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COMMENTATIONES MATHEMATICAE UNIVERSITATIS CAROLINAE

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INITIAL-BOUNDARY VALUE PROBLEMS DESCRIBING MOBILE CARRIER TRANSPORT IN SEMICONDUCTOR DEVICES K. GRÖGER

Abstract: In this paper the system of partial differential equations describing mobile carrier transport in semiconductor devices with constant or varying densities of ionized impurities is investigated. Under appropriate assumptions there are indicated proofs of the global existence, uniqueness and the exponential stability of solutions to corresponding systems.

Key words: Initial-boundary value problem, asymptotic behaviour of solutions, van Roosbroeck s equations, semiconductors, carrier transport, varying densities of ionized impurities.

Classification: 35Q20, 35D05, 35B40

Introduction. These lectures consist of two parts. In Part I we shall be concerned with a system of partial differential equations proposed in 1950 by van Roosbroeck [17] as a model for the transport of mobile carriers in a semiconductor device. A large number of numerical experiments has shown that this model is quite useful for purposes of device design and device analysis (see, e.g.,[3]). Its analytical investigation started rather late with a series of papers of M.S. Mock [12, 13, 14]. Mock also tried to justify some of the commonly adopted numerical methods, and he summed up his results in a book [15] that appeared in 1983. Further results were obtained by Seidman [18] and Gajewski [4,5,6]. In our presentation we follow closely a recent paper of Gajewski-Gröger [7] dealing with global existence, uniqueness, and asymptotic behaviour of solutions to van

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- 75 -

Roosbroeck's equations under reasonable initial and boundary conditions.

Van Roosbroeck's model assumes that the densities of ionized impurities in the semiconductor are known and do not vary during the process under consideration. In Part II we shall deal with a generalization of van Roosbroeck's model allowing the densities of ionized impurities to change according to simple kinetic equations. The results of this part are new. Since their proofs are similar to the proofs of the results of Part I we shall indicate only the necessary modifications.

I. <u>Semiconductors with constant densities of ionized</u> <u>impurities</u>

I.1. <u>Provisional formulation of the problem</u>. Let $G \subset \mathbb{R}^N$, N ≤ 3 , be the domain occupied by a semiconductor device. We are looking for functions u_1 , u_2 , and v of t $\in \mathbb{R}_+ := [0, +\infty)$ and x $\in G$ satisfying van Roosbroeck's equations

(1)
$$\frac{\partial u_{1}}{\partial t} + \operatorname{div} j_{1}(u_{1}, v) + R(u) = 0, \quad i=1,2,$$

- div (ε grad v) = $f + u_{1} - u_{2}$,

where

a...

 $u=(u_1,u_2)$ represents the densities of holes and electrons, v is the electrostatic potential, $j_i(u_1,v) = -D_i(\text{grad } u_i + q_i u_i \text{grad } v)$, i=1,2, $q_1=-q_2 = 1$, are the hole and the electron current densities, D_1 , D_2 are the diffusion coefficients of holes and electrons, R(u) is the net recombination rate, ε is the dielectric permittivity of the semiconductor material, f is the net density of the charge of impurities. The equations (1) are to be supplemented by appropriate side conditions. We assume that the boundary ∂G is the union of two disjoint parts $\widetilde{\Gamma}$ and Γ and that

$$u = \widetilde{u} = (\widetilde{u}_1, \widetilde{u}_2), v = \widetilde{v} \text{ on } \mathbb{R}_+ \times \widetilde{\Gamma},$$

(2)

$$j_1(u_1,v)\cdot v \neq j_2(u_2,v)\cdot v = 0, \frac{\partial v}{\partial v} + av = g \text{ on } \mathbb{R}_+ \times \Gamma_,$$

(3) $u(0,x) = u^{0}(x), x \in G.$

Here \vee denotes the outward unit normal at a point of Γ , and \widetilde{u} , \widetilde{v} , a, and g are functions representing the interaction of the semiconductor device with its environment.

