PERGAMON

International Journal of Heat and Mass Transfer 44 (2001) 863–865

International Journal of HEAT and MASS TRANSFER

www.elsevier.com/locate/ijhmt

Technical Note

Spatial extrema of advected scalars

G.D. McBain*

School of Engineering, James Cook University, Townsville, Qld 4811, Australia

Received 4 January 2000; received in revised form 3 April 2000

Abstract

Scalar fields satisfying the stationary advection–diffusion equation with no source or sink terms cannot have strong local extrema. This can be deduced from the elliptical nature of the equation. Here, however, an alternative, original and more physically motivated proof is offered. It highlights the positive role of diffusion in preventing extrema and the inability of advection to create them. Application is made to the theory of energy transfer by species interdiffusion and some anomalous numerical solutions from the literature are identified.

1. Introduction

This note concerns stationary solutions of the advection–diffusion equation without source or sink terms; for example, the steady-state temperature field in a pure fluid or ideal mixture when viscous dissipation, radiation, work against external forces, the Dufour effect, etc. may be neglected. Multiple advecting flows, which occur in multicomponent mixtures, are explicitly included.

The fact that no such scalar field can possess a strong relative maximum or minimum at an interior point of its domain of existence follows from the positive role of diffusion in eliminating them and the inability of advection to create them. This is reflected mathematically in the positive tensorial character of the diffusivity and the elliptic nature of the equation. The result is easily deduced from Hopf's Maximum Principle. Here, however, an alternative original and quite different proof is presented which, by avoiding the artifice of a comparison function and using vectorial and tensorial concepts rather than a general calculus of several variables, is, it is hoped, more conducive to physical intuition. The use of vectors also frees the result from any particular coordinate system. Since it adds little extra complexity, an anisotropic diffusivity is considered; $\mathbf{A}\cdot\nabla s$ being replaced by $A\nabla s$ in the special case of isotropy.

2. Definitions

A *divergence-free* vector field, $\mathbf{u}$, satisfies $\nabla\cdot\mathbf{u}=0$.
A *positive* tensor, $\mathbf{A}$, is one for which $\mathbf{u}\cdot(\mathbf{A}\cdot\mathbf{u})\geq 0$ for all vectors $\mathbf{u}$, with equality implying $u=\mathbf{0}$.

If the N scalar functions $h_{(i)}$, divergence-free vector fields $\mathbf{v}_{(i)}$ and the positive tensor field $\mathbf{A}$ are all continuously differentiable then

$$\nabla\cdot\left[-\mathbf{A}\cdot\nabla s+\sum_{i=1}^{N}h_{(i)}(s)\mathbf{v}_{(i)}\right]=0 \tag{1}$$

is the *steady-state advection–diffusion* equation for the scalar field, s.

A *regular solution* of a partial differential equation is

* Tel.: +61-7-47-81-55-12; fax: +61-7-47-81-46-60.
E-mail address: megdm@jcu.edu.au (G.D. McBain).

0017-9310/01/$ - see front matter
PII: S0017-9310(00)00136-8

one for which all the partial derivatives occurring in the equation exist and are continuous [1].

A *strong local maximum* of a scalar field is a point with a neighborhood in which the value of the field at every point is less than that at the maximum. Minima are defined analogously.

3. Theorem

No regular solution of the steady-state advection–diffusion equation possesses a strong local extremum.

4. Proof

The idea for this proof, suggested by Prof. Bob Street (1999, personal communication), is to recast the equation in quasilinear elliptic form, for which the result is known.

On carrying out the divergence,

$$\mathbf{A}{:}\nabla(\nabla s) + (\nabla \cdot \mathbf{A}) \cdot \nabla s - \sum_{i=1}^{N} \mathbf{v}_{(i)} \cdot h'_{(i)}(s)\nabla s = 0 \tag{2}$$

or

$$\mathbf{A}{:}\nabla(\nabla s) + \mathbf{v} \cdot \nabla s = 0 \tag{3}$$

where

$$\mathbf{v} \equiv \nabla \cdot \mathbf{A} - \sum_{i=1}^{N} h'_{(i)}(s)\mathbf{v}_{(i)} \tag{4}$$

and $h'_{(i)}(s)$ is the derivative of $h_{(i)}(s)$.

In Cartesian tensor notation with the summation convention in force, this is

$$A_{jk}s_{,jk} + v_j s_{,j} = 0, \tag{5}$$

which is of the form for which Hopf's Maximum Principle is shown to hold in treatises on partial differential equations [2]. The key here is that $\mathbf{A}$ is positive.

5. Alternative proof

The new proof is by contradiction: assume that there does exist an interior relative extremum. For definiteness, and without loss of generality, take this to be a minimum.

Construct a family of rays originating at the minimum and terminating when they encounter either:

(i) a boundary point of the domain; or
(ii) a stationary point, with respect to the ray, of s; i.e. $\hat{\boldsymbol{r}} \cdot \nabla s = 0$, where $\boldsymbol{r}$ is the unit radial vector from the minimum.

Except at the origin, and possibly the rays' termini, s is strictly increasing along the rays:

$$\hat{\boldsymbol{r}} \cdot \nabla s > 0, \tag{6}$$

by the definitions of a minimum and the rays (ii). Choose a value s_1 of s between that at the minimum and the least of those at the rays' termini. Let S be the set of points with $s = s_1$ passed through by the rays.

