Zeitschrift für Analysis
und ihre Anwendungen
Bd. 4 (3) 1985, S. 207–213

A Note on Optimal Domains in a Reaction-Diffusion Problem

C. Bandle

Es wird untersucht, welches Gefäß für eine chemische Reaktion optimal ist im Sinne, daß keine toten Zonen auftreten und daß der „Wirkungsgrad" möglichst groß wird. Es zeigt sich, daß bei vorgegebenem Volumen das Gefäß möglichst dünn sein muß. Der Beweis stützt sich auf die Methode der Ober- und Unterlösungen und auf die Abschätzung für die Lösung des Dirichletproblems, die vom Inkugelradius abhängt.

Исследуется, какой сосуд при химической реакции оптимален в таком смысле, что нет мертвых зон и что „коэффициент полезного действия" как можно больше. Оказывается, что при данном обьеме сосуд должен быть наиболее тонким. Доказательство опирается на метод вверхних и нижних решений и на оценки решений задачи Дирихле, зависящей от радиуса вписанного шара.

A simple model for a chemical reaction is considered. The vessel where the reaction takes place is optimal if no dead core appears and if effectiveness is high. By means of the method of upper and lower solutions it is shown that, independent of the volume, sufficiently thin domains have this property. The proof is based on an estimate for the solution of the Dirichlet problem.

1. Introduction

Set $D \subset \mathbf{R}^N$ be a bounded domain, $x = (x_1, x_2, \ldots, x_N)$ a generic point and

$$A = \sum_{i,j=1}^{N} \frac{\partial}{\partial x_i} \left[a_{ij}(x) \frac{\partial}{\partial x_j} \right]$$

a uniformly, elliptic operator such that

$$a_{ij} = a_{ji} \in C^1(\overline{D}) \quad \text{and} \quad \sum_{i,j=1}^{N} a_{ij}(x)\, \xi_i \xi_j \geqq \sum_{i=1}^{N} \xi_i^2 \quad \text{in } D. \tag{1.1}$$

This note deals with the problem

$$\begin{cases} \dfrac{\partial u}{\partial t} - Au = \lambda g(u) & \text{in } D \times \mathbf{R}^+, \quad \lambda \in \mathbf{R}^+ \\ u = 0 & \text{on } \partial D \times \mathbf{R}^+, \\ u(x, 0) = 0 & \end{cases} \tag{P}$$

the function $g = g(\sigma)$ being subject to the following conditions

(C-1) $g > 0$ in $(-\infty, 1)$, $g \in C^0(\mathbf{R})$ and $g \in C^1(-\infty, 1)$,
(C-2) g is non-increasing in $(-\infty, 1)$,
(C-3) $g(0) = 1$,
(C-4) $g(\sigma) = 0$ for $\sigma \geqq 1$,
(C-5) $g(\sigma) = g_0(\sigma)\,(1-\sigma)_+^{\,p}$ for some p, $0 < p < 1$, with $g_0(1-0) > 0$ and $g_0'(1-0) < \infty$ ($\sigma_+ := \max\{\sigma, 0\}$).

Such problems occur in simple models for reaction-diffusion processes [1, 4, 9] in the case where the reactions are endothermic or isothermal. Here D represents the domain where the reaction takes place, and $1 - u = c$ is the concentration of the reactant. A considerable amount of work has been devoted recently to these equations [1, 3–5, 9, 10].

