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SELF–SIMILAR PROBLEMS FOR MODELING THE SURFACE CHEMICAL REACTIONS WITH THE GRAVITATION

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ABSTRACT

The mathematical model of a chemical reaction which takes place on the surface of the uniformly moving vertically imbedded glass fibre material is considered. The effect of gravitation is taken into account. Boussinesq's and boundary layer fittings allow to derive boundary value problems for self–similar systems of ordinary differential equations.

1. INTRODUCTION

We propose improvement of the mathematical model which was considered in our previous report [1]. The main purpose of this development is to take into account the effect of gravitation. The main result is that all conclusions and recomendations which were done in [1] remain valid.

2. MATHEMATICAL MODEL

Let x_1, x_2 be the spatial coordinates in the lengthwise and the normal directions of the glass fibre material;
u_1, u_2 are the velocity components of the acid solution flow in the directions corresponding to axes x_1, x_2; $u = (u_1, u_2)$,
ν is the coefficient of kinematic viscosity, g is the acceleration of gravitation,
ρ is the density of solution, p is the pressure of the solution.
Then the stationary plane-parallel flow of solution taking into account the effect of gravitation is described by a system of Navier–Stokes equations (see,

for example, [5])

$$u\nabla u_i = \nu \triangle u_i - \frac{1}{\rho}\frac{\partial p}{\partial x_i} + \gamma g = 0, \quad i = 1,2, \tag{2.1}$$

$$\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} = 0, \tag{2.2}$$

where $\gamma = 1$, if the direction of the gravitation force is the same as the direction of x_1 axis, $\gamma = -1$, if this direction is opposite.

Let ρ_i, m_i respectively are the density and the mass concentration of acid ($i = 1$) and alkaline metal salt ($i = 2$), ρ_0 is the density of water, $m = (m_1, m_2)$, then

$$\rho = \rho(m) = \left(\frac{\rho_0 - \rho_1}{\rho_0\rho_1}m_1 + \frac{\rho_0 - \rho_2}{\rho_0\rho_2}m_2 + \frac{1}{\rho_0}\right)^{-1}.$$

Partly we denote by m_j^* values of the mass concentrations outside of the reaction zone and $\rho^* = \rho(m^*)$.

Let us also assume that the density ρ is not depending on the pressure p and $p = p^* + \tilde{p}, \rho = \rho^* + \tilde{\rho}$, where p^*, ρ^* satisfy the hydrostatic equations

$$\frac{1}{\rho^*}\frac{\partial p^*}{\partial x_i} = \gamma g, \quad i = 1,2,$$

and the perturbations $\tilde{p}, \tilde{\rho}$ are small (Boussinesq's fitting). Folloving [5] we obtain equality

$$\frac{1}{\rho}\frac{\partial p}{\partial x_1} = \gamma g(1 + \alpha\varphi_1 - \beta\varphi_2),$$

where $\alpha = \frac{m_1^*}{\rho^*}\left(\frac{\partial \rho}{\partial m_1}\right)^*, \beta = \frac{1}{\rho^*}\left(\frac{\partial \rho}{\partial m_2}\right)^*, \varphi_1 = \frac{m_1^* - m_1}{m_1^*}, \varphi_2 = m_2 - m_2^*, \varphi = (\varphi_1, \varphi_2)$.

If we assume the inequality of the hydrodynamics boundary layer fitting

$$\frac{\partial^2 u_i}{\partial x_1^2} \ll \frac{\partial^2 u_i}{\partial x_2^2},$$

then we can rewrite the first equation (2.1) in the following form

$$u\nabla u_1 = \nu\frac{\partial^2 u_1}{\partial x_2^2} - \gamma g(\alpha\varphi_1 - \beta\varphi_2). \tag{2.3}$$

We note also that succeeding [4] for the hydrodynamics boundary layer fitting are true the equality for the two last additives in the differential equation (2.1)

$$\gamma g - \frac{1}{\rho}\frac{\partial p}{\partial x_1} = -\gamma g F(m), \tag{2.4}$$

where $F(m) = \frac{\rho^* - \rho}{\rho^*}$.

