactor includes into itself (*i*) external casing; (*ii*) keeper of substrate with a substrate; (*iii*) spiral around the shell in the region. The spiral generats an induction heating to activate chemical reactions. The heating activate chemical reactions between materials during epitaxy. A mixture of reagents in gas phase enter to inlet of the reaction chamber in atmosphere of a gas-carrier. Our aim framework this paper is analysis of changing growth process with changing of physical parameters and parameters of technological process. An accompany aim of our paper is accounting of natural convection and chemical reaction. The third aim of our paper is development of analytical approach for prognosis of growth process to increase adequateness of the prognosis. It should be noted, that analytical approach for modeling are usually more demonstrative in comparison with numerical one and leads to decrease calculation time.
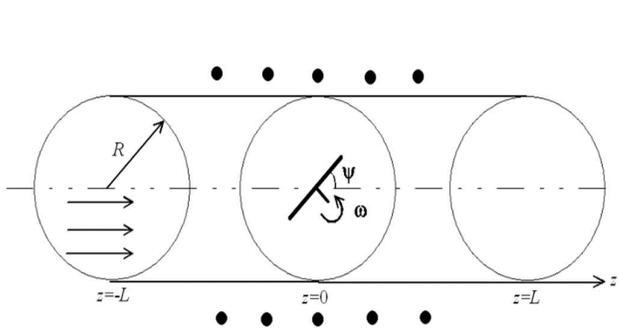
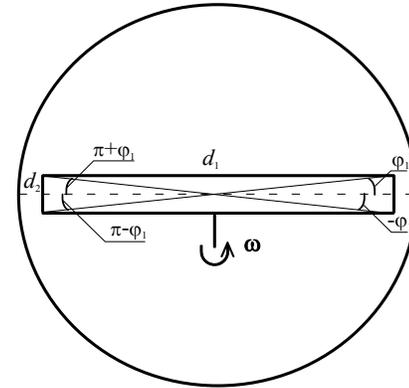Figure 1 (a). Structure of the considered reactor for epitaxy from gas phase with sloping keeper of substrate

Figure 1 (b). View of keeper of substrate from side with approximation of the keeper by sloping lines with angle of sloping φ_1

2. METHOD OF SOLUTION

We solve our aims by determination and analysis of spatio-temporal distribution of temperature and concentrations of reagents in the considered reactor. The spatio-temporal variation of temperature was obtained by induction heating due to electric current in spiral around keeper of substrate with a substrate to activate of chemical reactions gas-reagents before substrate during formation of required epitaxial layer on the substrate. We determined the considered temperature by solution of the following boundary value problem [13].

$$c \frac{\partial T(r,\phi,z,t)}{\partial t} = div\{\lambda \cdot grad[T(r,\phi,z,t)] - [\vec{v}(r,\phi,z,t) - \vec{\bar{v}}(r,\phi,z,t)] \cdot c(T) \cdot T(r,\phi,z,t) \cdot C_\Sigma(r,\phi,z,t)\} + p(r,\phi,z,t), \tag{1}$$

Here is the flow velocity of the gases-reagents; c is the heat capacity of the system; $T(r,,z,t)$ is the distribution of temperature in space and time; $p(r,,z,t)$ is the heat power density in the considered reactor; r, φ, z and t are the current cylindrical coordinates and time; $C_\Sigma(r,,z,t)$ is the distribution of the concentration of the mixture of reagents in space and time (we assume, that two reagents with concentrations of inlet in reactor with concentrations $C_1(r,,z,t)$ and $C_2(r,,z,t)$); $C_3(r,,z,t)$ is the material of the epitaxial layer in the gas phase; λ is the thermal conductivity coefficient, value of this coefficient has been determined by following relation: $\lambda = \vec{v}\bar{l}c_v\rho/3$, here $\bar{v} = \sqrt{2kT/m}$ describes modulus of the mean-square gas molecules velocity; $\bar{l}$ describes mean free path of gas molecules between collisions, c_v is the heat capacity of the gas at constant volume, ρ is the gas density.

To solve above equations we shall to take into account moving and quantity of reagents. In this situation we shall to solve equation of Navier-Stokes with the second equation of Fick. We assume that the radius of the substrate holder R larger, than diffusion and boundary layers thickness. We also assume that the flow of gas is laminar. In this case the above equations could be written in the form

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla)\vec{v} = -\nabla\left(\frac{P}{\rho}\right) + \nu\Delta\vec{v}, \tag{2}$$

$$\frac{\partial C_1(r,\phi,z,t)}{\partial t} = div\{D_1 \cdot grad[C_1(r,\phi,z,t)] - [\vec{v}(r,\phi,z,t) - \vec{\bar{v}}] \cdot C_1(r,\phi,z,t)\} - k_1(r,\phi,z,t) \cdot C_1(r,\phi,z,t), \tag{3a}$$

$$\frac{\partial C_2(r,\phi,z,t)}{\partial t} = div\{D_2 \cdot grad[C_2(r,\phi,z,t)] - [\vec{v}(r,\phi,z,t) - \vec{\bar{v}}] \cdot C_2(r,\phi,z,t)\} - k_2(r,\phi,z,t) \cdot C_2(r,\phi,z,t), \tag{3b}$$

$$\frac{\partial C_3(r,\phi,z,t)}{\partial t} = div\{D_3 \cdot grad[C_3(r,\phi,z,t)] - [\vec{v}(r,\phi,z,t) - \vec{\bar{v}}] \cdot C_3(r,\phi,z,t)\} + k_3(r,\phi,z,t) \cdot C_3(r,\phi,z,t), \tag{3c}$$

Here D_i are the coefficients of diffusion of reagents of the considered reagents. As an example of reagents, we consider trimethylgallium $(CH_3)_3Ga$ and arsenic hydride AsH_3. As result of reaction we consider $GaAs$. As gas-carrier we consider hydrogen. P describes pressure of gas in the reactor; ν describes kinematic viscosity of reagents. We assume, that all molecules will deposit on substance. Based on this assumption we used the following boundary and initial conditions. We also assume, that reactor is cylindrical and $d_2 \ll d_1$. In this situation we can write

