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Approximate solutions to a nonlinear diffusion equation

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Abstract. Approximate similarity solutions to the porous-medium equation, $c_t = \nabla \cdot (c^m \nabla c)$, are obtained in one and two dimensions. The problems considered arise in the modelling of dopant diffusion in semiconductors, the two-dimensional problems corresponding to diffusion under a mask edge.

1. Introduction

Dopant may be introduced into a semiconductor by various means, including ion-implantation followed by diffusion and by the diffusion of the dopant into the material from a source at the semiconductor surface. In the former process the total amount of dopant is fixed, whereas the latter may be modelled by a constant concentration boundary condition on the semiconductor surface (see, for example, Ghandhi [10]).

At fairly high concentrations the diffusivity of many dopants is known to be well represented by

$$D(c) = D_0 c^m \tag{1.1}$$

where D_0 and m are constants. Examples include: $m = 1$ for arsenic and boron in silicon (see Sze [22]); $m = 2$ for phosphorus in silicon (see Sze [22]); $m = 2$ or 3 for zinc in gallium arsenide (see Luque et al. [18]).

It should be noted that (1.1) is an accurate description of the diffusion coefficient only at high concentrations, the diffusivity remaining bounded away from zero as c drops. Hence the results of this paper based on (1.1) should be regarded as giving the first term in an outer expansion for the concentration. The models of Weisberg and Blanc [27] and Luque et al. [18] for zinc diffusion in gallium arsenide may be written in non-dimensional form as

$$c_t = ((c^m + \varepsilon^m)c_x)_x,$$

with $\varepsilon \ll 1$. In an inner region of low concentration occurring near $x = s(t; \varepsilon)$ (which is determined by matching) we rescale as follows:

$$c = \varepsilon p, \quad x = s + \varepsilon^m z,$$

to obtain

$$\varepsilon^m p_t - \dot{s} p_z = ((1 + p^m)p_z)_z,$$

so that, writing

$$p = p_0 + o(1), \quad s = s_0 + o(1),$$

we have

$$\ln p_0 + \frac{1}{m} p_0^m = -\dot{s}_0 z.$$

For a detailed analysis of the case $m = 1$, see King [14]. The usually assumed diffusion coefficient for arsenic leads to an algebraically more complicated problem, but a similar analysis holds (see King [15]). Because the inner region is asymptotically narrow this analysis carries over to higher dimensions.

In this paper we first consider one-dimensional similarity solutions corresponding to constant surface concentration. The initial concentration is taken to be zero everywhere which accurately models many of the constant-source diffusions in semiconductor fabrication, as well as having other physical applications. We obtain asymptotic results for small and large m, and a power-series solution for general m. Since the instantaneous-source similarity solution (relevant to the diffusion of implanted dopant) is available in closed form (see Barenblatt [3]) we need not discuss it here.

Secondly we consider both constant- and instantaneous-source problems in two dimensions corresponding to diffusion under a mask edge (a common process in semiconductor fabrication). In this case explicit solutions are available only in the limits of small and large m, but useful qualitative information may be obtained from these solutions.

2. One-dimensional similarity solutions

We consider the problem

$$\begin{aligned} &c_t = D_0(c^m c_x)_x, \\ &\text{at } t = 0: \quad c = 0, \\ &\text{at } x = 0: \quad c = c_0, \\ &\text{as } x \to +\infty: \quad c = 0. \end{aligned} \tag{2.1}$$

No closed-form solution to (2.1) is available, although it is easy to prove the following result for the centre of mass:

$$\int_0^\infty x c \, \mathrm{d}x = \frac{D_0 c_0^{m+1}}{m+1} t.$$

Problem (2.1) has been studied numerically for $m = 1$, 2 and 3 by Weisberg and Blanc [27]. Approximation procedures have been suggested by Tuck [25] and by Anderson and

Lisak [2], and approximate solutions have been proposed for arsenic by Nakajima et al. [19] and for boron by Fair [9]. Our purpose here is to propose more systematic (and simpler) procedures for obtaining approximate solutions to (2.1).

We introduce the variables

$$\eta = x/(D_0 c_0^m t)^{1/2}, \quad u = (c/c_0)^m$$

to obtain the free-boundary problem

$$-\tfrac{1}{2}\eta u_\eta = u u_{\eta\eta} + \frac{1}{m} u_\eta^2,$$

$$\text{at } \eta = 0: \quad u = 1, \tag{2.2}$$

$$\text{at } \eta = \eta_0: \quad u = 0, \quad u_\eta = -\frac{m}{2}\eta_0,$$

where η_0 must be found as part of the solution.

We now reduce (2.2) to an initial-value problem by introducing

$$\xi = 1 - \eta/\eta_0, \quad v = u/(\eta_0^2 m),$$

and obtain

$$m v v_{\xi\xi} + v_\xi^2 = \tfrac{1}{2}(1 - \xi)v_\xi,$$

$$\text{at } \xi = 0: \quad v = 0, \quad v_\xi = 1/2. \tag{2.3}$$

η_0 is then given by

$$\eta_0 = (mv(1))^{-1/2}. \tag{2.4}$$

Clearly such a procedure will work for more general similarity solutions to the porous medium equation.

