



Zentrum für Technomathematik
Fachbereich 3 – Mathematik und Informatik

**A Note on Global Weak Solutions for
Semilinear Parabolic Systems modelling
Equilibrium Reactions (Part 1)**

Michael Böhm

Report 13–05

Berichte aus der Technomathematik

Report 13–05

September 2013

A Note on Global Weak Solutions for Semilinear Parabolic
Systems modelling Equilibrium Reactions (Part 1)

by

Michael Böhm

Universität Bremen, FB 3, Zentrum für Technomathematik,

Bibliotheksstraße 1, 28213 Bremen, Germany.

E-Mail: mbohm@math.uni-bremen.de

August 2013

Abstract: In this note we show well posedness for a relatively general semilinear parabolic system under nonhomogeneous Neumann conditions and semi-linearities of (some) equilibrium-reaction type. The result weakens previously made by Kräutle and Mahato ([Kra08,11] and [Mah12a,b], resp.) on the coefficients of the elliptic operator as well as on the boundary conditions considerably.

1. Introduction Even very simple semi-linear parabolic equation can have merely local solutions, i.e. solutions in some perhaps small neighbourhood of the initial time. The same applies to coupled systems of more than one, say m , such equations for the unknowns u_k , $k = 1, \dots, m$. Therefore it takes some special structure of the nonlinearities to guarantee the existence of *global* solutions, i.e. solutions on any given time interval. Nonlinearities modelling *equilibrium* reactions bear some potential for producing global solutions since positive productions are accompanied by negative ones. Kräutle [Kra08,11] shows that the production rates of a large class of m_1 equilibrium reactions of m species can be reduced to the following setting: Let $\Omega \subset \mathbb{R}^N$ be a bounded domain with C^2 -boundary Γ , $S := (0, T)$ - a time interval,

$$E \in M(m \times m_1) \text{ with } \text{rank}(E) = m_1, k_j^\pm > 0, s_{ij} \in \{0\} \cup [1, \infty), \quad (1)$$
$$j = 1, \dots, m_1, i = 1, \dots, m,$$

and set

$$R_j(u) := R_j^+(u) - R_j^-(u) := k_j^+ \prod_{i=1}^m u_j^{s_{ij}} - k_j^- \prod_{i=1}^m u_j^{s_{ij}}, \quad (2)$$
$$R = (R_1, \dots, R_m)^T, u = (u_1, \dots, u_m)^T,$$

$$\widehat{f}(u) = ER(u). \quad (3)$$

Furthermore, let

$$D_i \in L^\infty(\Omega; Sym(N)), \quad D = (D_1, \dots, D_m), \quad (4)$$

$$\mathbf{q} : S \times \Omega \rightarrow \mathbb{R}^N \text{ sufficiently smooth, } \operatorname{div} \mathbf{q} = 0 \text{ (incompressibility)} \quad (5)$$

$$A_{0i}(D, u) \quad : \quad = \operatorname{div}(\mathbf{j}_i), \quad i = 1, \dots, m, \quad A_0 := \operatorname{diag}(A_{01}, \dots, A_{0m}), \quad \text{where} \quad (6)$$

$$\mathbf{j}_i \quad : \quad = -D_i \nabla u_i + \mathbf{q} u_i \quad (= \text{diffusion flux} + \text{advection}) \quad (7)$$

$$\begin{aligned} B_{0i}(D, u) &:= -a_i D_i \frac{\partial u_i}{\partial n} + \mathbf{q} u_i \text{ on } \Gamma, \quad i = 1, \dots, m, \\ B_0 &:= \operatorname{diag}(B_{01}, \dots, B_{0m}), \end{aligned} \quad (8)$$

$n = n(x)$ is the unit outward normal on $\partial\Omega$, $a_i = a_i(x) \in \{0, 1\}$ and $\theta \in (0, 1]$ are given (cf. text following (12)) below). In Kräutle's as well as Mahato's settings, advection and diffusion, the latter modelled by Fick's law (cf. (7)), are the transport mechanisms.

