Boundary Value Multidimensional Problems in Fast Chemical Reactions

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Communicated by R. ARIS

1. Introduction

In a recent paper [1] J. R. CANNON & C. D. HILL studied the movement of the interface between two diffusing substances which undergo a chemical reaction, the products of which do not take part in the diffusion process. This is a simplified picture of a fast chemical reaction between two diffusing substances in a solution with precipitation after the reaction. Many other phenomena (see [1] for references) can be described by this scheme, which leads to the multidimensional analytical model described below.

Adopting the symbols of [1] we let G be a bounded domain in R^n with a smooth boundary ∂G. Setting $G(t)=G\times\{t\}$ and $\partial G(t)=\partial G\times\{t\}$ for each $t\in[0, T]$, $T>0$, we shall consider the cylinder $\Omega=\bigcup_{0<t\leqq T} G(t)$ and its lateral surface $S=\bigcup_{0<t\leqq T}\partial G(t)$. Then we shall define a surface Γ (the free boundary), separating Ω into two parts Ω_1, Ω_2, in the following way. Let $\Phi\in C^1(\overline{\Omega})$ be such that $\Phi<0$ in Ω_1 and $\Phi>0$ in Ω_2; we set $\Gamma(t)=\{(x, t)\in\overline{G(t)}: \Phi(x, t)=0\}$ and $\Gamma=\bigcup_{0<t\leqq T}\Gamma(t)$, assuming that grad $\Phi(x, t)\neq 0$* on Γ. $G_1(0)$ and $G_2(0)$ will denote the regions into which $G(0)$ is divided by $\Gamma(0)$. Finally, we define $S_i=\overline{\Omega}_i\cap S$ $(i=1, 2)$. Further considerations about the geometry of the problem are found in [1].

Now let $\tilde{u}_1, \tilde{u}_2$ denote the concentrations of the reacting substances, with initial values $\tilde{h}_1, \tilde{h}_2$ in $G_1(0)$, $G_2(0)$. The problem studied in [1] was to find $\tilde{u}_1, \tilde{u}_2$ in Ω_1, Ω_2 and, of course, the interface Γ (that is, a function Φ defining Γ) under the assumption that no flow occurs at the boundaries S_i. More precisely, we have the following set of equations:

$$(1.1)\qquad \alpha_i(\tilde{u}_i)\frac{\partial\tilde{u}_i}{\partial t}=\operatorname{div}[k_i(\tilde{u}_i)\operatorname{grad}\tilde{u}_i]\quad \text{in } \Omega_i\ (i=1,2),$$

$$(1.2)\qquad \tilde{u}_i=\tilde{h}_i,\quad \tilde{h}_i>0\quad \text{in } G_i(0)\ (i=1,2),$$

$$(1.3)\qquad k_i(\tilde{u}_i)\frac{\partial\tilde{u}_i}{\partial n}=0\quad \text{on } S_i\ (i=1,2),$$

* Throughout the paper the operators grad and div refer only to the space variables.

(1.4) $$\tilde{u}_i = 0 \quad \text{on } \Gamma \quad (i=1,2),$$

(1.5) $$\nu k_1(\tilde{u}_1) \operatorname{grad} \Phi \cdot \operatorname{grad} \tilde{u}_1 = -k_2(\tilde{u}_2) \operatorname{grad} \Phi \cdot \operatorname{grad} \tilde{u}_2 \quad \text{on } \Gamma,$$

where $\partial/\partial n$ is the derivative along the outer normal to S, ν is a positive constant related to the mass ratio in the reaction and $\alpha_i(u)$, $k_i(u)$ are positive and bounded functions defined for $u \geqq 0$.

Uniqueness, existence, qualitative properties and compatibility of suitably defined *weak solutions* of problems (1.1)–(1.5) were investigated in [1]. In this paper similar results will be given concerning the more general second boundary value problem obtained by replacing (1.3) by

(1.3′) $$k_i(\tilde{u}_i) \frac{\partial \tilde{u}_i}{\partial n} = \tilde{\psi}_i(x,t) \geqq 0 \quad \text{on } S_i^0 \ (i=1,2)$$

with $S_i^0 = S_i - \Gamma \cap S$, and also concerning the first boundary value problem where (1.3) is replaced by

(1.3″) $$\tilde{u}_i(x,t) = \tilde{f}_i(x,t) > 0 \quad \text{on } S_i^0 \ (i=1,2).$$

We shall refer to these problems as problem A and problem B respectively. A somewhat delicate question arises in the proper statement of conditions (1.3′): Are the surfaces S_i^0 in (1.3′) meant to be known? Consider now the case in which G is a cube in which a given flow of the two substances occurs at two opposite faces σ_1, σ_2, not intersecting $\Gamma(0)$, while the other ones are insulated (i.e., here we have $\tilde{\psi}_i = 0$). In this case some parts of S_1^0, S_2^0, namely, $\sigma_1 \times [0,T]$, $\sigma_2 \times [0,T]$, are really known while $\Gamma \cap S$ still has to be determined.

Thus we are led to the following remark.

Remark 1. In the conditions (1.3′) only those parts of S_i^0 on which $\tilde{\psi}_i$ is essentially positive are understood to be given.