We now consider the asymptotic solution of (2.3) in the limits $m \to 0$ and $m \to +\infty$, and give a power-series solution for general m.

2.1. *The limit $m \to 0$*

It is well-known that for $m = 0$ (linear diffusion) the solution to (2.1) is given by

$$c = c_0 \operatorname{erfc}(\eta/2).$$

In this section we consider the case $m \ll 1$, a limit in which the porous medium equation was first considered by Kath and Cohen [12]. We note that in order to obtain the first-order term for c we must obtain v correct to $O(m)$.

Posing the expansion

$$v \sim v_0 + mv_1 + m^2 v_2, \tag{2.5}$$

we find

$$\begin{aligned} v_0 &= \tfrac{1}{4}(1 - (1 - \xi)^2), \\ v_1 &= -\tfrac{1}{8}(1 - (1 - \xi)^2) - \tfrac{1}{4} \ln (1 - \xi), \\ v_2 &= \tfrac{1}{16}(1 - (1 - \xi)^2) + \tfrac{1}{8}\left(1 - \frac{1}{(1 - \xi)^2}\right) + \tfrac{1}{8} \ln^2 (1 - \xi) - \tfrac{1}{8} \ln (1 - \xi). \end{aligned} \tag{2.6}$$

Since the expansion (2.5) breaks down at $1 - \xi = O(m^{1/2})$ there is a boundary layer in which we rescale:

$$\xi = 1 - m^{1/2}\zeta, \quad v = \tfrac{1}{4} - \tfrac{1}{8} m \ln m + mw,$$

so that

$$w_\zeta^2 + (\tfrac{1}{4} - \tfrac{1}{8}\, m \ln m + mw) w_{\zeta\zeta} = -\tfrac{1}{2}\zeta\, w_\zeta.$$

Posing $w = w_0 + o(1)$, with $q_0 = \frac{1}{4} \ln w_0$, we have

$$q_{0\zeta\zeta} = -2\zeta q_{0\zeta},$$

so that

$$w_0 = \tfrac{1}{4} \ln (\operatorname{erfc} (\zeta)) + \tfrac{1}{8} (\ln \pi - 1),$$

where the constant of integration has been determined by matching with (2.6).
(2.4) becomes

$$\eta_0 \sim 2m^{-1/2}(1 + \tfrac{1}{4} m \ln m - \tfrac{1}{4} m(\ln \pi - 1)).$$

In $\xi = O(1)$ we have

$$v^{1/m} \sim \{\tfrac{1}{4}(1 - (1 - \xi)^2)\}^{1/m} \exp\left(-\frac{1}{2} - \frac{\ln (1 - \xi)}{1 - (1 - \xi)^2}\right),$$

while in $\zeta = O(1)$

$$v^{1/m} \sim \{\tfrac{1}{4}\}^{1/m} \pi^{1/2} m^{-1/2} e^{-1/2} \operatorname{erfc} (\zeta),$$

so that a uniformly valid expression for c is given by

$$c \begin{cases} \sim c_0(1 - m\zeta^2)^{1/m}(m^{1/2}\zeta)^{-(m\zeta^2)/(1-m\zeta^2)}\, e^{\zeta^2}\, \mathrm{erfc}\,(\zeta), & \zeta < m^{-1/2} \\ = 0, & \zeta > m^{-1/2} \end{cases}$$

with $\zeta = \eta/\eta_0 m^{1/2} \sim \eta/2$.

We finally note in this context that the approximation suggested by Anderson and Lisak [2] for small m does not have compact support and is therefore of very limited value.

2.2. *The limit $m \to +\infty$*

The limit in which m becomes large has been considered for constant total mass by Elliott et al. [7], solutions being characterized by a "mesa" region in which c is almost uniform, while outside the mesa c remains at almost its initial value. Similar behaviour occurs for the constant-surface-concentration case.

Posing the regular expansion

$$v \sim v_0 + \frac{1}{m} v_1 + \frac{1}{m^2} v_2,$$

we find

$$v_0 = \xi/2,$$

$$v_1 = -\xi^2/2,$$

$$v_2 = \xi^2/4 + \xi^3/24,$$

so that as $m \to +\infty$

$$c \begin{cases} \sim c_0(1 - \eta/\eta_0)^{1/m}, & \eta < \eta_0 \\ = 0, & \eta > \eta_0 \end{cases}$$

where $\eta_0 \sim (2/m)^{1/2}$.

Note that for $\eta < \eta_0$, $c \approx c_0$ until η becomes very close to η_0 when c drops rapidly to zero.

2.3. *General m*

When m is neither large nor small, analytic progress seems possible only by means of a power-series expansion about the point where c drops to zero. It turns out that for $m = O(1)$ only a few terms in the expansion are non-negligible, so that a truncated expansion may be expected to form a useful approximation to the true solution.