An important tool in the study of problem (P) is the method of upper and lower solutions. A function $\overline{u} = \overline{u}(x, t)$ is called a *upper solution*, if

$$\overline{u}_t - A\overline{u} \geqq \lambda g(\overline{u}) \text{ in } D \times \mathbf{R}^+, \quad \overline{u} \geqq 0 \text{ on } \partial D \times \mathbf{R}^+, \quad \overline{u}(x, 0) \geqq 0.$$

Conversely, $\underline{u} = \underline{u}(x, t)$ is a *lower solution* if the inequality signs are reversed. The theorem [8] states that, if there exist upper solutions such that $\underline{u} \leqq \overline{u}$ in $D \times [0, T]$, then the problem (P) possesses a solution u with $\underline{u} \leqq u \leqq \overline{u}$ in $D \times [0, T]$. In our case the assumptions are satisfied for $\overline{u} \equiv 1$ and $\underline{u} \equiv 0$. Consequently problem (P) has a solution u such that $0 \leqq u(x, t) \leqq 1$, which is unique by virtue of the monotonicity of g (C-2). Observing that $u(x, t + \Delta t) =: \overline{u}(x, t)$ is an upper solution for problem (P) we conclude that

$$u(x, t_1) \leqq u(x, t_2) \quad \text{for} \quad t_1 \leqq t_2. \tag{1.2}$$

Furthermore, by standard arguments we have $\lim\limits_{t \to \infty} u(x, t) = U(x)$, where $U(x)$ is the solution of the stationary problem.

The set $\Omega(t) := \{x \in D: u(x, t) = 1\}$ is called the *dead core*. It represents the region where no reaction takes place at the time t. We shall write $\Omega(\infty)$ for the dead core of $U(x)$. The special feature about our problem is that für λ sufficiently large, $\Omega(t)$ is non empty if $t \geqq \tau(\lambda)$ [4]. From (1.2) it follows that

$$\Omega(t_1) \subset \Omega(t_2) \subset \Omega(\infty) \quad \text{for} \quad t_1 \leqq t_2. \tag{1.3}$$

Clearly, $\Omega(t)$ depends on the geometry of D and on λ. We have for example [4]

$$\begin{aligned} &\text{(i)} \quad \Omega_{D_1}(t) \subset \Omega_{D_2}(t) \quad \text{for} \quad D_1 \subset D_2 \text{ and } \lambda \text{ fixed},\\ &\text{(ii)} \quad \Omega_{\lambda_1}(t) \subset \Omega_{\lambda_2}(t) \quad \text{for} \quad \lambda_1 \leqq \lambda_2 \text{ and } D \text{ fixed}. \end{aligned} \tag{1.4}$$

A comparison result of a different nature was obtained by means of rearrangement methods [4] and is expressed as follows.

Theorem I: *Let $\Omega^*(t)$ be the dead core corresponding to problem* (P) *with A replaced by the Laplacian and D by the sphere $D^* := \{x: |x| < R, \text{vol } D = \text{vol } D^*\}$ of the same volume as D. Then* meas $\Omega(t) \leqq$ meas $\Omega^*(t)$.

Another quantity of physical interest is the so called *effectiveness* defined by

$$\eta(t) = \frac{1}{\text{vol } D} \int_D g[u(x, t)]\, dx \leqq 1.$$

It is the ratio of the actual average reaction rate in a region to the rate corresponding to reference values of reactant concentration and temperature. Rearrangement techniques yield [5, 3].

Theorem II: *Let η^* be the effectiveness corresponding to problem* (P) *with* $A = \Delta$ *and $D = D^*$. If in addition to* (C-1)–(C-5) *g is concave, then $\eta \geqq \eta^*$. In the stationary case $\big(\eta(\infty)\big)$ no concavity on g is required.*

For practical purposes it is desirable to have a small dead core and a high effectiveness.

If we restrict ourselves to the case where $A = \Delta$, then the Theorems I and II imply the following extremal properties of the sphere:

(i) *Among all domains of given volume the volume of the dead core is biggest for the sphere.*

(ii) *Among all domains of given volume the sphere has the smallest effectiveness.*

The sphere is in some sense the worst region. In the "International Meeting on Optimization Techniques" at the Wartburg 1983, Professor R. Klötzler asked the question: is there a best domain? Since the worst domain is fat, the best domain, provided it exists, has to be thin. In fact, it turns out that for any fixed λ there is always a domain of given volume such that $\Omega(\infty)$ is empty. Moreover there exists a sequence of domains $\{D_k\}_{k=1}^{\infty}$ such that

$$\operatorname{vol} D_k = V \quad \text{and} \quad \lim_{k\to\infty} \eta_{D_k}(t) = 1.$$

Those statements follow from counterparts of Theorem I and II, which will be formulated in Section 3.