Now we define what we shall mean by classical solutions of problems A or B: a set $\{\tilde{u}_1, \tilde{u}_2, \phi\}$ satisfying (1.1), (1.2), (1.3′), (1.4), (1.5) is a classical solution of problem A if $\tilde{u}_i$ and $\operatorname{grad} \tilde{u}_i$ are continuous in $\bar{\Omega}_i$ and $\Delta \tilde{u}_i$ and $\partial \tilde{u}_i/\partial t$ are continuous in Ω_i; similar conditions are required for classical solutions of problem B, with the exception that $\operatorname{grad} \tilde{u}_i$ are continuous only on $\Omega_i \cup \Gamma$.

The definition of weak solutions of problems A and B will be given in the next section. Uniqueness and existence of the weak solution to problem A will be investigated in Section 3, while Section 4 is devoted to the study of stability, monotone dependence on the data, and regularity of such solutions. In Sections 5 and 6 a parallel study will be made for weak solutions of problem B. The last section deals with some complementary remarks concerning the disappearance of one or both the reacting substances and the compatibility of approximate solutions. The results of [1] and the techniques of [2] will be used extensively.

2. Generalized Formulations of Problems A and B

In order to give a generalized formulation of problem A we make even extensions to $u<0$ of the functions $\alpha_i(u)$, $k_i(u)$ and, following [1], we define the odd functions

$$A_i(u)=\int_0^u \alpha_i(\xi)\,d\xi, \qquad K_i(u)=\int_0^u k_i(\xi)\,d\xi \qquad (i=1,2)$$

and set

$$u_1=\tilde{u}_1,\ u_2=-\tilde{u}_2; \qquad h_1=\tilde{h}_1,\ h_2=-\tilde{h}_2; \qquad \psi_1=\tilde{\psi}_1,\ \psi_2=-\tilde{\psi}_2.$$

Thus problem (A) takes the form

$$\frac{\partial}{\partial t}A_i(u_i)=\operatorname{div}\operatorname{grad}K_i(u_i) \quad \text{in } \Omega_i\ (i=1,2), \tag{2.1}$$

$$u_1=h_1>0 \quad \text{in } G_1(0), \qquad u_2=h_2<0 \quad \text{in } G_2(0), \tag{2.2}$$

$$\frac{\partial}{\partial n}K_i(u_i)=\psi_i \quad \text{on } S_i\ (i=1,2), \tag{2.3}$$

$$u_i=0 \quad \text{on } \Gamma\ (i=1,2), \tag{2.4}$$

$$v\operatorname{grad}\Phi\cdot\operatorname{grad}K_1(u_1)=\operatorname{grad}\Phi\cdot\operatorname{grad}K_2(u_2) \quad \text{on } \Gamma. \tag{2.5}$$

We now introduce the test functions for problem A as smooth functions ϕ in R^{n+1} vanishing on $G(T)$ and such that $\partial\phi/\partial n=0$ on S. We shall denote the space of such functions by Θ_A.

Selecting a test function from Θ_A, multiplying each of (2.1) by it, performing elementary calculations similar to [1], and taking into account (2.2)–(2.5), we obtain

$$\begin{aligned}&\iint_{\Omega_1}\left[vA_1(u_1)\frac{\partial\phi}{\partial t}+vK_1(u_1)\Delta\phi\right]dx\,dt\\ &+\iint_{\Omega_2}\left[A_2(u_2)\frac{\partial\phi}{\partial t}+K_2(u_2)\Delta\phi\right]dx\,dt+\int_{G_1(0)}vA_1(h_1)\phi\,dx\\ &+\int_{G_2(0)}A_2(h_2)\phi\,dx+\int_0^T\int_{\partial G_1(t)}v\psi_1\phi\,dS_x\,dt+\int_0^T\int_{\partial G_2(t)}\psi_2\phi\,dS_x\,dt=0.\end{aligned} \tag{2.6}$$

Then, defining

$$u=\begin{cases}u_1 & \text{in } \Omega_1\\ 0 & \text{on } \Gamma,\\ u_2 & \text{in } \Omega_2\end{cases} \qquad h=\begin{cases}h_1>0 & \text{in } G_1(0)\\ 0 & \text{on } \Gamma(0),\\ h_2<0 & \text{in } G_2(0)\end{cases} \qquad \psi=\begin{cases}v\psi_1 & \text{on } S_1^0\\ \psi_2 & \text{on } S_2^0,\end{cases}$$

and

$$a(u)=\begin{cases}vA_1(u), & u\geqq 0\\ A_2(u), & u<0,\end{cases} \qquad b(u)=\begin{cases}vK_1(u), & u\geqq 0\\ K_2(u), & u<0,\end{cases}$$

we get from (2.6)

$$\iint_{\Omega}\left[a(u)\frac{\partial\phi}{\partial t}+b(u)\Delta\phi\right]dx\,dt+\int_{G(0)}a(h)\phi\,dx+\int_S\psi\phi\,dS=0. \tag{2.7}$$

Definition 1. *A bounded measurable function u in Ω satisfying* (2.7) *for all $\phi\in\Theta_A$ is called a weak solution of problem A.*

The definition of weak solution of problem B can be given similarly. First of all it is necessary to formulate problem B in a form analogous to (2.1)–(2.5). Obviously, (2.3) must be replaced by

$$(2.3') \qquad K_i(u_i)=K_i(f_i) \quad \text{on } S_i^0 \ (i=1,2).$$

Then a different class of test functions is needed. We define the space Θ_B of test functions for problem B as the space of smooth functions in R^{n+1} vanishing on $G(T)\cup S$.