Assuming the expansion

$$\rho = \rho^* + \left(\frac{\partial \rho}{\partial m_1}\right)^* (m_1 - m_1^*) + \left(\frac{\partial \rho}{\partial m_2}\right)^* (m_2 - m_2^*)$$

we obtain $F(m) = \alpha\varphi_1 - \beta\varphi_2$ and so simultaneously the equation (2.3).

The differential equations of chemical substances transport (see, for example, [1]) are given by

$$\rho u \nabla m_i = D_i \left(\frac{\partial}{\partial x_1} \left(\rho \frac{\partial m_i}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left(\rho \frac{\partial m_i}{\partial x_2} \right) \right), \quad i = 1, 2,$$

where D_i are the corresponding diffusion coefficients of the chemical substances. Assuming the inequalities of the mass concentrations boundary layer fitting

$$\frac{\partial^2 m_i}{\partial x_1^2} \ll \frac{\partial^2 m_i}{\partial x_2^2}, \quad i = 1, 2,$$

yields the equations

$$u \nabla \varphi_i = D_i \frac{\partial^2 \varphi_i}{\partial x_2^2} + \frac{D_i}{\rho} \nabla \rho \nabla \varphi_i, \quad i = 1, 2. \tag{2.5}$$

Naturally we have the boundary conditions

$$\varphi(0, x_2) = 0, \quad \varphi(x_1, d) = 0, \tag{2.6}$$

if $d > \delta_1$, where δ_1 is the thickness of the mass concentrations boundary layer.

The boundary conditions determined by the surface chemical reactions are discussed in [1] and we can add the equalities

$$D_i \frac{\partial m_i(x_1, 0)}{\partial x_2} = \frac{A}{M_1} m_1(x_1, 0) \left(\kappa_i M_i + \kappa_3 M_3 m_i(x_1, 0) \right), \quad i = 1, 2,$$

where $M_j, \kappa_j, \quad j = 1, 2, 3$ respectively are the molecular weights and stochiometric coefficients of the chemical substances involved in the reaction, index 3 corresponds to the alkaline metal oxide which is situated on the surface of the glass fibre material, but A is the Arrhenius rate of the reaction. Of course, we must perceive the expressions

$$m_1 = m_1^*(1 - \varphi_1), \quad m_2 = m_2^* + \varphi_2,$$

and then we have the following form of these boundary conditions

$$\begin{aligned} -\tfrac{\partial \varphi_1(x_1, 0)}{\partial x_2} &= F_1(\kappa_1 M_1 + \kappa_3 M_3 m_1^*(1 - \varphi_1(x_1, 0)), \\ \tfrac{\partial \varphi_2(x_1, 0)}{\partial x_2} &= F_2 m_1^*(\kappa_2 M_2 + \kappa_3 M_3 (m_2^* + \varphi_2(x_1, 0)), \end{aligned} \tag{2.7}$$

where $F_i = \frac{A}{M_1 D_i}(1 - \varphi_1(x_1, 0))$

Finally we add the boundary conditions implied by the acid solution flow:

$$u_1(x_1, 0) = w_0, \quad u_2(x_1, 0) = 0, \quad u(0, x_2) = 0, \quad u(x_1, d) = 0, \tag{2.8}$$

where w_0 is the velocity of the glass fibre material uniformly pulling.

Therefore we obtain the mathematical model of the considered process as the boundary value problem (2.2)–(2.8). This problem could be numerically solved by modifying the finite difference method which was proposed in [5].

