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ON MAXIMUM PRINCIPLES FOR DIFFUSION IN THE PRESENCE OF THREE DIFFUSION PATHS

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Abstract

This note examines maximum principles for systems of parabolic partial differential equations describing diffusion in the presence of three diffusion paths. The particular system under consideration arises from a random walk model. For a more general system constraints on the various constants are given which guarantee maximum principles. Remarkably, the physical system arising from the random walk model automatically satisfies these constraints.

1. Introduction

The diffusion of ions and point defects in metals which are comprised of a continuous distribution of high-diffusivity paths such as grain boundaries and dislocations has recently been modelled by Aifantis [1, 2]. In the general theory it is assumed that each point of the medium is simultaneously occupied by n diffusion paths and the concentrations in each diffusion path are governed by a system of n parabolic partial differential equations. Recently, Hill [8] presented a simple discrete random walk model for diffusion which, in the continuous limit, gives rise to this system of partial differential equations. Extensive study has been completed for diffusion in the presence of two diffusion paths and the reader is referred to Aifantis and Hill [3], Hill and Aifantis [10] and Hill [9]. Further applications for this system of parabolic differential equations, when $n = 2$, arise in the theories of seepage of homogeneous liquids in fissured rocks (Barenblatt, Zheltov and Kochina [4]), the conduction of heat in heterogeneous media (Rubinstein [13]), and the transport of water through plant tissue (Molz [12]). In this

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note maximum principles are examined for the system of equations which describes diffusion in the presence of three diffusion paths, namely

$$\left.\begin{aligned}\partial u_1/\partial t &= D_1\nabla^2 u_1 - (a_{21} + a_{31})u_1 + a_{12}u_2 + a_{13}u_3,\\ \partial u_2/\partial t &= D_2\nabla^2 u_2 + a_{21}u_1 - (a_{12} + a_{32})u_2 + a_{23}u_3,\\ \partial u_3/\partial t &= D_3\nabla^2 u_3 + a_{31}u_1 + a_{32}u_2 - (a_{13} + a_{23})u_3,\end{aligned}\right\} \tag{1.1}$$

for $u_1(\mathbf{x}, t)$, $u_2(\mathbf{x}, t)$ and $u_3(\mathbf{x}, t)$ which are concentrations and taken to be non-negative. The diffusivities D_1, D_2 and D_3 are non-negative constants. The constants a_{ij} $(i, j = 1,2,3;\ i \neq j)$ represent transition probabilities in the random walk model of Hill [8] and are therefore non-negative.

In this note we develop maximum principles for the more general non-conservative system given by

$$\left.\begin{aligned}\partial u_1/\partial t &= D_1\nabla^2 u_1 - a_{11}u_1 + a_{12}u_2 + a_{13}u_3,\\ \partial u_2/\partial t &= D_2\nabla^2 u_2 + a_{21}u_1 - a_{22}u_2 + a_{23}u_3,\\ \partial u_3/\partial t &= D_3\nabla^2 u_3 + a_{31}u_1 + a_{32}u_2 - a_{33}u_3,\end{aligned}\right\} \tag{1.2}$$

where a_{11}, a_{22} and a_{33} are further non-negative constants. We show that sufficient conditions on the constants which guarantee maximum principles for the system (1.2) are contained in

$$\left.\begin{aligned}a_{ii}a_{jj} &\geqslant a_{ij}a_{ji},\\ (a_{ii}a_{jj} - a_{ij}a_{ji})(a_{ii}a_{kk} - a_{ik}a_{ki}) &\geqslant (a_{ii}a_{jk} + a_{ik}a_{ji})(a_{ii}a_{kj} + a_{ij}a_{ki})\end{aligned}\right\} \tag{1.3}$$

for $i, j, k = 1,2,3;\ i \neq j,\ j \neq k,\ k \neq i$. For the system (1.1) we find that these inequalities are trivially satisfied upon substituting in (1.3)

$$a_{ii} = \sum_{\substack{j=1\\ j\neq i}}^{3} a_{ji} \qquad (i = 1,2,3). \tag{1.4}$$

Thus, remarkably, a maximum principle is available for the physical system (1.1) without imposing any further conditions on the constants a_{ij}. These results are given as theorems in the following section.