Now define $f_1=\tilde{f}_1, f_2=-\tilde{f}_2$ and

$$f=\begin{cases} vK_1(f_1) & \text{on } S_1^0,\\ K_2(f_2) & \text{on } S_2^0,\end{cases}$$

and it follows from analysis similar to that above that

$$(2.8) \qquad \iint_\Omega \left[a(u)\frac{\partial\phi}{\partial t}+b(u)\Delta\phi\right] dx\,dt+\int_{G(0)} a(h)\phi\,dx-\int_S f\frac{\partial\phi}{\partial n}dS=0.$$

Definition 2. *A weak solution of problem B is a bounded measurable function u satisfying* (2.8) *for all* $\phi\in\Theta_B$.

Obviously, any classical solution of problem A or B is also a weak solution. Conversely, it is easy to show that a weak solution of problem A or B possessing the smoothness requirements of a classical solution is actually a classical solution.

3. Uniqueness and Existence Theorems for Problem A

The uniqueness of the solution of problem A can be established in exactly the same way as in the case $\psi\equiv 0$ of reference [1]. The following assumptions are required:

(i) G is bounded and ∂G is of class $C^{2+\alpha}$ $(\alpha>0)$ (see [3], p. 86);

(ii) the functions $\alpha_i(u)$, $k_i(u)$ $(i=1,2)$ are continuous and there exist two positive constants γ_0, γ_1 such that

$$(3.1) \qquad \gamma_0<\alpha_i(u)<\gamma_1, \quad \gamma_0<k_i(u)<\gamma_1, \quad i=1,2.$$

We shall now prove the following existence theorem.

Theorem 1. *Under assumptions* (i) *and* (ii), *together with*

(iii) *the initial datum h is a bounded and measurable function in* $G(0)$;

(iv) $h\in H^1(G)$ *(see* [3], p. 272); *and*

(v) ψ, ψ_t *are summable over S and* ψ *is bounded;*

a weak solution of problem A exists in $H^1(\Omega)$.

The assumptions on h and ψ will be considerably weakened in the next section. This will obviously reduce the regularity of u.

Proof of Theorem 1. Let us take sequences $\{a_m(u)\}$, $\{b_m(u)\}$ of $C^\infty(R^1)$ functions uniformly convergent on compact subsets of R^1 to $a(u)$ and $b(u)$ respectively. Recalling (3.1) and the definitions of $a(u)$ and $b(u)$, we may choose $\{a_m\}$, $\{b_m\}$ in such a way that $a_m(0)=b_m(0)=0$ and that

$$0<\gamma_2\leqq a'_m(u)\leqq\gamma_3, \quad 0<\gamma_2\leqq b'_m(u)\leqq\gamma_3, \tag{3.2}$$

hold for all m, where γ_2 and γ_3 are fixed constants.

Next consider a sequence $\{h_m(x)\}$, with $h_m\in C^\infty(\bar{G})$ and $\max_{\bar{G}}|h_m|\leqq \operatorname{ess\,sup}_G |h|$, converging to h with respect to the $H^1(G)$-norm.

Finally, let us introduce a sequence $\{\psi_m(x,t)\}$ of smooth functions defined on S such that

$$\sup_S|\psi_m|\leqq \operatorname{ess\,sup}_S|\psi|, \quad \psi_m(x,0)=\left.\frac{\partial b_m(h_m)}{\partial n}\right|_{\partial G},$$

and $\lim_{m\to\infty}\int_S\{|\psi_m-\psi|+|\psi_{mt}-\psi_t|\}\,dS=0$.

Consider now the problems

$$\frac{\partial a_m(u_m)}{\partial t}=\operatorname{div}\operatorname{grad} b_m(u_m) \quad \text{in } \Omega, \tag{3.3}$$

$$u_m=h_m \quad \text{in } G(0), \tag{3.4}$$

$$\frac{\partial}{\partial n}b_m(u_m)=\psi_m \quad \text{on } S, \tag{3.5}$$

which by means of the transformation

$$v_m=b_m(u_m) \tag{3.6}$$

can be readily put into the forms

$$\frac{\partial v_m}{\partial t}=c_m(v_m)\Delta v_m \quad \text{in } \Omega, \tag{3.7}$$

$$v_m=b_m(h_m) \quad \text{in } G(0), \tag{3.8}$$

$$\frac{\partial v_m}{\partial n}=\psi_m \quad \text{on } S, \tag{3.9}$$

where c_m is the $C^\infty(R^1)$ function defined by

$$c_m(v_m)=\{a'_m[\xi_m(v_m)]\,\xi'_m(v_m)\}^{-1} \tag{3.10}$$

and $\xi_m(v_m)$ is the inverse of the function $b_m(u_m)$, that is, $u_m=\xi_m(v_m)$. By virtue of (3.2) we have

$$0<\gamma_2/\gamma_3\leqq c_m\leqq\gamma_3/\gamma_2, \quad m=1,2,\ldots. \tag{3.11}$$

Multiplying both sides of (3.9) by $c_m(v_m)$, one sees that problem (3.7)–(3.9) is a special case of the initial-boundary value problem for quasilinear parabolic equations treated in [2] (see problem (7.1)–(7.3), p. 475–476). The results of [2] concerning this problem were also applied in [1], but in our case special care is needed due to the non-homogeneous boundary condition.