$C_1\ (r,\varphi,-L,t) = C_2\ (r,\varphi,-L,t) = C_0,\ C_3\ (r,\varphi,-L,t) = 0;\ C_i\ (r,-\varphi_1,z,t) = C_i\ (r,\varphi_1,z,t) = C_i\ (r,\pi-\varphi_1,z,t) = C_i\ (r,\pi +\varphi_1,z,t);\ C_1\ (r,\varphi,z,0) = C_2\ (r,\varphi,z,0) = C_0\delta\ (z+L),\ C_3\ (r,\varphi,z,0) = 0;\ C_i\ (0,\varphi,z,t) \neq \infty;\ C_i(r,\phi,z,t)|_S = 0;\ T\ (r,-\varphi_1,z,t) = T\ (r,\varphi_1,z,t) = T\ (r,\pi-\varphi_1,z,t) = T\ (r,\ \pi+\varphi_1,z,t);\ T\ (r,\varphi,z,0) = T_r;$
$-\lambda \left.\frac{\partial T(r,\phi,z,t)}{\partial r}\right|_S = \sigma T^4(R,\phi,z,t);\quad \left.\frac{\partial T(r,\phi,z,t)}{\partial \phi}\right|_{\phi=0} = \left.\frac{\partial T(r,\phi,z,t)}{\partial \phi}\right|_{\phi=2\pi};\quad \left.\frac{\partial v_r(r,\phi,z,t)}{\partial r}\right|_{r=R} = 0;$
$\left.\frac{\partial C_i(r,\phi,z,t)}{\partial r}\right|_{r=R} = 0;\ -\lambda\left.\frac{\partial T(r,\phi,z,t)}{\partial z}\right|_S = \sigma T^4(r,\phi,-L,t);\ \left.\frac{\partial v_r(r,\phi,z,t)}{\partial r}\right|_{r=0} = 0;\ v_r\ (r,-\varphi_1,z,t) = v_r\ (r,\varphi_1,z,t)$
$= v_r\ (r,\pi-\varphi_1,z,t) = v_r\ (r,\pi+\varphi_1,z,t);\ T\ (0,\varphi,z,t) \neq \infty;\ v_\varphi\ (r,-\varphi_1,z,t) = v_\varphi\ (r,\varphi_1,\ z,t) = v_\varphi\ (r,\pi-\varphi_1,z,t) = v_\varphi$
$(r,\pi+\varphi_1,z,t);\ v_z\ (r,-\varphi_1,z,t) = v_z\ (r,\varphi_1,z,t) = v_z\ (r,\pi-\varphi_1,z,t) = v_z\ (r,\pi+\varphi_1,z,t);\ v_r\ (r,\varphi,-L,t) = 0;\ v_r(r,\varphi,L,t) =$
$0;\ v_r\ (0,\varphi,z,t) \neq \infty;\ v_z(r,\varphi,-L,t) = V_0;\ v_z(r\pm d_2/2,\varphi,z\in[-d_2/2,d_2/2],0) = \omega\ z\cdot cos\ (\psi)\cdot tg\ (\varphi_1);\ v_\varphi\ (r,\varphi,L,t) = 0;\ v_\varphi(0,\varphi,z,t) \neq \infty;\ v_z(r,\varphi,0,t) = 0;\ v_z(r,\varphi,L,t) = V_0,\ v_z(r,\varphi,L,t) = V_0,\ v_z(0,\varphi,z,t) \neq \infty;\ v_r(r,\varphi,z,0) = 0;$
$v_\varphi(r,\varphi,z,0) = 0;\ v_\varphi(r,\varphi,0,t) = \omega\ r,$ (4)

Here $\sigma = 5{,}6710^{-8}$ W$m^{-2}K^{-4}$, T_r describes room temperature, ω describes frequency of rotation of substrate. Using cylindrical system of coordinate leads to the following form of equations for projections of reagents velocity

$$\frac{\partial v_r}{\partial t} = \nu\left\{\frac{1}{r}\frac{\partial}{\partial r}\left[r\frac{\partial v_r(r,\phi,z,t)}{\partial r}\right] + \frac{1}{r^2}\frac{\partial^2 v_r(r,\phi,z,t)}{\partial \phi^2} + \frac{\partial^2 v_r(r,\phi,z,t)}{\partial z^2}\right\} - v_r\frac{\partial v_r}{\partial r} - \frac{v_\phi}{r}\frac{\partial v_\phi}{\partial \phi} - v_z\frac{\partial v_z}{\partial z} - \frac{\partial}{\partial r}\left(\frac{P}{\rho}\right) \quad (5a)$$

$$\frac{\partial v_r}{\partial t} = \nu\left\{\frac{1}{r}\frac{\partial}{\partial r}\left[r\frac{\partial v_\phi(r,\phi,z,t)}{\partial r}\right] + \frac{1}{r^2}\frac{\partial^2 v_\phi(r,\phi,z,t)}{\partial \phi^2} + \frac{\partial^2 v_\phi(r,\phi,z,t)}{\partial z^2}\right\} - v_r\frac{\partial v_r}{\partial r} - \frac{v_\phi}{r}\frac{\partial v_\phi}{\partial \phi} - v_z\frac{\partial v_z}{\partial z} - \frac{1}{r}\frac{\partial}{\partial \phi}\left(\frac{P}{\rho}\right) (5b)$$

$$\frac{\partial v_z}{\partial t} = \nu\left\{\frac{1}{r}\frac{\partial}{\partial r}\left[r\frac{\partial v_z(r,\phi,z,t)}{\partial r}\right] + \frac{1}{r^2}\frac{\partial^2 v_z(r,\phi,z,t)}{\partial \phi^2} + \frac{\partial^2 v_z(r,\phi,z,t)}{\partial z^2}\right\} - v_r\frac{\partial v_r}{\partial r} - \frac{v_\phi}{r}\frac{\partial v_\phi}{\partial \phi} - v_z\frac{\partial v_z}{\partial z} - \frac{\partial}{\partial z}\left(\frac{P}{\rho}\right). \quad (5c)$$

Now we will calculate solution of (5) by method of averaging functional corrections [14-19]. Equations for first-order approximations v_{r1}, $v_{1\varphi}$, v_{z1} of the considered components takes the form

$$\frac{\partial v_{1r}}{\partial t} = -\frac{\partial}{\partial r}\left(\frac{P}{\rho}\right), \frac{\partial v_{1\phi}}{\partial t} = -\frac{1}{r}\frac{\partial}{\partial \phi}\left(\frac{P}{\rho}\right), \frac{\partial v_{1z}}{\partial t} = -\frac{\partial}{\partial z}\left(\frac{P}{\rho}\right). \tag{6}$$