Assuming

$$v \sim \sum_{n=1}^{\infty} a_n \xi^n \quad \text{as} \quad \xi \to 0,$$

we obtain from (2.3) the recurrence relation

$$\tfrac{1}{2}(n+1)(1+mn)a_{n+1} = -\tfrac{1}{2}na_n - \sum_{p=1}^{n-1}(p+1)(n+1+p(m-1))a_{n-p+1}a_{p+1}, \tag{2.7}$$

with $a_1 = 1/2$.

Hence

$$a_2 = -\frac{1}{4(m+1)},$$

$$a_3 = \frac{m}{12(2m+1)(m+1)^2},$$

$$a_4 = \frac{m(m+3)}{48(3m+1)(2m+1)(m+1)^3}.$$

This series expansion may be shown to be consistent with the large and small m results of the previous sections. The coefficients decay particularly quickly with n when m is large. Particular cases include:

$$\begin{aligned} m &= 1: \quad v \sim \tfrac{1}{2}\xi - \tfrac{1}{8}\xi^2 + \tfrac{1}{144}\xi^3 + \tfrac{1}{1152}\xi^4, \\ m &= 2: \quad v \sim \tfrac{1}{2}\xi - \tfrac{1}{12}\xi^2 + \tfrac{1}{270}\xi^3 + \tfrac{1}{4536}\xi^4, \\ m &= 3: \quad v \sim \tfrac{1}{2}\xi - \tfrac{1}{16}\xi^2 + \tfrac{1}{448}\xi^3 + \tfrac{1}{19968}\xi^4. \end{aligned} \tag{2.8}$$

In each of these cases the first three terms may be expected to give much better than 1% accuracy for $\xi \in [0, 1]$. We do not, however, have a convergence proof for the asymptotic expansion.

Of particular importance in semiconductor applications is the value of η_0 since this determines the position of the n–p junction where the net dopant concentration changes type. From (2.8) we obtain (correct to three decimal places):

m	η_0	η_{WB}
1	1.616	1.616
2	1.090	1.092
3	0.871	0.872

The final column gives the numerical values obtained by Weisberg and Blanc [27]. In each case η_0 is given correct to two significant figures by just two terms of the power series. For $m = 2.5$ we obtain $\eta_0 \approx 0.963$, indicating that the interpolated estimate of 0.940 used by Luque et al. [18] is somewhat in error.

3. Two-dimensional diffusions

Important steps in the fabrication of many integrated circuits involve the diffusion of dopant under a mask, which is a fully two-dimensional process. Further background to the processes, together with constant- and instantaneous-source solutions for linear diffusion, are given in Kennedy and O'Brien [13]. Numerical solutions to the time-dependent problem for the full diffusion coefficients for arsenic and boron, together with experimental work, are given in Warner and Wilson [26]. Another reference for numerical work is Tielert [23], while Sheng and Marcus [21] give experimental observations.

3.1. Constant-source solutions

In this section we consider processes which may be modelled by the following boundary-value problem

$$
\begin{aligned}
&c_t = \nabla \cdot (D(c)\nabla c), \\
&\text{on } y = 0,\ x > 0: && c = c_0, \\
&\text{on } y = 0,\ x < 0: && c_y = 0, \\
&\text{as } y \to +\infty \text{ or } x \to -\infty: && c \to 0, \\
&\text{as } x \to +\infty: && c_x \to 0, \\
&\text{at } t = 0: && c = 0.
\end{aligned} \tag{3.1}
$$

Here $y = 0$ is the silicon surface, with $x < 0$ covered by a diffusion mask which is impervious to dopant, while $x > 0$ is held at constant concentration.

It was noted by Warner and Wilson [26] that the solution to (3.1) is self-similar. However, they did not appear to recognize that in the high-concentration limit ($D \sim D_0 c^m$) not only may the time-dependence be taken out of the problem but (for given m) all the process parameters may be scaled out.

To achieve this we introduce similarity variables

$$\xi = \frac{m^{1/2} x}{2(D_0 c_0^m t)^{1/2}}, \quad \eta = \frac{m^{1/2} y}{2(D_0 c_0^m t)^{1/2}},$$

and define

$$g \equiv (c/c_0)^m$$

to obtain

$$
\begin{aligned}
&-2(\xi g_\xi + \eta g_\eta) = mg(g_{\xi\xi} + g_{\eta\eta}) + g_\xi^2 + g_\eta^2, \\
&\text{on } \eta = 0, \quad \xi > 0: \qquad g = 1, \\
&\text{on } \eta = 0, \quad \xi < 0: \qquad g_\eta = 0, \\
&\text{on } \eta = G(\xi): \qquad g = 0,\ g_\xi^2 + g_\eta^2 = -2(\xi g_\xi + \eta g_\eta), \\
&\text{as } \eta \to +\infty \text{ or } \xi \to -\infty: \quad g \to 0, \\
&\text{as } \xi \to +\infty: \qquad g_\xi \to 0,
\end{aligned} \tag{3.2}
$$

where $\eta = G(\xi)$ denotes the free boundary.

Further analytic progress to (3.2) does not seem to be possible for general m and we shall restrict the discussion here to the limits of small and large m.