First of all we have to ascertain that problem (3.7)–(3.9) fulfills the assumptions of Theorem 7.3, p. 487 of [2], listed under (7.34). This will be a basic result in the proof of the existence theorem since a bound independent of m will be derived for $\max_{\bar{\Omega}} |v_m|$ and, consequently, for $\max_{\bar{\Omega}} |u_m|$.

By virtue of (3.11), most of (7.34) of [2] are satisfied. It remains only to prove that we can choose two non-negative constants γ_4, γ_5 such that

$$v_m c_m(v_m) \psi_m(x,t) \leqq \gamma_4 v_m^2 + \gamma_5 \quad \text{for all } (x,t) \in S. \tag{3.12}$$

Set $\Psi \equiv \operatorname{ess\,sup}_S |\psi|$. Since

$$v_m c_m(v_m) \psi_m \leqq (\gamma_3/\gamma_2) \Psi v_m \qquad \text{for } v_m \geqq 0$$

and

$$v_m c_m(v_m) \psi_m \leqq -(\gamma_3/\gamma_2) \Psi v_m \qquad \text{for } v_m < 0,$$

condition (3.12) is satisfied if

$$\gamma_4 v_m^2 - (\gamma_3/\gamma_2) \Psi v_m + \gamma_5 \geqq 0 \qquad \text{for } v_m \geqq 0$$

and

$$\gamma_4 v_m^2 + (\gamma_3/\gamma_2) \Psi v_m + \gamma_5 \geqq 0 \qquad \text{for } v_m < 0.$$

These inequalities are both valid if

$$\gamma_4 \gamma_5 \geqq \tfrac{1}{4} (\gamma_3/\gamma_2)^2 \Psi^2.$$

Thus γ_4 and γ_5 can be chosen independent of m. An application of the maximum principle [2, p. 487] yields

$$\max_{\bar{\Omega}} |v_m(x,t)| \leqq \lambda_1 e^{\lambda T} \max\left(\sqrt{\gamma_5}, \max_{\bar{G}} b_m(h_m)\right), \tag{3.13}$$

with λ_1, λ dependent only on the constants γ_2, γ_3, γ_4 and the boundary S.

By virtue of the assumptions made on b_m, h_m, (3.13) leads to the estimate

$$\max_{\bar{\Omega}} |v_m(x,t)| \leqq C_1, \qquad m = 1, 2, \ldots,$$

where the constant C_1 depends on the data of problem A, but not on m. Recalling (3.6) and (3.2), we obtain the estimate

$$\max_{\bar{\Omega}} |u_m(x,t)| \leqq C_2, \qquad m = 1, 2, \ldots, \tag{3.14}$$

with $C_2 = C_1/\gamma_2$.

It is worthwhile to remark for further applications of (3.14) that the constant C_2 is independent of $\|\psi_t\|_{L^1(S)}$ and $\|\operatorname{grad} h\|_{L^2(G)}$.

By reducing problem (3.2)–(3.9) to a problem with zero initial value by means of the transformation $w_m = v_m - b_m(h_m)$ and applying Theorem 7.4, p. 491 in [2], existence and uniqueness of v_m is established.

Now we shall obtain a uniform bound for the functions u_m in the norm of $H^1(\Omega)$. Multiplying both sides of equation (3.3) by $\partial b_m/\partial t$, integrating over $G(t)$ and performing an integration by parts on the right hand side, we obtain

$$\int_{G(t)} a_m'(u_m) b_m'(u_m) \left|\frac{\partial u_m}{\partial t}\right|^2 dx = \int_{\partial G(t)} \frac{\partial b_m}{\partial t} \frac{\partial b_m}{\partial n} dS_x - \frac{1}{2} \int_{G(t)} \frac{\partial}{\partial t} |\operatorname{grad} b_m(u_m)|^2 dx.$$

Now we take into account (3.5) and integrate with respect to time. Next, we interchange the order of the integrations in the right hand side and integrate the first term by parts. We obtain

$$\int_0^t \int_{G(\tau)} a_m' b_m' \left|\frac{\partial b_m}{\partial \tau}\right|^2 dx\, d\tau = \tfrac{1}{2} \int_{G(0)} (b_m')^2 |\operatorname{grad} h_m|^2 dx$$
$$-\tfrac{1}{2} \int_{G(t)} (b_m')^2 |\operatorname{grad} u_m|^2 dx + \int_{\partial G(t)} b_m \psi_m dS_x$$
$$-\int_{\partial G(0)} b_m \psi_m dS_x - \int_0^t \int_{\partial G(\tau)} b_m \frac{\partial \psi_m}{\partial \tau} dS_x\, d\tau, \quad 0<t\leqq T.$$

Next we recall that a_m', b_m' have lower and upper bounds independent of m (see (3.2)) and that (3.14) implies an m-independent bound for $b_m(v_m)$: $|b_m(v_m)| \leqq \gamma_3 C_2$ in $\bar{\Omega}$. Hence we arrive at the inequality

$$\gamma_2^2 \int_0^t \int_{G(\tau)} \left|\frac{\partial u_m}{\partial t}\right|^2 dx\, d\tau + \tfrac{1}{2}\gamma_2^2 \int_{G(t)} |\operatorname{grad} u_m|^2 dx$$
$$\leqq \tfrac{1}{2}\gamma_3^2 \int_{G(0)} |\operatorname{grad} h_m|^2 dx + 2\gamma_3 C_2 \Psi \operatorname{mes}(\partial G) + \gamma_3 C_2 \left\|\frac{\partial \psi_m}{\partial t}\right\|_{L^1(S)}, \quad 0<t\leqq T.$$

Since $h_m \to h$ in the norm of $H^1(G)$ and $\frac{\partial \psi_m}{\partial t} \to \frac{\partial \psi}{\partial t}$ in the norm of $L^1(S)$, the right hand side of this inequality is in turn dominated by a constant independent of m. Thus we have proved that

$$\|u_m\|_{H^1(\Omega)} \leqq C_3, \tag{3.15}$$

where C_3 is dependent only on the data of problem A.