Now we integrate both sides of the above equations. The result of integration could be written as

$$v_{1r} = -\frac{\partial}{\partial r}\int_0^t \frac{P}{\rho}d\tau, v_{1\phi} = -\frac{1}{r}\frac{\partial}{\partial \phi}\int_0^t \frac{P}{\rho}d\tau, v_{1z} = -\frac{\partial}{\partial z}\int_0^t \frac{P}{\rho}d\tau. \tag{7}$$

Equations of the second-order approximations of the velocity projections v_{r1}, $v_{1\varphi}$, v_{z1} could be written in the form by using standard procedure of method of averaging functional corrections

$$\frac{\partial v_{2r}}{\partial t} = \nu\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_{1r}}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 v_{1r}}{\partial \phi^2} + \frac{\partial^2 v_{1r}}{\partial z^2}\right] - \frac{\partial}{\partial r}\left(\frac{P}{\rho}\right) - (\alpha_{2r} + v_{1r})\frac{\partial v_{1r}}{\partial r} - \frac{(\alpha_{2\phi}+v_{1\phi})}{r}\frac{\partial v_{1r}}{\partial \phi} - (\alpha_{2z} + v_{1z})\frac{\partial v_{1r}}{\partial z}, \tag{8a}$$

$$\frac{\partial v_{2\phi}}{\partial t} = \nu\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_{1\phi}}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 v_{1\phi}}{\partial \phi^2} + \frac{\partial^2 v_{1\phi}}{\partial z^2}\right] - \frac{1}{r}\frac{\partial}{\partial \phi}\left(\frac{P}{\rho}\right) - (\alpha_{2r} + v_{1r})\frac{\partial v_{1\phi}}{\partial r} - \frac{(\alpha_{2\phi}+v_{1\phi})}{r}\frac{\partial v_{1\phi}}{\partial \phi} - (\alpha_{2z} + v_{1z})\frac{\partial v_{1\phi}}{\partial z}, \tag{8b}$$

$$\frac{\partial v_{2z}}{\partial t} = \nu\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_{1z}}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 v_{1z}}{\partial \phi^2} + \frac{\partial^2 v_{1z}}{\partial z^2}\right] - \frac{\partial}{\partial z}\left(\frac{P}{\rho}\right) - (\alpha_{2r} + v_{1r})\frac{\partial v_{1z}}{\partial r} - \frac{(\alpha_{2\phi}+v_{1\phi})}{r}\frac{\partial v_{1z}}{\partial \phi} - (\alpha_{2z} + v_{1z})\frac{\partial v_{1z}}{\partial z}. \tag{8c}$$

Integration of the above equations on time t leads to the following result

$$v_{2r} = \nu \int_0^t \left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_{1r}}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 v_{1r}}{\partial \phi^2} + \frac{\partial^2 v_{1r}}{\partial z^2}\right] d\tau - \frac{\partial}{\partial r}\left(\int_0^t \frac{P}{\rho} d\tau\right) - \int_0^t (\alpha_{2r} + v_{1r})\frac{\partial v_{1r}}{\partial r} d\tau -$$
$$\int_0^t \frac{(\alpha_{2\phi} + v_{1\phi})}{r}\frac{\partial v_{1r}}{\partial \phi} d\tau - \int_0^t (\alpha_{2z} + v_{1z})\frac{\partial v_{1r}}{\partial z} d\tau, \tag{8d}$$

$$v_{2\phi} = \nu \int_0^t \left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_{1\phi}}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 v_{1\phi}}{\partial \phi^2} + \frac{\partial^2 v_{1\phi}}{\partial z^2}\right] d\tau - \frac{1}{r}\frac{\partial}{\partial \phi}\left(\int_0^t \frac{P}{\rho} d\tau\right) - \int_0^t (\alpha_{2r} + v_{1r})\frac{\partial v_{1\phi}}{\partial r} d\tau -$$
$$\int_0^t \frac{(\alpha_{2\phi} + v_{1\phi})}{r}\frac{\partial v_{1\phi}}{\partial \phi} d\tau - \int_0^t (\alpha_{2z} + v_{1z})\frac{\partial v_{1\phi}}{\partial z} d\tau, \tag{8e}$$

$$v_{2z} = V_0 + \nu \int_0^t \left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_{1z}}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 v_{1z}}{\partial \phi^2} + \frac{\partial^2 v_{1z}}{\partial z^2}\right] d\tau - \frac{\partial}{\partial z}\left(\int_0^t \frac{P}{\rho} d\tau\right) - \int_0^t (\alpha_{2r} + v_{1r})\frac{\partial v_{1z}}{\partial r} d\tau -$$
$$\int_0^t \frac{(\alpha_{2\phi} + v_{1\phi})}{r}\frac{\partial v_{1z}}{\partial \phi} d\tau - \int_0^t (\alpha_{2z} + v_{1z})\frac{\partial v_{1z}}{\partial z} d\tau. \tag{8f}$$

Average values α_{2r}, $\alpha_{2\varphi}$, α_{2z} have been calculated by the following standard relations

$$\alpha_{2r} = \frac{1}{\pi \theta R^2 L}\int_0^\theta \int_0^R r \int_0^{2\pi}\int_{-L}^L (v_{2r} - v_{1r}) dz d\phi dr dt, \qquad \alpha_{2\phi} = \frac{1}{\pi \theta R^2 L}\int_0^\theta \int_0^R r \int_0^{2\pi}\int_{-L}^L (v_{2\phi} -$$
$$v_{1\phi}) dz d\phi dr dt, \; \alpha_{2z} = \frac{1}{\pi \theta R^2 L}\int_0^\theta \int_0^R r \int_0^{2\pi}\int_{-L}^L (v_{2z} - v_{1z}) dz d\phi dr dt, \tag{9}$$

