Similarity, attraction and initial conditions in an example of nonlinear diffusion

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Abstract

Similarity solutions play an important role in many fields of science. The recent book of Barenblatt [2] discusses many examples. Often, outstanding unresolved issues are whether a similarity solution is dynamically attractive, and if it is, to what particular solution does the system evolve. By recasting the dynamic problem in a form to which centre manifold theory may

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be applied, based upon a transformation by Wayne [10], we may resolve these issues in many cases. For definiteness we illustrate the principles by discussing the application of centre manifold theory to a particular nonlinear diffusion problem arising in filtration. Theory constructs the similarity solution, confirms its relevance, and determines the correct solution for any compact initial condition. The techniques and results we discuss are applicable to a wide range of similarity problems.

Contents

1 Introduction

Consider the nonlinear diffusion problem with a step in the diffusivity discussed by Barenblatt [2, §3.2] which in nondimensional form is

$$\theta_t = \begin{cases} \theta_{xx}\,, & \theta_t \geq 0 \\ (1+\epsilon)\theta_{xx}\,, & \theta_t \leq 0 \end{cases}\,, \tag{1}$$

where $\theta(x,t)$ is the evolving concentration of some spatially distributed substance. Such a problem, with its nonlinear step in the diffusivity, arises in theory of filtration of an elastic fluid in an elasto-plastic porous media (see the discussion in [2, §3.2.1]). It describes the diffusion in one spatial dimension x which is assumed here to be effectively of infinite extent.

We write and analyse (1) as a perturbation of the basic linear diffusion problem, namely

$$\theta_t = \theta_{xx} + f(\theta,\epsilon)\,, \tag{2}$$

where, since θ_t has the same sign as θ_{xx},

$$f = \begin{cases} 0\,, & \theta_{xx} \geq 0 \\ \epsilon\theta_{xx}\,, & \theta_{xx} \leq 0 \end{cases}\,. \tag{3}$$

The term $f(\theta,\epsilon)$ acts as a nonlinear perturbation to the basic diffusion of

$$\theta_t = \theta_{xx} \tag{4}$$

on an infinite domain. Of course ϵ need not be small but we shall treat it so.

We apply centre manifold theory to help understand and solve this problem. But on the infinite spatial domain there is no clear cut centre eigenspace for (4). However, following Wayne [10, 9] we transform the problem to one of seeking $\phi(\xi, \tau)$ where

$$\tau = \log t\,, \quad \xi = \frac{x}{\sqrt{t}}\,, \quad \theta = \frac{1}{\sqrt{t}}\phi(\tau, \xi)\,. \tag{5}$$

Then the dependence upon the scaled space variable ξ causes the Gaussian spread from a point release,

$$\theta = \frac{a}{2\sqrt{\pi t}} e^{-x^2/(4t)}\,, \tag{6}$$

to correspond to a fixed point of the dynamics for ϕ, namely

$$\phi_* = \frac{a}{2\sqrt{\pi}} e^{-\xi^2/4}\,. \tag{7}$$

Also, the algebraic decay in t from any compact release to the Gaussian (6) transforms to an exponentially quick decay in τ to the fixed point (7). Centre manifold theory is applied in Section 2 to justify the self-similar Gaussian (6) as a valid approximation to the long-term dynamics of the non-constant diffusivity problem (1). Then the centre manifold analysis, as extended in Section 3, determines that the amplitude a of the decaying Gaussian evolves like

$$a \approx a_0 t^{-\epsilon/\sqrt{2\pi e}} \tag{8}$$

in accordance with the result reported by Barenblatt for $\epsilon \neq 0$. In addition to this confirmation of earlier results, centre manifold theory [3] immediately guarantees the attraction of the similarity solution. That is, this approach easily establishes the relevance of the similarity solution to the long-term dynamics of this nonlinear diffusion and we expect it to be able to analogously justify the relevance of similarity solutions for other problems.

The amplitude of the spreading Gaussian not only decays in time, it also is a function of the initial distribution $\theta(x, 1)$ of the substance (note that the initial release is assumed to occur at $t = 1$ corresponding to the transformed time $\tau = 0$). Qualitatively, the long term behaviour is similar for all initially compact releases. However, the specific evolution of the model does depend on the specific initial conditions. In other words, we need to determine a_0 in (8). Naively we may expect that the total amount of substance in the model, given by a in (6), will be the same as that at the instant of release and so use

$$a_0 = \int_{-\infty}^{\infty} \theta(x, 1)\, dx\,. \tag{9}$$

However, this is only a leading order approximation and needs correction depending upon other details of the release distribution $\theta(x, 1)$. The corrections cannot be determined by scaling law arguments, but require a knowledge of the dynamics of approach to the similarity solution. Recently developed theory [7, 8] is used in Section 4 to determine the proper choice of the initial conditions for the model amplitude a.

For any given release of substance, the assumed origin of space-time may not be the best location for the origin of the similarity solution. In Section 5 we show how the translational degrees of freedom in the coordinate system can be incorporated into the model for it to represent better the solution of the original diffusion problem. Numerical solutions reported in Section 6 confirm the effectiveness of the correct choice of a_0 as well as of time and space origins of the model.

Finally we comment that the example discussed in detail here is just one of a wide class of nonlinear advection-reaction-diffusion problems. Centre manifold theory may be successfully applied to many of these problems and not only create the similarity solution, but also justify its relevance as an attractive manifold, and determine the correct initial amplitude for the similarity solutions. One class of nonlinear reaction-diffusion problems was similarly analysed by Gene Wayne [10]. Some of the similarity solutions of the nonlinear advection diffusion problems discussed by Doyle and Englefeld [5] are also amenable to this centre manifold approach.