From this point the proof of Theorem 1 is strictly similar to the existence theorem of [1].

4. Properties of Weak Solutions to Problem A

Theorem 2 (Stability). *If u, $\hat{u}$ are weak solutions to problem A with the respective data h, ψ, $\hat{h}$, $\hat{\psi}$ satisfying the assumptions of Theorem 1, then*

$$\|u-\hat{u}\|_{L^2(\Omega)} \leqq C_4 \{\|h-\hat{h}\|_{L^2(G)} + \|\psi-\hat{\psi}\|_{L^1(S)}\}. \tag{4.1}$$

In (4.1) C_4 is a constant depending on T and on $\max(C_2, \hat{C}_2)$, C_2, $\hat{C}_2$ being the constants in (3.14) corresponding to h, ψ and $\hat{h}$, $\hat{\psi}$ respectively. The proof can be carried out following the method given in [1] with no important modifications.

Theorem 2 can be used to show the existence of a weak solution of problem A for $h \in L^2(\Omega)$ and $\psi \in L^1(S)$. As in [1] it suffices here to take a sequence of functions $\bar{h}_m$ satisfying (iii), (iv), converging to h in $L^2(G)$, and a sequence of functions $\bar{\psi}_m$ satisfying (v), converging to ψ in $L^1(S)$. Considering a sequence of weak solutions $\{\bar{u}_m\}$ which satisfy

$$\iint_\Omega \left\{a(\bar{u}_m)\frac{\partial \phi}{\partial t} + b(\bar{u}_m)\Delta\phi\right\} dx\, dt + \int_{G(0)} a(\bar{h}_m)\phi\, dx + \int_S \bar{\psi}_m \phi\, dS = 0 \tag{4.2}$$

and using the fact that the constant C_4 in (4.1) does not depend on $\|\bar{h}_m\|_{H^1(G)}$ and $\|\bar{\psi}_{m\,t}\|_{L^1(S)}$ (see the remark made about (3.14)), we find that the sequence $\{\bar{u}_m\}$ is a Cauchy sequence in $L^2(\Omega)$ and therefore it has a bounded limit $u \in L^2(\Omega)$ which is a weak solution to problem A with data h, ψ.

As a corollary and by similar arguments, Theorem 2 can be demonstrated for $h \in L^2(\Omega)$ and $\psi \in L^1(S)$. For Theorems 3 and 4 below, we assume only that $h \in L^2(\Omega)$ and $\psi \in L^1(S)$.

Theorem 3 (Monotone dependence). *If $h \geqq \hat{h}$ a.e. in G and $\psi \geqq \hat{\psi}$ a.e. on S, then $u \geqq \hat{u}$ a.e. in Ω.*

Theorem 4 (Regularity). *If Ω' is a subdomain of Ω separated from $S \cup \overline{G(0)}$ by a positive distance d, the weak solution u of problem A belongs to $C^{\alpha,\alpha/2}(\Omega')$ for some α with a Hölder coefficient depending on the data and d.*

We shall omit the proofs of these theorems because they are strictly similar to the corresponding ones in [1]. However, we remark that the demonstration of Theorem 4 is based upon a uniform Hölder estimate in Ω' (that is, in the norm of $C^{\alpha,\alpha/2}(\Omega')$) of the solutions of the following problems:

$$\frac{\partial w_m}{\partial t} = \operatorname{div}\{D_m(w_m)\operatorname{grad} w_m\} \quad \text{in } \Omega, \tag{4.3}$$

$$w_m = a_m(h_m) \quad \text{in } G(0), \tag{4.4}$$

$$D_m(w_m)\frac{\partial w_m}{\partial n} = \psi_m \quad \text{on } S, \ m = 1, 2, \dots, \tag{4.5}$$

which are obtained from problems (3.3)–(3.5) by means of the transformation $w_m = a_m(u_m)$. The coefficients $D_m(w_m)$ are given by $D_m(w_m) = \dfrac{b'_m(\eta_m(w_m))}{a'_m(\eta_m(w_m))}$, with $\eta_m(w_m) = u_m$. Since an estimate of $\max\limits_{\bar{\Omega}} |w_m|$ independent of m is easily deduced by (3.15), all the assumptions of Theorem 1.1 of [2], Chapter V are fulfilled and this gives an estimate of the norm of w_m in $C^{\alpha,\alpha/2}(\Omega')$ which is independent of m.

5. Uniqueness and Existence Theorems for Problem B

Theorem 5. *Under assumptions* (i), (ii), *problem B has at most one weak solution.*

Due to the different space of test functions entering the definition of weak solutions to problem B, the proof of the uniqueness theorem of [1] cannot be immediately extended to the present case. Nevertheless, some results of [1] will be utilized. One of these is the following: if (ii) is satisfied, the function

$$e(x,t) = \begin{cases} \dfrac{b(u)-b(v)}{a(u)-a(v)}, & u \neq v, \\ 0, & u = v \end{cases} \tag{5.1}$$

defined for any pair of functions $u=u(x,t)$, $v=v(x,t)$, satisfies the inequalities

$$0 \leqq e(x,t) \leqq C_5$$

where C_5 is a positive constant dependent on γ_0, γ_1.