2. Maximum principles

In this section maximum principles are obtained for the systems (1.1) and (1.2). The concentrations u_1, u_2 and u_3 are defined over a bounded domain Ω in the $\mathbf{x}$-space and for the finite time interval, $0 \leqslant t \leqslant T$. This region of $\mathbf{x} - t$ space is denoted by

$$\mathbf{R} = \{(\mathbf{x}, t) : \mathbf{x} \in \Omega \cup \partial\Omega, 0 \leqslant t \leqslant T\}, \tag{2.1}$$

where $\partial\Omega$ is the piecewise continuously differentiable surface of Ω. Theorem 2.1 states that for particular conditions on the concentrations, at least one of the concentrations in the system (1.2) must attain its maximum on the boundary of **R**, whenever conditions (1.3) hold. Theorem 2.2 is the corresponding result for the system (1.1). The following lemma and definition are required.

LEMMA. *Let A, B and $b_{ij}(i, j = 1, 2)$ be positive constants. If*

$$-b_{11}A + b_{12}B > 0 \quad \text{and} \quad b_{21}A - b_{22}B > 0, \tag{2.2}$$

then

$$b_{12}b_{21} - b_{11}b_{22} > 0. \tag{2.3}$$

PROOF. The first of (2.2) implies $B > b_{11}b_{12}^{-1}A$. The second of (2.2) implies $A > b_{22}b_{21}^{-1}B$. The elimination of either A or B gives $b_{11}b_{22}b_{12}^{-1}b_{21}^{-1} < 1$. This implies (2.3).

DEFINITION. *We say that $\{u_1, u_2, u_3\} \in H$ in S if and only if*
(i) $\{u_1, u_2, u_3\} \in C^2$ *in S, and*
(ii) $\{u_1, u_2, u_3\}$ *satisfy* (1.2) *in S,*
where S is an arbitrary region of the $\mathbf{x} - t$ space, and C^2 denotes the set of functions which are continuous together with their derivatives up to second order.

THEOREM 2.1. *At least one of u_1, u_2 and u_3 attains its maximum on the boundary of* **R** *if the following hold*:
(i) $\{u_1(\mathbf{x}, t), u_2(\mathbf{x}, t), u_3(\mathbf{x}, t)\} \in H$ *if* $\mathbf{x} \in \Omega, 0 < t < T$,
(ii) $\{u_1(\mathbf{x}, t), u_2(\mathbf{x}, t), u_3(\mathbf{x}, t)\}$ *are continuous if* $(\mathbf{x}, t) \in \mathbf{R}$,
(iii) $\{u_1(\mathbf{x}, t), u_2(\mathbf{x}, t), u_3(\mathbf{x}, t)\} \geqslant 0$ *if* $(\mathbf{x}, t) \in \mathbf{R}$,
(iv) $a_{11}a_{22} > a_{12}a_{21}, a_{11}a_{33} > a_{13}a_{31}$,
(v) $(a_{11}a_{22} - a_{12}a_{21})(a_{11}a_{33} - a_{13}a_{31}) \geqslant (a_{11}a_{23} + a_{13}a_{21})(a_{11}a_{32} + a_{12}a_{31})$.