2 Similarity solutions form a centre manifold

Now investigate the centre manifold analysis in more detail. The transformation (5) changes (2) to

$$\phi_\tau = \mathcal{L}\phi + f(\phi, \epsilon)\,, \tag{10}$$

where the linear operator

$$\mathcal{L}\phi = \phi_{\xi\xi} + \frac{1}{2}\xi\phi_\xi + \frac{1}{2}\phi\,. \tag{11}$$

Adjoin the trivial equation

$$\epsilon_\tau = 0\,. \tag{12}$$

Then observe that for $\epsilon = 0$ the Gaussian (7) describes a fixed point of (10)–(12) for all amplitudes a. Thus the centre manifold we construct will be global in a and local only in ϵ. Now the linear operator $\mathcal{L}$ has a spectrum of

$$\lambda = -n/2\,, \quad n = 0, 1, 2, \ldots\,. \tag{13}$$

This is straightforwardly shown by looking for eigensolutions in the form

$$e^{\lambda_n \tau - \xi^2/4} H_n(\xi)\,,$$

where H_n are Hermite polynomials [1]. With two zero eigenvalues, one from (13) and one trivially from (12), and the rest strictly negative, centre manifold theory asserts there exists a two dimensional centre manifold for (10)–(12), $\mathcal{M}_c$, which is exponentially attractive to nearby trajectories.

Thus by Theorem 2 in [3, p.4], centre manifold theory immediately proves the attraction to the asymptotic similarity solution, albeit only for small enough ϵ. (Contrast the ease of obtaining this result with Barenblatt's stability analysis [2, §8.3.2].) In agreement with Barenblatt's equation (8.67), from the spectrum (13), we immediately deduce that the longest-lasting transient in the approach to the similarity solution will be of relative magnitude approximately $e^{-\tau/2} = 1/\sqrt{t}$.

We now approximate $\mathcal{M}_c$, parameterized by a and ϵ, and the evolution thereon by

$$\phi = a(\tau)\left[\psi_0(\xi) + \epsilon\psi_1(\xi) + \epsilon^2\psi_2(\xi) + \mathcal{O}\left(\epsilon^3\right)\right]\,, \quad \text{where} \quad \psi_0 = \frac{e^{-\xi^2/4}}{2\sqrt{\pi}}\,, \tag{14}$$

$$\text{s.t.} \quad \dot{a} = ag = a\left[\epsilon g_1 + \epsilon^2 g_2 + \mathcal{O}\left(\epsilon^3\right)\right] \tag{15}$$

(ψ_0 is normalised such that $\int_{-\infty}^{\infty} \psi_0 \, d\xi = 1$ and the overdot denotes $d/d\tau$). Substituting (14) and (15) into (10) and equating all terms of $\mathcal{O}(\epsilon)$ we need to solve

$$\mathcal{L}\psi_1 = \psi_0 g_1 - D_{\xi_0}\psi_0 \,, \tag{16}$$

where for any s

$$D_s = \begin{cases} 0\,, & \xi \notin [-s, s] \\ \frac{\partial^2}{\partial \xi^2}\,, & \xi \in [-s, s] \end{cases} . \tag{17}$$

Here $\xi_0 = \sqrt{2}$ is such that $\psi_{0\xi\xi}(-\xi_0) = \psi_{0\xi\xi}(\xi_0) = 0$. But $\mathcal{L}$ is singular as it has a zero eigenvalue; so we choose g_1 to put the remaining terms in the range of $\mathcal{L}$—this is the solvability condition. In order to do this we take the inner product of equation (16) with the solution z of the adjoint problem

$$\mathcal{L}^\dagger z \equiv z_{\xi\xi} - \frac{1}{2}\xi z_\xi = 0 \,, \tag{18}$$

where the adjoint is obtained using the obvious inner product

$$\langle u, v\rangle \equiv \int_{-\infty}^{\infty} uv \, d\xi \,. \tag{19}$$

For a reason discussed later in the paper we normalise the adjoint eigenvector such that $\langle z, \psi_0 \rangle = 1$. It is straightforward to check that the adjoint eigenvector satisfying this normalisation is $z = 1$.

Finally, applying the solvability condition we find that

$$g_1 = 2\psi_{0\xi}(\xi_0) = -\frac{1}{\sqrt{2\pi e}}\,. \tag{20}$$

(As usual, we do not need to find ψ_1 to determine the leading order evolution.) The leading order centre manifold model $\dot{a} \approx -\epsilon a/\sqrt{2\pi e}$ then has solution

$$a = a_0 e^{-\epsilon\tau/\sqrt{2\pi e}} = a_0 t^{-\alpha/2}\,, \quad \text{where} \quad \alpha = \epsilon\sqrt{\frac{2}{\pi e}}\,, \tag{21}$$

in agreement with Barenblatt [2, pp175–6]. The constant a_0 is determined by the initial conditions for the full original problem and will be determined in Section 4.

3 The next-order correction matches earlier results

Before proceeding to the next order approximation for the evolution on the centre manifold we need to find ψ_1.