The semi-linear problem is: Let g and h be given and find $u : \bar{S} \times \bar{\Omega} \rightarrow \mathbb{R}^m$ such that

$$\theta \frac{\partial u}{\partial t} + A_0(D, u) \quad = \quad \hat{f}(u) \quad \text{in } (0, T) \times \Omega \quad (9)$$

$$u(0, \cdot) \quad = \quad g \quad \text{on } \Omega \quad (10)$$

$$B_0(D, u) \quad = \quad h \quad \text{on } (0, T) \times \Gamma \quad (11)$$

Kräutle's solution $u(t, \cdot)$ lives in $W^{2,p}(\Omega)^m$ for a.a. t , where $p > N + 1$. Since he deals with diffusion and reaction in porous media, in his setting the porosity θ might be different from one. Mahato considers a free flow - and thus $\theta = 1$. Kräutle splits Γ in two disjoint parts Γ_{in} and Γ_{out} , the in- and outflow boundary parts, and specifies (11) as

$$-\mathbf{q} \cdot n \geq 0 \text{ on } \Gamma_{in}, \quad -\mathbf{q} \cdot n \leq 0 \text{ on } \Gamma_{out} \text{ and } -D_i \frac{\partial u_i}{\partial n} = 0 \text{ on } \Gamma_{out}, \quad (12)$$

$$h = 0 \quad (13)$$

i.e. the outflow is entirely advective ([Kra08,11]). In order to model the third condition in (12), we choose $a_i(x) := 0$ on Γ_{out} . The existence proof is based on L^∞ -estimates obtained via a Ljapunov functional, a fixed-point argument and classical $W^{2,p}$ theory for linear parabolic systems. An essential drawback is that - in their approach - the diffusion coefficients need to be the same for all species. For a diffusion setting in a porous medium this can be justified by the observation that - usually - the advective flux dominates the diffusive one by order of magnitudes. Although not being completely uncommon in some practical applications with large Peclet number, $Pe \gg 8$ (cf. [Bet08]), in

general this is a serious restriction, in particular for free flows. A less serious restriction is $h = 0$ in (11) since this excludes some (technical) applications in which there is might be an injection or take-out of substance from the outside. Mahato extends this setting in several directions; among others he obtains global and unique *weak* solutions with $u(t, \cdot) \in W^{1,p}(\Omega)^m$, $p > N + 2$, under far less restrictive assumptions on the initial data, but still with one and the same scalar diffusion coefficient for all species ([Mah13a]). His approach also allows for some non-mooth dissolution from (parts of) $\partial\Omega$ contributing to the species in Ω and $h \neq 0$ ([MaB13c]).

In this note we address the issue of identical diffusion coefficients and show that the unique existence of weak solutions can still be guaranteed under the following assumptions: Let

$$\begin{aligned} D_0^* &= \text{const.} > 0, \quad D_{0k} := \text{diag}(D_0^*, \dots, D_0^*) \in \text{Sym}(N), \\ D_0 &:= (D_{01}, \dots, D_{0m}) \in \text{Sym}(N)^m \end{aligned}$$

and

$$h_0 \in L^q(\partial\Omega)^m. \quad (14)$$

Then there is an $L^\infty(\Omega; \text{Sym}(N))$ -neighbourhod of D_0^* , $U = U(D_0^*)$, such that for all $D \in U$ there is a unique weak solution of (10).

Remark: In this note we do not directly employ the particular structure (1) - (3) of the reaction rates incorporated into $\widehat{f}(u)$, rather we use (15) in theorem 1 below the proof of which is based on this structure. All we need here is - in (3) -

$$\widehat{f} \in C^1(\mathbb{R})^m. \quad (15)$$

For ease of notation we assume

$$\# \text{ of unknown concentrations} = \# \text{ of reactions, i.e. } m = m_1. \quad (16)$$

2. Technical preliminaries

Spaces Let $p, q \in [1, \infty]$, $\frac{1}{r} + \frac{1}{s} = 1$, $\lambda \in [0, 1]$, $\Omega \subset \mathbb{R}^N$ - a bounded Lipschitz domain.

$\text{Sym}(N)$ is the set of all real symmetric matrices $A = (A_{ij})$ normed by $|A|_{\text{Sym}(N)} := \max_{i,j=1,\dots,N} |A_{ij}|$.