For a detailed discussion of these equations see [15,3]. We remark only that $j_1(u_1,v) = -D_1u_1$ grad ξ_1 if we define $\xi_1 := \log u_1 + q_1v$. The variables ξ_1 , i=1,2, are to be interpreted as the electrochemical potentials of holes and electrons, respectively.

I.2. <u>Precise formulation of the problem</u>. If E is any Banach space and S an interval of the real axis then $C(S;E), C^{1}(S;E), L^{p}(S;E)$, $L^{p}_{loc}(S;E)$, $1 \leq p \leq \infty$, denote the usual spaces of E-valued functions defined on S. If E carries a natural lattice structure then we denote by E_{+} the positive cone in E, and for $u \in E$ we define u^{+} := sup {u,0}, u^{-} := sup {-u,0}.

In what follows we assume that

D₁>0, D₂>0,
$$\varepsilon$$
>0, q₁ = -q₂ = 1, a∈ L[∞]₊(Γ), g∈ L[∞](Γ),
(5)
f∈ L[∞](G), R(u) = k(u₁u₂ - 1), k≥0,

(6)
$$\widetilde{\mathbf{v}} \in \mathbb{H}^1(\mathbb{G}) \wedge \mathbb{L}^{\infty}(\mathbb{G}), \widetilde{\mathfrak{u}}_1 = e^{\overbrace{i}^{\widetilde{\mathbf{v}}_1 - \mathfrak{q}_1}\widetilde{\mathbf{v}}}, \widetilde{\boldsymbol{\xi}}_1 \in \mathbb{W}^{1,\infty}(\mathbb{G}), i=1,2.$$

The last assumption means that the boundary values on $\widetilde{\Gamma}$ appearing in (2) can be extended to sufficiently nice functions on G.

Let $V := \{ w \in H^1(G) : w \mid \widetilde{\Gamma} = 0 \}$, and let V^* be its dual. We define $A_i : (H^1(G) \cap L^{\infty}(G)) \times H^1(G) \longrightarrow V^*$, i=1,2, and $B: H^1(G) \longrightarrow V^*$ by

$$\langle A_1(w,v),h \rangle := \int_G D_1(\text{grad } w + q_1 w \text{ grad } v) \text{grad } h dx,$$

(7)
$$\langle Bv,h \rangle := \int_{G} \varepsilon \operatorname{grad} v \operatorname{grad} h \, dx + \int_{\Gamma} (av-g) \, dG,$$

 $w \in H^{1}(G) \cap L^{\infty}(G), v \in H^{1}(G), h \in V.$

Purthermore, we introduce $F_1 = F_2$; L^{∞}(G; |R²) $\longrightarrow V^*$ by

(8)
$$\langle F_{i}(u),h \rangle := \int_{G} k(1-u_{1}u_{2})h \, dx, u \in L^{\infty}(G; \mathbb{R}^{2}), h \in V,$$

i=1,2.

(By $L^p(G; \mathbb{R}^n)$, $n \in \mathbb{N}$, $1 \le p \le \infty$, we denote the usual space of \mathbb{R}^n -valued functions defined on G.) Finally, let

(9)
$$u^{o} \in L^{\infty}_{+}(G; \mathbb{R}^{2}).$$

The problem (1)-(3) can now be written precisely as follows: $\forall t > 0: u'_i(t) + A_i(u_i(t), v(t)) = F_i(u(t)),$

(I)
$$Bv(t) = t + (u_1 - u_2)(t), u_1 - \widetilde{u}_1 \in L^2_{loc}(\mathbb{R}_+; V) \cap L^{\infty}_{loc}(\mathbb{R}_+; L^{\infty}(G)),$$

 $u_1 \in L^2_{loc}(\mathbb{R}_+; V^*), i=1,2, u(0) = u^0, v - \widetilde{v} \in C(\mathbb{R}_+; V),$

where u_i denotes the derivative of u_i with respect to time in the sense of V*-valued distributions. It is easy to check that sufficiently smooth functions u, v are a solution to (I) if and only if they satisfy (1)-(3).