Here Θ is the continuance of technological process. Using of the first- and the second-order approximations of the velocity projections in the above relation leads to necessity of solution of the algebraic system of equations, which is presented bellow

$$\begin{cases} A_1\alpha_{2r} + B_1\alpha_{2\phi} + C_1\alpha_{2z} = D_1 \\ A_2\alpha_{2r} + B_2\alpha_{2\phi} + C_2\alpha_{2z} = D_2 \\ A_3\alpha_{2r} + B_3\alpha_{2\phi} + C_3\alpha_{2z} = D_3 \end{cases} \tag{10}$$

where,

$$A_1 = 1 + \int_0^\theta (\Theta - t)\int_0^R r \int_0^{2\pi}\int_{-L}^L \frac{\partial v_{1r}}{\partial r} dz d\phi dr dt, \; B_1 = \int_0^\theta (\Theta - t)\int_0^R r \int_0^{2\pi}\int_{-L}^L \frac{\partial v_{1r}}{\partial \phi} dz d\phi dr dt, \; C_1 =$$
$$C_2 = \frac{\pi}{2}\Theta^2 R^2 V_0, D_1 = \nu \times \int_0^\theta (\Theta - t)\int_0^R r \int_0^{2\pi}\int_{-L}^L \left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_{1r}}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 v_{1r}}{\partial \phi^2} + \frac{\partial^2 v_{1r}}{\partial z^2}\right] dz d\phi dr dt -$$
$$\int_0^\theta (\Theta - t)\int_0^R r \int_0^{2\pi}\int_{-L}^L v_{1r}\frac{\partial v_{1r}}{\partial r} dz d\phi dr dt - \frac{\pi}{8}\Theta^2 R^2 V_0^2 - \int_0^\theta (\Theta - t)\int_0^R r \int_0^{2\pi}\int_{-L}^L v_{1\phi}\frac{\partial v_{1r}}{\partial \phi} dz d\phi dr dt,$$
$$A_2 = \int_0^\theta (\Theta - t)\int_0^R r \int_0^{2\pi}\int_{-L}^L \frac{\partial v_{1r}}{\partial r} dz d\phi dr dt, \; B_2 = 1 + \int_0^\theta (\Theta - t)\int_0^R r \int_0^{2\pi}\int_{-L}^L \frac{\partial v_{1r}}{\partial \phi} dz d\phi dr dt,$$
$$D_2 = \nu \int_0^\theta (\Theta - t)\int_0^R r \int_0^{2\pi}\int_{-L}^L \left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_{1\phi}}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 v_{1\phi}}{\partial \phi^2} + \frac{\partial^2 v_{1\phi}}{\partial z^2}\right] dz d\phi dr dt - \int_0^\theta (\Theta -$$
$$t)\int_0^R r \int_0^{2\pi}\int_{-L}^L v_{1r}\frac{\partial v_{1r}}{\partial r} dz d\phi dr dt - \frac{\pi}{8}\Theta^2 R^2 V_0^2 - \int_0^\theta (\Theta - t)\int_0^R \int_0^{2\pi}\int_{-L}^L v_{1\phi}\frac{\partial v_{1r}}{\partial \phi} dz d\phi dr dt,$$
$$C_3 = 1 + \frac{\pi}{2}\Theta^2 R^2 V_0, \; A_3 = \int_0^\theta (\Theta - t)\int_0^R r \int_0^{2\pi}\int_{-L}^L \frac{\partial v_{1z}}{\partial r} dz d\phi dr dt,$$
$$B_3 = \int_0^\theta (\Theta - t)\int_0^R r \times \int_0^{2\pi}\int_{-L}^L \frac{\partial v_{1z}}{\partial \phi} dz d\phi dr dt,$$
$$D_3 = \nu \int_0^\theta (\Theta - t)\int_0^R r \int_0^{2\pi}\int_{-L}^L \left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_{1z}}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 v_{1z}}{\partial \phi^2} + \frac{\partial^2 v_{1z}}{\partial z^2}\right] dz d\phi dr dt - \frac{\pi}{8}\Theta^2 R^2 V_0^2 -$$
$$\int_0^\theta (\Theta - t)\int_0^R r \int_0^{2\pi}\int_{-L}^L v_{1r}\frac{\partial v_{1z}}{\partial r} dz d\phi dr dt - \int_0^\theta (\Theta - t)\int_0^R r \int_0^{2\pi}\int_{-L}^L v_{1\phi}\frac{\partial v_{1z}}{\partial \phi} dz d\phi dr dt.$$

Solution of the above equations could be obtained by standard approaches [20] and written in the form

$$\alpha_{2r} = \Delta_r/\Delta, \; \alpha_{2\phi} = \Delta_\phi/\Delta, \; \alpha_{2z} = \Delta_z/\Delta, \tag{11}$$

where

$$\Delta = A_1(B_2 C_3 - B_3 C_2) - B_1(A_2 C_3 - A_3 C_2) + C_1(A_2 B_3 - A_3 B_2),$$
$$\Delta_r = D_1(B_2 C_3 - B_3 C_2) - B_1(D_2 C_3 - D_3 C_2) + C_1(D_2 B_3 - D_3 B_2),$$
$$\Delta_\phi = D_1(B_2 C_3 - B_3 C_2) - B_1(D_2 C_3 - D_3 C_2) + C_1(D_2 B_3 - D_3 B_2),$$
$$\Delta_z = A_1(B_2 D_3 - B_3 D_2) - B_1(A_2 D_3 - A_3 D_2) + D_1(A_2 B_3 - A_3 B_2).$$

In this section, we calculate the required projections of the considered velocity by the method of method of averaging functional corrections. Usually, the such approximation is enough to obtain main results of analysis [15-19].

Now we will analyze distributions of temperature and concentrations of components of gas-reagents in space and time. In this section we will consider (1) and (3) by using cylindrical system coordinate

$$c\frac{\partial T(r,\phi,z,t)}{\partial t} = \lambda\frac{\partial^2 T(r,\phi,z,t)}{\partial r^2} + \lambda\frac{1}{r^2}\frac{\partial^2 T(r,\phi,z,t)}{\partial\phi^2} + \lambda\frac{\partial^2 T(r,\phi,z,t)}{\partial z^2} + p(r,\phi,z,t) - c\cdot\frac{\partial}{\partial r}\{[v_r(r,\phi,z,t) - \bar{v}_r(r,\phi,z,t)]\cdot C_\Sigma(r,\phi,z,t)\cdot T(r,\phi,z,t)\} - \frac{c}{r}\frac{\partial}{\partial\phi}\{[v_\phi(r,\phi,z,t) - \bar{v}_\phi(r,\phi,z,t)]\cdot C_\Sigma(r,\phi,z,t)\cdot T(r,\phi,z,t)\} - c\cdot\frac{\partial}{\partial z}\{[v_z(r,\phi,z,t) - \bar{v}_z(r,\phi,z,t)]\cdot C_\Sigma(r,\phi,z,t)\cdot T(r,\phi,z,t)\}, \qquad (12)$$

