MMCA–97 Conference, pp. 41–47
R. Čiegis (Ed)

QUALITATIVE INVESTIGATIONS OF BOUNDARY VALUE PROBLEM FOR SELF-SIMILAR SECOND ORDER SYSTEM WHICH ARISES FROM MODELING OF SURFACE CHEMICAL REACTIONS

JĀNIS CEPĪTIS

University of Latvia, Department of Mathematics,
Zeļļu ielā 8, Rīga, Latvia, LV-1002,
e-mail: cepitis@fmf.lu.lv

1. INTRODUCTION

The mathematical model of chemical reactions which are taking place on the surface of the glass fibre material, if it is pulled through bathes filled with acid solution, was constructed and partly numerically investigated in the article [1]. The urgency of this investigation was caused by necessity to minimize substance of alkaline metal oxides in the glass fibre material and thus magnify its thermal strength. The two point boundary value problem for system of two self-similar ordinary differential equations with quadratic right side in respect to derivatives of unknown functions under some partial assumptions was carried out in [1]. We offer some qualitative investigations of this boundary value problem in the present article. At the same time our observations are interesting from the point of view of the mathematical modeling.

2. MATHEMATICAL MODEL

The full mathematical model of considered technological process consists of:

a) differential equations of hydrodynamics (equation of flow continuity and equations of momentum conservation in the directions of coordinate axes),

b) differential equations of substances transport in the acid solution,

c) boundary conditions determined by chemical reactions on the surface of the glass fibre material.

Of course, these are steady-state differential equations since the industrial process is continued and established.

For the sake of simplicity let us consider that only one oxide of alkaline metal was involved in the surface chemical reaction. Then the differential equations of substances transport taking into account the differential equations of hydrodynamics are following

$$\rho(u_1\frac{\partial m_j}{\partial x_1}+u_2\frac{\partial m_j}{\partial x_2})=D_j(\frac{\partial}{\partial x_1}(\rho\frac{\partial m_j}{\partial x_1})+\frac{\partial}{\partial x_2}(\rho\frac{\partial m_j}{\partial x_2})),j=1,2;$$

where x_1, x_2 respectively is the spatial coordinates in the lengthwise and the normal directions of the glass fibre material,

u_1, u_2 are velocity components of the acid solution flow in the directions corresponding to axes x_1, x_2,

ρ_i, m_i, D_i respectively are density, mass concentration and diffusion coefficient of acid ($i=1$) and alkaline metal salt ($i=2$) formed by the surface chemical reaction in the acid solution flow,

ρ_0 is the density of water and

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

is the density of the acid solution.

If axis x_1 is located on the surface of the glass fibre material and R_i are the Arrhenius rates of the chemical reaction for species $i=0,1,2$, then boundary conditions which are determined by the chemical reaction on the surface of the glass fibre material ($x_2=0$) are following

$$-D_j\rho\frac{\partial m_j}{\partial x_2}=R_j-(R_0+R_1+R_2)m_j,\ j=1,2.$$

Let $R_i=-\kappa_i M_i A\frac{\rho m_1}{M_1}(\frac{\bar\rho m_3}{M_3})^\alpha, i=0,1,2$, where $\bar\rho$ is the area density of the glass fibre material, m_3 is the mass concentration of alkaline metal oxide in the glass fibre material, $\kappa_j, M_j (j=0,1,2,3)$ respectively are the stochiometric coefficients in the equation of the chemical reaction and the molecular weights of substances,

A is the Arrhenius coefficient of proportionality, $\alpha>0$ is a chosen exponent.

Then the mentioned boundary conditions obtain the following form

$$D_j\frac{\partial m_j}{\partial x_2}=\frac{A}{M_1}(\frac{\bar\rho m_3}{M_3})^\alpha m_1(\kappa_3 M_3 m_j+\kappa_j M_j),j=1,2.$$

Furthermore, let us assume that for the velocity profile of the acid solution

$$u_1=\nu_0=const,u_2=0,\frac{\partial^2 m_j}{\partial x_1^2}\ll\frac{\partial^2 m_j}{\partial x_2^2},j=1,2.$$