The stationary problem corresponding to (I) reads as follows:

- 78 -

(II)

$$A_{1}(u_{1}^{*}, \nabla^{*}) = P_{1}(u^{*}), u_{1}^{*} = \widetilde{u}_{1} \overset{\mu_{1}}{\bullet}, (u_{1}^{*} \in \nabla \cap L^{\infty}(G), 1=1,2, D^{*})$$

$$Bv^{*} = f + u_{1}^{*} - u_{2}^{*}, v^{*} - \widetilde{\forall} \in V.$$

I.3. Results

<u>Theorem 1</u>. Let the conditions (4)-(9) be satisfied. Then there exists a unique solution (u,v) to the initial-boundary value problem (I). This solution has the property $u \ge 0$.

(10) Theorem 2. Suppose that (4)-(8) hold and that in addition $\tilde{\xi}_1 = 0, i=1,2, \quad \tilde{\xi}_1 + \tilde{\xi}_2 = 0.$

Then there exists a unique solution (u*,v*) to the boundary value problem (II). This solution has the properties

$$u_{1}^{*} = e^{i_{1} - q_{1} v^{*}}$$
, $j_{1}(u_{1}^{*}, v^{*}) = 0$, $i=1,2, R(u^{*}) = k(u_{1}^{*}u_{2}^{*}-1) = 0$.

<u>Theorem 3</u>. Suppose that (4)-(10) hold. Furthermore, let (11) $u_i^0 \leq \text{const} > 0$, i=1,2.

If (u,v) and (u^*,v^*) are the solutions to (I) and (II), respectively, then there exist $\mathcal{A} > 0$, c > 0, $c_0 > 0$, $c_1 < \infty$ such that $\forall t \in \mathbb{R}_+: c_0 \leq u_1(t) \leq c_1$, i=1,2,

$$\| u(t) - u^{*} \|_{L^{2}(G;\mathbb{R}^{2})} + \| v(t) - v^{*} \|_{H^{1}(G) \cap L^{\infty}(G)} \leq c e^{-\lambda t}.$$

<u>Remarks</u>. 1. The main result of Theorem 1 is the global existence of the solution despite the quadratic nonlinearity of the operators A_i and F_i . Of interest is also the boundedness property of the densities u_i since the equations (1) are inacceptable if the u_i become too large.

2. Condition (10) means that the driving forces for the flows of holes and electrons and for the net recombination rate vanish at the ohmic contacts of the device. By Theorem 2 this implies that the flows and the net recombination rate

- 79 -

vanish everywhere in G.

3. We presented a result on the stationary problem (II) only as a preparation for Theorem 3. An existence result for Problem (II) avoiding the hypothesis (10) can be found in Gajewski [5].

4. In his papers Mock considered only the case a = g = 0, thus excluding contacts called gates. He never proved that u_i belongs to $L_{loc}^{\infty}(R_{+i}L^{\infty}(G))$ or to $L^{\infty}(R_{+i}L^{\infty}(G))$, not even in the context of asymptotic behaviour. He assumed that for some p > Nthe relations Bv = h, $h \in L^p(G)$, $v - \tilde{v} \in V$ imply that $v \in W^{2,p}(G)$. This assumption clearly restricts the considerations to special geometries (see, e.g., Grisvard [9]). Similar assumptions were made by Seidman [18] and Gajewski [4-6].

5. The results stated above remain true if the constants k, D_i are replaced by k(u, v) and $D_i^0 + D_i^1(igrad v)$, where $k: |\mathbb{R}^2 \times \mathbb{R} \longrightarrow |\mathbb{R}_+$ is Lipschitzian and $D_i^1: \mathbb{R}_+ \longrightarrow |\mathbb{R}_i$ is such that $y \longmapsto D_i^1(y)y$, $y \in |\mathbb{R}_+$, is Lipschitzian and bounded.