Let $\{e_m\}$ be a sequence of $C^\infty(\bar{\Omega})$ functions such that

$$\frac{1}{m} \leqq e_m(x,t) \leqq C_6 \tag{5.2}$$

for some constant C_6 independent of m and let us look for an m-independent bound for the solutions ϕ_m of the following parabolic problems:

$$\frac{\partial \phi_m}{\partial t} + e_m \Delta \phi_m = F \quad \text{in } \Omega, \tag{5.3}$$

$$\phi_m(x,T) = 0 \quad \text{in } G(T), \tag{5.4}$$

$$\phi_m = 0 \quad \text{on } S,\ m=1,2,\dots, \tag{5.5}$$

where $F \in C_0^\infty(\Omega)$. Existence and uniqueness of smooth solutions to (5.3)–(5.5) under the assumption (i) are well known classical results (see, for example, [2], [3]). Note that $\phi_m \in \Theta_B$, $m=1,2,\dots$.

Lemma 1. *There is a constant C_7 depending only on T and $\max_{\bar{\Omega}} |F|$ such that*

$$\max_{\bar{\Omega}} |\phi_m| \leqq C_7, \qquad m=1,2,\dots. \tag{5.6}$$

Proof. The estimate (5.6) is readily obtained by the maximum principle. Since the functions $z_m^\pm(x,t) = A(T-t) \pm \phi_m(x,t)$, with $A > \max_{\bar{\Omega}} |F|$, satisfy the inequalities

$$\frac{\partial z_m^\pm}{\partial t} + e_m \Delta z_m^\pm = -A \pm F < 0; \qquad z_m^\pm \geqq 0 \quad \text{on } G(T) \cup S,$$

then $|\phi_m(x,t)| \leqq A(T-t)$ in $\bar{\Omega}$. Hence, (5.6) follows with $C_7 = T \max_{\bar{\Omega}} |F|$.

The following estimate is also needed.

Lemma 2. *There is a constant C_8 depending on Ω and F such that*

$$\|e_m^{1/2} \Delta \phi_m\|_{L^2(\Omega)} \leqq C_8. \tag{5.7}$$

Proof. We multiply both sides of (5.3) by $\Delta \phi_m$ and integrate to get

$$\iint_\Omega \frac{\partial \phi_m}{\partial t} \Delta \phi_m \, dx\, dt + \iint_\Omega e_m |\Delta \phi_m|^2 \, dx\, dt = \iint_\Omega F \Delta \phi_m \, dx\, dt.$$

An integration by parts in the first integral yields:

$$\iint_\Omega \frac{\partial \phi_m}{\partial t} \Delta \phi_m \, dx\, dt = \int_0^T \int_{\partial G(t)} \frac{\partial \phi_m}{\partial t} \frac{\partial \phi_m}{\partial n} \, dS_x \, dt - \int_0^T \int_{\partial G(t)} \frac{1}{2} \frac{\partial}{\partial t} |\operatorname{grad} \phi_m|^2 \, dx\, dt.$$

It follows from (5.4) and (5.5) that

$$\iint_{\Omega} \frac{\partial \phi_m}{\partial t} \Delta \phi_m \, dx\, dt = \tfrac{1}{2} \int_{G(0)} |\operatorname{grad} \phi_m(x,0)|^2 \, dx.$$

Moreover, the membership of F in $C_0^\infty(\Omega)$ yields

$$\iint_{\Omega} F \Delta \phi_m \, dx\, dt = \iint_{\Omega} \phi_m \Delta F \, dx\, dt,$$

thus,

$$\tfrac{1}{2} \int_{G(0)} |\operatorname{grad} \phi_m(x,0)|^2 \, dx + \iint_{\Omega} e_m |\Delta \phi_m|^2 \, dx\, dt = \iint_{\Omega} \phi_m \Delta F \, dx\, dt$$

which implies (5.7).

Now, if $u(x,t)$, $v(x,t)$ are two weak solutions of problem B, consider the function $e(x,t)$ defined by (5.1) and introduce $C^\infty(\bar{\Omega})$ approximations $\bar{e}_m$ to e such that $0 \leqq \bar{e}_m \leqq C_5$ and $\|e - \bar{e}_m\|_{L^2(\Omega)} < \frac{1}{m}$, $m = 1, 2, \ldots$. Assume $e_m = \bar{e}_m + \frac{1}{m}$; then Lemmas 1 and 2 and the same argument given for Lemma 5 in [1] imply that $\|e/e_m\|_{L^2(\Omega)}$ is bounded independently of m.

As in [1], the following equation is derived from (2.8) and (5.3):

$$\iint_{\Omega} [a(u) - a(v)] F \, dx\, dt = \iint_{\Omega} (e_m - e) \Delta \phi_m \, dx\, dt.$$

Hence,

$$\left| \iint_{\Omega} [a(u) - a(v)] F \, dx\, dt \right| \leqq \bar{C} \iint_{\Omega} |e_m - e| \, |\Delta \phi_m| \, dx\, dt$$

where $\bar{C}$ is independent of m. The right hand side of this inequality tends to zero as $m \to \infty$. Since F can be arbitrarily chosen in $C_0^\infty(\Omega)$, $a(u) = a(v)$ a.e. in Ω. Hence, $u = v$ a.e. in Ω. This completes the proof of Theorem 5.