Then by variable $\eta = x_2\sqrt{\frac{\nu_0}{x_1 D_1 D_2}}$ the differential equations of substances transport we can alter in the following form

$$f_j'' + \frac{D_1 D_2}{D_j}\frac{\eta}{2} f_j' = \frac{1 + \frac{\eta^2 D_1 D_2}{4\nu_0 x_1}}{\frac{1}{\rho_0} + \frac{\rho_0 - \rho_1}{\rho_0\rho_1} f_1 + \frac{\rho_0 - \rho_2}{\rho_0\rho_2} f_2}\left(\frac{\rho_0 - \rho_1}{\rho_0\rho_1} f_1' f_j' + \frac{\rho_0 - \rho_2}{\rho_0\rho_2} f_2' f_j'\right), \quad (1)$$

where $f_j(\eta) = m_j, j = 1, 2$, but from the boundary conditions determined by the chemical reaction on the surface of the glass fibre material we obtain

$$f_j'(0) = A_j f_1(0)(\kappa_3 M_3 f_j(0) + \kappa_j M_j), j = 1, 2, \quad (2)$$

where $A_j = \frac{A}{M_1}(\frac{\bar{\rho} m_3}{M_3})^\alpha \sqrt{\frac{x_1 D_1 D_2}{\nu_0 D_j^2}}$. Note, that if x_1 is fixed, then $A_j = const$ because we are considering the established process.

In addition the conditions for the mass concentrations of the acid and the salt at the beginning of process of surface chemical reaction ($x_1 = 0$) give the boundary conditions in the infinity

$$f_1(\infty) = m_1^*, f_2(\infty) = 0, \quad (3)$$

where m_1^* is the mass concentration of acid at the beginning of process.

The right side of the differential equations (1), which we shall denote by $g(\eta, f, f')$, are quadratic with respect to first derivatives and therefore did not satisfied the classical Bernstein-Nagumo-Opial condition (see, for example, [2])

$$| g(\eta, f, f') | \le p(1 + | f' |^2 \, b(| f' |)),$$

$$p \ge 0, \lim_{s\to\infty} b(s) = 0, b(s) > 0, \frac{d}{ds}(s^2 b(s)) \ge 0, s \in [0, \infty),$$

which implies the a priori estimate for the first derivative of bounded solutions of the system (1). It should be noted also that boundary value problem (1)-(3) has nonlinear boundary conditions. So, the solvability of this boundary value problem causes clearly mathematical interest.

3. EXISTENCE OF SOLUTIONS

Let us consider k-dimensional generalization of obtained boundary value problem (1)-(3)

$$f_j'' + \beta_j \eta f_j' = \frac{(1 + \sigma\eta^2)}{\frac{1}{\rho_0} + \sum_{i=1}^{k} \alpha_i f_i} \sum_{i=1}^{k} \alpha_i f_i' f_j', \quad (4)$$

$$f_j'(0) = A_j f_1(0)(\lambda_{k+1} f_j(0) + \lambda_j), f_j(\infty) = m_j^*, \quad (5)$$

$$f_j(\infty) = m_j^*, \tag{6}$$

where $j = 1, \ldots, k, \beta_j = \frac{1}{2D_j} \prod_{i=1}^{k} D_i, \alpha_j = \frac{\rho_0 - \rho_j}{\rho_0 \rho_j}, \sigma = \frac{1}{4\nu_0 x_1} \prod_{i=1}^{k} D_i, D_j, \nu_0,$ $x_1 > 0,$

$$m_j^* \in [0,1], \sum_{j=1}^{k} m_j^* \leq 1, A_j > 0, \lambda_j \in R, \lambda_{k+1} \in (-\infty, 0).$$

THEOREM 1. [Existence theorem]. *If for all $j = 1, \ldots, k$ inequalities*

$$\rho_j > \rho_0, \tag{7}$$

$$\mid \lambda_j \mid -2\lambda_{k+1} \leq \frac{1}{A_j} \sqrt{\frac{\beta_j}{2\pi}} \min \left\{ (1 + m_j^*, 2 - m_j^*) \right\}, \tag{8}$$

are true, then the boundary value problem (4)-(6) has the solution f and exist monotone functions $h_{ji} : [0, \infty) \to R, j = 1, \ldots, k; i = 1, 2,$ such, that

$$\lim_{\eta \to \infty} h_{ji}(\eta) = m_i^*$$

and components $f_j, j = 1, \ldots, k,$ of this solution have the estimates

$$h_{j1}^{(0)}(\eta) \leq f_j(\eta) \leq h_{j2}^{(0)}(\eta), \tag{9}$$

$$\frac{d}{d\eta} h_{j1}^{(0)} \leq f_j'(\eta) \leq \frac{d}{d\eta} h_{j2}^{(0)}(\eta) \tag{10}$$

in the domain $[0, \infty)$.