Since the operator $\mathcal{L}$ is singular the solution is not unique and we are free to impose one additional condition on the solution to fix it. It is convenient to require that

$$\int_{-\infty}^{\infty} \psi_1\, d\xi = 0\,. \tag{22}$$

Physically this implies that the total amount of the diffused substance is given completely by the leading order approximation of the solution, and as $\int_{-\infty}^{\infty} \psi_0\, d\xi =$

1, the total amount is simply a. Under this condition the continuous, up to the second derivative, solution to (16) becomes

$$\begin{aligned}\psi_1 &= e^{-\xi^2/4}\Bigg\{c_3 + \frac{i}{2\sqrt{2e}}\left(\operatorname{erf}(\frac{|\xi|}{2}) - 1\right)\operatorname{erf}\left(\frac{i|\xi|}{2}\right) \\ &\quad - \frac{i}{2\sqrt{2\pi e}}\int_0^\xi \operatorname{erf}\left(\frac{iy}{2}\right)e^{-y^2/4}dy \\ &\quad + \left[\frac{\xi^2-2}{8\sqrt{\pi}} + \frac{i}{2\sqrt{2e}}\left(\operatorname{erf}\left(\frac{i|\xi|}{2}\right) - \operatorname{erf}\left(\frac{i}{\sqrt{2}}\right)\right)\right] \\ &\quad \times \left(H(\xi+\xi_0) - H(\xi-\xi_0)\right)\Bigg\}\,, \end{aligned} \tag{23}$$

where H denotes the Heaviside function and

$$\begin{aligned} c_3 &= \frac{1}{2\pi\sqrt{2e}}\left[1 + i\pi\operatorname{erf}\left(\frac{1}{\sqrt{2}}\right)\operatorname{erf}\left(\frac{i}{\sqrt{2}}\right) - i\sqrt{\pi}\left(I_1 + I_2 - \frac{I_3}{\sqrt{\pi}}\right)\right] \\ &\approx -0.1076980691\,. \end{aligned} \tag{24}$$

The integrals entering the definition of c_3 are:

$$I_1 = \int_0^{\xi_0} e^{-\frac{\xi^2}{4}}\operatorname{erf}\left(\frac{\xi}{2}\right)\operatorname{erf}\left(\frac{i\xi}{2}\right)d\xi \approx 0.2262196880i\,, \tag{25}$$

$$I_2 = \int_{\xi_0}^{\infty} e^{-\frac{\xi^2}{4}}\left[\operatorname{erf}\left(\frac{\xi}{2}\right) - 1\right]\operatorname{erf}\left(\frac{i\xi}{2}\right)d\xi \approx -0.1358229603i\,, \tag{26}$$

$$I_3 = \int_0^{\infty} e^{-\frac{\xi^2}{4}}\int_0^{\xi} e^{-\frac{y^2}{4}}\operatorname{erf}\left(\frac{iy}{2}\right)dy\,d\xi \approx 0.6931471806i\,. \tag{27}$$

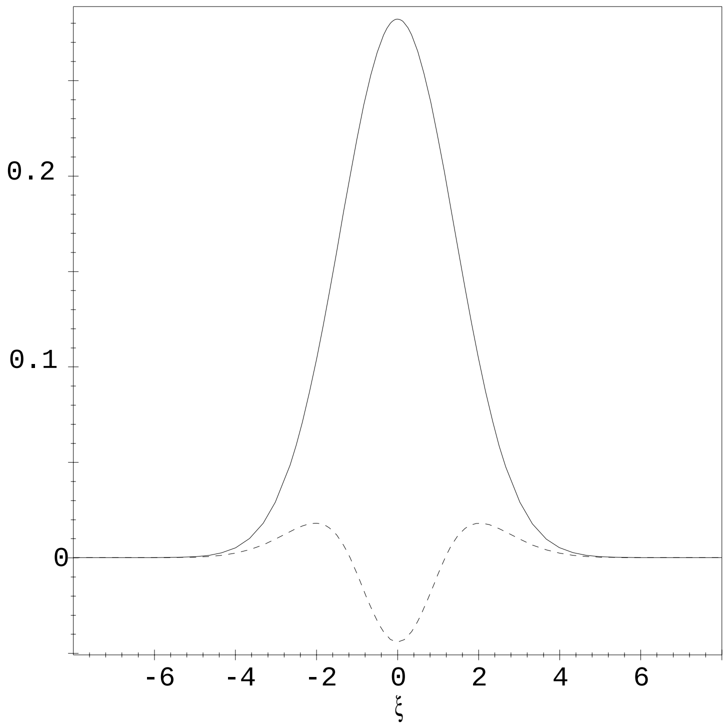

FIGURE 1. Solutions $\psi_0(\xi)$ (solid line) showing the Gaussian shape of the basic similarity solution, and $\psi_1(\xi)$ (dashed line) showing that the Gaussian is flattened and broadened by the nonlinear diffusion.

As expected the first order correction, ψ_1, is an even function of ξ, see Figure 1.

Let $\psi_{\xi\xi}(\bar{\xi}) = 0$. Then $\bar{\xi} = \xi_0 + \epsilon\xi_1 + \mathcal{O}\left(\epsilon^2\right)$ where, as is deduced from (14) and (23),

$$\xi_1 = -\frac{\psi_{1\xi\xi}(\xi_0)}{\psi_{0\xi\xi\xi}(\xi_0)} \approx 0.5665706981\,. \tag{28}$$

Collecting terms of $\mathcal{O}\left(\epsilon^2\right)$ we obtain

$$\mathcal{L}\psi_2 = \psi_1 g_1 + \psi_0 g_2 - \left(D_{\xi_0+\epsilon\xi_1} - D_{\xi_0}\right)\psi_0 - D_{\xi_0}\psi_1\,. \tag{29}$$