3. SELF-SIMILAR PROBLEMS

Let us introduce the flow function Φ by the equalities

$$u_1 = \frac{\partial \Phi}{\partial x_2}, \quad u_2 = -\frac{\partial \Phi}{\partial x_1},$$

and choose the new variables as it was done in [4]:

$$\eta = \left(\frac{g}{4\nu^2 x_1}\right)^{\frac{1}{4}} x_2, \quad f(\eta) = \frac{\Phi}{(4x_1)^{\frac{3}{4}}(g\alpha)^{\frac{1}{4}}\nu^{\frac{1}{2}}}.$$

Then the differential equation (2.2) becomes as the identity, and we can rewrite the differential equation (2.3) in the form

$$f''' + 3ff'' - 2(f')^2 = \gamma(\varphi_1 - \frac{\alpha}{\beta}\varphi_2) \tag{3.1}$$

and we can rewrite the differential equations (2.5) as

$$\varphi_i'' + 3Pr_i f\varphi_i' = \rho\left(1 + \frac{\nu\eta^2}{8g^{\frac{1}{2}}x_1^{\frac{3}{2}}}\right)\Psi_i, \quad i = 1, 2, \tag{3.2}$$

where

$$Pr_i = \frac{\nu}{D_i}, \quad \Psi_i = \frac{\rho_0 - \rho_1}{\rho_0\rho_1}\varphi_1'\varphi_i' + \frac{\rho_0 - \rho_2}{\rho_0\rho_2}\varphi_2'\varphi_i', \quad i = 1, 2.$$

The boundary conditions (2.6)-(2.8) and hydrodynamics boundary layer fitting assumptions yields the following boundary conditions:

$$f(0) = f'(\infty) = \varphi(\infty) = 0, \quad f'(0) = a, \tag{3.3}$$

$$-D_1\varphi_1'(0) = F_1(\kappa_3 M_3 m_1^*(1-\varphi_1(0)) + \kappa_1 M_1),$$
$$D_2\varphi_2'(0) = F_2 m_1^*(\kappa_3 M_3 \varphi_2(0) + \kappa_2 M_2), \tag{3.4}$$

where

$$a = \frac{w_0}{2(g\alpha x_1)^{\frac{1}{2}}}, \quad F_i = \frac{bA}{M_1 D_i}(1-\varphi_1(0)), \quad i=1,2, \quad b = \left(\frac{4\nu^2 x_1}{g\alpha}\right)^{\frac{1}{4}},$$

and $m_2^* = 0$ as it is essentially in the practice.

Since $w_0 \neq 0$ we can also use the new variables [1]

$$\eta = x_2\left(\frac{w_0}{\nu x_1}\right)^{\frac{1}{2}}, \quad f(\eta) = \Phi(\nu x_1 w_0)^{-\frac{1}{2}}.$$

Then we can rewrite the differential equations (2.3),(2.5)

$$f''' + \frac{1}{2}ff'' = \gamma\frac{g x_1}{w_0^2}(\alpha\varphi_1 - \beta\varphi_2), \tag{3.5}$$

$$\varphi_i'' + \frac{Pr_i}{2}f\varphi_i' = \rho\left(1 + \frac{\nu\eta^2}{4w_0 x_1}\right)\Psi_i, \quad i=1,2, \tag{3.6}$$

but the boundary conditions (2.6)–(2.8) become the boundary conditions (3.3),(3.4) with $a=1, b=\left(\frac{x_1\nu}{w_0}\right)^{\frac{1}{2}}$.

If the effect of gravitation is not taken into account ($\alpha = \beta = 0$) and we have the Quetta flow, which without assumptions of the hydrodynamics boundary layer implies the boundary condition $f'(\infty) = 1$, the boundary value problem (3.3)-(3.6) has the solution $f(\eta) = \tilde{f}(\eta) = \eta$. From (3.6) we obtain the differential equation

$$\varphi_i'' + \frac{Pr_i}{2}\eta\varphi_i' = \rho\left(1 + \frac{\nu\eta^2}{4w_0 x_1}\right)\Psi_i, \quad i=1,2,$$

which together with the boundary conditions was numerically and qualitatively investigated in our previous papers [1], [2]. If

$$D_1 = D_2 = D, \quad Pr_1 = Pr_2 = Pr, \tag{3.7}$$

then it is possible to use the variables

$$\eta = x_2\left(\frac{w_0}{Dx_1}\right)^{\frac{1}{2}}, \quad f(\eta) = \Psi(Dx_1 w_0)^{-\frac{1}{2}}.$$