P r o o f. The linear homogenous boundary value problems

$$f'' + \beta_j \eta f' = 0, f'(0) = 0, f(\infty) = 0, j = 1, \ldots, k,$$

have Green's functions, which can be written in the following form:

$$G_j(\eta, \xi) = \begin{cases} \int\limits_{\xi}^{\infty} \exp(\frac{\beta_j(\xi^2 - \tau^2)}{2}) d\tau, 0 \leq \eta \leq \xi, \\ \int\limits_{\eta}^{\infty} \exp(\frac{\beta_j(\xi^2 - \tau^2)}{2}) d\tau, \xi \leq \eta \leq \infty. \end{cases}$$

Let $p_{ji} = (-1)^{i+1} \times 2A_j(\mid \lambda_j \mid -2\lambda_{k+1})$ and define for arbitrary chosen $g_{j1} \in R, g_{j2} \in (g_{j1}, \infty), j = 1, \ldots, k; i = 1, 2$, the functions

$$h_{ji}^{(0)}(\eta) = \int_0^\infty G_j(\eta, \xi) g_{ji} d\xi + p_{ji} \int_0^\eta \exp(-\frac{\beta_j \tau^2}{2}) d\tau - p_{ji}\sqrt{\frac{\pi}{2\beta_j}} + m_j^*.$$

Furthermore we introduce also the functions

$$h_{ji}^{(1)}(\eta) = \frac{d}{d\eta} h_{ji}^{(0)}(\eta) = -\int_0^\eta \exp(\frac{\beta_j(\xi^2 - \eta^2)}{2}) g_{ji} d\xi + p_{ji} \exp(-\frac{\beta_j \eta^2}{2}).$$

Let $q = (q_{10}, q_{11}, q_{20}, q_{21}, \ldots, q_{k0}, q_{k1})$,

$$F_j(\eta, q) = \frac{1 + \sigma\eta^2}{\frac{1}{\rho_0} + \sum_{i=1}^k \alpha_i h_{iq_{i0}}^{(0)}} \sum_{i=1}^k \alpha_i h_{iq_{i1}}^{(1)} h_{jq_{j1}}^{(1)}$$

and $F_j^{(1)}(\eta) = \min_{q \in \{1,2\}^{2k}} F_j(\eta, q), F_j^{(2)}(\eta) = \max_{q \in \{1,2\}^{2k}} F_j(\eta, q)$. According to the modification of methods based on the a priori estimates, which was applied for particular boundary value problem in the article [3] and was formulated in more general form in the work [4], the sufficient conditions for the solvability of the boundary value problem (4),(5) are fulfillment of the inequalities

$$(-1)^i F_j^{(i)}(\eta) \leq (-1)^i g_{ji}, \eta \in [0, +\infty), \tag{11}$$

for certain $g_{j1} \in R, g_{j2} \in (g_{j1}, \infty), j = 1, \ldots, k$.

Due to relations $\alpha_j < 0, j = 1, \ldots, k$, which are true since the assumptions (7), we have the possibility to find numbers g_{j1}, g_{j2} providing the inequalities (11). Furthermore, let for $x, y, z \in R$,

$$\delta(x, y, z) = 2^{-1}(x + \mid x - y \mid + \mid y - z \mid + z),$$

$r \to \eta_r$ is an arbitrary chosen sequence of numbers such, that $\lim_{r \to \infty} \eta_r = +\infty$,

$$\bar{m}_j^* \in [h_{j1}^{(0)}(\eta_r), h_{j2}^{(0)}(\eta_r)], \sum_{i=1}^k \bar{m}_j^* < 1,$$