Each ray intersects S exactly once, and since s possesses at least two continuous spatial derivatives, S is closed and smooth enough to have a well-defined unit outward normal, $\hat{\boldsymbol{n}}$. No ray is tangent to S, since then the ray should have terminated, by (ii); thus,

$$\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{n}} > 0. \tag{7}$$

Now, by definition of the vector triple product,

$$\hat{\boldsymbol{r}} \times (\hat{\boldsymbol{n}} \times \nabla s) = (\hat{\boldsymbol{r}} \cdot \nabla s)\hat{\boldsymbol{n}} - (\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{n}})\nabla s, \tag{8}$$

but $\hat{\boldsymbol{n}} \times \nabla s = 0$, since the normal of a level surface is parallel to the gradient; therefore,

$$\hat{\boldsymbol{n}} \cdot (\mathbf{A} \cdot \nabla s) = \frac{(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{n}})}{(\hat{\boldsymbol{r}} \cdot \nabla s)} \nabla s \cdot (\mathbf{A} \cdot \nabla s) > 0 \tag{9}$$

by Eqs. (6), (7) and since $\mathbf{A}$ is positive. Thus, the inward diffusive flux is positive over the entire surface.

Integrate the steady-state advection–diffusion equation (1) over the volume V enclosed by S:

$$\iiint_V \nabla \cdot \left[-\mathbf{A} \cdot \nabla s + \sum_{i=1}^{N} h_{(i)}(s)\mathbf{v}_{(i)} \right] \mathrm{d}V. \tag{10}$$

Applying the divergence theorem gives:

$$\sum_{i=1}^{N} \iint_S \hat{\boldsymbol{n}} \cdot h_{(i)}(s)\mathbf{v}_{(i)} \, \mathrm{d}S = \iint_S \hat{\boldsymbol{n}} \cdot \mathbf{A} \cdot \nabla s \, \mathrm{d}S, \tag{11}$$

of which the right-hand side is positive by Eq. (9). The left-hand side, however, vanishes;

$$\iint_S \hat{\boldsymbol{n}} \cdot h_{(i)}(s)\mathbf{v}_{(i)} \, \mathrm{d}S = h_{(i)}(s_1) \iint_S \hat{\boldsymbol{n}} \cdot \mathbf{v}_{(i)} \, \mathrm{d}S \tag{12}$$

$$= h_{(i)}(s_1) \iiint_V \nabla \cdot \mathbf{v}_{(i)} \, \mathrm{d}V = 0; \tag{13}$$

by virtue of the hypotheses on the $\mathbf{v}_{(i)}$.

This is a contradiction, so the theorem is proved.

6. Notes

- The alternative proof may be summarized as follows. The existence of a strong local extremum would imply the existence of a closed level surface on which the normal component of the gradient, and so the normal component of the diffusive flux, must be of a single sign. Thus, there would always be a net diffusion through the surface, but the net advection would vanish.
- The application to the multicomponent energy equation is clear (cf. [3]). The variables s, $\mathbf{A}$, $h_{(i)}$ and $\mathbf{v}_{(i)}$ are the temperature, (tensor) conductivity, partial specific enthalpies and absolute species fluxes, respectively. The required assumption is that the partial specific enthalpies are independent of pressure and composition. The absolute species fluxes are divergence-free because the species they represent are conserved.
- For many common fluids, the diffusivity is isotropic; i.e. a product of a (positive) scalar field and the Kronecker delta; and so is symmetric and positive definite, as required.
- In the special case $\mathbf{v}_{(i)} = \mathbf{0}$ and $A_{ij} = A\delta_{ij}$, where A is a constant, the steady-state advection–diffusion equation (1) reduces to Laplace's equation, for which the corresponding result is classical [4].
- The diffusivity and velocities can depend on s, so that the equation is only quasilinear. In the proof, s is assumed to be given, so that $\mathbf{A}$ and the $\mathbf{v}_{(i)}$ can be re-expressed as functions of position.
- Completely analogous theorems hold in one and two dimensions.
- One can conclude that the minimum temperature apparent in the two-dimensional numerical solutions of Weaver and Viskanta [5,6], and attributed to interdiffusion (the advection of enthalpy by the diffusive flux of multiple species), was erroneous. The source of the error is the inconsistent treatment of whether the mixture enthalpy did or did not depend on the composition. The *sine qua non* of interdiffusion is the difference in specific heat capacities of the different species, and interdiffusion only arises from a (frequently convenient) repartitioning of the enthalpy fluxes due to the N species fluxes into a bulk advective flux and $N-1$ interdiffusion fluxes. It is essential, therefore, to treat the mixture enthalpy or specific heat capacity, consistently in the bulk advection and interdiffusion terms. A concise consistent derivation of the energy equation for a binary mixture may be found in Ref. [7]; a lengthier discussion has been given elsewhere [8].
- Extrema might occur if there were source or sink terms in the equations, such as, for the case of the energy equation when the scalar is temperature, one or more of the components changed phase in the domain; the Dufour effect was appreciable; or there were viscous heating.
- Extrema are, of course, possible in transient advection–diffusion, as, for example, they may be specified in the initial conditions. An interesting but as yet (to my knowledge) unanswered question is whether strong local extrema can arise in the evolution of a scalar field; this was predicted in the two-dimensional numerical solutions of Bergman and Hyun [9] for the mass fraction of tin in a non-isothermal amalgam with lead.

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