PROOF. The substitution of the new concentrations

$$\left.\begin{aligned} u_1^* &= u_1 + \varepsilon e^{x(a_{11}/D_1)^{1/2}}, \\ u_2^* &= u_2 + \varepsilon e^{x(a_{22}/D_2)^{1/2}}, \\ u_3^* &= u_3 + \varepsilon e^{x(a_{33}/D_3)^{1/2}}, \end{aligned}\right\} \tag{2.4}$$

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for $\varepsilon > 0$, into (1.2) yields

$$\left.\begin{aligned} &D_1\nabla^2 u_1^* - \partial u_1^*/\partial t - a_{11}u_1^* + a_{12}u_2^* + a_{13}u_3^* \\ &\qquad = \varepsilon\left[a_{12}e^{x(a_{22}/D_2)^{1/2}} + a_{13}e^{x(a_{33}/D_3)^{1/2}}\right] > 0, \\ &D_2\nabla^2 u_2^* - \partial u_2^*/\partial t + a_{21}u_1^* - a_{22}u_2^* + a_{23}u_3^* \\ &\qquad = \varepsilon\left[a_{21}e^{x(a_{11}/D_1)^{1/2}} + a_{23}e^{x(a_{33}/D_3)^{1/2}}\right] > 0, \\ &D_3\nabla^2 u_3^* - \partial u_3^*/\partial t + a_{31}u_1^* + a_{32}u_2^* - a_{33}u_3^* \\ &\qquad = \varepsilon\left[a_{31}e^{x(a_{11}/D_1)^{1/2}} + a_{32}e^{x(a_{22}/D_2)^{1/2}}\right] > 0. \end{aligned}\right\} \tag{2.5}$$

Assume that u_1^*, u_2^* and u_3^* all attain their maximum values in the interior of **R**, respectively at the points $(\mathbf{x}_1, t_1)$, $(\mathbf{x}_2, t_2)$ and $(\mathbf{x}_3, t_3)$. Therefore

$$\left.\frac{\partial u_i^*}{\partial t}\right|_{(\mathbf{x}_i, t_i)} = 0, \qquad \left.\nabla^2 u_i^*\right|_{(\mathbf{x}_i, t_i)} \leqslant 0, \qquad (i = 1, 2, 3). \tag{2.6}$$

It is observed that if u_i^* has a maximum on $\Omega \times (t = T)$, then $\partial u_i^*/\partial t \geqslant 0$ there. This only serves to strengthen the following inequalities. The substitution of (2.6) into (2.5) yields

$$\left.\begin{aligned} -a_{11}u_1^*(\mathbf{x}_1, t_1) + a_{12}u_2^*(\mathbf{x}_1, t_1) + a_{13}u_3^*(\mathbf{x}_1, t_1) > 0, \\ a_{21}u_1^*(\mathbf{x}_2, t_2) - a_{22}u_2^*(\mathbf{x}_2, t_2) + a_{23}u_3^*(\mathbf{x}_2, t_2) > 0, \\ a_{31}u_1^*(\mathbf{x}_3, t_3) + a_{32}u_2^*(\mathbf{x}_3, t_3) - a_{33}u_3^*(\mathbf{x}_3, t_3) > 0. \end{aligned}\right\} \tag{2.7}$$

The assumption that u_1^*, u_2^* and u_3^* attain their maximum values at $(\mathbf{x}_1, t_1)$, $(\mathbf{x}_2, t_2)$ and $(\mathbf{x}_3, t_3)$ respectively, implies

$$u_i^*(\mathbf{x}_i, t_i) \geqslant u_i^*(\mathbf{x}_j, t_j), \qquad (i, j = 1, 2, 3). \tag{2.8}$$

Inequalities (2.8) can be used to strengthen inequalities (2.7) to obtain

$$\left.\begin{aligned} a_{11}u_1^*(\mathbf{x}_1, t_1) < a_{12}u_2^*(\mathbf{x}_2, t_2) + a_{13}u_3^*(\mathbf{x}_3, t_3), \\ a_{22}u_2^*(\mathbf{x}_2, t_2) < a_{21}u_1^*(\mathbf{x}_1, t_1) + a_{23}u_3^*(\mathbf{x}_3, t_3), \\ a_{33}u_3^*(\mathbf{x}_3, t_3) < a_{31}u_1^*(\mathbf{x}_1, t_1) + a_{32}u_2^*(\mathbf{x}_2, t_2). \end{aligned}\right\} \tag{2.9}$$