$$\frac{\partial C_1(r,\phi,z,t)}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[rD_1\frac{\partial C_1(r,\phi,z,t)}{\partial r}\right] + \frac{1}{r^2}\frac{\partial}{\partial\phi}\left[D_1\frac{\partial C_1(r,\phi,z,t)}{\partial\phi}\right] - \frac{1}{r}\frac{\partial}{\partial r}\{rC_1(r,\phi,z,t)\cdot[v_r(r,\phi,z,t) - \bar{v}_r(r,\phi,z,t)]\} - +\frac{\partial}{\partial z}\left[D_1\frac{\partial C_1(r,\phi,z,t)}{\partial z}\right] - \frac{1}{r}\frac{\partial}{\partial\phi}\{rC_1(r,\phi,z,t)\cdot[v_\phi(r,\phi,z,t) - \bar{v}_\phi(r,\phi,z,t)]\} - k_1(r,\phi,z,t)\cdot C_1(r,\phi,z,t) - \frac{\partial}{\partial z}\{C_1(r,\phi,z,t)\cdot[v_z(r,\phi,z,t) - \bar{v}_z(r,\phi,z,t)]\}, \qquad (13a)$$

$$\frac{\partial C_2(r,\phi,z,t)}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[rD_2\frac{\partial C_2(r,\phi,z,t)}{\partial r}\right] + \frac{1}{r^2}\frac{\partial}{\partial\phi}\left[D_2\frac{\partial C_2(r,\phi,z,t)}{\partial\phi}\right] - \frac{1}{r}\frac{\partial}{\partial r}\{rC_2(r,\phi,z,t)\cdot[v_r(r,\phi,z,t) - \bar{v}_r(r,\phi,z,t)]\} + \frac{\partial}{\partial z}\left[D_2\frac{\partial C_2(r,\phi,z,t)}{\partial z}\right] - \frac{1}{r}\frac{\partial}{\partial\phi}\{rC_2(r,\phi,z,t)\cdot[v_\phi(r,\phi,z,t) - \bar{v}_\phi(r,\phi,z,t)]\} - k_2(r,\phi,z,t)\cdot C_2(r,\phi,z,t) - \frac{\partial}{\partial z}\{C_2(r,\phi,z,t)\cdot[v_z(r,\phi,z,t) - \bar{v}_z(r,\phi,z,t)]\}, \qquad (13b)$$

$$\frac{\partial C_3(r,\phi,z,t)}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[rD_3\frac{\partial C_3(r,\phi,z,t)}{\partial r}\right] + \frac{1}{r^2}\frac{\partial}{\partial\phi}\left[D_3\frac{\partial C_3(r,\phi,z,t)}{\partial\phi}\right] - \frac{1}{r}\frac{\partial}{\partial r}\{rC_3(r,\phi,z,t)\cdot[v_r(r,\phi,z,t) - \bar{v}_r(r,\phi,z,t)]\} + \frac{\partial}{\partial z}\left[D_3\frac{\partial C_3(r,\phi,z,t)}{\partial z}\right] - \frac{1}{r}\frac{\partial}{\partial\phi}\{rC_3(r,\phi,z,t)\cdot[v_\phi(r,\phi,z,t) - \bar{v}_\phi(r,\phi,z,t)]\} - k_3(r,\phi,z,t)\cdot C_3(r,\phi,z,t) - \frac{\partial}{\partial z}\{C_3(r,\phi,z,t)\cdot[v_z(r,\phi,z,t) - \bar{v}_z(r,\phi,z,t)]\}. \qquad (13c)$$

To calculate distributions of temperature and concentration of reagents in space and time, we use the same method of averaging functional corrections as for solution of (2). We used the same algorithm of method of averaging functional corrections to solve (12) and (13). The result of calculation of the first- order approximations $T_1(r,,z,t)$ and $C_{i1}(r,,z,t)$ of considered distributions could be written as

$$T_1(r,\phi,z,t) = T_r + \int_0^t \frac{p(r,\phi,z,\tau)}{c}d\tau - \alpha_{1T}\alpha_{1C}\int_0^t \frac{\partial[v_r(r,\phi,z,\tau) - \bar{v}_r(r,\phi,z,\tau)]}{\partial r}d\tau - \frac{\alpha_{1T}\alpha_{1C}}{r}\int_0^t \frac{\partial[v_\phi(r,\phi,z,\tau) - \bar{v}_\phi(r,\phi,z,\tau)]}{\partial\phi}d\tau - \alpha_{1T}\alpha_{1C}\int_0^t \frac{\partial[v_z(r,\phi,z,\tau) - \bar{v}_z(r,\phi,z,\tau)]}{\partial z}d\tau, \qquad (14)$$

$$C_{11}(r,\phi,z,t) = -\frac{\alpha_{11C}}{r}\int_0^t \frac{\partial\{r[v_r(r,\phi,z,\tau) - \bar{v}_r(r,\phi,z,\tau)]\}}{\partial r}d\tau - \alpha_{11}\int_0^t k_1(r,\phi,z,\tau)d\tau + C_0 - \frac{\alpha_{11C}}{r}\int_0^t \frac{\partial[v_\phi(r,\phi,z,\tau) - \bar{v}_\phi(r,\phi,z,\tau)]}{\partial\phi}d\tau - \alpha_{11C}\int_0^t \frac{\partial[v_z(r,\phi,z,\tau) - \bar{v}_z(r,\phi,z,\tau)]}{\partial z}d\tau, \qquad (15a)$$

$$C_{21}(r,\phi,z,t) = -\frac{\alpha_{21C}}{r}\int_0^t \frac{\partial\{r[v_r(r,\phi,z,\tau) - \bar{v}_r(r,\phi,z,\tau)]\}}{\partial r}d\tau + C_0 - \alpha_{21C}\int_0^t k_2(r,\phi,z,\tau)d\tau - \frac{\alpha_{21C}}{r}\int_0^t \frac{\partial[v_\phi(r,\phi,z,\tau) - \bar{v}_\phi(r,\phi,z,\tau)]}{\partial\phi}d\tau - \alpha_{21C}\int_0^t \frac{\partial[v_z(r,\phi,z,\tau) - \bar{v}_z(r,\phi,z,\tau)]}{\partial z}d\tau, \qquad (15b)$$