$(\cdot, \cdot)_{p,\lambda}$ and $[\cdot, \cdot]_\lambda$ stand for the real- and complex-interpolation functor, resp. (cf. [Tri78]),

$L^p(\Omega)$, $H^{1,p}(\Omega)$, $W^{2,p}(\Omega)$, $C^\lambda(\overline{\Omega})$ - (standard) Lebesgue, Sobolev- and Hölder spaces, resp., with their any of their standard norms (cf. [AdF03], [Tri78]).

" \hookrightarrow " denotes a continuous imbedding.

Let Y be a normed space. $L^p(S; Y)$ and $H^{1,p}(S; Y)$ are the (standard) Bochner and Sobolev-Bochner spaces (cf. [Eme04], [Wlo87]).

Y^* stands for the dual of Y , the product $Y := Y_1 \times \dots \times Y_m$ of normed spaces Y_k is normed by $\|(y_1, \dots, y_m)\|_Y = \sum_{k=1}^m \|y_k\|_{Y_k}$ unless required otherwise. If X and Y are normed spaces, then $Iso(X; Y)$ stands for the set of all top-linear isomorphisms from $\mathfrak{L}(X; Y)$.

From here on we assume

$$p > N + 2 \text{ - fixed.} \quad (17)$$

The imbedding $L^p(\Omega)^m \hookrightarrow (H^{1,q}(\Omega)^*)^m$ is given by

$$\begin{aligned} L^p(\Omega)^m \ni w &\mapsto L_h : \\ \langle L_h, w \rangle &:= \sum_{i=1}^m \int_{\Omega} h_{0i}(x) w_i(x) dx, \quad w \in (H^{1,q}(\Omega))^m. \end{aligned} \quad (18)$$

We set

$$F_p := F_p(\Omega) := L^p(S; H^{1,p}(\Omega)) \cap H^{1,p}(S; (H^{1,q}(\Omega)^*)),$$

normed by

$$\|u\|_{F_p} := \|u\|_{L^p(S; H^{1,p}(\Omega))} + \|u\|_{L^p(S; (H^{1,q}(\Omega)^*)^*)} + \|u'\|_{L^p(S; (H^{1,q}(\Omega)^*)^*)}. \quad (19)$$

u' is the distributional derivative of u . The solution space of the system under consideration is

$$\mathfrak{F} = \mathfrak{F}(\Omega) := F_p(\Omega)^m.$$

Note that

$$F_p \subset C(\bar{S}; (H^{1,q}(\Omega)^*, H^{1,p}(\Omega))_{1-\frac{1}{p}, p}) \quad (20)$$

and

$$F_p \subset C(\bar{S}; C(\bar{\Omega})) \quad (21)$$

(cf. [Mah13a]).

For abbreviation, set

$$\begin{aligned} V &:= H^{1,p}(\Omega)^m, \quad W := (H^{1,q}(\Omega))^m, \\ V_0 &:= ((H^{1,q}(\Omega)^*, H^{1,p}(\Omega))_{1-\frac{1}{p}, p})^m \text{ and } V_{\partial\Omega} := L^q(\partial\Omega)^m. \end{aligned}$$

Thus

$$\mathfrak{F} = L^p(S; V) \cap H^{1,p}(S; W^*) \subset C(\bar{S}; V_0). \quad (22)$$

We introduce

$$E_1 := L^\infty(\Omega; Sym(N))^m, \quad E_2 := \mathfrak{F}_p^u, \quad E := E_1 \times E_2, \quad (23)$$

Let $D = (D_1, \dots, D_m) \in E_1$. E_1 is normed by

$$|D|_{E_1} := \max_{\substack{i=1, \dots, N, \\ k=1, \dots, m}} |D_{kij}|_{L^\infty(\Omega)}, \cdot$$

Finally, let

$$\begin{aligned} Z_1 &:= L^p(S; W^*) \text{ ("time-derivative space"),} \\ Z_2 &:= V_0 \text{ ("initial value space"),} \quad Z := Z_1 \times Z_2. \end{aligned} \quad (24)$$

Note: If $D_k = \text{diag}(D^*, D^*, \dots, D^*)$, $D^* = \text{const.} \in \mathbb{R}$ for all k , then $|D|_{E_1} = |D^*|_{L^\infty(\Omega)}$.