I.4. Essential steps of the proofs. We shall outline the main ideas of the proofs of Theorem 1 - Theorem 3. For details we refer to Gajewski-Gröger [7].

1. The existence of a solution to (I) has been proved as follows: The operators A_i and F_i have been replaced by $A_i^{(r)}$, $F_i^{(r)}$, where r > 0 is a regularization parameter and

 $\langle A_{1}^{(r)}(w,v),h \rangle := \int_{G} D_{1}(\text{grad } w+q_{1} \min \{w^{+},r\} \text{grad } v) \text{grad } h dx,$ $\langle F_{1}^{(r)}(u),h \rangle := \int_{G} k(1 - \min \{(u_{1}u_{2})^{+},r^{2}\})h dx,$ $w \in H^{1}(G), v \in H^{1}(G), u \in L^{2}(G, \mathbb{R}^{2}), h \in V.$

The solvability of the regularized problem has been shown by means

- 80 -

of Schauder's fixed point theorem. Next by methods to be described below there were derived a-priori estimates for u_i in $L_{loc}^{\infty}(\mathbb{R}_+;L^{\infty}(G))$ uniformly with respect to r. Thus, for a given compact interval S = [0,T] one can choose r > 0 so large that a solution to the regularized problem is a solution to the original problem on S. The uniqueness of a solution to (I) can be proved by standard arguments.

For the sake of simplicity we describe the proof of a-priori estimates only for the original problem (I). At first one proves $u_i \ge 0$ by means of the test function u_i^- . Next one uses the function $H: L^2_+(G; \mathbb{R}^2) \times H^1(G) \longrightarrow \mathbb{R}$ defined by

$$H(u,v) := \int_{\mathcal{G}} \sum_{i=1}^{2} \int_{\widetilde{u}_{i}}^{u_{i}} \log \frac{v}{u_{i}} \, dy \, dx + \frac{1}{2} \langle Bv - B\vec{v}, v - \vec{v} \rangle$$

(cf. Gajewski [4]). Almost the same function had been introduced already by Gokhale [8]. Corresponding functions were used also in the theory of reaction systems and diffusion-reaction systems (see Horn-Jackson [11], Gröger [10]). If (u,v) is a solution to (I) such that $u_i \ge \text{const} > 0$ then

$$-\frac{\mathrm{d}}{\mathrm{d}t} H(u(t),v(t)) = \frac{2}{5 + 1} \langle u_{i}(t), \xi_{i}(t) - \xi_{i} \rangle,$$

and this is the dissipation rate of the system. Under the assumptions of Theorem 3 the semiconductor device is a closed system in the sense of thermodynamics. Hence one would expect in this case H to be decreasing along the trajectories of the system. Indeed, one can prove

Lemma 1. If (u,v) is a solution to (I) then for $t \ge s \ge 0$ H(u(t),v(t)) \le H(u(s),v(s)) + c $\int_{\lambda}^{b} (1+H(u(\tau),v(\tau))) d\tau$. If (10) is satisfied then this inequality holds with c = 0.

- 81 -

From Lemma 1 and the properties of H it follows that

$$\begin{array}{c} \forall t \in \mathbb{R}_+: \|u(t)\| & \neq \ \mathcal{J} e^{ct}, \\ L^1(G_{4}\mathbb{R}^2) & H^1(G) \end{array}$$

where \mathcal{T} , c depend only on the data of the problem and c = 0 if (10) is satisfied.

Lemma 2. If (u, v) is a solution to (I) and S = [0,T] then $\|u\|_{L^{\infty}(S;L^{\infty}(G;\mathbb{R}^{2}))} \stackrel{\leq}{=} C(\|u\|_{L^{\infty}(S;L^{1}(G;\mathbb{R}^{2}))}, \|v\|_{L^{\infty}(S;H^{1}(G))}),$

where C is a continuous function of its arguments depending only on the data of the problem.