In order to prove the existence of a weak solution of problem B we will make the following assumptions on the initial and boundary data:

(vi) f and h are bounded measurable functions in their respective domains of definition and there exists a bounded measurable function g defined in Ω and belonging to $W_2^{2,1}(\Omega)$*, such that $g|_S = f$, $g|_{G(0)} = h$.

Lemma 3.4 of [2], Chapter II, specifies the regularity properties of f and h satisfying (vi).

Theorem 6. *Under assumptions* (i), (ii) *and* (vi), *problem B possesses a weak solution* $u \in H^1(\Omega)$.

After having proved a stability theorem (Section 6) we will be able to assert that a weak solution exists in $L^2(\Omega)$ for any pair of data $h \in L^2(G)$, $f \in L^2(S)$.

Proof of Theorem 6. Take a sequence of $C^\infty(\bar{\Omega})$ functions $\{g_m\}$ converging to g in the norm of $W_2^{2,1}(\Omega)$ and such that $\max_{\bar{\Omega}} |g_m| \leqq \operatorname{ess\,sup}_{\Omega} |g|$. Next, consider the approximating problems

$$(5.8) \qquad \frac{\partial a_m(u_m)}{\partial t} = \operatorname{div} \operatorname{grad} b_m(u_m) \quad \text{in } \Omega,$$

* See [2], Chapter I, for the definition of the space $W_2^{2,1}(\Omega)$.

(5.9) $$u_m = h_m \quad \text{in } G(0),$$

(5.10) $$w_m = f_m \quad \text{on } S,\ m=1,2,\ldots,$$

where the sequences $\{a_m\}$ and $\{b_m\}$ are the ones introduced in Section 3 and $h_m = g_m|_{G(0)}$, $f_m = g_m|_S$. Using the symbols of Section 3, we rewrite (5.8)–(5.10) in the form

(5.11) $$\frac{\partial v_m}{\partial t} = c_m(v_m)\,\Delta v_m \quad \text{in } \Omega,$$

(5.12) $$v_m = b_m(h_m) \quad \text{in } G(0),$$

(5.13) $$v_m = b_m(f_m) \quad \text{on } S,\ m=1,2,\ldots.$$

Using Theorem 9.1, Chapter IV, of [2], we obtain

(5.14) $$\|v_m\|_{W_2^{2,1}(\Omega)} \leqq C_9, \qquad m=1,2,\ldots,$$

where the constant C_9 depends only upon Ω, $\|g\|_{W_2^{2,1}(\Omega)}$ and the upper bound γ_3 for b_m'.

The chain of inequalities

$$\|v_m\|_{W_2^{2,1}(\Omega)} \geqq \|v_m\|_{H^1(\Omega)} \geqq \gamma_2\,\|u_m\|_{H^1(\Omega)}$$

leads to the estimate

(5.15) $$\|u_m\|_{H^1(\Omega)} \leqq C_9/\gamma_2, \qquad m=1,2,\ldots.$$

Moreover, the estimate

(5.16) $$\max_{\bar\Omega} |u_m| \leqq C_{10}, \qquad m=1,2,\ldots,$$

follows from an application of the maximum principle to (5.11)–(5.13). Here C_{10} depends only on γ_2 and $\operatorname*{ess\,sup}_{\Omega} |g|$.

This being shown, the proof is completed in a similar manner to that of Section 3.

6. Properties of Weak Solutions of Problem B

Let $u, \hat u$ be two weak solutions of problem B corresponding to the pairs of data h, f; $\hat h, \hat f$, respectively. Recalling the definition (5.1) of $e(x,t)$ and replacing v by $\hat u$, we have

(6.1) $$\begin{aligned}&\iint_\Omega [a(\hat u) - a(u)]\left\{\frac{\partial \phi}{\partial t} + e\,\Delta\phi\right\} dx\,dt \\ &\quad = \int_{G(0)} [a(h) - a(\hat h)]\,\phi\,dx + \int_S (\hat f - f)\,\frac{\partial\phi}{\partial n}\,dS\end{aligned}$$

for any $\phi \in \Theta_B$.

Now take $\phi = \phi_m$, where ϕ_m is defined by (5.3)–(5.5). It follows from Lemmas 1 and 2 of Section 5, the method of proof in [1], and (6.1) that for any $F \in C_0^\infty(\Omega)$

there exists a constant C_{11}, dependent only on Ω and $\max_{\bar\Omega}|F|$, such that

$$\begin{aligned}(6.2)\qquad &\Big|\iint_{\Omega}[a(u)-a(\hat u)]F\,dx\,dt\Big|\\ &\leqq C_{11}\left\{\int_{G(0)}|a(h)-a(\hat h)|\,|\phi_m|\,dx+\int_S|f-\hat f|\left|\frac{\partial\phi_m}{\partial n}\right|dS\right\}+\varepsilon_m\end{aligned}$$

where $\lim \varepsilon_m=0$. Since the difference $a(u)-a(\hat u)$ is bounded and measurable, it can be approximated in $L^2(\Omega)$ by a sequence of $C_0^\infty(\Omega)$ uniformly bounded functions $\{F^j\}$. Then, assuming $F=F^j$ in (6.2) and taking the independent limits for $j\to\infty$ and $m\to\infty$, we obtain a stability theorem from uniform bounds for $|\phi_m|$ and $|\partial\phi_m/\partial n|_S$. The bound for $|\phi_m|$ is given by (5.6). By virtue of the uniform boundedness of $\max_{\bar\Omega}|F^j|$, the bound for the $|\partial\phi_m/\partial n|_S$ is obtained by means of a straight-forward application of Theorem 9.2 of [2], Chapter IV, along with Lemma 3.4 of [2], Chapter II.