Operators and forms

For functions $v = v(t, x), t \in \bar{S}, x \in \bar{\Omega}$, we set $v(t) := v(t, \cdot)$. $D_k G := \frac{\partial G}{\partial x_k}$ is

the partial F-derivative of $G = G(\xi_1, \dots, \xi_n)$, $DH(\xi)$ - the F-derivative of $H = H(\xi)$,

$\hat{f} \in C^1(\mathbb{R}^m, \mathbb{R}^m)$ (production-rate vector, cf. (3) and (15)),

$f : V \rightarrow W^*$, $\langle f(u), v \rangle := \int_{\Omega} \hat{f}(u(x))^T v(x) dx$ (the V -realisation of \hat{f}),

$F : \mathfrak{F} \rightarrow L^p(S; W^*)$, $\langle (F(u))(t), v \rangle := \int_{\Omega} \hat{f}(u(t, x))^T v(x) dx$ a.a.t $\in S$,

$A_{01}(D, u) := -(\operatorname{div}(D_1 \nabla u_1), \dots, \operatorname{div}(D_m \nabla u_m))^T$, $A_{02}(D, u) := (\operatorname{div} u_1 \mathbf{q}, \dots, \operatorname{div} u_m \mathbf{q})^T$
for $u = (u_1, \dots, u_m)^T \in C^2(\bar{\Omega})^m$, $D = (D_1, \dots, D_m) \in E_1$ (cf. (23)),

$A_0 := A_{01} + A_{02}$.

$A(D, \cdot)$ is the V -realisation of $A_0(D, \cdot)$, i.e. $A : E_1 \times V \rightarrow W^*$, where

$$\begin{aligned} A(D, u) & : = A_1(D, u) + A_2(u) + B(h), \\ \langle A_1(D, u), v \rangle & : = \sum_{k=1}^m \int_{\Omega} D_k \nabla u_k(t, \cdot) \cdot \nabla v_k, \quad u \in V, v \in W, \\ \langle A_2(u), v \rangle(t) & : = \sum_{k=1}^m \int_{\Omega} u_k(t, \cdot) \mathbf{q}(t, \cdot) \cdot \nabla v_k dx, \quad u \in V, v \in W, \\ \langle B(h), v \rangle & = \sum_{k=1}^m \int_{\partial\Omega} h_k(t, \cdot) v_k d\sigma, v \in V. \end{aligned}$$

The corresponding extensions for time dependent $u = u(t)$ is, with the same notation, given by $A(D, u)(t) := A(D, u(t))$. Similarly we proceed with A_1, A_2 and B and obtain

$$A, A_1, A_2 : E_1 \times E_2 \rightarrow Z_1, \quad B : L^q(S; V_{\partial\Omega}) \rightarrow Z_1.$$

$h \neq 0$ corresponds to non-homogeneous flux boundary conditions.

Finally set

$$G_1(D, u) : = u' + A(D, u) + B(D, h_0) - F(u), \quad (25)$$

$$G_2(D, u) : = u(0) - g_0, \quad (26)$$

$$G : = (G_1, G_2)^T.$$

Weak solutions Let $D \in E_1$. u is called a weak solution of problem (9) - (12), if

$$\begin{aligned} u & \in \mathfrak{F}, \\ u'(t) + A(D, u(t)) + B(h(t)) & = F(u)(t) \quad \text{in } W^* \text{ for a.a.t } \in S, \\ u(0) & = u_0. \end{aligned} \quad (27)$$

Alternatively: u is a weak solution if

$$G(D, u) = 0 \quad \text{in } Z := Z_1 \times Z_2, \quad u \in \mathfrak{F} \quad (28)$$

We will make use of the following simple

Lemma 1 Let P_k and Q_k be normed spaces and $P_1 \hookrightarrow Q_1$, $Q_2 \hookrightarrow P_2$, $W \subset P_1 \times P_2$, $M : Q_1 \rightarrow Q_2$ - F-differentiable and $\overline{M} := M/P_1$. Then:

$$\mathfrak{L}(Q_1; Q_2) \hookrightarrow \mathfrak{L}(P_1; P_2), \quad (29)$$

$$C(W; \mathfrak{L}(Q_1; Q_2)) \hookrightarrow C(W; \mathfrak{L}(P_1; P_2)) \quad (30)$$