The proof of this lemma is rather complicated. It uses an iteration technique introduced by Moser [16] (cf. also Alikakos [1]). One derives for n=1,2,... bounds for the norm $\|u_i\|$ by means of the test function $((u_i-M)^+)^{2^n-1}$, M $L^{\infty}(S_{\xi}L^{2^n}(G))$ sufficiently large. Lemma 2 completes the proof of the a-priori estimates.

2. If (u^*, v^*) is a solution to (II) then one proves by means of the test function $\log(u_1^*/\tilde{u}_1)$ that $A_1(u_1^*, v^*) = F_1(u^*) = 0$, $u_1^* = \sum_{i=1}^{\tilde{k}_1 - q_1} v^*$ = $e^{\tilde{k}_1 - q_1} v^*$, i=1,2, and

(12) $Bv^* = f + e^{\int_{x_1}^{x_1} - v^*} - e^{\int_{x_2}^{x_2} + v^*}, v^* - \tilde{v} \in V.$

Conversely, using standard maximum principle and monotone operator arguments one can show that (12) has a unique solution. This leads to the unique solvability of Problem (II).

3. By an iteration technique similar to that in the proof of Lemma 2 one obtains $u_1 \ge \text{const} > 0$ under the hypotheses of Theorem 3. This can be used to show that $\frac{d}{dt} H(u(t),v(t)) \le -\lambda H(u(t)v(t))$ for sufficiently small $\lambda > 0$, if H is defined by means of u_1^{\star}

- 82 -

instead of \widetilde{u}_1 . Hence H decreases exponentially along the trajectory (u,v). The assertions of Theorem 3 are easy consequences of this fact.

II. <u>Semiconductors with varying densities of ionized</u> <u>impurities</u>

II.1. The kinetics of impurities, holes, and electrons.

In Part I there was no need to distinguish between different impurities. In this part we have to take into account that the densities of some of the ionized impurities may vary during the process under consideration.

Let X_j , j=1,...,m, be species taking part in the process as impurities. By e⁺ and e⁻ we denote holes and electrons considered as species. If X_j is a donor and X_j^+ the corresponding ion then the reactions taking place can be written symbolically as follows:

(13)
$$\mathbf{e}^+ + \mathbf{x}_j \xrightarrow{\mathbf{k}_j} \mathbf{x}_j^+, \ \mathbf{e}^- + \mathbf{x}_j^+ \xrightarrow{\mathbf{m}_j} \mathbf{x}_j^-, \mathbf{e}^- \mathbf{x}_j^+ \xrightarrow{\mathbf{m}_j} \mathbf{x}_j^-,$$

This means that we have mass action kinetics with reaction constants as assigned to the reaction arrows. For the sake of simplicity we assume that each molecule supplies only one electron. Similarly, if X_j is an acceptor and X_j^- its ion then the reactions are

(14)
$$e^+ + X_j^- \xrightarrow{k_j} X_j, e^- + X_j \xrightarrow{m_j} X_j^-, x_j^-$$

Due to the choice of units made tacitly already in Part I we have $K_jM_j = 1$ (K_jM_j is the square of the intrinsic carrier density). If X_j is a donor (an acceptor) we denote by u_{2j+1} the density of

- 83 -

 X_j (of X_j) and by u_{2j+2} the density of X_j^+ (of X_j). Accordingly we define

$$\mathbf{q_{2j+1}} := \begin{cases} 0 \text{ if } \mathbf{X}_j \text{ is a donor} \\ -1 \text{ if } \mathbf{X}_j \text{ is an acceptor} \end{cases}, \mathbf{q_{2j+2}} := 1 + \mathbf{q_{2j+1}} \\ \end{cases}$$