3.1.1. Linear diffusion ($m \doteq 0$)

For $D \equiv D_0$ we define

$$\xi = \frac{x}{2(D_0 t)^{1/2}}, \quad \eta = \frac{y}{2(D_0 t)^{1/2}}, \quad q = \frac{c}{c_0},$$

so that

$$
\begin{aligned}
&-2(\xi q_\xi + \eta q_\eta) = q_{\xi\xi} + q_{\eta\eta}, \\
&\text{on } \eta = 0,\ \xi > 0: \qquad q = 1, \\
&\text{on } \eta = 0,\ \xi < 0: \qquad q_\eta = 0, \\
&\text{as } \eta \to +\infty \text{ or } \xi \to -\infty: \quad q \to 0, \\
&\text{as } \xi \to +\infty: \qquad q \to \operatorname{erfc}(\eta).
\end{aligned} \tag{3.3}
$$

The linear case corresponds to dopant diffusion at low concentrations and has been solved in this context by Kennedy and O'Brien [13] and Cherednichenko et al. [5] (see also Townsend and Strachan [24]). The same problem has also occurred and been solved in other contexts – it is one of the heat-conduction problems discussed by Jaeger [11], and has arisen in models of electrochemical transport (Oldham [20]), random walks (Boersma and Wiegel [4]), and etching (Kuiken [17]).

In the next section we shall require an asymptotic result of Boersma and Wiegel [4], namely

$$q \sim \frac{1}{2^{1/2}\pi} \frac{\cos\theta/2}{\cos\theta} r^{-2} e^{-r^2} \quad \text{as} \quad r \to \infty, \quad \text{for} \quad 0 \leqslant \theta < \frac{\pi}{2}, \tag{3.4}$$

where $\xi = -r\cos\theta$, $\eta = r\sin\theta$.

3.1.2. The limit $m \to 0$

We now consider the case $m \ll 1$ and pose

$$
\begin{aligned}
g &= g_0 + o(1), \\
G &= G_0 + o(1), \quad \text{as } m \to 0.
\end{aligned}
$$

Hence (3.2) gives

$$
\begin{aligned}
& g_{0\xi}^2 + g_{0\xi}^2 = -2(\xi g_{0\xi} + \eta g_{0\eta}), \\
& \text{on } \eta = 0, \xi > 0: \quad g_0 = 1, \\
& \text{on } \eta = 0, \xi < 0: \quad g_{0\eta} = 0, \\
& \text{on } \eta = G_0(\xi): \qquad g_0 = 0.
\end{aligned}
$$

Using Charpit's equations (see, for example, Chester [6]) we may derive:

$$
g_0 = \begin{cases} 1 - \eta^2, & \eta < 1, \xi \geqslant 0, \\ 1 - \xi^2 - \eta^2, & \eta^2 + \xi^2 < 1, \xi < 0, \\ 0, & \text{otherwise}, \end{cases}
$$

and

$$
G_0 = \begin{cases} 1, & \xi > 0, \\ (1 - \xi^2)^{1/2}, & -1 < \xi < 0. \end{cases}
$$

At higher orders we require boundary layers at $\xi = 0$, and at $\eta = 0$ for $\xi < 0$. There are five regions to consider and we have the following results (writing $X = m^{-1/2}\xi$, $Y = m^{-1/2}\eta$):

(i) $\xi > 0$, $\xi = O(1)$, $\eta = O(1)$:

$$
\begin{aligned}
g &\sim 1 - \eta^2 + \tfrac{1}{2} m \ln m + \tfrac{1}{2} m(\eta^2 - \ln \pi - 2 \ln \eta), \\
G &\sim 1 + \tfrac{1}{4} m \ln m + \tfrac{1}{4} m(1 - \ln \pi); \qquad (3.5)
\end{aligned}
$$

(ii) $\xi > 0$, $\xi = O(1)$, $Y = O(1)$:

$$
g \sim 1 + m \ln(\operatorname{erfc}(Y));
$$

(iii) $X = O(1)$, $Y = O(1)$:

$$
g \sim 1 + m \ln q,
$$

where q is the solution to (3.3);

(iv) $X = O(1)$, $\eta = O(1)$:

$$g \sim 1 - \eta^2 + \tfrac{1}{2} m \ln m + m g_0^*,$$

where g_0^* satisfies

$$-2(X g_{0X}^* - \eta g_{0\eta}^*) = (1 - \eta^2)(g_{0XX}^* - 2) + g_{0X}^{*2};$$

(v) $\xi < 0$, $\xi = O(1)$, $\eta = O(1)$:

$$g \sim 1 - r^2 + m \ln m + m\left\{r^2 - 2 \ln r + \ln\left(\frac{\cos\theta/2}{2^{1/2}\pi\cos\theta}\right)\right\},$$

and the free boundary is given by

$$r = R(\theta) \sim 1 + \tfrac{1}{2} m \ln m + \tfrac{1}{2}\left\{1 + \ln\left(\frac{\cos\theta/2}{2^{1/2}\pi\cos\theta}\right)\right\}, \tag{3.6}$$

where $\xi = -r\cos\theta$, $\eta = r\sin\theta$ and we have made use of (3.4) in performing the matching.

