ROCKY MOUNTAIN
JOURNAL OF MATHEMATICS
Volume 17, Number 3, Summer 1987

ON THE NONNEGATIVITY OF SOLUTIONS OF REACTION DIFFUSION EQUATIONS

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ABSTRACT. Consider the system of reaction diffusion equations

$$(*) \qquad \frac{\partial u}{\partial t} = A\Delta u + f(u, \nabla_x u, x, t)$$

where A is a $p \times p$ matrix, $u(x,t)$ is a p-dimensional vector with components $u^{(j)}(x,t), j = 1, \cdots, p$ and where $(x,t) \in R^n \times (0,\infty)$. Motivated by phenomena modeled by (*) in which off-diagonal entries of the matrix A are specifically included, we study the circumstances under which solutions of the initial boundary value problem for (*) in $\Omega \times (0,T)$ (Ω a bounded domain) with either homogeneous Dirichlet or Neumann boundary conditions holding on $\partial\Omega \times (0,T)$, have the property that starting out from nonnegative initial data, they will remain nonnegative for all subsequent times. For the simplest equation modeling multicomponent diffusion [**4**] which corresponds to $f \equiv 0 : \frac{\partial u}{\partial t} = A\Delta u$ with A a constant positive definite matrix, we show that the property of persistence of nonnegativity for solutions cannot hold unless the off-diagonal entries of A are not present. To obtain a result assuring the persistence of nonnegativity with the off-diagonal entries a_{jk} of A present, we assume that these entries depend on u and $\nabla_x u$ as follows:

$$a_{jk} = u^{(j)}\alpha_{jk}(u, \nabla_x u, x, t) \quad (j \neq k)$$

while the diagonal entries are assumed to be positive and f is suitably structured. This result is applicable to the equations used by Keller and Segel [**10**] to model slime mold aggregation; as well as to more sophisticated models for multicomponent diffusion accompanied by a reaction such as appear in the most general formulation of combustion theory.

1. Introduction.

Equations of the form

$$(1.1) \qquad \frac{\partial u}{\partial t} = A\Delta u + f(u, \nabla_x u, x, t),$$

Received by the editors on August 20, 1984 and in revised form on August 22, 1985.

where $u = u(x,t) = [u^{(1)}(x,t), \ldots, u^{(p)}(x,t)]$ is a p-dimensional vector function of $(x,t) \in R^n \times (0,\infty)$ with components $u^{(j)}(x,t), (j = 1, \ldots, p), A = [a_{jk}]_{j,k=1}^{p}$ is a $p \times p$ matrix, and f is a vector function mapping $(u, \nabla_x u, x, t)$ into R^p have been used extensively to model various chemical and biological phenomena (see, e.g., [**1**], [**3**], [**5**], [**7**], [**13**], and [**14**]). In that case the components of $u(x,t)$ represent either chemical concentrations or biological population densities; and one would then like to study the evolution of $u(x,t)$ from a given initial state $u(x,0) = u_0(x)$ in a cylindrical space time domain of $R^n \times (0,\infty)$ under a variety of boundary conditions. In view of the phenomena being modeled by (1.1) it is natural to inquire into the circumstances under which solutions to such initial boundary value problems have the property that starting out from nonnegative initial data they will remain nonnegative for all subsequent times. When this happens we will say, for brevity, that the solutions of our problem preserve nonnegativity.

Conditions guaranteeing the preservation of nonnegativity are known in case A is a diagonal matrix (see, for example [**5**, p. 29]). However, the situation in which A is not not necessarily diagonal does not seem to have attracted a great deal of attention, although equations of this type have been considered for modeling purposes (see [**4**], [**6**], [**9**], [**10**]. [**12**], [**16**], [**18**] and [**19**].) It is the aim of this paper to consider the question of preservation of nonnegativity for solutions of equations of the form (1.1), allowing for the appearance of the off-diagonal terms in the matrix A.