The elimination of $u_1^*(\mathbf{x}_1, t_1)$ from (2.9) yields

$$\left.\begin{aligned} (a_{12}a_{21} - a_{11}a_{22})u_2^*(\mathbf{x}_2, t_2) + (a_{13}a_{21} + a_{11}a_{23})u_3^*(\mathbf{x}_3, t_3) > 0, \\ (a_{12}a_{31} + a_{11}a_{32})u_2^*(\mathbf{x}_2, t_2) + (a_{13}a_{31} - a_{11}a_{33})u_3^*(\mathbf{x}_3, t_3) > 0. \end{aligned}\right\} \tag{2.10}$$

Conditions (iv) of the theorem ensure that (2.10) is of the form (2.2). Application of the lemma to (2.10) gives

$$(a_{11}a_{22} - a_{12}a_{21})(a_{11}a_{33} - a_{13}a_{31}) < (a_{11}a_{23} + a_{13}a_{21})(a_{11}a_{32} + a_{12}a_{31}). \tag{2.11}$$

Inequality (2.11) constitutes a contradiction of condition (v) of the theorem. Therefore the assumption that u_1^*, u_2^* and u_3^* all attain their maximum values in the interior of **R** is invalid. Hence at least one of the following holds,

$$u_1^* \leqslant \max_{\partial \mathbf{R}} u_1^*, \qquad u_2^* \leqslant \max_{\partial \mathbf{R}} u_2^*, \qquad u_3^* \leqslant \max_{\partial \mathbf{R}} u_3^*, \tag{2.12}$$

where $\partial\mathbf{R}$ denotes the boundary of **R**. By returning to the original concentrations we see that at least one of the following holds:

$$\left.\begin{aligned} u_1 &\leqslant u_1 + \varepsilon e^{x(a_{11}/D_1)^{1/2}} \leqslant \max_{\partial \mathbf{R}} u_1 + \varepsilon \max_{\partial \mathbf{R}} e^{x(a_{11}/D_1)^{1/2}}, \\ u_2 &\leqslant u_2 + \varepsilon e^{x(a_{22}/D_2)^{1/2}} \leqslant \max_{\partial \mathbf{R}} u_2 + \varepsilon \max_{\partial \mathbf{R}} e^{x(a_{22}/D_2)^{1/2}}, \\ u_3 &\leqslant u_3 + \varepsilon e^{x(a_{33}/D_3)^{1/2}} \leqslant \max_{\partial \mathbf{R}} u_3 + \varepsilon \max_{\partial \mathbf{R}} e^{x(a_{33}/D_3)^{1/2}}. \end{aligned}\right\} \tag{2.13}$$

Letting ε approach zero yields

$$u_1 \leqslant \max_{\partial \mathbf{R}} u_1 \quad \text{or} \quad u_2 \leqslant \max_{\partial \mathbf{R}} u_2 \quad \text{or} \quad u_3 \leqslant \max_{\partial \mathbf{R}} u_3, \tag{2.14}$$

concluding the proof of the theorem.

Theorem 2.1 also holds if conditions (iv) and (v) are replaced by either of the following two sets of conditions:

$$\left.\begin{aligned} &(\text{iv})_1 \quad a_{11}a_{22} > a_{12}a_{21}, \qquad a_{22}a_{33} > a_{23}a_{32}, \\ &(\text{v})_1 \quad (a_{11}a_{22} - a_{12}a_{21})(a_{22}a_{33} - a_{23}a_{32}) \\ &\qquad\qquad \geqslant (a_{22}a_{13} + a_{23}a_{12})(a_{22}a_{31} + a_{21}a_{32}), \end{aligned}\right\} \tag{2.15}$$

or

$$\left.\begin{aligned} &(\text{iv})_2 \quad a_{11}a_{33} > a_{13}a_{31}, \qquad a_{22}a_{33} > a_{23}a_{32}, \\ &(\text{v})_2 \quad (a_{11}a_{33} - a_{13}a_{31})(a_{22}a_{33} - a_{23}a_{32}) \\ &\qquad\qquad \geqslant (a_{33}a_{12} + a_{32}a_{13})(a_{33}a_{21} + a_{31}a_{23}). \end{aligned}\right\} \tag{2.16}$$

As a direct consequence of substituting (1.4) into the above theorem, the corresponding maximum principle is obtained for (1.1). It has already been noted that conditions (iv) and (v) of Theorem 2.1 are trivially satisfied upon this substitution. Therefore the corresponding maximum principle for diffusion in the presence of three diffusion paths is as follows.