Of particular importance in semiconductor applications is the aspect ratio of the free boundary defined by

$$a = \frac{R(0)}{G(\infty)},$$

which is the ratio of lateral to vertical junction depths. The lateral junction depth determines the channel length (which is the distance between the source and drain of a MOSFET, a common semiconductor device (see, for example, Sze [22])).

From (3.5) and (3.6) we obtain

$$a \sim 1 + \tfrac{1}{4} m \ln m + \tfrac{1}{4} m(1 - \ln(2\pi)) \quad \text{as } m \to 0, \tag{3.7}$$

which is consistent with observations (see Ghandhi [10]) that a decreases with increasing nonlinearity.

3.1.3. The limit $m \to \infty$

For large m we pose

$$g = g_0 + o(1) \quad \text{as } m \to \infty,$$

and obtain

$$g_{0\xi\xi} + g_{0\eta\eta} = 0.$$

Laplace's equation arises for the limit $m \to \infty$ of the porous medium in general situations in which the concentration is held constant on part of the boundary. This is in contrast to constant-total-mass problems where a source term arises due to the changing height of the mesa, leading to a Poisson equation (see Elliott et al. [7]).

It turns out that this limit may be solved explicitly following the introduction of a Baiocchi transformation. We first return to the time-dependent problem for general m and introduce

$$u = c/c_0, \quad \hat{x} = x/(D_0 c_0^m)^{1/2}, \quad \hat{y} = y/(D_0 c_0^m)^{1/2},$$

and define the moving boundary to be $t = \omega(\hat{x}, \hat{y})$. Next we introduce the Kirchhoff variable

$$v = \frac{1}{m+1} u^{m+1},$$

and the Baiocchi transformation

$$w = \int_\omega^t v(\hat{x}, \hat{y}, t')\,\mathrm{d}t'$$

(note that a similar procedure applies to more general $D(c)$ for which the solution has a moving boundary).

In general w satisfies

$$\begin{aligned} ((m+1)w_t)^{1/(m+1)} &= w_{\hat{x}\hat{x}} + w_{\hat{y}\hat{y}} \\ \text{on } t = \omega: \quad w &= w_n = 0, \end{aligned} \tag{3.8}$$

and for the case discussed here we have in addition

$$\text{on } \hat{y} = 0, \hat{x} > 0: \quad w = \frac{1}{m+1} t,$$

$$\text{on } \hat{y} = 0, \hat{x} < 0: \quad w_{\hat{y}} = 0.$$

We now introduce similarity variables

$$\xi = m^{1/2}\hat{x}/(2t^{1/2}), \quad \eta = m^{1/2}\hat{y}/(2t^{1/2}), \quad w = \frac{1}{m+1} t\, W(\xi, \eta),$$

so that

$$4\left(\frac{m+1}{m}\right)(W - \tfrac{1}{2}\xi W_\xi - \tfrac{1}{2}\eta W_\eta)^{1/(m+1)} = W_{\xi\xi} + W_{\eta\eta},$$

$$\text{on } \eta = 0, \xi > 0: \quad W = 1,$$

$$\text{on } \eta = 0,\ \xi < 0: \quad W_\eta = 0,$$

$$\text{on } F(\xi, \eta) = 0: \quad W = W_n = 0,$$

where $F(\xi, \eta) = 0$ denotes the free boundary.

Writing

$$W = W_0 + o(1), \quad F = F_0 + o(1), \quad \text{as } m \to \infty,$$

we then obtain

$$W_{0\xi\xi} + W_{0\eta\eta} = 4,$$

$$\text{on } \eta = 0,\ \xi > 0: \quad W_0 = 1,$$

$$\text{on } \eta = 0,\ \xi < 0: \quad W_{0\eta} = 0,$$

$$\text{as } \eta \to +\infty \text{ or } \xi \to -\infty: \quad W_0 \to 0, \tag{3.9}$$

$$\text{as } \xi \to +\infty: \quad W_0 \to \begin{cases} (1 - \sqrt{2}\,\eta)^2, & 0 \leqslant \eta < 1/\sqrt{2}, \\ 0, & \eta > 1/\sqrt{2}, \end{cases}$$

$$\text{on } F_0(\xi, \eta) = 0: \quad W_0 = W_{0n} = 0.$$

Problem (3.9) is one of a class of problems which may be solved explicitly (see King and Howison [16] for details).

Introducing

$$\phi = \frac{1}{2\sqrt{2}} W_{0\xi}, \quad \psi = \sqrt{2}\eta - \frac{1}{2\sqrt{2}} W_{0\eta},$$

η may easily be obtained as a function of ϕ and ψ. Writing

$$z = \xi + i\eta, \quad q = \phi + i\psi,$$

we obtain

$$z = \frac{1}{\sqrt{2}}\left(q - \frac{2}{\pi}(1 + q \tan^{-1} q)\right).$$

In order to evaluate the concentration we require

$$W_0 = 2\eta^2 + \operatorname{Re}\left(q^2 - \frac{2}{\pi}(q + (q^2 - 1)\tan^{-1} q)\right),$$

so that

$$u \sim \left(\frac{2}{\pi} \operatorname{Re}(\tan^{-1} q)\right)^{1/m}$$

The free boundary is given by

$$\xi = -\frac{\sqrt{2}}{\pi} + \eta \left(\frac{2}{\pi} \tanh^{-1} \sqrt{2}\eta\right),$$

so that the aspect ratio is

$$a \sim \frac{2}{\pi} \approx 0.637. \tag{3.10}$$

It seems likely that $2/\pi$ is a lower bound on a for all m.