Now, using Schwartz's inequality in the right hand side of (6.2) and recalling again (3.2), we arrive at the following conclusion:

Theorem 7. *For any two weak solutions $u, \hat u$ of problem B with data satisfying the assumption of Theorem 6, we have*

$$(6.3)\qquad \|u-\hat u\|_{L^2(\Omega)}\leqq C_{12}\{\|h-\hat h\|_{L^2(G)}+\|f-\hat f\|_{L^2(S)}\}.$$

In (6.3), C_{12} depends on Ω, on the upper bounds C_{10}, $\hat C_{10}$ for $u, \hat u$ (see (5.16)) and on γ_3. By the arguments of Section 4, one can show the existence of a weak solution of problem B in $L^2(\Omega)$ for any pair of data $h\in L^2(G)$, $f\in L^2(S)$ and the validity of (6.3) for $h, \hat h\in L^2(G)$; $f, \hat f\in L^2(S)$.

Under the same weakened assumptions the following theorem holds.

Theorem 8. *If $h\geqq\hat h$ a.e. in G and $f\geqq\hat f$ a.e. on S, then $u>\hat u$ a.e. in Ω.*

Proof. The proof of Theorem 8 is similar to the proof of the corresponding Theorem 3. Hence, we omit it.

The regularity of weak solutions of problem B can be discussed in a similar manner to that of Theorem 4 and the same conclusions are reached.

Remark 2. The solution u turns out to be continuous in $\bar\Omega-\partial G(0)$ if f and h are continuous on S and $G(0)$ respectively. Indeed, in this case we can choose the sequence $\{g_m\}$ in such a way that $f_m\to f$ and $h_m\to h$ in the maximum norm. Thus the convergence of u_m to u will be uniform in each closed subset of $\bar\Omega-\partial G(0)$.

7. Complementary Remarks

I. Disappearance of One or Both of the Reacting Substances

We shall give here an extension of the results of [1]. Let us consider the function

$$(7.1)\qquad H(t)\equiv\int_{G(0)}a(h)\,dx+\int_0^t\int_{\partial G(\tau)}\psi\,dS_x\,d\tau.$$

We shall refer to the substance 1 and the substance 2 according to the symbols in Section 1. The following theorem holds:

Theorem 9. *If* $H(t_0)>0$ $(H(t_0)<0)$ *for a given* $t_0\in(0,T)$, *then the substance* 1 (*the substance* 2) *cannot disappear at* $t=t_0$; *if* $H(t_0)=0$ *and the substance* 1 (2) *disappears at* $t=t_0$, *then the substance* 2 (1) *must also disappear at the same instant.*

Proof. Following the argument in [1], it can be shown that

$$\int_{G(t)} a(u)\phi\,dx=\int_{G(0)} a(h)\phi\,dx+\int_0^t\int_{\partial G(\tau)} \psi\phi\,dS_x\,d\tau + \int_0^t\int_{G(\tau)}\left[a(u)\frac{\partial\phi}{\partial\tau}+b(u)\Delta\phi\right]dx\,d\tau \tag{7.2}$$

for $0\leqq t<T$ and any $\phi\in\Theta_A$. Choosing $\phi=1$ on $G\times[0,t]$, it follows from (7.2) that

$$\int_{G(t)} a(u)\,dx=H(t),\qquad 0\leqq t<T. \tag{7.3}$$

Suppose now $H(t_0)>0$ for some $t_0\in(0,T)$: if the concentration of the substance 1 were zero at $t=t_0$, we should have $\int_{G(t_0)} a(u)\,dx\leqq 0$, which contradicts (7.3). Similar arguments apply to the case $H(t_0)<0$. If $H(t_0)=0$ and the concentration of the substance 1 is zero at $t=t_0$, the eventual persistence of the substance 2 would imply $\int_{G(t_0)} a(u)\,dx<0$ and the same contradiction would be reached.

II. Computability of Approximate Solutions

The solutions of the approximating problems can be calculated by means of classical finite difference schemes or via the techniques of J. Douglas & T. Dupont [4] for nonlinear parabolic equations.

This research was supported in part by the National Science Foundation, the NATO Senior Fellowship Program, and the Gruppo Nazionale per la Fisica Matematica of the Consiglio Nazionale delle Ricerche.

References

1. Cannon, J. R., & C. D. Hill, On the movement of a chemical reaction interface. Indiana Math. J. **20**, 429–454 (1970)
2. Ladyzenskaja, O. A., V. A. Solonnikov & N. N. Ural'ceva, Linear and quasilinear equations of parabolic type. A.M.S., Providence, R.I. (1968)
3. Friedman, A., Partial Differential Equations of Parabolic Type. Englewood Cliffs, N.J.: Prentice-Hall (1964)
4. Douglas, J., & T. Dupont, Galerkin methods for parabolic equations. SIAM J. Numer. Anal. **7**, 575–626 (1970)

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(Received March 27, 1973)