and consider the boundary value problem

$$f_j'' + \beta_j \eta f_j' = \delta(g_{j1}, \frac{1+\sigma\eta^2}{\frac{1}{\rho_0} + \sum_{i=1}^{k} \alpha_i f_i} \sum_{i=1}^{k} \alpha_i f_i' f_j', g_{j2}),$$

$$f_j'(0) = \delta(p_{j2}, A_j f_1(0)(\lambda_{k+1} f_j(0) + \lambda_j), p_{j1}),$$

$$f_j(\eta_r) = \bar{m}_j^*, j = 1, \ldots, k.$$

As it is well known (see,for example, [2]) these quasilinear boundary value problems for any natural number r have the solutions $f^{[r]}$.

For components $f_j^{[r]}, j = 1, \ldots, k$, of these solutions are true the estimates

$$h_{j1}^{(0)}(\eta) \leq f_j^{[r]}(\eta) \leq h_{j2}^{(0)}(\eta), h_{j1}^{(1)}(\eta) \leq \frac{d}{d\eta} f_j^{[r]} \leq h_{j2}^{(1)}(\eta), \eta \in [0, \eta_r), \tag{12}$$

and according to assumptions (8) also the following inequalities

$$p_{j2} \leq A_j f_1^{[r]}(0)(\lambda_{k+1} f_j^{[r]}(0) + \lambda_j) \leq p_{j1}. \tag{13}$$

The estimates (12) together with the inequalities (11) for every natural number r imply

$$g_{j1} \leq \frac{1+\sigma\eta^2}{\frac{1}{\rho_0} + \sum_{i=1}^{k} \alpha_i f_i^{[r]}} \sum_{i=1}^{k} \alpha_i (f_i^{[r]})'(f_j^{[r]})\prime \leq g_{j2}, j = 1, \ldots, k.$$

So, the functions $f^{[r]} : [0, \eta_r) \to R^n$ are also the solutions of the differential equation system (4) and the inequalities (13) provide that the functions $f^{[r]}$ satisfy the boundary condition (5).

Later we have the possibility to select from the sequence of solutions $r \to f^{[r]}$ the convergent subsequence which converge to solution f of the boundary value problem (4)-(6). Of course, components f_j of this solution also satisfy the estimates (9), (10). The theorem is proved.

Remark. It is interesting to pay attention to the physical significance of the assumptions (7). These inequalities mean that density of each chemical substance which solution contains and which is involved in the chemical reactions no less like the density of water.

Extensions. The formulated existence theorem is possible to extend to some classes of boundary value problems which generalize the boundary value problem (4)-(6). For example, it remains valid if in place of the differential equation (4)is considered more general differential equation

$$f_j'' + \beta_j \eta f_j' = \frac{\phi_j(\eta)}{c_0 + \sum\limits_{i=1}^{k} \gamma_i f_i} \sum_{i=1}^{k} \sum_{l=1}^{k} \alpha_{jil} f_i' f_l', j = 1, \ldots, k,$$

where $\beta_j > 0, \gamma_j, \alpha_{jil} \in R, i, j, l = 1, \ldots, k; c_0 \in (0, +\infty)$

$$\sum_{i=1}^{k} \gamma_i < 0, \sum_{i,j,l=1}^{k} \alpha_{jil} < 0,$$

and $\phi_j\colon [0, \infty) \to (0, \infty)$ are continuous functions.

REFERENCES

[1] J. Cepītis, J. Kalis. A certain mathematical model of the glass fibre material production, *In Book "Progress in Industrial Mathematics at ECMI 96"*, B.G.Teubner, Stutgart, 1997, P. 166–173.

[2] N.I.Vasilyev, Ju.A.Klokov. Foundations of the theory of boundary value problems for ordinary differential equations, *Zinātne*, Rīga, 1978 (In Russian).

[3] J.Cepītis. On the solvability of boundary value problem arising in the investigation of fluid motion between two rotating discs, *Latv. Mat. Ezhegodnik*, **25**, 1981, P. 102–108. (In Russian).

[4] J.Cepītis. The boundary value problem for system of differential equations with separated boundary conditions, *Mat. conf. "VIII school on the theory of operators in the functional spaces"*, Rīga, Univ. Latvia, part 2, 1983, P. 114–115. (In Russian).