With this notation the reaction equations for the impurities take the form (see, e.g., [2])

$$\frac{\partial u_i}{\partial t} = F_i(u), i=3,...,n,$$

where n = 2m + 2, $u = (u_1, ..., u_n)$, and

$$F_{2j+1}(u) := k_{j}(-u_{1}u_{2j+1}+k_{j}u_{2j+2}) + m_{j}(u_{2}u_{2j+2}-M_{j}u_{2j+1}),$$
(15)
$$F_{2j+2} := -F_{2j+1}, j=1, \dots, m.$$

Simultaneously we have to redefine \mathbf{F}_1 , \mathbf{F}_2 as follows:

(16)

$$F_{1}(u) := k(1-u_{1}u_{2}) + \sum_{j=1}^{\infty} k_{j}(-u_{1}u_{2j+1} + K_{j}u_{2j+2}),$$

$$F_{2}(u) := k(1-u_{1}u_{2}) + \sum_{j=1}^{\infty} m_{j}(-u_{2}u_{2j+2} + M_{j}u_{2j+1}).$$

II.2. Formulation of the problem. Let again (4)-(7) be satisfied, and let

$$\begin{array}{l} \mathbf{m} \in \mathbb{N}, \ \mathbf{n} := \ 2\mathbf{m} + 2; \ \mathbf{q}_{2j+1} = 0 \ \text{or} \ \mathbf{q}_{2j+1} = -1, \ \mathbf{q}_{2j+2} = \ 1 + \mathbf{q}_{2j+1}, \\ (17) \\ \mathbf{k}_{j} > 0, \ \mathbf{m}_{j} > 0, \ \mathbf{K}_{j} > 0, \ \mathbf{K}_{j} \mathbf{M}_{j} = 1, \ j = 1, \dots, \mathbf{m}. \end{array}$$

The mappings F_1 , F_2 defined by (16) will be considered as mappings from $L^{\infty}(G_1 | \mathbb{R}^n)$ to ∇^* (cf. (8)), whereas F_3, \ldots, F_m will be considered as mappings from $L^{\infty}(G_1 | \mathbb{R}^n)$ to $L^{\infty}(G)$. Let

(18)
$$u^{O} \in L^{\infty}_{+}(G; \mathbb{R}^{n}).$$

The evolution of the system under consideration is described by the following equations and side conditions:

- 84 -

$$\forall t > 0: \ u_{1}^{\prime}(t) + A_{1}(u_{1}(t), v(t)) = F_{1}(u(t)),$$

$$u_{1}^{\prime} - \widetilde{u}_{1}^{\prime} \in L_{loc}^{2}(R_{+}; V) \wedge L_{loc}^{\infty}(R_{+}; L^{\infty}(G)),$$

$$(III) \quad u_{1}^{\prime} \in L_{loc}^{2}(R_{+}; V^{*}), \ i=1,2; \ u_{1}^{\prime}(t) = F_{1}(u(t)),$$

$$u_{1}^{\prime} \in C^{1}(R_{+}; L^{2}(G)) \wedge L_{loc}^{\infty}(R_{+}; L^{\infty}(G)), \ i=3,...,n,$$

$$u(0) = u^{0}, \ Bv(t) = f + \sum_{i=1}^{\infty} q_{1}u_{1}(t), \ v - \forall \in C(R_{+}; V).$$

The function f takes into account that we may still have fixed ionized impurities. The corresponding stationary problem reads as follows:

$$\begin{aligned} A_{i}(u_{1}^{*},v^{*}) &= F_{i}(u^{*}), \ u_{1}^{*} &= \widetilde{u}_{1}e^{u_{1}^{*}}, \ u_{1}^{*} \in V \cap L^{\infty}(G), \ i=1,2; \\ (IV) &F_{i}(u^{*}) &= 0, \ u_{1}^{*} \in L^{\infty}_{+}(G), \ i=3,...,n, \\ Bv^{*} &= f + \sum_{i=1}^{m} q_{1}u_{1}^{*}, \ v^{*} - \widetilde{v} \in V. \end{aligned}$$