Similarly to the previous section, the application of the solvability condition, upon making use of (22), leads to

$$\begin{aligned} g_2 &= 2\left(\psi_{1\xi}(\xi_0+\epsilon\xi_1) + \psi_{0\xi}(\xi_0+\epsilon\xi_1) - \psi_{0\xi}(\xi_0)\right) \\ &= 2\psi_{1\xi}(\xi_0) + \mathcal{O}\left(\epsilon\right) \\ &\approx 0.06354624322 + \mathcal{O}\left(\epsilon\right)\,, \end{aligned} \tag{30}$$

where the even symmetry of ψ_0 and ψ_1 is taken into account. The numerical results given in (28) and (30) coincide with the ones reported by Cole and Wagner in their paper [4, p.167] though our values are given with more significant digits. Consequently, the next order centre manifold model is

$$\dot{a} \approx a(\epsilon g_1 + \epsilon^2 g_2) \tag{31}$$

with solution

$$a = a_0 t^{-\alpha'/2}\,, \quad \text{where} \quad \alpha' = 2\epsilon\left(\frac{1}{\sqrt{2\pi e}} - \epsilon g_2\right)\,. \tag{32}$$

4 The correct initial condition ensures fidelity of the model

The correct projection of initial conditions onto a centre manifold, first developed in [7] and recently refined in [8], should approximately determine the "functional of the initial conditions" mentioned by Barenblatt near the top of p.202 [2], but not previously found. Here we follow the procedure outlined in [8] to give the proper initial conditions a_0 for the centre manifold model (32) when the initial conditions for the original problem are given by $\theta = \theta_0(x)$ at $t = 1$ corresponding to $\tau = 0$. We expect that $a|_{\tau=0} = \int_{-\infty}^{\infty} \theta_0 \, dx$, but this is only a first approximation. The more careful analysis corrects this approximation.

As used in previous sections, the special form of (10) implies that its solution is to be found in the separable form

$$\phi(\tau, \xi; \epsilon) = a(\tau)\psi(\xi; \epsilon) \,, \quad \text{where} \quad \dot{a} = a(\tau) g(\epsilon) \,. \tag{33}$$

Then "vectors" locally tangent to the centre manifold are found to be

$$\mathbf{e}_1 = (a\partial\psi/\partial\epsilon, 1) \quad \text{and} \quad \mathbf{e}_2 = (\psi, 0) \,.$$

According to [8] we need to find "vectors" $\mathbf{z}_1$ and $\mathbf{z}_2$ satisfying

$$\mathcal{D}\mathbf{z}_j - \sum_{k=1}^{2} \langle \mathcal{D}\mathbf{z}_j, \mathbf{e}_k \rangle \, \mathbf{z}_k = \mathbf{0} \,, \quad j = 1, 2 \tag{34}$$

and normalisation $\langle \mathbf{z}_j, \mathbf{e}_k \rangle = \delta_{jk}$ where the dual operator $\mathcal{D}$ is defined as

$$\mathcal{D} \equiv \frac{\partial}{\partial \tau} + \mathcal{I}^\dagger \,, \tag{35}$$

the adjoint

$$\mathcal{I}^\dagger = \begin{bmatrix} \mathcal{L}^\dagger + \epsilon D_{\bar{\xi}}^\dagger & 0 \\ D_{\bar{\xi}}\phi + \epsilon D_{\bar{\xi}}\frac{\partial \phi}{\partial \epsilon} & 0 \end{bmatrix} \tag{36}$$

and

$$D_{\bar{\xi}}^\dagger \equiv D_{\bar{\xi}} + 2\left(\delta(\xi + \bar{\xi}) - \delta(\xi - \bar{\xi})\right)\frac{\partial}{\partial \xi} + \delta'(\xi + \bar{\xi}) - \delta'(\xi - \bar{\xi}) \,, \tag{37}$$

in which δ and δ' denote the Dirac delta function and its derivative, respectively. The normalisation conditions give that

$$\begin{bmatrix} z_1^{(1)} \\ z_1^{(2)} \end{bmatrix} = \begin{bmatrix} \frac{1}{a} r_1^{(1)}(\xi) \\ r_1^{(2)}(\xi) \end{bmatrix} , \quad \begin{bmatrix} z_2^{(1)} \\ z_2^{(2)} \end{bmatrix} = \begin{bmatrix} r_2^{(1)}(\xi) \\ a r_2^{(2)}(\xi) \end{bmatrix} , \tag{38}$$

$$\begin{array}{ll} \int_{-\infty}^{\infty} r_1^{(1)}\psi \, d\xi = 0 \,, & \int_{-\infty}^{\infty}\left(r_1^{(1)}\frac{\partial \psi}{\partial \epsilon} + r_1^{(2)}\right) d\xi = 1 \,, \\ \int_{-\infty}^{\infty} r_2^{(1)}\psi \, d\xi = 1 \,, & \int_{-\infty}^{\infty}\left(r_2^{(1)}\frac{\partial \psi}{\partial \epsilon} + r_2^{(2)}\right) d\xi = 0 \,. \end{array} \tag{39}$$

We look for the solution of (34) satisfying $\mathcal{D}\mathbf{z}_1 = \mathbf{0}$, *i.e.*

$$\begin{bmatrix} -\frac{g}{a} r_1^{(1)} \\ 0 \end{bmatrix} = -\begin{bmatrix} \frac{1}{a}\left(\mathcal{L}^\dagger + \epsilon D_{\bar{\xi}}\right) r_1^{(1)} \\ \left(D_{\bar{\xi}}\psi + \epsilon D_{\bar{\xi}}\frac{\partial \psi}{\partial \epsilon}\right) r_1^{(1)} \end{bmatrix} . \tag{40}$$

Hence we immediately deduce that $r_1^{(1)} = 0$. Consequently, the second of normalisation conditions (39) is transformed to $\int_{-\infty}^{\infty} r_1^{(2)} d\xi = 1$. Then from the projection of initial conditions

$$\frac{1}{a|_{\tau=0}} \left\langle r_1^{(1)}, \theta_0 - a|_{\tau=0}\psi \right\rangle + (\epsilon_0 - \epsilon) \left\langle r_1^{(2)}, 1 \right\rangle = 0 \tag{41}$$

and we deduce that $\epsilon \equiv \epsilon_0$. This result, that the parameter ϵ remains unchanged between the model and the original problem, is expected at the outset, but we have just demonstrated how it is obtained in the context of the developed theory for the projection of initial conditions.