We will first consider this question for the simplest equation of this type, namely,

$$\frac{\partial u}{\partial t} = A\Delta u \tag{1.2}$$

where A is a constant matrix and which has been used as an approximative model for the simultaneous diffusion of several chemical species, a situation which is frequently referred to as "multicomponent diffusion" (see [**4**], [**18**] and [**19**]). Assuming that A is a positive definite matrix (which assures that the various initial-boundary value problems mentioned above are well-posed) we will show that the solutions of (1.2) in $\Omega \times (0,T)$ (with Ω a bounded domain in R^n) subject to either homogeneous Dirichlet or Neumann boundary conditions preserve nonnegativity if and only if A is a diagonal matrix.

These negative results suggest that in order to obtain a theorem assuring the preservation of nonnegativity with the inclusion of the off-diagonal terms $a_{jk}\Delta u^{(k)}, j \neq k$, in (1.1), we will have to allow the off-diagonal coefficients a_{jk} to depend on u and possibly also the first order spatial derivatives of u. Such a result is indeed possible, as we will show, when a_{jk} has the form

$$a_{jk} = u^{(j)}\alpha_{jk}(u, \nabla_x u, x, t) \quad j \neq k, \tag{1.3}$$

with the diagonal coefficients a_{jj} assumed to be positive and provided that the term $f(u, \nabla_x u, x, t)$ in (1.1) is then suitably structured. This result turns out to be applicable to the equations considered by Keller and Segel in [**10**] to model slime mold aggregation. It is also applicable to the more sophisticated model involving (1.1) for diffusion of several chemical species with a reaction in which the diffusion coefficients, the a_{jk} in (1.1), are assumed to be concentration dependent. Such models are discussed by Aris [**1**] and Hasse [**9**] from a general point of view; in particular, the most comprehensive formulation of combustion theory employs such a model (see Buckmaster and Ludford [**2**]).

2. Preservation of nonnegativity for the multicomponent diffusion equation. In this section we will discuss the preservation of nonnegativity for the simplest model, utilizing equation (1.2), of multicomponent diffusion. Our principal result is

THEOREM 2.1. *Consider the equations*

$$\frac{\partial u}{\partial t} = A\Delta u \tag{2.1}$$

where A is a constant positive definite matrix. Then classical solutions of the initial boundary value problem for (2.1) in $\Omega \times (0,T)$ under either homogeneous Dirichlet or Neumann boundary conditions preserve nonnegativity if and only if A is a diagonal matrix.

REMARK. The same conclusion also holds for solutions of the Cauchy problem for (2.1) in $R^n \times (0,T)$ (with the same proof for the necessity but a different proof for the sufficiency).

PROOF. If A is a diagonal, the preservation of nonnegativity is an immediate consequence of the maximum principle for the heat equation.

To prove the converse, assume that $A = [a_{jk}]_{j,k=1}^{p}$ is not diagonal; there is then an off-diagonal entry in the matrix A which is not zero. Relabelling, if necessary, we may assume this entry to be a_{12}.

Consider now the equation for $u^{(1)}(x,t)$:

$$\frac{\partial u^{(1)}}{\partial t}(x,t) = \sum_{k=1}^{p} a_{1k}\Delta u^{(k)}(x,t), \tag{2.2}$$

$(x,t) \in \Omega \times (0,T)$. To show that nonnegativity is not preserved, choose the initial data $u_o(x) = [u^{(1)}(x), \dots, u_o^{(p)}(x)]$ in Ω $U_0^{(1)}(X)$ so that

$$u_o^{(k)}(x) \equiv 0 \quad \text{for } k \neq 2, \; x \in \Omega, \tag{2.3}$$

while taking $u_o^{(2)}(x)$ to be a $C_o^{\infty}(\Omega)$ function with

$$u_o^{(2)}(x) \geq 0 \quad \text{for } x \in \Omega \tag{2.4}$$

and

$$a_{12}\Delta u_o^{(2)}(x_o) < 0, \tag{2.5}$$

x_o being a fixed but arbitrary point in Ω. Since $a_{12} \neq 0$, such a choice is clearly possible.