$$C_{31}(r,\phi,z,t) = -\frac{\alpha_{31C}}{r}\int_0^t \frac{\partial\{r[v_r(r,\phi,z,\tau) - \bar{v}_r(r,\phi,z,\tau)]\}}{\partial r}d\tau + \alpha_{31C}\int_0^t k_3(r,\phi,z,\tau)d\tau - \frac{\alpha_{31C}}{r}\int_0^t \frac{\partial[v_\phi(r,\phi,z,\tau) - \bar{v}_\phi(r,\phi,z,\tau)]}{\partial\phi}d\tau - \alpha_{31}\int_0^t \frac{\partial[v_z(r,\phi,z,\tau) - \bar{v}_z(r,\phi,z,\tau)]}{\partial z}d\tau. \qquad (15c)$$

where α_{1T} and α_{i1C} are the average values of the considered approximations. Now let us calculate these average values by using the following relations

$$\alpha_{1T} = \frac{1}{\pi\Theta^2 L}\int_0^\Theta \int_0^R r\int_0^{2\pi}\int_{-L}^L T_1(r,\phi,z,\tau)dzd\phi drdt,$$
$$\alpha_{i1C} = \frac{1}{\pi\Theta^2 L}\int_0^\Theta \int_0^R r\int_0^{2\pi}\int_{-L}^L C_{i1}(r,\phi,z,\tau)dzd\phi drdt \qquad (16)$$

We calculate average values α_{1T} and α_{i1C} by using the following standard relations

$$\alpha_{iC} = C_0/L \cdot \left\{1 + \frac{1}{\pi\Theta RL}\int_0^\Theta (\Theta - t)\int_0^{2\pi}\int_{-L}^{L}[v_r(R,\phi,z,t) - \bar{v}_r(R,\phi,z,t)]dzd\phi dt + \frac{\Theta V_0}{RL}\right\},$$

$$\alpha_{1T} = \left[T_r + \frac{1}{\pi\Theta R^2 L}\int_0^\Theta (\Theta - t)\int_0^R r\int_0^{2\pi}\int_{-L}^{L}\frac{p(r,\phi,z,t)}{c}dzd\phi drdt\right]\left(1 + \frac{C_0}{\pi\Theta}\left\{\int_0^\Theta (\Theta - t)\int_0^{2\pi}\int_{-L}^{L}[v_r(R,\phi,z,\tau) - \bar{v}_r(R,\phi,z,t)]dzd\phi dt + \frac{V_0}{2} - \frac{1}{\pi\Theta R^2}\int_0^\Theta (\Theta - t)\int_0^R\int_0^{2\pi}\int_{-L}^{L}[v_r(r,\phi,z,t) - \bar{v}_r(r,\phi,z,t)]dzd\phi drdt\right\}\frac{1}{RL^2}\times (\Theta - t)dt \frac{1}{\pi\Theta RL} + \frac{\Theta V_0}{RL} + 1\right\}^{-1}\right).$$

We calculate approximations of temperature and concentrations of gases with the second-order by method of averaging of function corrections [14-19]. The result of calculation could be written as

$$c \cdot T_2(r,\phi,z,t) = \lambda\int_0^t \frac{\partial^2 T_1(r,\phi,z,\tau)}{\partial r^2}d\tau - c\cdot\frac{\partial}{\partial r}\int_0^t\{[v_r(r,\phi,z,\tau) - \bar{v}_r(r,\phi,z,\tau)]\cdot[\alpha_{2C} + C_{\Sigma1}(r,\phi,z,\tau)]\cdot[\alpha_{2T} + T_1(r,\phi,z,\tau)]\}d\tau + \lambda\frac{1}{r^2}\int_0^t\frac{\partial^2 T_1(r,\phi,z,\tau)}{\partial\phi^2}d\tau - \frac{c}{r}\frac{\partial}{\partial\phi}\int_0^t\{[\alpha_{2C} + C_{\Sigma1}(r,\phi,z,\tau)]\cdot[v_\phi(r,\phi,z,\tau) - \bar{v}_\phi(r,\phi,z,\tau)]\cdot[\alpha_{2T} + T_1(r,\phi,z,\tau)]\}d\tau + T_r +$$
(16)

$$+\lambda\int_0^t\frac{\partial^2 T_1(r,\phi,z,\tau)}{\partial z^2}d\tau - c\cdot\frac{\partial}{\partial z}\int_0^t\{[v_z(r,\phi,z,\tau) - \bar{v}_z(r,\phi,z,\tau)]\cdot[\alpha_{2C} + C_{\Sigma1}(r,\phi,z,\tau)]\cdot[\alpha_{2T} + T_1(r,\phi,z,\tau)]\}d\tau + \int_0^t p(r,\phi,z,\tau)d\tau, C_{21}(r,\phi,z,t) = \frac{1}{r}\frac{\partial}{\partial r}\int_0^t rD\frac{\partial C_{11}(r,\phi,z,\tau)}{\partial r}d\tau + \frac{1}{r^2}\frac{\partial}{\partial\phi}\int_0^t D\frac{\partial C_{11}(r,\phi,z,\tau)}{\partial\phi}d\tau + \frac{\partial}{\partial z}\int_0^t D\frac{\partial C_{11}(r,\phi,z,\tau)}{\partial z}d\tau + C_0\delta(z+L) - -\alpha_{12C}\int_0^t k_1(r,\phi,z,\tau)[\alpha_{12C} + C_{11}(r,\phi,z,\tau)]d\tau - \frac{1}{r}\frac{\partial}{\partial r}\left\{r\int_0^t[\alpha_{12C} + C_{11}(r,\phi,z,\tau)]\cdot[v_r(r,\phi,z,\tau) - \bar{v}_r(r,\phi,z,\tau)]d\tau\right\} -$$
(17a)

$$-\frac{1}{r}\frac{\partial}{\partial\phi}\int_0^t[\alpha_{12C} + C_{11}(r,\phi,z,\tau)]\cdot[v_\phi(r,\phi,z,\tau) - \bar{v}_\phi(r,\phi,z,\tau)]d\tau - \frac{\partial}{\partial z}\int_0^t[\alpha_{12C} + C_{11}(r,\phi,z,\tau)]\cdot[v_z(r,\phi,z,\tau) - \bar{v}_z(r,\phi,z,\tau)]d\tau, C_{22}(r,\phi,z,t) = \frac{1}{r}\frac{\partial}{\partial r}\int_0^t rD\frac{\partial C_{11}(r,\phi,z,\tau)}{\partial r}d\tau + \frac{1}{r^2}\frac{\partial}{\partial\phi}\int_0^t D\frac{\partial C_{11}(r,\phi,z,\tau)}{\partial\phi}d\tau + \frac{\partial}{\partial z}\int_0^t D\frac{\partial C_{11}(r,\phi,z,\tau)}{\partial z}d\tau + C_0\delta(z+L) - \alpha_{22C}\int_0^t k_1(r,\phi,z,\tau)[\alpha_{22C} + C_{21}(r,\phi,z,\tau)]d\tau - \frac{1}{r}\frac{\partial}{\partial r}\left\{r\int_0^t[\alpha_{22C} + C_{21}(r,\phi,z,\tau)]\cdot[v_r(r,\phi,z,\tau) - \bar{v}_r(r,\phi,z,\tau)]d\tau\right\} -$$
(17b)