Thus the proper initial condition for the amplitude $a|_{\tau=0}$ is given by

$$\left\langle r_2^{(1)}, \theta_0 - a|_{\tau=0}\psi \right\rangle = 0\,, \tag{42}$$

or, equivalently, since the problem is linear in amplitude a and the normalisation conditions (39) are used, by

$$a|_{\tau=0} = \left\langle r_2^{(1)}, \theta_0 \right\rangle\,. \tag{43}$$

Thus the problem of finding the proper initial condition is reduced to solving for $r_2^{(1)}$ which satisfies the following equation deduced from (34)

$$\left(\mathcal{L}^\dagger + \epsilon D_\xi^\dagger\right) r_2^{(1)} = \left\langle \left(\mathcal{L}^\dagger + \epsilon D_\xi^\dagger\right) r_2^{(1)}, \psi \right\rangle r_2^{(1)}\,. \tag{44}$$

Performing integration by parts in the right-hand side of (44) and using the normalisation (39) we obtain

$$\left(\mathcal{L}^\dagger + \epsilon D_\xi^\dagger\right) r_2^{(1)} - g r_2^{(1)} = 0, \quad \left\langle r_2^{(1)}, \psi \right\rangle = 1\,. \tag{45}$$

We solve (45) assuming $r_2^{(1)} = p_0(\xi) + \epsilon p_1(\xi) + \mathcal{O}\left(\epsilon^2\right)$ and recollecting that $g \approx -\epsilon/\sqrt{2\pi e} + \mathcal{O}\left(\epsilon^2\right)$ and $\psi = \psi_0 + \epsilon\psi_1 + \mathcal{O}\left(\epsilon^2\right)$. At $\mathcal{O}\left(\epsilon^0\right)$ we obtain

$$\mathcal{L}^\dagger p_0 = 0, \quad \langle p_0, \psi_0\rangle = 1 \tag{46}$$

with solution $p_0 = z = 1$. Thus at leading order $a|_{\tau=0} = \int_{-\infty}^{\infty} \theta_0(\xi) d\xi$.

At $\mathcal{O}\left(\epsilon^1\right)$ we obtain

$$\mathcal{L}^\dagger p_1 + \delta'(\xi+\xi_0) - \delta'(\xi-\xi_0) + \frac{1}{\sqrt{2\pi e}} = 0\,, \quad \langle p_1, \psi_0\rangle = 0\,. \tag{47}$$

The solution, presented in Figure 2, has the following algebraic form

$$\begin{aligned} p_1(\xi) = \; & c_4 + \left(1 + i\sqrt{\tfrac{\pi}{2e}}\,\mathrm{erf}\left(\tfrac{i}{\sqrt{2}}\right)\right)\left(H(\xi-\xi_0) - H(\xi+\xi_0)\right) \\ & - \tfrac{i}{\sqrt{2e}} \textstyle\int_0^\xi \mathrm{erf}\left(\tfrac{iy}{2}\right) e^{-y^2/4} dy \\ & + i\sqrt{\tfrac{\pi}{2e}}\left(1 + \mathrm{erf}(\tfrac{\xi}{2}) - H(\xi+\xi_0) - H(\xi-\xi_0)\right)\,\mathrm{erf}\left(\tfrac{i\xi}{2}\right)\,, \end{aligned} \tag{48}$$

where

$$\begin{aligned} c_4 = \; & \tfrac{i}{\sqrt{2\pi e}}\left(I_3 - \sqrt{\pi}(I_2 + I_1)\right) + \left(1 + i\sqrt{\tfrac{\pi}{2e}}\,\mathrm{erf}\left(\tfrac{i}{\sqrt{2}}\right)\right)\,\mathrm{erf}\left(\tfrac{1}{\sqrt{2}}\right) \\ \approx \; & 0.0589390531\,. \end{aligned} \tag{49}$$

Finally we then have that the proper initial condition for the centre manifold model (31) is given by

$$a|_{\tau=0} = \int_{-\infty}^{\infty}\left(1 + \epsilon p_1(\xi) + \mathcal{O}\left(\epsilon^2\right)\right)\theta_0\left(\xi\right)\,d\xi \tag{50}$$