II.3. Results

<u>Theorem 4</u>. Let the conditions (4)-(7), (15)-(18) be satisfied. Then there exists a unique solution to Problem (III). If (u,v) is this solution then $u \ge 0$ and

(19)
$$\forall t \in \{R_{+}: (u_{2j+1}+u_{2j+2})(t) = u_{2j+1}^{0}+u_{2j+2}^{0}, j=1, \dots, m.$$

<u>Theorem 5.</u> Suppose that (4)-(7),(10), and (15)-(17) hold. Moreover, let $f_j \in L^{\infty}_+(G)$, $j=1,\ldots,m$, be given. Then there exists a unique solution (u^*,v^*) to Problem (IV) such that $u^*_{2j+1} + u^*_{2j+2} = f_j$, $j=1,\ldots,m$. For this solution it holds

$$u_{i}^{*} = e^{\hat{s}_{i} - q_{i}v^{*}}, \quad i=1,2; \quad u_{1}^{*}u_{2}^{*} = 1,$$
$$u_{2j+1}^{*} = f_{j}(1 + M_{j}u_{1}^{*})^{-1}, \quad j = 1,...,m.$$

<u>Theorem 6</u>. Let (4)-(7), (10), (11), and (15)-(18) be satisfied. If (u,v) is the solution to (III) and (u^*,v^*) is the

- 85 -

solution to (IV) such that

 $u_{2j+1}^{\#} + u_{2j+2}^{\#} = f_{j} = u_{2j+1}^{0} + u_{2j+2}^{0}$, $j=1,\ldots,m$, then there exist $\lambda > 0$, c > 0, $c_{0} > 0$, $c_{1} < \infty$ such that

 $\forall t \in R_{+}: c_0 \leq u_1(t) \leq c_1, i=1,2,$

$$\|u(t)-u^*\|_{L^2(G_{\mathfrak{g}}\mathbb{R}^n)} + \|v(t)-v^*\|_{H^1(G) \cap L^{\infty}(G)} \leq c e^{-\lambda t}.$$

<u>Remarks</u>. 1. If (u^*, v^*) is a solution to Problem (IV) under the hypotheses of Theorem 5 then we have equilibrium for each pair of reactions in (13),(14) and $R(u^*) = 0$.

2. Another natural choice of P_{2i+1} is

$$F_{2j+1}(u,v) := k_j (-e^{k_1 + k_2} j + 1 + k_j e^{k_2} j + 2}) + m_j (e^{k_2 + k_2} j + 2 - k_j e^{k_2} j + 1}) = k_j e^{q_2 j + 2^v} (-u_1 u_{2j+1} + k_j u_{2j+2}) + m_j e^{q_2 j + 1^v} (u_2 u_{2j+2} - M_j u_{2j+1}),$$

where $k_j := \log u_j + q_j v$ and the constants in this definition satisfy the conditions (17). Therefore it is of interest that the results of Theorem 4 - Theorem 6 remain true if the constants k_j , m_j are replaced by strictly positive locally Lipschitz-ien functions of u and v.

3. If the ions of impurities can accept or supply more than one electron then one has to modify the definition of the functions \mathbf{F}_i somewhat, but the results are essentially the same.

II.4. <u>Comments on the proofs</u>. The proofs of Theorem 4 -Theorem 6 are similar to those of Theorem 1 - Theorem 3. We restrict ourselves to short comments.