$$-\frac{1}{r}\frac{\partial}{\partial\phi}\int_0^t[\alpha_{22C} + C_{21}(r,\phi,z,\tau)]\cdot[v_\phi(r,\phi,z,\tau) - \bar{v}_\phi(r,\phi,z,\tau)]d\tau - \frac{\partial}{\partial z}\int_0^t[\alpha_{22C} + C_{21}(r,\phi,z,\tau)]\cdot[v_z(r,\phi,z,\tau) - \bar{v}_z(r,\phi,z,\tau)]d\tau, C_{32}(r,\phi,z,t) = \frac{1}{r}\frac{\partial}{\partial r}\int_0^t rD\frac{\partial C_{31}(r,\phi,z,\tau)}{\partial r}d\tau + \frac{1}{r^2}\frac{\partial}{\partial\phi}\int_0^t D\frac{\partial C_{31}(r,\phi,z,\tau)}{\partial\phi}d\tau + \frac{\partial}{\partial z}\int_0^t D\frac{\partial C_{31}(r,\phi,z,\tau)}{\partial z}d\tau + \alpha_{32C}\int_0^t k_3(r,\phi,z,\tau)[\alpha_{32C} + C_{31}(r,\phi,z,\tau)]d\tau - \frac{1}{r}\frac{\partial}{\partial r}\left\{r\int_0^t[\alpha_{32C} + C_{31}(r,\phi,z,\tau)]\cdot[v_r(r,\phi,z,\tau) - \bar{v}_r(r,\phi,z,\tau)]d\tau\right\} - \frac{1}{r}\frac{\partial}{\partial\phi}\int_0^t[\alpha_{32C} + C_{31}(r,\phi,z,\tau)]\cdot[v_\phi(r,\phi,z,\tau) - \bar{v}_\phi(r,\phi,z,\tau)]d\tau - \frac{\partial}{\partial z}\int_0^t[\alpha_{32C} + C_{31}(r,\phi,z,\tau)]\cdot[v_z(r,\phi,z,\tau) - \bar{v}_z(r,\phi,z,\tau)]d\tau.$$
(17c)

Average values of the above approximations were determined by standard relations

$$\alpha_{2T} = \frac{1}{\pi\Theta R^2 L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^{L}(T_2 - T_1)dzd\phi drdt,$$

$$\alpha_{2C} = \frac{1}{\pi\Theta R^2 L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^{L}(C_2 - C_1)dzd\phi drdt.$$
(18)

We calculate average values α_{2T} and α_{i2C} by using the following standard relations

$$\alpha_{2T} = \left(\frac{\lambda\sigma}{c\pi\Theta RL}\int_0^\Theta (\Theta - t)\int_0^{2\pi}\int_{-L}^{L}T^4(R,\phi,z,t)dzd\phi dt - \frac{\lambda}{c\pi\Theta R^2 L}\int_0^\Theta (\Theta - t)\int_0^{2\pi}\int_{-L}^{L}T_1(R,\phi,z,t)dzd\phi dt + \frac{\lambda}{c\pi\Theta R^2 L}\times\int_0^\Theta (\Theta - t)\int_0^{2\pi}\int_{-L}^{L}T_1(0,\phi,z,t)dzd\phi dt - \frac{1}{\pi\Theta RL}\int_0^\Theta (\Theta - t)\int_0^{2\pi}\int_{-L}^{L}\{T_1(R,\phi,z,t)[\alpha_{2C} + C_{\Sigma1}(R,\phi,z,t)] - \alpha_{1T}\alpha_{1C}\}\times[v_r(R,\phi,z,t) - \bar{v}_r(R,\phi,z,t)]dzd\phi dt - \int_0^\Theta (\Theta - t)\int_0^R\int_0^{2\pi}\int_{-L}^{L}\{[\alpha_{2C} + C_{\Sigma1}(r,\phi,z,t)] - \alpha_{1T}\alpha_{1C}\}\cdot[v_r(r,\phi,z,t) - \bar{v}_r(r,\phi,z,t)]\times T_1(r,\phi,z,t)dzd\phi drdt\frac{1}{\pi\Theta R^2 L} - \frac{V_0}{\pi\Theta R^2 L}\int_0^\Theta (\Theta - t)\int_0^R r\int_0^{2\pi}[T_1(r,\phi,L,t)(\alpha_{2C} + C_0) - \alpha_{1T}\alpha_{1C}]d\phi drdt\left\{\int_0^\Theta (\Theta - t)\times\int_0^{2\pi}\int_{-L}^{L}[v_r(R,\phi,z,t) - \bar{v}_r(R,\phi,z,t)]\sum_i[\alpha_{i2C} +\right.$$

$C_{i1}(R,\phi,z,t)]\,dzd\phi dt\,\frac{1}{\pi\theta RL}+1-\int_0^\theta\int_0^R r\int_0^{2\pi}\int_{-L}^L[v_r(r,\phi,z,t)-\bar{v}_r(r,\phi,z,t)]\cdot\sum_i[\alpha_{i2C}+$

$C_{i1}(R,\phi,z,t)]\,dzd\phi dr(\Theta-t)dt\,\frac{1}{\pi\theta R^2 L}+2\Theta(\sum_i\alpha_{2iC}+C_0)\frac{V_0}{L}\}^{-1},\,\alpha_{2iC}=\frac{1}{\pi\theta R^2 L}\int_0^\theta(\Theta-$

$t)\int_0^R r\int_0^{2\pi}[C_{2i}(r,\phi,z,\tau)-C_{1i}(r,\phi,z,\tau)]d\phi dr dt.$