3.2. Instantaneous-source solutions

We now consider the following problem, relevent to diffusion from a narrow implant close to the silicon surface:

$$\begin{aligned}
&c_t = D_0((c^m c_x)_x + (c^m c_y)_y), \\
&\text{on } y = 0: \qquad c_y = 0, \\
&\text{as } y \to +\infty \text{ or } x \to -\infty: \quad c \to 0, \\
&\text{as } x \to +\infty: \qquad c_x \to 0, \\
&\text{at } t = 0: \qquad c = Q\delta(y)H(x).
\end{aligned} \tag{3.11}$$

Here $y = 0, x > 0$ denotes a mask to the implantation of dopant atoms, H is the Heaviside step function and Q is the dose in a cross-section far away from the mask.

The solution to (3.11) is expressed terms of the similarity variables

$$\xi = \frac{x}{D_0^{1/2} a\, t^{1/(m+2)}}, \quad \eta = \frac{y}{D_0^{1/2} a\, t^{1/(m+2)}}, \quad c = a^{2/m} t^{-1/(m+2)} d^{1/m}(\xi, \eta),$$

where a is given by

$$Q = D_0^{1/2} \frac{\sqrt{\pi}}{2} \frac{\Gamma\left(\frac{m+1}{m}\right)}{\Gamma\left(\frac{3m+2}{2m}\right)} a^{(m+2)/m} \left(\frac{m}{2(m+2)}\right)^{1/m}.$$

Then d satisfies

$$-\frac{m}{m+2}d - \frac{1}{m+2}(\xi d_\xi + \eta d_\eta) = d(d_{\xi\xi} + d_{\eta\eta}) + \frac{1}{m}(d_\xi^2 + d_\eta^2),$$

$$\text{on } \eta = 0: \qquad d_\eta = 0,$$

$$\text{on } \eta = G(\xi): \qquad d = 0,\ d_\xi^2 + d_\eta^2 = -\frac{m}{m+2}(\xi d_\xi + \eta d_\eta), \tag{3.12}$$

$$\text{as } \eta \to +\infty \text{ or } \xi \to -\infty: \quad d \to 0,$$

$$\text{as } \xi \to +\infty, \quad \eta < 1: \qquad d \sim \frac{m}{2(m+2)}(1-\eta^2),$$

where $\eta = G(\xi)$ denotes the free boundary. For given m all process parameters have again been scaled out.

3.2.1. The limit $m \to 0$

For small m we must introduce

$$g = m^{-1}d,$$

and again using Charpit's equations and defining $X = m^{-1/2}\xi$ we obtain the following regions:

(i) $\xi > 0$, $\xi = O(1)$:

$$g \sim \tfrac{1}{4}(1-\eta^2) - \frac{m}{8}(1-\eta^2),$$

$$G \sim 1;$$

(ii) $X = O(1)$:

$$g \sim \tfrac{1}{4}(1-\eta^2) + mg_0^*$$

where g_0 satisfies

$$-\tfrac{1}{2}(Xg_{0_X}^* - \eta g_{0_\eta}^*) = \tfrac{1}{4}(1-\eta^2)g_{0XX}^* + \tfrac{1}{8}\eta^2 + g_{0X}^{*2}.$$

In this case there is no boundary layer for small η, but g_0^* satisfies

$$g_0^* \sim \tfrac{1}{4}\ln q \quad \text{as } \eta \to 0$$

where $q = \tfrac{1}{2}e^{-1/2}\operatorname{erfc} X$. This result enables us to match into $\xi < 0$.

(iii) $\xi < 0$, $\xi = O(1)$:

$$g \sim \tfrac{1}{4}(1 - r^2) + \tfrac{1}{8} m \ln m + m\left(\frac{r^2}{4} - \tfrac{1}{4}\ln(r\cos\theta) - \tfrac{1}{8} - \tfrac{1}{4}\ln 2\sqrt{\pi}\right),$$

$$R(\theta) \sim 1 + \tfrac{1}{4} m \ln m + \tfrac{1}{4} m(1 - 2\ln(\cos\theta) - 2\ln 2\sqrt{\pi}).$$

where $\xi = -r\cos\theta$, $\eta = r\sin\theta$. Also

$$a = \frac{R(0)}{G(\infty)} \sim 1 + \tfrac{1}{4} m \ln m + \tfrac{1}{4} m(1 - 2\ln 2\sqrt{\pi}). \qquad (3.13)$$

3.2.2. The limit $m \to \infty$

Writing $d_0 = d_0 + o(1)$, (3.11) becomes $d_{0\xi\xi} + d_{0\eta\eta} = -1$. We now introduce

$$u = c/a^{2/m} \quad \hat{x} = x/(D_0^{1/2} a), \quad \hat{y} = y/(D_0^{1/2} a).$$