I'm indebted to Prof. R. Klötzler for having suggested this problem.

2. Preliminary bounds for the solution of a Dirichlet problem

2.1 We proceed now to derive bounds for the solution of the Dirichlet problem

$$A\psi + 1 = 0 \text{ in } D, \qquad \psi = 0 \text{ on } \partial D. \tag{2.1}$$

For $N = 2$ and $A = \Delta$, ψ coincides up to a constant factor, with the warping function in the torsion problem of a cylindrical beam. A number of inequalities relating $\psi_{\max}$ to several geometrical quantities has been derived (cf. [2, 14—16] and the literature cited there). The following lemma extends an inequality of PAYNE [14]. Its proof is very similar and will be given for the sake of completeness.

Lemma 2.1: *Let ω_N be the volume of the unit sphere and let A satisfy* (1.1). *Then we have for the solution of* (2.1)

$$\psi_{\max}^{1+N/2} \leqq \frac{2+N}{2\omega_N} (2N)^{-N/2} \int_D \psi \, dx.$$

Equality holds for $D = D^*$ and $A = \Delta$.

Proof: The proof is based on rearrangement techniques developed in [2, 17]. For this purpose let us introduce the notation

$$D(\tilde{\psi}) = \{x \in D : \tilde{\psi}(x) \geqq \tilde{\psi}\}, \qquad a(\tilde{\psi}) = \operatorname{meas} D(\tilde{\psi}).$$

By Schwarz's inequality and (1.1) we have

$$\left\{\frac{1}{d\tilde{\psi}} \int_{D(\tilde{\psi})-D(\tilde{\psi}+d\tilde{\psi})} |\nabla\psi| \, dx\right\}^2 \leqq \left\{\frac{1}{d\tilde{\psi}} \int_{D(\tilde{\psi})-D(\tilde{\psi}+d\tilde{\psi})} |\nabla\psi|^2 \, dx \, \frac{a(\tilde{\psi}) - a(\tilde{\psi}+d\tilde{\psi})}{d\tilde{\psi}}\right\}$$

$$\leqq \left\{\frac{1}{d\tilde{\psi}} \int_{D(\tilde{\psi})-D(\tilde{\psi}+d\tilde{\psi})} \left(\sum_{i,j=1}^{N} a_{ij}\psi_{x_i}\psi_{x_j}\right) dx \, \frac{a(\tilde{\psi}) - a(\tilde{\psi}+d\tilde{\psi})}{d\tilde{\psi}}\right\}. \tag{2.2}$$

In view of Fleming-Rishel's formula

$$-\frac{d}{d\tilde{\psi}} \int_{D(\tilde{\psi})} |\nabla\psi| \, dx = P(\tilde{\psi}), \tag{2.3}$$

where $P(\tilde\psi)$ is the perimeter of $D(\tilde\psi)$ in the sense of de Giorgi. In addition

$$\frac{d}{d\tilde\psi}\int\limits_{D(\tilde\psi)}\left(\sum_{i,j=1}^{N} a_{ij}\psi_{x_i}\psi_{x_j}\right)dx = \int\limits_{D(\tilde\psi)} A\psi\,dx = -a(\tilde\psi). \tag{2.4}$$

If we let $d\tilde\psi$ tend to zero, then (2.2) combined with (2.3) and (2.4) yields

$$P^2(\tilde\psi) \leqq -a(\tilde\psi)\,a'(\tilde\psi) \quad \text{for almost all } \tilde\psi. \tag{2.5}$$