3. RESULTS AND DISCUSSION

Now we analyzed redistribution of reagents and temperature in the considered reactor during growth of films to formulate conditions for improvement of properties of films. Figure 2 illustrates dependence of concentrations of reagents on substrate's rotation frequency. Curve 1 shows such dependence at atmospheric pressure without accounting natural convection. Curve 2 shows such dependence of concentrations of reagents on substrate's rotation frequency at decreased in 10 times pressure. Curve 3 describes the dependence of the concentration of reagents on substrate's rotation frequency at atmospheric pressure with account natural convection. The figure shows, that increasing of rotation frequency leads to increasing of homogeneity of epitaxial layer. Figure 3 illustrates dependence of concentration of reagents on diffusion coefficient D in gas-carrier. Curve 1 shows dependence of the concentration of reagents at atmospheric pressure without accounting natural convection. Curve 2 shows dependence of the concentration of reagents at decreased in 10 times pressure without accounting natural convection. Curve 3 shows dependence of the concentration of reagents at atmospheric pressure with accounting natural convection. This figure describes monotonous decreasing of considered concentration. Figure 4 illustrates dependence of concentration of kinematic viscosity of gas-carrier without accounting natural convection. Curves, analogous corves 2 and 3 on previous figures, have small differences with the presented curve. Figure 5 illustrates dependence of concentration of reagents on velocity of mixture of reagents and gas-carrier at the entrance to the reaction zone V_0. Curve 1 shows dependence of the concentration of reagents at atmospheric pressure without accounting natural convection. Curve 2 shows dependence of the concentration of reagents at decreased in 10 times pressure without accounting natural convection. Curve 3 shows dependence of the concentration of reagents at atmospheric pressure with accounting natural convection. This figure describes monotonous decreasing of considered concentration.
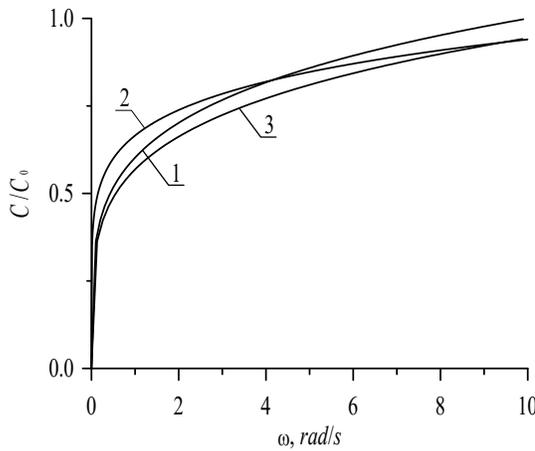
Figure 2. The dependence of the concentration of the mixture of gases on the frequency of rotation of the substrate
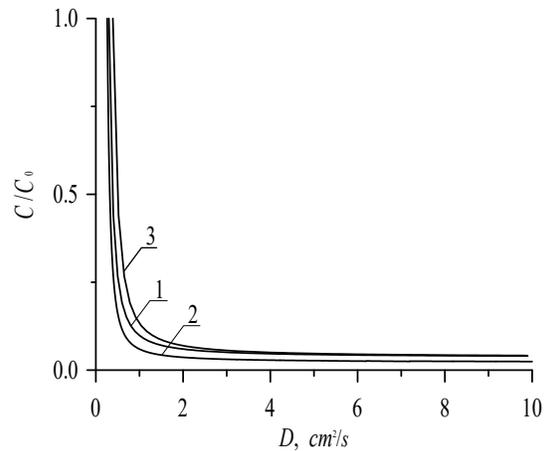
Figure 3. The dependence of the concentration of the mixture of gases from its diffusion coefficient
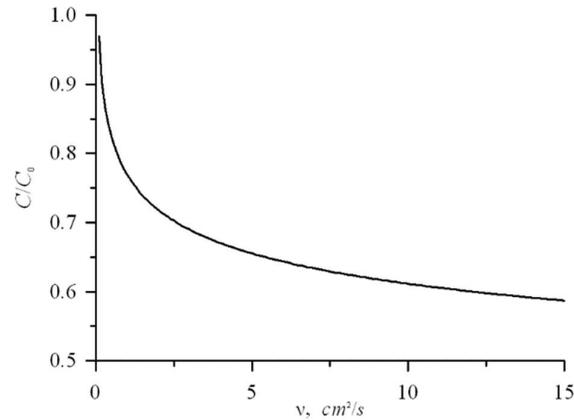
Figure 4. The dependence of the concentration of the mixture of gases from the kinematic viscosity
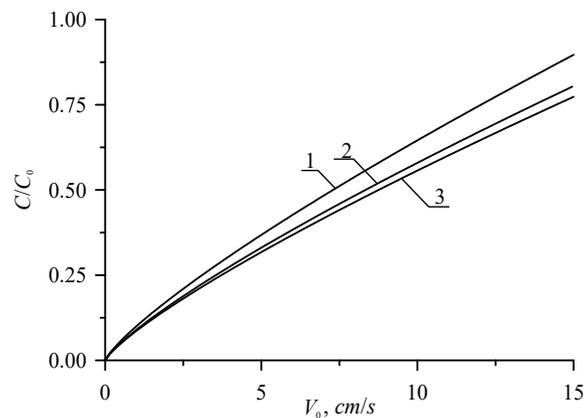

Figure 5. The dependence of the concentration of the mixture of gases from its input velocity

It is attracted an interest choosing of power of induction heating of reaction zone. This choosing should compensate losses of heat due to convective heat transfer [21]. In this situation relaxation time of temperature could be estimate by using recently introduced criterion [22]. This time is equal to $\vartheta \approx (6\pi - 1)$ $R^2/24\lambda_0$, where λ_0 is the average value of the thermal conductivity coefficient. In this case, the power required to compensate for the cooling of the region of the formation of the epitaxial layer can be estimated from the following relation

$$\int_0^R r \cdot p(r,\phi,z,t)dr \approx \sigma \cdot T^4(R,\phi,z,t) + \Theta \cdot v_z(R,\phi,z,t)/4\pi LR^2 \ [16].$$

4.   CONCLUSION

In this paper based on considered analytical approach for analysis of mass and heat transfer during film growth in reactors for gas phase epitaxy we analyzed this growth with account natural convection and chemical interaction between reagents. In this situation we analytically analyzed growth of films from gas phase in more common case in comparison with cited references to increase predictability of this technological process (it should be noted, that analytical approach for modeling are usually more demonstrative in comparison with numerical one and leads to decrease calculation time). As a result of this analysis, the obtain conditions to increase homogeneity of the grown epitaxial layers with changing of values of parameters of growth process with higher exactness.

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