As in Section 3.1.3 we write

$$v = \frac{1}{m+1} u^{m+1}, \quad w = \int_\omega^t v(\hat{x}, \hat{y}, t')\,dt'$$

so that w again satisfies (3.8). In this case the extra conditions are

$$\text{on } \hat{y} = 0, \hat{x} > 0: \quad w_{\hat{y}} = -\frac{\sqrt{\pi}}{2}\left(\frac{m}{2(m+2)}\right)^{1/m} \frac{\Gamma\left(\dfrac{m+1}{m}\right)}{\Gamma\left(\dfrac{3m+2}{2m}\right)},$$

$$\text{on } \hat{y} = 0, \hat{x} < 0: \quad w_{\hat{y}} = 0.$$

We now introduce similarity variables

$$\xi = \hat{x}/t^{1/(m+2)}, \quad \eta = \hat{y}/t^{1/(m+2)}, \quad w = t^{1/(m+2)} W(\xi, \eta),$$

so that

$$\left(\left(\frac{m+1}{m+2}\right)(W - \xi W_\xi - \eta W_\eta)\right)^{1/(m+1)} = W_{\xi\xi} + W_{\eta\eta},$$

$$\text{on } \eta = 0, \xi > 0: \qquad W_\eta = -\frac{\sqrt{\pi}}{2}\left(\frac{m}{2(m+2)}\right)^{1/m} \frac{\Gamma\left(\dfrac{m+1}{m}\right)}{\Gamma\left(\dfrac{3m+2}{2m}\right)},$$

on $\eta = 0,\ \xi < 0$: $\quad W_\eta = 0,$

on $\xi \to -\infty$ or $\eta \to +\infty$: $\quad W \to 0,$

as $\xi \to +\infty$:
$$W \sim \left(\frac{m+2}{m+1}\right)\left(\frac{m}{2(m+2)}\right)^{(m+1)/m}(1-\eta^2)^{(m+1)/m} \tag{3.14}$$
$$-\frac{\sqrt{\pi}}{2}\left(\frac{m}{2(m+2)}\right)^{1/m}\frac{\Gamma\left(\frac{m+1}{m}\right)}{\Gamma\left(\frac{3m+2}{2m}\right)}\eta + \tfrac{1}{2}\left(\frac{m}{2(m+2)}\right)^{1/m}\eta\, B_{\eta^2}\left(\frac{1}{2}, \frac{m+1}{m}\right),$$

on $F(\xi, \eta) = 0$: $\quad W = W_n = 0,$

where B is the incomplete Beta function (see Abramowitz and Stegun [1], p. 263) and $F(\xi, \eta) = 0$ denotes the free boundary.

We now write

$$W = W_0 + o(1), \quad F = F_0 + o(1), \quad \text{as } m \to \infty,$$

and obtain

$$W_{0\xi\xi} + W_{0\eta\eta} = 1,$$

on $\eta = 0,\ \xi > 0$: $\quad W_{0\eta} = -1,$

on $\eta = 0,\ \xi < 0$: $\quad W_{0\eta} = 0,$

as $\xi \to -\infty$ or $\eta \to +\infty$: $\quad W_0 \to 0,$ (3.15)

as $\xi \to +\infty$: $\quad W_0 \sim \tfrac{1}{2}(1 - \eta^2),$

on $F_0(\xi, \eta) = 0$: $\quad W_0 = W_{0n} = 0.$

(3.15) could be obtained directly from the formulation of Elliott et al. [7] for general constant-total-mass problems for the porous-medium equation in the limit $m \to \infty$.

Again η can easily be obtained as a function of

$$\phi = W_{0\xi}, \quad \text{and} \quad \psi = \eta - W_{0\eta},$$

and we find

$$z = -\frac{2}{\pi}\ln\left(1 + e^{-\pi q}\right)$$

where

$$z = \xi + \mathrm{i}\eta, \quad q = \phi + \mathrm{i}\psi.$$

Hence

$$W_0 = \frac{1}{2}\eta^2 + \frac{1}{6} - \frac{2}{\pi}\operatorname{Re}\left(q \ln(1 + \mathrm{e}^{-\pi q}) + \frac{1}{\pi}L(\mathrm{e}^{-\pi q})\right),$$

and

$$u \sim t^{-1/(m+2)}\left(\frac{1}{6} - \frac{1}{2}\eta^2 - \frac{2}{\pi^2}\operatorname{Re}(L(\mathrm{e}^{-\pi q}))\right)^{1/m},$$

where

$$L(\omega) = \int_0^\omega \frac{\ln(\omega' + 1)}{\omega'}\,\mathrm{d}\omega' = -f(\omega + 1),$$

and f is the dilogarithm (see Abramowitz and Stegun [1], p. 1004).
$\hat{L} = \operatorname{Re}(L)$ is easily calculated from

$$0 < r < 1: \quad \hat{L}(r\mathrm{e}^{\mathrm{i}\theta}) = \sum_{m=1}^{\infty}(-1)^{m+1}\frac{r^m \cos m\theta}{m^2}, \quad (\text{with } -\pi < \theta \leqslant \pi),$$

$$r = 1: \quad \hat{L} = \frac{\pi^2}{12} - \frac{\theta^2}{4},$$

$$r > 1: \quad \hat{L} = \frac{1}{2}\ln^2 r - \frac{\theta^2}{2} + \frac{\pi^2}{6} - \sum_{m=1}^{\infty}(-1)^{m+1}\frac{r^{-m}\cos m\theta}{m^2}.$$