From the isoperimetric inequality $P(\tilde\psi) \geqq N\omega_N{}^{1/N}a(\tilde\psi)^{1-1/N}$, it follows that $N^2\omega_N{}^{2/n} \times a^{1-2/N} \leqq -a'(\tilde\psi)$. Integration gives $\tilde\psi \geqq \psi_{\max} - \left(\frac{a}{\omega_N}\right)^{2/N}\cdot\frac{1}{2N}$. Since $\tilde\psi = 0$ for $a = A$, we get

$$\psi_{\max} \leqq \left(\frac{A}{\omega_N}\right)^{2/N}\cdot\frac{1}{2N}. \tag{2.6}$$

Hence, setting $\tilde\psi(t) := \inf\{\tilde\psi : a(\tilde\psi) < t\}$ we find

$$\int\limits_0^A \tilde\psi\,da \geqq \int\limits_0^\gamma \tilde\psi\,da \geqq \int\limits_0^\gamma \left\{\psi_{\max} - \left(\frac{a}{\omega_N}\right)^{2/N}\cdot\frac{1}{2N}\right\}da; \qquad \gamma = (2N\psi_{\max})^{N/2}\,\omega_N.$$

From

$$\int\limits_0^\gamma \left\{\psi_{\max} - \left(\frac{a}{\omega_N}\right)^{2/N}\cdot\frac{1}{2N}\right\}da = (2N)^{N/2}\,\omega_N\,\frac{2}{N+2}\,\psi_{\max}^{1+N/2}$$

and

$$\int\limits_0^A \tilde\psi\,da = \int\limits_D \psi\,dx$$

the assertion follows ∎

If we multiply (2.1) by ψ and integrate we obtain, observing (1.1),

$$\int\limits_D \psi\,dx = \int\limits_D \left(\sum_{i,j=1}^{N} a_{ij}\psi_{x_i}\psi_{x_j}\right)dx \geqq \int\limits_D |\nabla\psi|^2\,dx. \tag{2.7}$$

Schwarz's inequality together with (2.7) implies

$$\int\limits_D \psi\,dx \leqq \frac{\left(\int\limits_D \psi\,dx\right)^2}{\int\limits_D |\nabla\psi|^2\,dx} \leqq V\,\frac{\int\limits_D \psi^2\,dx}{\int\limits_D |\nabla\psi|^2\,dx},$$

where V stands for the volume of D. Moreover by the Rayleigh principle

$$\int\limits_D \psi^2\,dx \leqq \frac{1}{\lambda_1}\int\limits_D |\nabla\psi|^2\,dx,$$

where λ_1 is the smallest eigenvalue of

$$\Delta w + \lambda_1 w = 0 \text{ in } D, \qquad w = 0 \text{ on } \partial D. \tag{2.8}$$

This leads to the following estimate for $\psi_{\max}$

$$\psi_{\max}^{1+N/2} \leqq \frac{2+N}{2\omega_N}\,(2N)^{-N/2}\,\frac{V}{\lambda_1}.$$

Remark: This inequality is never sharp. Clearly any lower bound for λ_1 will provide an upper bound for $\psi_{\max}$.

In the next section we describe classes of domains of fixed volume whose first eigenvalue exceeds any given number.

2.2 The best known bound for λ_1 is obtained from the Rayleigh-Faber-Krahn inequality [2, 15]

$$\lambda_1 \geqq \left(\frac{\omega_N}{V}\right)^{2/N} \cdot j_{(N-2/2)} \qquad (j_k \text{ first zero of the Bessel function } J_k),$$

equality holding only for the sphere. Obviously this estimate is not of great use for our purpose. The only chance to achieve our goal is to restrict ourselves to "thin" domains.

Let us now introduce the following classes of domains

$\mathcal{P} = \{D \subset \mathbf{R}^N$ lying between two parallel $(N-1)$-dimensional hyperplane at a distance 2ϱ, that is all domains of breadth $\leqq 2\varrho\}$,

$\mathcal{C}_N = \{$convex domains in $\mathbf{R}^N$ of inradius $\varrho\}$,

$\mathcal{A}_k = \{$plane domains of inradius ϱ and connectivity $k\}$.