Because of the smoothness of our initial data, the solution of (2.1) under consideration will then, together with its second order spatial derivatives, be continuous down to $t = 0$ (see [**11**, p. 616, Thm. 10.1]). Hence, from (2.2), (2.3) and (2.5) it follows that $\frac{\partial u^{(1)}}{\partial t}(x_o, 0) < 0$; and this together with (2.3) implies that $u^{(1)}(x_0, t)$ will be negative for all sufficiently small positive values of t. Since our initial data $u_o(x)$ is nonnegative, this proves that nonnegativity is not preserved.

3. A theorem assuring preservation of nonnegativity. The objective of this section is to consider the following result which guarantees preservation of nonnegativity for solutions of equations of the form (1.1) in which we specifically allow for the inclusion of the off diagonal terms in $A\Delta u$. For the purposes of stating and proving this result it will be more convenient to write it out in component form.

THEOREM 3.1. *Let the components $u^{(j)}(x,t), j = 1,\dots,p$, of $u(x,t)$ satisfy the system of equations*

$$(3.1)\quad \frac{\partial u^{(j)}}{\partial t} = \sum_{k=1}^{p} a_{jk}\Delta u^{(k)} + \sum_{\ell=1}^{n} b_{j\ell}\frac{\partial u^{(j)}}{\partial x_\ell} + \sum_{k=1}^{p} c_{jk}u^{(k)} \quad (j = 1,\dots,p)$$

in $\Omega \times (0,T)$ where we assume that

$$(3.2)\qquad a_{jk} = u^{(j)}\alpha_{jk}(u, \frac{\partial u}{\partial x}, x, t) \quad (j \neq k);$$

$$(3.3)\qquad a_{jj} = a_{jj}(u, \frac{\partial u}{\partial x}, x, t) > 0;$$

$$(3.4)\qquad c_{jk} = c_{jk}(u, \frac{\partial x}{\partial x}, xt) \geq 0 \quad (j \neq k),$$

with α_{jk}, a_{jj} and c_{jk} being well-defined continuous functions for $u \in R^p, \frac{\partial u}{\partial x} \in R^{np}$ and $(x,t) \in \overline{\Omega} \times [0,T]$. Now let u be a smooth classical solution of (3.1) satisfying either homogeneous Dirichlet or Neumann boundary conditions with

$$(3.5)\qquad \sup_{(x,t)\in\Omega\times(0,T)} [|u| + |\frac{\partial u}{\partial x}| + |\Delta u|] < \infty.$$

Then, for such solutions of (3.1), non-negativity is preserved.

REMARK 1. The same conclusion may be obtained with the boundary conditions replaced more generally by either

$$(3.6)\qquad u^{(j)} \geq 0 \text{ on } \partial\Omega \times (0,T), \quad (j = 1,\dots,p),$$

$$(3.7)\qquad \frac{\partial u^{(j)}}{\partial n} \geq 0 \text{ on } \partial\Omega \times (0,T), \quad (j = 1,\dots,p),$$

or

$$(3.8)\quad \frac{\partial u^{(j)}}{\partial n} + \beta_j u^{(j)} \geq 0 \text{ on } \partial\Omega \times (0,T), \quad (j = 1,\dots,p), \text{ with } \beta_j \geq 0,$$

where in the last two conditions, $\frac{\partial}{\partial n}$ denotes the exterior normal derivative on $\partial\Omega$.