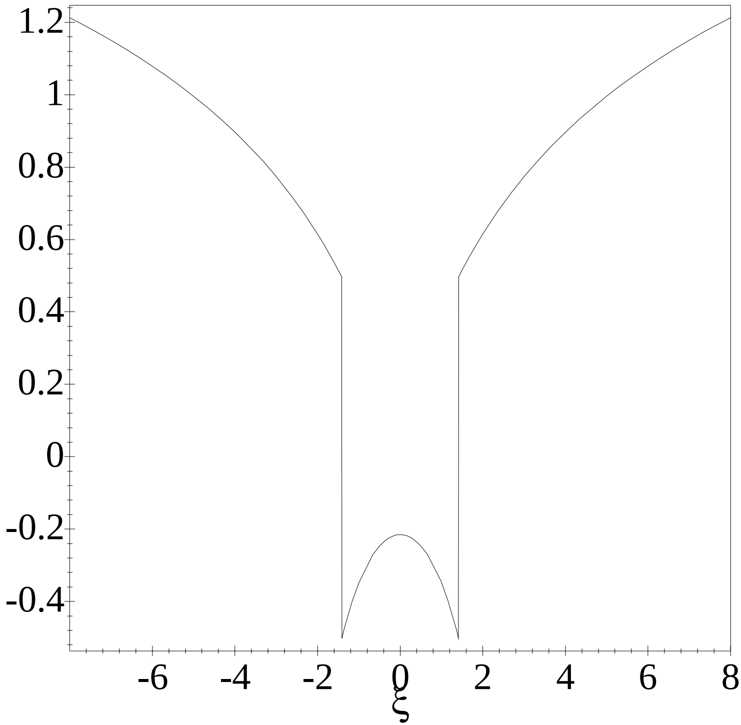

FIGURE 2. $\mathcal{O}(\epsilon)$ initial condition projection function $p_1(\xi)$.

Note that $p_1 \sim [2/(\pi e)]^{1/2} \log(|\xi|)$ as $|\xi| \to \infty$ and, consequently, the integral (43) converges only for a sufficiently compact initial distribution θ_0. This emphasises that the projection of the initial conditions is local in its nature and it is applicable only if the initial conditions for the original problem are, in some sense, close to the centre manifold.

5 Choose an optimal origin in time and space

It follows from the transformation of space and time variables (5) that the diffusion from a localised initial release of arbitrary form occurring in the original problem at $t = 1$ is modelled by the evolution from the initial state of a point release, a delta function, at $x = t = 0$. On the other hand the original partial differential equation (1) is invariant with respect to translations in time and space. Thus there is freedom to choose the time and space origins for the model to suit best the actual distribution of the initial θ. To account for these inherit degrees of freedom in the original problem we generalise the coordinate transformation (5) to

$$\tau = \log\left(t + t_0\right), \quad \xi = \frac{x - x_0}{\sqrt{t + t_0}}, \quad \theta = \frac{\phi(\tau, \xi)}{\sqrt{t + t_0}}, \tag{51}$$

where $t_0 > 0$. Now the localised release $\theta_0(x)$ occurring in the original problem at time $t = 0$ (not at $t = 1$ as assumed in the previous sections) is modelled by some Gaussian centred at x_0 rather than by the delta function at $x = 0$. The width of the model Gaussian at the moment of the actual release $t = 0$ is determined by t_0

which also determines the location of the virtual origin in time for the model. Generalisation (51) does not affect the analysis of the previous sections. In particular, the model dynamics (31) is unchanged because the general long-term dynamics are independent of the space-time origin. However, the generalisation provides a two-parameter family of model solutions to the original problem (1) rather than just the unique model described earlier. Thus here the general projection of initial condition (50) becomes

$$a_0 = t_0^{\alpha'/2} \int_{-\infty}^{\infty} \left[1 + \epsilon p_1 \left(\frac{x - x_0}{\sqrt{t_0}} \right) + \mathcal{O}\left(\epsilon^2\right) \right] \theta_0(x)\, dx\,. \tag{52}$$

One is free to choose parameters x_0 and t_0 entering (52) in such a way that the model possess certain additional properties. For instance, we choose t_0 such that the contribution of the ϵ-dependent terms in (52) is zero—this choice should ensure that the model a most closely matches the solution θ for the original problem in the short-term as well as the long-term evolution. In essence this is equivalent to considering all the centre manifolds (in a and ϵ) parameterized by t_0 and x_0, and choosing that centre manifold whose isochrons are linearly "vertical" and hence make the definition of a match the projection. It is always possible to make this choice since physical initial distributions θ_0 are non-negative functions while the mean of p_1 is zero. Thus require

$$I = \int_{-\infty}^{\infty} p_1 \left(\frac{x - x_0}{\sqrt{t_0}} \right) \theta_0(x)\, dx = 0\,, \tag{53}$$

which we view as implicitly defining t_0 as a function of x_0.

The value of x_0 is then fixed to minimise t_0. We feel this is desirable since it minimises the spread of the model's Gaussian at the initial instant of release and so maximises the information content of the model. (It is also the only distinguished x_0.) Differentiating (53) with respect to x_0 we obtain

$$\frac{dI}{dx_0} = -\frac{1}{\sqrt{t_0}} \int_{-\infty}^{\infty} p_1'\left(\frac{x-x_0}{\sqrt{t_0}}\right)\theta_0(x)\left[1+\frac{x-x_0}{2t_0}\frac{dt_0}{dx_0}\right]dx = 0\,, \tag{54}$$

where prime denotes differentiation with respect to the argument. At the point of extremum $dt_0/dx_0 = 0$ and the second term in the brackets in (54) vanishes. Thus we solve

$$\int_{-\infty}^{\infty} p_1'\left(\frac{x-x_0}{\sqrt{t_0}}\right)\theta_0(x)\,dx = 0\,. \tag{55}$$

in conjunction with (53) to define x_0 and t_0. As an aside it follows from the above discussion that such chosen x_0 and t_0 guarantee that $I = 0$ is a minimum contribution to the ϵ-correction of initial conditions for the model. If θ_0 is symmetric, say about $x = q$, then, owing to the even symmetry of p_1, the choice of $x_0 = q$ guarantees that (55) is satisfied. Thus for symmetric θ_0 the best choice for the centre of the Gaussian spread of the model is the point of symmetry.