and

$$D\overline{M}(u) = DM(u)/P_1 \in \mathfrak{L}(P_1; P_2). \quad (31)$$

Proof. Follows directly from the definitions. \triangle

4. Result

Theorem Let $D_0^* = \text{const.} > 0$ and let $D_0 := (D_{01}, \dots, D_{0m}) \in (\mathbb{R}^N)^m$ be the vector of identical diagonal matrices with identical entries

$$D_{0k} = \text{diag}(D_0^*, \dots, D_0^*) \in \text{Sym}(N), \quad k = 1, \dots, m,$$

assume for the initial function

$$g \in V_0 \text{ such that for all components: } g_i \geq 0,$$

$$h \in Z_1$$

and let (12) be satisfied. Then there is a neighbourhood $U = U(D_0)$ in $L^\infty(\Omega; \text{Sym}(N)^m)$ such that (28) is uniquely solvable for all $D \in U$. The components of the solutions are non-negative.

Note: The proof of the implicit function theorem provides estimates for the size of $U(D_0)$. Here we do not yet go into detail.

5. Proof of the theorem We employ the (classic version of the) implicit function theorem (cf. [Wlo71], e.g.):

By [Ma13a],[MaB13b] there is a unique solution $u_0 \in \mathfrak{F}$ of

$$G(D_0, u_0) = 0 \quad \text{in } Z. \quad (32)$$

The components of u are non-negative. We show

$$\langle \langle DF(u(t), v), \varphi \rangle \rangle = \int_\Omega D_u f(u(t, x)) v(x) \varphi(x) dx \quad (33)$$

for a.a. $t \in S$, $u, v \in \mathfrak{F}$, $\varphi \in W$,

$$\langle D_1G(D, u), \bar{D} \rangle = (A_1(\bar{D}, u), 0)^T, \quad (34)$$

$$\langle D_2G(D, u), v \rangle = (v' + A(D, v) - \langle DF(u), v \rangle, v(0))^T \text{ for } u, v \in \mathfrak{F}, \quad (35)$$

$$G \in C^1(E_1 \times E_2; Z) \quad (36)$$

and

$$L := D_2G(D_0, u_0) \in Iso(E_2, Z). \quad (37)$$

Re. (33) Set

$$\begin{aligned} P_1 &:= E_2 (= \mathfrak{F}!), \quad P_2 := Z_1 (= L^p(S; (H^{1,q}(\Omega)^*)^m)), \\ Q_1 &:= C(S; C(\bar{\Omega})^m), \quad Q_2 := L^p(S; C(\bar{\Omega})^m). \end{aligned}$$

Since $f \in C^1(\mathbb{R}^m)^m$, $DF(u) \in \mathfrak{L}(Q_1; Q_2)$ exists and the restriction F/P_1 is differentiable with $D(F/P_1)(u) \in \mathfrak{L}(P_1; P_2)$ for all $u \in P_1$. Therefore, $\langle DF(u), v \rangle$ exists in (35). The verification of the rest of (35) follows right away by using the linearity of the corresponding expressions.

In order to **see (36)** we note that $DF(\cdot) \in C(E_1; \mathfrak{L}(Q_1; Q_2))$ and, by (30), $DF/P_1 \in \mathfrak{L}(P_1; P_2)$. This implies (36).

Given the linearity of the corresponding terms, **(34)** is straightforward. Therefore $D_1G(D, u)$ exist. To see the continuity of $D_2G(\cdot, \cdot)$ we note, that $E_1 \ni D \mapsto A_1(D, u) \in Z_1$ is linear and continuous, thus Lipschitz. Therefore $E_1 \ni D \mapsto D_2G(D, u) \in \mathfrak{L}(E_2; Z)$ is Lipschitz. This and the continuity of $\mathfrak{F} \ni u \mapsto D_2G(D, u) \in \mathfrak{L}(E_2; Z)$ imply the continuity of $E \ni (D, u) \mapsto D_2G(D, u) \in \mathfrak{L}(E_2; Z)$. Having the continuity of one partial derivative ($D_2G(\cdot, \cdot)!$) of a total of two, we obtain the existence of $DG(\cdot, \cdot)$. The estimate

$$\|A_1(\bar{D}, u)\|_{Z_1} \leq |\bar{D}|_{E_1} \|u\|_{L^p(S, V)} \leq |\bar{D}|_{E_1} \|u\|_{E_2} \text{ (definition of } W \text{ !)}$$

implies

$$\|D_1G(D, u)\|_{\mathfrak{L}(E_1, Z)} \leq |\bar{D}|_{E_1} \|u\|_{E_2}. \quad (38)$$

The continuity of both D_1G and D_2G imply the continuity of DG .