REMARK 2. The equations considered by Keller and Segel in [**10**] to model slime mold aggregation are, in the notation of [**17**; pp. 163-165, eq. (10) and eq. (11)],

$$\tag{3.9} \begin{cases} \frac{\partial a}{\partial t} = \frac{\partial}{\partial x}(\mu \frac{\partial a}{\partial x} - X a \frac{\partial p}{\partial x}) \\ \frac{\partial p}{\partial t} = D \frac{\partial^2 p}{\partial x^2} - kp + fa \end{cases}$$

where $a = a(x,t)$ represents the population density of an ameobae culture with the dimension of x-space, for simplicity, assumed to be 1; and $p = p(x,t)$ represents the concentration of a certain chemical attractant for the amoebae which they themselves secrete; the remaining parameters μ, χ, D, k and f appearing in these equations are all assumed to be positive constants. Differentiating out the right side of the equation for $\frac{\partial a}{\partial t}$, we see that (3.9) becomes

$$\begin{cases} \frac{\partial a}{\partial t} = \mu \frac{\partial^2 a}{\partial x^2} - \chi a \frac{\partial^2 p}{\partial x^2} - (\chi \frac{\partial p}{\partial x}) \frac{\partial a}{\partial x} \\ \frac{\partial p}{\partial t} = D \frac{\partial^2 p}{\partial x^2} - kp + fa \end{cases}$$

which is precisely of the form (3.1) with the coefficients satisfying conditions (3.2)-(3.4).

REMARK 3. In the more exact theory of multicomponent diffusion for several chemical species, with or without reaction, modelled by equation (1.1), the a_{jk}'s are diffusion coefficients which are generally to be regarded as depending on the concentrations $u = [u^{(1)}, \ldots, u^{(p)}]$ in such a way that a_{jk} should vanish when $u^{(j)}$ vanishes for $j \neq k$ (see [**8**, p. 283] and [**16**, p.1991]). If the a_{jk} vanishes to a sufficiently high order with $u^{(j)}$, then Theorem 3.1 guarantees that the $u^{(j)}$'s will be nonnegative as long as the solution lasts.

PROOF OF THEOREM 3.1. Under the assumptions made, the j^{th} equation of the system (3.1) can be re-written as

$$\tag{3.10} \frac{\partial u^{(j)}}{\partial t} = a_{jj} \Delta u^{(j)} + \sum_{\ell=1}^{n} b_{j\ell} \frac{\partial u^{(j)}}{\partial x_\ell} + \sum_{k=1}^{p} q_{jk} u^{(k)} \quad (j = 1, \ldots, p),$$

where

$$q_{jj}(x,t) = \sum_{\substack{k=1 \\ k\neq j}}^{p} \alpha_{jk}(u, \frac{\partial u}{\partial x}, x, t)\Delta u^{(k)} + c_{jj}(u, \frac{\partial u}{\partial x}, x, t)$$

and

$$q_{jk}(x,t) = c_{jk}(u, \frac{\partial u}{\partial x}, x, t) \geq 0 \quad \text{for } j \neq k, \tag{3.11}$$

and where we are regarding the solution and its derivatives as known functions of x and t.

Once the equations are recognized to be of the form (3.10) with, according to (3.11), the coefficients $q_{jk} \geq 0$ for $j \neq k$, the desired results follow by applying standard theorems for solutions of parabolic inequalities, see e.g., [**15**, pp. 188-190]. In order to be able to apply these theorems on parabolic inequalities, it is essential to know that the coefficients q_{jk} are all bounded in $\Omega \times (0,T)$ and this is a consequence of our continuity assumptions on the coefficients α_{jk} and c_{jk} together with the assumption (3.5).

Finally, as a further variation on the method used here, we want to point out that precisely the same proof works if, in place of (3.2), we assume that the off diagonal coefficients have the form

$$a_{jk} = u^{(j)}\alpha_{jk}(u, \frac{\partial u}{\partial x}, x, t) + \sum_{\ell=1}^{n} \beta_{j\ell}^{k}(u, \frac{\partial u}{\partial x}, x, t)\frac{\partial u^{(j)}}{\partial x_\ell} \quad (j \neq k).$$

Acknowledgement. The author wishes to thank Professor Paul Fife for suggesting some helpful simplifications and interesting additions.

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