If the variations of density are neglected instead of the differential equations (2.3),(2.5) we have the differential equations

$$Prf''' + \frac{1}{2}ff'' = \gamma\frac{x_1 g}{w_0^2}(\alpha\varphi_1 - \beta\varphi_2), \tag{3.8}$$

$$\varphi_i'' + \frac{1}{2}f\varphi_i' = 0, \quad i = 1, 2, \tag{3.9}$$

but we have $a = 1, \quad b = \left(\frac{x_1 D}{w_0}\right)^{\frac{1}{2}}$ in the boundary conditions (3.3),(3.4).

Finally, if the equality (2.4) takes place, using the new variables from (2.3) we obtain the differential equation

$$Prf''' + \frac{1}{2}ff'' = \gamma\frac{x_1 g}{w_0^2}F(\varphi), \tag{3.10}$$

where

$$F(\varphi) = 1 - \frac{1}{\rho^*}\left(\frac{\rho_0 - \rho_1}{\rho_0\rho_1}m_1^*(1 - \varphi_1) + \frac{\rho_0 - \rho_2}{\rho_0\rho_2}(\varphi_2 + m_2^*) + \frac{1}{\rho_0}\right)^{-1}.$$

4. CALCULATIONS

We solved numerically the boundary value problems (2.2)–(2.8); (3.1)–(3.4); (3.3)–(3.6); (3.3), (3.4), (3.8), (3.9) and (3.3), (3.4), (3.9), (3.10), using the real parameters from technological process or those which were identified in our previous work [1]. For the sake of determination all computations were done for $\gamma = 1$, although we must acknowledge that in the case $\gamma = -1$ the offered algorithms converge more slowly.

The assumption (3.7) is realiable, so the main conclusion of our investigations shows that the qualitative physical and chemical picture can be obtained by solving the boundary value problem (3.3), (3.4), (3.8), (3.9).

If $Pr = 1, \alpha = \beta = 0$, we have obtained that the symbol of infinity in the boundary conditions (3.3) can be replaced by number $L \approx 8$.

For the sake of brevity let denote $u_2^*(\eta) = u_2(\eta)\left(\frac{x_1}{Dw_0}\right)^{\frac{1}{2}}$, and let $f = \tilde{f}(\eta)$ (case A) or f is calculated from the differential equation (3.8) (case B). If $L = 8, \quad , Pr = 1, \quad \alpha = \beta = 0$, we have obtained:

$$\varphi_1'(0) = -0.564, \quad \varphi_2'(0) = -0.1123, \quad \varphi_2(0) = 0.2052, \quad \text{(case A)},$$

$$\varphi_1'(0) = -0.445, \quad \varphi_2'(0) = -0.0886, \quad \varphi_2(0) = 0.1896 \quad \text{(case B)}.$$

These results show that the chemical reaction on the surface of the glass fibre material coursing slowly in the influence of gravitation.

Moreover, table 1 shows that the process goes rapidly if the hydrodynamics boundary layer is formed.

Table 1.

	A	A	B	B	B
η	$m_1(\eta)$	$m_2(\eta)$	$m_1(\eta)$	$m_2(\eta)$	$f'(\eta)$
0.8	0.0642	0.1199	0.0510	0.1219	0.6631
1.6	0.1113	0.0575	0.0906	0.0692	0.4014
2.4	0.1365	0.0240	0.1166	0.0347	0.2298
3.2	0.1464	0.0108	0.1320	0.0143	1.282

Comparing the thickness of the mass concentration boundary layer turns out that it is greater in the case A ($\delta_1 = 7$) against the case B ($\delta_1 = 4$).