If we compare the first eigenvalue of a domain $D \in \mathcal{P}$ with the corresponding eigenvalue for the "strip" and use the monotonicity of the eigenvalues with respect to the domain [6] we get

$$\lambda_1(D) \geqq \left(\frac{\pi}{2\varrho}\right)^2 \quad \text{for} \quad D \in \mathcal{P}. \tag{2.10}$$

As HERSCH [12] observed the same result holds for convex domains in the plane, that is

$$\lambda_1(D) \geqq \left(\frac{\pi}{2\varrho}\right)^2 \quad \text{for} \quad D \in \mathcal{C}_2. \tag{2.11}$$

Using Cheeger's method OSSERMAN [13] proved that

$$\lambda_1(D) \geqq \left(\frac{1}{2\varrho}\right)^2 \quad \text{for} \quad D \in \mathcal{C}_N \tag{2.12}$$

and

$$\lambda_1(D) \geqq \left(\frac{1}{2\varrho}\right)^2 \quad \text{for} \quad D \in \mathcal{A}_1 \quad \text{and} \quad D \in \mathcal{A}_2. \tag{2.13}$$

The best result at the time for $D \in \mathcal{A}_k$, $k > 2$, is due to CROKE [7], namely

$$\lambda_1(D) \geqq \frac{1}{2k\varrho^2} \quad \text{for} \quad D \in \mathcal{A}_k, \qquad k \geqq 2. \tag{2.14}$$

Little is known for higher dimensions except that, no lower bound depending only on the inradius ϱ can be expected to hold without further assumption on the geometry of D. As HAYMAN [11] points out, the first eigenvalue of a ball doesn't change much if narrow, inward pointing spiches are removed, whereas ϱ tends to zero.

Inserting these estimates into (2.9) we get the

Theorem 2.1: *Let A satisfy* (1.1), ψ *be the solution of* (2.1) *and D be a domain of volume V. Then the following estimates hold.*

(i) $\psi_{\max}^{1+N/2} \leqq \frac{(4+2N)\,(2N)^{-N/2}}{\pi^2 \omega_N} V\varrho^2$ *for all D in $\mathcal{P}$ or in $\mathcal{C}_2$.*

(ii) $\psi_{\max}^{1+N/2} \leqq \frac{4+2N}{\omega_N} (2N)^{-N/2} \cdot V\varrho^2$ *for all D in $\mathcal{A}_1$, $\mathcal{A}_2$ and $\mathcal{C}_N$.*

(iii) $\psi_{\max}^{1+N/2} \leqq \frac{k(2+N)}{\omega_N} (2N)^{-N/2} \cdot V\varrho^2$ *for all D in $\mathcal{A}_k$ $(k > 2)$.*

Remark: In the case $A \doteq \Delta$, SPERB [16] derived the estimate

$$\psi_{\max} \leqq \frac{\varrho^2}{2} \quad \text{for all } D \in \mathcal{C}_2. \tag{2.15}$$

Clearly (2.15) is not comparable to Theorem 2.1 (i).

3. Main results

Let us go back to problem (P) with the assumptions made in Section 1. It is immediate that $\overline{u} = \lambda\psi(x)$, ψ being the solution of (2.1), is an upper solution for problem (P) and thus

$$u(x, t) \leqq \lambda\psi_{\max} \quad \text{for all} \quad (x, t) \in D \times \mathbf{R}^+. \tag{3.1}$$

This inequality together with the estimates of Theorem 2.1 yields

Theorem 3.1: *Let D belong to either classes $\mathcal{P}$, $\mathcal{C}_N$ or $\mathcal{A}_k$. Then*

$$\max_{x \in \overline{D}} u(x, t) \leqq cV\varrho^2,$$

where c depends only on the number of dimensions N and on λ. There exists therefore a value $\varrho_0 = \varrho_0(\lambda, N, V)$ such that

$$\text{meas}\, \Omega(t) \leqq \text{meas}\, \Omega(\infty) = 0 \quad \textit{for} \quad \varrho \leqq \varrho_0.$$

As an immediate consequence we have the

Theorem 3.2: *Let the assumptions of the previous theorem hold and suppose that* vol $D = V$. *Then $\eta(t) \to 1$ as $\varrho \to 0$.*

An optimal domain has to be thin in the sense that its inradius is small.