These series converge most slowly near $r = 1$, where the expressions

$$\theta \neq \pi: \quad \hat{L} = \frac{\pi^2}{12} - \frac{\theta^2}{4} + \ln(2\cos\tfrac{1}{2}\theta)(r - 1)$$
$$+ \sum_{m=1}^{\infty}\frac{(-1)^{m+1}}{m+1}(a_m - \ln(2\cos\tfrac{1}{2}\theta))(r - 1)^{m+1},$$

$$\theta = \pi: \quad \hat{L} = -\frac{\pi^2}{6} + \sum_{m=0}^{\infty}\frac{(-1)^m}{m+1}\left(\ln|r - 1| - \frac{1}{m+1}\right)(r - 1)^{m+1},$$

may be used. Here

$$a_m = \sum_{k=1}^{m}\frac{\cos\dfrac{k\theta}{2}}{k(2\cos\frac{1}{2}\theta)^k}$$

(so that $a_\infty = \ln(2\cos\frac{1}{2}\theta)$ for $-2\pi/3 < \theta < 2\pi/3$).

The free boundary is given by

$$\xi = -\frac{2}{\pi}\ln(2\cos\pi\eta), \tag{3.16}$$

so that $a \sim (2\ln 2)/\pi \approx 0.441$.

We again expect this to be a lower bound for all m. Since (3.13) and (3.16) are smaller than (3.7) and (3.10) respectively, this work strongly indicates that for all m the aspect ratio is smaller for the instantaneous-source problem than for the constant-source problem.

3.2.3. Integral invariants

In practice the initial data corresponding to an implant is clearly not given by a δ-function, but the similarity solution discussed in this section gives the large-time behaviour for fairly general initial data. The first two terms in the large-time expansion will take the form

$$c \sim a^{2/m} t^{-1/(m+2)} \left\{ d^{1/m}(\xi, \eta) + \frac{x_0 t^{-1/(m+2)}}{D_0^{1/2} a} \frac{\partial}{\partial \xi}(d^{1/m}(\xi, \eta)) \right\} \tag{3.17}$$

where x_0 is a constant. The second term in this expansion simply represents a shift in the origin of x and may be eliminated by replacing ξ by

$$\hat{\xi} = \frac{x - x_0}{D_0^{1/2} a\, t^{1/(m+2)}}.$$

It is therefore useful to have a relationship which determines the value of x_0 in terms of the initial data.

We now introduce

$$I_0(t) = \int_0^\infty \int_{-\infty}^\infty (c - c^* H(x))\, dx\, dy,$$

where $c \to c^*(y, t)$ as $x \to +\infty$. It is straightforward to show that

$$\frac{dI_0}{dt} = 0,$$

so that (3.17) implies

$$x_0 = I_0(0)/Q$$

where $Q = \int_0^\infty c^*\, dy$; in other words the origin of x should be chosen so that

$$I_0 \equiv 0.$$

Introducing

$$I_1 = \int_0^\infty \int_{-\infty}^\infty x(c - c^* H(x))\, dx\, dy$$

it is also straightforward (using

$$x\nabla \cdot (c^m \nabla c) = \nabla \cdot \left(x c^m \nabla c - \frac{1}{m+1} c^{m+1} \hat{\boldsymbol{x}} \right),$$

where $\hat{\boldsymbol{x}}$ is the unit vector in the x direction) to show that

$$\frac{\mathrm{d}}{\mathrm{d}t} I_1 = \frac{1}{m+1} \int_0^\infty c^{*m+1} \, \mathrm{d}y,$$

a relationship which may be used to give some indication of the extent of lateral diffusion.

4. Discussion

In this paper we have obtained approximate similarity solutions to the porous-medium equation in one and two-dimensions.

The results of Section 2 include a power-series solution for the one-dimensional constant-source problem. For $m = O(1)$ the terms of this series rapidly become negligible, though for small m convergence is slow close to $\xi = 1$, as would be expected from the boundary-layer behaviour which occurs for small m. Such approximate (rather than numerical) solutions are desirable not only because they reveal trends and avoid the need for interpolation, but also because they are easily manipulated in order to obtain the dependence on the processing conditions of various quantities which are important in device operation (see Fair [8]) and because they facilitate the construction of uniformly valid expansions for cases in which (1.1) describes only the first-order term in one region of a singular perturbation problem (see King [15]). The approximation given here has the further advantage that its accuracy can easily be improved by taking more terms in series.

In Section 3 we considered physically important two-dimensional situations in which the problem for $m = O(1)$ requires numerical solution, which is not discussed here. However, the limiting cases considered, while not of direct practical relevance, not only provide useful test cases for numerical schemes but also give a fair amount of qualitative information.

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