DEFINITION. *We say that* $\{u_1, u_2, u_3\} \in H^1$ *in S if and only if*

(i) $\{u_1, u_2, u_3\} \in C^2$ *in S, and*

(ii) $\{u_1, u_2, u_3\}$ *satisfy* (1.1) *in S*,

where S is an arbitrary region of the $\mathbf{x} - t$ *space, and* C^2 *denotes the set of functions which are continuous together with their derivatives up to second order.*

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THEOREM 2.2. *At least one of* u_1, u_2 *and* u_3 *attains its maximum on the boundary of* **R** *if the following hold*:

(i) $\{u_1(\mathbf{x}, t), u_2(\mathbf{x}, t), u_3(\mathbf{x}, t)\} \in H^1$ *if* $\mathbf{x} \in \Omega$, $0 < t < T$,

(ii) $\{u_1(\mathbf{x}, t), u_2(\mathbf{x}, t), u_3(\mathbf{x}, t)\}$ *are continuous if* $(\mathbf{x}, t) \in \mathbf{R}$,

(iii) $\{u_1(\mathbf{x}, t), u_2(\mathbf{x}, t), u_3(\mathbf{x}, t)\} \geqslant 0$ *if* $(\mathbf{x}, t) \in \mathbf{R}$.

Theorem 2.1 can be extended to systems in which there are more than three diffusion paths. The details are involved and become more difficult for larger systems. For n diffusion equations, corresponding to the system (1.2), inequalities (2.9) may be generalized to

$$a_{ii}u_i^*(\mathbf{x}_i, t_i) < \sum_{\substack{j=1 \\ j\neq i}}^{n} a_{ij}u_j^*(\mathbf{x}_j, t_j), \tag{2.17}$$

for $i = 1, 2, \ldots, n$. For four diffusion paths a theorem similar to Theorem 2.1 can be proved in which conditions (iv) remain the same, condition (v) becomes a strict inequality, and if two further conditions are stipulated:

$$\left.\begin{aligned}
&(a_{11}a_{44} - a_{14}a_{41})(a_{11}a_{33} - a_{13}a_{31}) > (a_{41}a_{13} + a_{43}a_{11})(a_{31}a_{14} + a_{34}a_{11}),\\
&[(a_{11}a_{44} - a_{14}a_{41})(a_{11}a_{33} - a_{13}a_{31}) - (a_{41}a_{13} + a_{43}a_{11})(a_{31}a_{14} + a_{34}a_{11})]\\
&\times[(a_{11}a_{22} - a_{12}a_{21})(a_{11}a_{33} - a_{13}a_{31}) - (a_{13}a_{21} + a_{23}a_{11})(a_{12}a_{31} + a_{32}a_{11})]\\
&\geqslant[(a_{41}a_{12} + a_{42}a_{11})(a_{11}a_{33} - a_{13}a_{31}) + (a_{41}a_{13} + a_{43}a_{11})(a_{12}a_{31} + a_{32}a_{11})]\\
&\times[(a_{13}a_{21} + a_{23}a_{11})(a_{31}a_{14} + a_{34}a_{11}) + (a_{11}a_{33} - a_{13}a_{31})(a_{14}a_{21} + a_{24}a_{11})].
\end{aligned}\right\} \tag{2.18}$$

There exist similar sets of conditions under which a maximum principle holds for systems with four diffusion paths. For further results concerning maximum principles for coupled parabolic systems the reader is referred to Dow [5], Dow [6], Dow and Výborný [7] and McNabb [11].

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