Remark: The Theorems 3.1 and 3.2 hold also if $g(u)$ is replaced by $g(x, u)$. Of all assumptions (C-1)–(C-5) we have only used (C-3), (C-4), the fact that $g(\sigma)$ takes values in $[0, 1]$ for $\sigma \in [0, 1]$ and the continuity of g.

REFERENCES

[1] ARIS, R.: The mathematical theory of diffusion and reaction in permeable catalysts. Oxford: Clarendon Press 1975.

[2] BANDLE, C.: Isoperimetric Inequalities and Applications. Boston—London—Melbourne: Pitman Publ. 1980.

[3] Bandle, C., Sperb, R., and I. Stakgold: Diffusion-reaction with monotone kinetics. Nonlinear Analysis 8 (1984), 321—333.

[4] Bandle, C., and I. Stakgold: The formation of the dead core in parabolic reaction-diffusion problems. Trans. Amer. Math. Soc. 286 (1984), 275—293.

[5] Bandle, C., and I. Stakgold: Isoperimetric inequalities for the effectiveness in semilinear parabolic equations. In: General Inequalities 4 (ed.: W. Walter). Basel—Boston—Stuttgart: Birkhäuser Verlag ISNM 71 (1984).

[6] Courant, D., and D. Hilbert: Methoden der mathematischen Physik, Vol. 1 (Grundlehren d. math. Wiss.: Bd. 12). Berlin: Springer-Verlag 1924.

[7] Croke, C. B.: The first eigenvalue of the Laplacian for plane domains. Proc. Amer. Math. Soc. 81 (1981), 304—305.

[8] Deuel, J., and P. Hess: Nonlinear parabolic boundary value problems with upper and lower solutions. Israel J. Math. 29 (1978), 92—104.

[9] Diaz, J., and J. Hernandez: On the estimate of a free boundary for a class of reaction-diffusion systems. Mathematics Research-Center, University of Wisconsin-Madison Report 1981.

[10] Friedman, A., and D. Phillips: The free boundary of a semilinear elliptic equation. Trans. Amer. Math. Soc. 282 (1984) 153—182.

[11] Hayman, W. K.: Some bounds for principal frequency. Applicable Analysis 7 (1977/78), 247—254.

[12] Hersch, J.: Sur la fréquence fondamentale d'une membrane vibrante. Evaluation par défaut et principe du maximum. ZAMP 11 (1960), 387—413.

[13] Osserman, R.: Bonnesen-style inequalities. Amer. Math. Monthly 86 (1979), 1—29.

[14] Payne, L. E.: Some isoperimetric inequalities in the torsion problem for multiply connected regions. In: Studies in Mathematical Analysis and Related Topics: Essays in Honar of G. Pólya (eds.: S. Gilbarg a. o.). Stanford (California): Univ. Press 1962.

[15] Pólya, G., and G. Szegö: Isoperimetric inequalities in mathematical physics. Princeton: Univ. Press 1951.

[16] Sperb, R.: Maximum principles and their applications. New York: Acad. Press 1981.

[17] Talenti, G.: Elliptic equations and rearrangements. Ann. Scuola Norm. Sup. Pisa 3 (1976), 697—718.

Manuskripteingang: 27. 01. 1984

VERFASSER:

Prof. Dr. Catherine Bandle
Mathematisches Institut der Universität Basel
CH - 4051 Basel, Rheinsprung 21