Re. (37): Let $(f_1, g_1) \in Z$, $\kappa > 0$. In order to verify (37) it remains to show, that the problem

$$\text{Find } v \in E_2 (= \mathfrak{F}!) \text{ with} \quad (39)$$

$$v' + (A_1(D_0, v) + \kappa v) + B(h) - (\langle DF(u_0), v \rangle + \kappa v - A_2(v)) = f_1, \quad (40)$$

$$v(0) = g_1. \quad (41)$$

has a unique solution. The operator $A_1(D_0, \cdot) + \kappa \cdot$ (with flux-boundary conditions $h = 0$) possesses the maximal-regularity property on V in the L^p -sense (cf. [PrS01]; also cf. [KuL01]) and $-\langle DF(u_0), \cdot \rangle - \kappa \cdot + A_2 \cdot$ is a lower-order perturbation (with smooth coefficients). Therefore (39) - (41) is uniquely solvable.

∇

6. Extensions The approach from the previous sections can also be applied

to Kräutle's $W^{2,p}$ -setting. Modifying the setting (25), (26), (32) as

$$G_1(D, h, u) : = u' + A(D, u) + B(D, h) - F(u), \quad (42)$$

$$G_2(D, j, u) : = (u(0) - g_0, B_0(D, u) - h)^T \quad (43)$$

$$G : = (G_1, G_2)^T.$$

one can also deal with (perhaps small) nonhomogeneities h . Moreover, the size of neighbourhood $U(D_0)$ (cf. section 4) can be estimated. This will be addressed somewhere else.

7. References

- [AdF03] Adams, R.A., Fournier, J.F., Sobolev Spaces, Volume 140 of Pure and Applied Mathematics, Academic Press, Amsterdam, 2nd ed., 2003
- [Bet08] Bethke, C.M., Geochemical and biogeochemical reaction modeling. Cambridge Univ. Press, Cambridge, 2nd ed., 2008
- [Eme04] Emmrich, E.. Gewöhnliche und Operator-Differentialgleichungen. Vieweg, Wiesbaden, 2004
- [Kra08] Kräutle, S., General Multi-Species Reactive Transport Problems in Porous Media: Efficient Numerical Approaches and Existence of Global Solutions, Habilitation Thesis, University of Erlangen, Dept. of Mathematics, March 2008
- [Kra11] Kräutle, S., Existence of Global Solutions of Multicomponent Reactive Transportproblems with Mass Action Kinetics in Porous Media, J. Appl. Anal. and Comput., Vol. 1, Number 4, November 2011, pp. 497 - 515
- [Ma13a] Mahato, H-S, Homogenization of a system of semilinear multi-species diffusion-reaction equations with homogeneous Neuman boundary conditions in an $H^{1,p}$ -setting, Ph.D dissertation, University of Bremen, FB Mathematik und Informatik, May 2013
- [MaB13b+c] Mahato, H-S, Papers in preparation
- [HaR08] Haller-Dintelmann, R., Rehberg, J., Maximal parabolicregularity for divergence operators including mixed boundary conditions. Preprint No. 1288, Weierstrass-Institut für Angewandte Analysis und Stochastik, Berlin 2008
- [KuL01] Kunstmann, P. C., Weis, L., Perturbation theorems for maximal L_p -regularity, Annali della Scuola Norm. Sup. di Pisa. Classe die Scienze 4^e serie, t. 30, nr. 2, 2001, pp. 415 - 435

- [PrS01] Prüss, J., Schnaubelt, R, Solvability and Maximal Regularity of Parabolic Evolution Equations with Coefficients Continuous in Time, Journ. of Mathem. Analysis and Applications 256, pp. 405 - 430, 2001
- [Tri78] Triebel, H., Interpolation theory, function spaces, differential operators, North-Holland Publishibg Comp., 1978
- [Wlo87] Wloka, J., Partial Differential Equations, Cambridge University Press, 1987
- [Wlo71] Wloka, J., Funktionalanalysis und Anwendungen, de Gruyter, 1971