1. Let (u,v) be a solution to (III). The assertion $u \ge 0$ can be proved again by means of the test function $u_{\underline{i}}^-$. From $u \ge 0$ it follows immediately (cf. [191))

 $\|u_{2j+i}\|_{L^{\infty}(\mathbb{R}_{+};L^{\infty}(G))} \leq \|u_{2j+1}^{0}+u_{2j+2}^{0}\|_{L^{\infty}(G)}, j=1,\ldots,m, i=i,2.$

- 86 -

The main problem is once more to find bounds for u_1 , u_2 . One can prove an analogue to Lemma 1 if one defines

$$H(u, \mathbf{v}) := \int_{G} \sum_{i=1}^{\infty} \int_{\widetilde{u}_{i}}^{u_{i}} \log \frac{\mathbf{v}}{\widetilde{u}_{i}} \, d\mathbf{y} \, d\mathbf{x} + \frac{1}{2} \langle B\mathbf{v} - B\widetilde{\mathbf{v}}, \mathbf{v} - \widetilde{\mathbf{v}} \rangle,$$

for $u_i \in L^2_+(G; \mathbb{R}^n)$, $v \in H^1(G)$, where $\tilde{u}_i = e^{\alpha_i}$, $\alpha_i \in L^\infty(G)$,

i=3,...,n, are such that $\tilde{u}_1 \tilde{u}_{2j+1} = K_j \tilde{u}_{2j+2}$, j=1,...,m. Subsequently one can obtain bounds for $\|u_1(t)\|$, i=1,2, almost literally as under the hypotheses of Part I.

2. If (u^*, v^*) is a solution to (IV) satisfying the relations $u^*_{2j+1} + u^*_{2j+2} = f_j$, j=1,...,m, then by means of the test functions $\log(u^*_1/\tilde{u}_1)$ one can prove that $A_1(u^*_1, v^*) = 0$, i=1,2, $F_1(u^*) = 0$, i=1,...,n, and

$$u_{1}^{*} = e^{\underbrace{\tilde{s}}_{1} - q_{1} \nabla^{*}}, \ i=1,2, \ u_{2j+1}^{*} = f_{j}(1+M_{j} e^{\underbrace{\tilde{s}}_{1} - \nabla^{*}})^{-1}, \ j=1,\ldots,m,$$

By * = f + e^{\underbrace{\tilde{s}}_{1} - \nabla^{*}} - e^{\underbrace{\tilde{s}}_{2} + \nabla^{*}} f_{j}(q_{2j+2} - (1+M_{j} e^{\underbrace{\tilde{s}}_{1} - \nabla^{*}})^{-1}), \ \nabla^{*} - \nabla \in \nabla.

Conversely, the last equation can easily be handled by maximum principle and monotonicity arguments. This leads to the assertions of Theorem 5.

3. Under the hypotheses of Theorem 6 one proves at first as in Part I that $u_i(t) \ge const > 0$, i=1,2, t \ge 0. Next one shows that for every $t_0 > 0$ there exists $c_0 > 0$ such that

 $\forall t \geq t_0: u_{2j+i}(t) \geq c_0 f_j, j=1,\ldots,m, i=1,2,$

where $f_{j} := u_{2j+1}^{0} + u_{2j+2}^{0}$. Thus, for t>0 it makes sense to define $H(u(t), v(t)) := \frac{1}{2} \langle Bv(t) - Bv^{*}, v(t) - v^{*} \rangle + \int_{G} \sum_{i=1}^{2} \int_{u_{i}}^{u_{i}(t)} \log \frac{v}{u_{1}^{*}} dy dx +$ $+ \sum_{j=1}^{m_{v}} \int_{G_{j}} \left\{ \int_{u_{2j+1}}^{u_{2j+1}(t)} \log \frac{v}{u_{2j+1}^{*}} dy + \int_{u_{2j+2}}^{u_{2j+2}(t)} \log \frac{v}{u_{2j+2}^{*}} dy \right\} dx,$

- 87 -

where $G_{j} := \{x \in G : f_{j}(x) > 0\}$. If $t_{0} > 0$ and $\lambda > 0$ is sufficiently small then

 $\forall t \ge t_{\alpha}: \frac{d}{dt} H(u(t), v(t)) \le - \mathcal{A}H(u(t), v(t)).$

The proof of this inequality is, however, somewhat more complicated than the proof of the corresponding assertion of Part I.

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- 89 -