The results when the effect of gravitation was taken into account (case C; $Pr = 8400, \alpha = 0.0765, \beta = 0.6780, L = 10$) and without its influence (case D) are shown in table 2.

Table 2.

	C	C	C	C	D	D	D
η	$f'(\eta)$	$u_2^*(\eta)$	$m_1(\eta)$	$m_2(\eta)$	$f'(\eta)$	$u_2^*(\eta)$	$m_1(\eta)$
0	1.000	0.000	0.82E-8	0.196	1.000	0.000	0.68E-8
2	0.822	0.197	0.123	0.004	0.308	-0.031	0.105
4	0.719	0.004	0.149	0.001	0.077	-0.626	0.141
6	0.623	-0.266	0.150	0.000	0.026	-0.746	0.148

Moreover, we have obtained :

$$\varphi_1'(0) = -0.536, m_2'(0) = -0.1069, f''(0) = -0.140, u_2^*(L) = -0.7178 (\text{case C}),$$

$$\varphi_1'(0) = -0.444, m_2'(0) = -0.0877, f''(0) = -0.440, u_2^*(L) = -0.7876 (\text{case D}).$$

The thickness of the mass concentration boundary layer diminishes in the influence of the gravitation, but, on the other hand, the thickness of the hydrodynamics boundary layer increases if the number Pr increases.

It is seen, that the influence of gravitation increases the velocity component $u_1 = w_0 f'(\eta)$, but the velocity component u_2 in the boundary layer stands positive, has the positive maximum and then alternates. It means that there can appear vortexes.

So, the calculations have shown that the main conclusions which were done in [1] remained valid when we took into account the effect of gravitation.

5. QUALITATIVE INVESTIGATIONS

The self-similar differential equations, which were obtained from the differential equations of chemical substances mass transfer, are homogenous because we have neglected the variations of the density ρ. These differential equations become nonhomogenous if we take into account the variations of density. The self-similar boundary value problem which generalizes the modeled situation of chemical reactions on the surface of the glass fibre material in the acid solutions can be generalized in the following view:

$$f''' + qff'' - r(f')^2 = R(\rho), \tag{5.1}$$

$$m_i'' + \beta_i f m_i = \rho(\gamma_{1i} + \gamma_{2i}\eta^2)\sum_{j=1}^{k}\alpha_i m_i' m_j', \quad i = 1,\ldots,k,$$

$$m_i'(0) = A_i m_1(0)(\kappa_{k+1} m_i(0) + \kappa_i)$$

$$f(0) = 0, \quad f'(0) = \mu, \quad f'(\infty) = 0, \quad , m_i(\infty) = m_i^*, \quad , i = 1,\ldots,k,$$

where $A_i, \beta_i, \gamma_{1i}, \gamma_{2i}, q, \alpha_0 > 0; r \geq 0; \mu, \lambda_i \in R, \alpha_i, \lambda_{k+1} < 0, \quad i = 1,\ldots,k;$

$$m_i^* \in [0,1]; \sum_{i=1}^{k} m_i^* \leq 1; R \in C([0,+\infty)), \quad \rho = \left(\sum_{i=1}^{k}\alpha_i m_i + \alpha_0\right)^{-1}.$$

Note that in the differential equation (5.1) the parameters q and r can take the following values: $q = 3, r = 2$ or $q = \frac{1}{2}, r = 0$.

If we can show that the component of solution f has at most a linear growth, the proof of the existence theorem becomes possible using the procedures from the paper [2]. It seems like this if we are looking to the experimental results of the computing in the previous section. Much more, the certainty of this situation is provided by the observation that solution $\tilde{f}(\eta)$ which corresponds to the Quetta flow without the influence of gravitation is the majorant for f (see, for example, table 2).

The second significant matter of the qualitative investigations is the behavior of the function $u_2^*(\eta) = \eta f'(\eta) - f(\eta)$. As it is seen for the case without the influence of gravitation this function is monotone, but taking into account the effect of gravitation we have obtained a nonmonotone character of this function.

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