Finally, the initial amplitude is then given by

$$a_0 = t_0^{\alpha'/2}\int_{-\infty}^{\infty}\theta_0(x)\,dx \tag{56}$$

and the model solution written in the original variables becomes

$$\theta = \frac{a_0}{(t+t_0)^{(1+\alpha')/2}}\left[\psi_0\left(\frac{x-x_0}{\sqrt{t+t_0}}\right)+\epsilon\psi_1\left(\frac{x-x_0}{\sqrt{t+t_0}}\right)+\mathcal{O}\left(\epsilon^2\right)\right], \tag{57}$$

where t_0 and x_0 satisfy (53) and (55).

6 Numerical results demonstrate the accuracy of the model

We illustrate the correctness of the derived initial conditions by comparing the model predictions with the direct numerical integration of equation (1). Let the initial distribution of substance for the original problem at $t = 0$ be in the form of the Gaussian

$$\theta_0 = \sqrt{\frac{10}{\pi}} \exp(-10x^2)\,. \tag{58}$$

Numerical integration of (1) with initial distribution (58) was performed using IMSL routine DMOLCH [6] with the accuracy of 10^{-8}. Since the long term behaviour of the numerical solution was found to depend on the size of the computational domain, the preliminary test of the numerical solution was performed for $\epsilon = 0$ for which the analytic solution comes from (6). It was found that the non-reflecting boundary conditions $\theta_x(L)/\theta(L) = x/(2t)$ imposed at $L = 22.5$ eliminated such an influence for the time interval considered.

The resulting time evolution of the direct numerical solution for $\epsilon = 0.1$ at $x = 0$ is shown by a solid line in Figure 3. Because of the symmetry of initial distribution (58) with respect to the line $x = 0$, (55) gives the value $x_0 = 0$ for

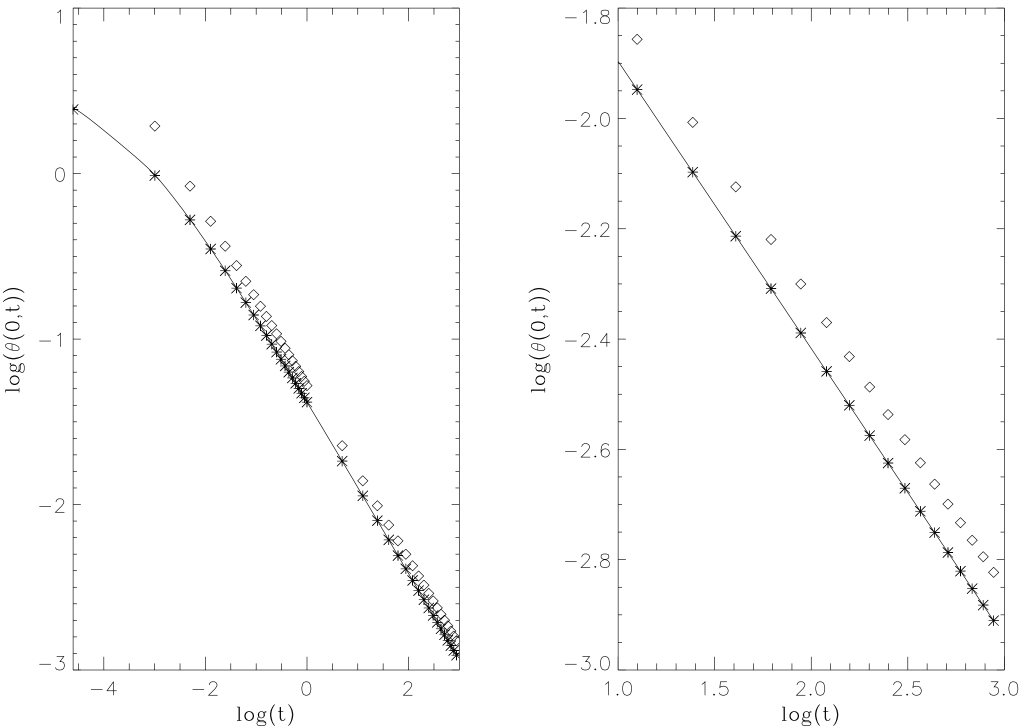

FIGURE 3. Numerical (solid line) solutions of equation (1) evaluated at $x = 0$ for $\epsilon = 0.1$ compared with the model (57) that uses the correct initial conditions (stars) and the previous model (59) (diamonds).

model (57). Numerical evaluation shows that condition (53) is satisfied for θ_0 given by (58) for $t_0 \approx 0.0250$. As seen from Figure 3(a) the model dynamics shown by star symbols virtually coincides with the one obtained from numerical integration for all time. In Figure 3(b) we compare the numerical and the proper model (57) solutions with the earlier proposed model [2, 4]

$$\theta = \frac{\int_{-\infty}^{\infty} \theta_0(x)\, dx}{t^{(1+\alpha')/2}} \left(\psi_0 \left(\frac{x}{\sqrt{t}} \right) + \epsilon \psi_1 \left(\frac{x}{\sqrt{t}} \right) + \mathcal{O}\left(\epsilon^2\right) \right) , \tag{59}$$

which uses naive initial condition (9)—shown by diamond symbols—for larger times. While the present model and numerical solution are virtually indistinguishable in their evolution, the model (59) based solely on scaling arguments is able to predict just a slope. The actual values of the distribution maximum it provides lies apart from the numerical curve for all time. Thus the correct initial conditions for the model are essential to avoid a permanent finite phase difference between the model and the actual full solutions.

In Figure 4 we show the difference $|\theta_n - \theta_m|$ between the numerical (θ_n) and model (θ_m) solutions as a function of space and time (the error is symmetric about $x = 0$). See that our model (57) agrees with a numerical solution much better than the previous (59): the the maximum discrepancy between our model and the numerical solution does not exceed the value of 0.4 while for the previous model it reaches the values up to 1.6. Our model deviates most from the numerical solution in the vicinity of the inflection point (the location of the discontinuity of the diffusion coefficient) shown by the red line in Figure 4, while for the previous model the largest error is in the over-prediction of the solution amplitude during the initial stages of evolution (lower left corner of the right plot in Figure 4).

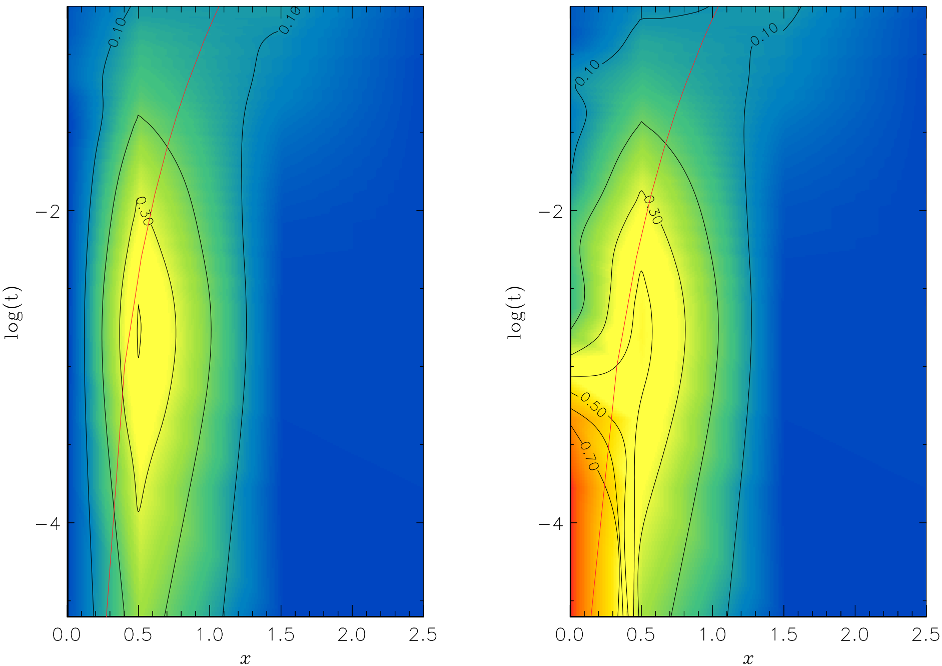

FIGURE 4. The difference between the numerical solution with the initial condition (58) and (left) our model (57) and (right) the previous model (59). The colour scale blue–red corresponds to the range of values from 0 to 0.8 and larger. The red line shows the location of the inflection points for the solutions.

The provision of correct initial conditions for the model are essential for accurate forecasts.

7 Conclusions

We have demonstrated that the centre manifold theory provides a straightforward and rigorous way of deriving not only the functional form of similarity solutions of nonlinear diffusion, but also the appropriate initial conditions for the model in terms of the initial distributions of the substance. This cannot be done using other modelling approaches such as, for example, scaling laws or the method of multiple scales. The correct provision of initial conditions also enables us to determine an optimal location for the virtual space-time origin for the model. The present technique may be successfully used for modelling a wide class of nonlinear filtration/diffusion problems.

References

[1] M. Abramowitz and I.A. Stegan, editors. Handbook of Mathematical Functions With Formulas, Graphs, and Mathematical Tables. Dover Publications, Inc., New York, 1972. E7

[2] G.I. Barenblatt. Scaling, self-similarity, and intermediate asymptotics. *Cam-* E1, E3, E3, E7, E9, E13, E23

bridge Texts in Applied Mathematics. Volume 14. CUP, 1996.

[3] J. Carr. Applications of Centre Manifold Theory. *Applied Mathematical Sciences*, 35, Springer-Verlag, 1980. E4, E7

[4] J.D. Cole and B.A. Wagner. On self-similar solutions of Barenblatt's nonlinear filtration equation. *Euro. Jnl of Applied Mathematics*, 7:151–167, 1996. E12, E23

[5] J. Doyle and M.J. Englefeld. Similarity solutions of a generalised Burgers equation *IMA J. of Appl. Math.*, 44:145–153, 1990. E6

[6] IMSL, Inc. *IMSL Mathematical Library, Version 1.1*. Houston, TX, USA, 1989. E21

[7] A.J. Roberts. Appropriate initial conditions for asymptotic descriptions of the long term evolution of dynamical systems. *J. Austral. Math. Soc. B*, 31:48–75, 1989. E5, E13

[8] A.J. Roberts. Computer algebra derives correct initial conditions for low-dimensional dynamical models. preprint, USQ, June 1997. E5, E13, E13, E13

[9] C.E. Wayne. Invariant manifolds and the asymptotics of parabolic equations in cylindrical domains. pp.314–325 in *Differential equations and applications*, ed. Bates, Chow, Lu and Pan, International Press, 1997. E4

[10] C.E. Wayne. Invariant manifolds for parabolic partial differential equations on unbounded domains. *Arch. Rat. Mech. Anal.*, to appear, 1997. E2, E4, E6