



On the Uniqueness Theorem for Advective–Diffusive Transport in Porous Media: A Canonical Proof

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Abstract. This paper presents a proof of the uniqueness theorem for the initial boundary value problem governing advective–diffusive transport of a chemical in a fluid-saturated non-deformable isotropic, homogeneous porous medium. The advective Darcy flow in the porous medium results from the gradient of a hydraulic potential, which is derived from a well-posed problem in potential theory. The paper discusses the relevant set of consistent boundary conditions applicable to the potential inducing the advective flow and to the concentration field, which ensures uniqueness of the solution.

Key words: advection–diffusion equation, uniqueness theorem, contaminant transport, diffusive phenomena, advective transport.

1. Introduction

The study of movement of hazardous chemicals and contaminants in fluid-saturated porous geological media is of considerable importance to environmental geosciences. In environmental engineering in particular, the evaluation of the concentration of such earth borne chemicals leads to a better assessment of related environmental risk. The mechanisms associated with the transport processes are generally quite complicated and usually involve both advective and diffusive processes, governed, respectively, by flow velocities and concentration gradients. Also, depending upon the micro-structural morphology of the porous medium, the physico-chemical characteristics of the porous medium, the saturating fluid and the species that are being transported, these basic modes of transport can be highly non-linear. The linear theories of advective–diffusive transport therefore provide a useful first approximation for the study of chemical and contaminant migration in fluid-saturated porous media. The extent to which either advection or diffusion dominates the overall transport process, will depend on the Peclet number $Pe = VL/D$, where V is a characteristic velocity, L is a characteristic length and D is a diffusion coefficient. When Pe exceeds unity, advective phenomena will dominate and when Pe is less than unity, the dominant transport mechanism will

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be diffusive. The objective of this paper is to present a brief exposition of the uniqueness theorem applicable to the initial boundary value problem governing the classical advective–diffusive transport problem, which, as far as the author is aware, is perhaps the most direct and elementary way of establishing the proof of the theorem.

2. Governing Equations

The partial differential equation governing the combined advective and diffusive transport of a chemical species in a porous medium has been presented in a number of textbooks dealing with both mathematical modelling and engineering applications of geo-environmental transport processes (Bear, 1972; Freeze and Cherry, 1979; Dagan, 1989; Bear and Verruijt, 1990; Philips, 1991; Bear and Bachmat, 1992; Bear *et al.*, 1993; Fetter, 1993; Banks, 1994; Sun, 1996; Bedient *et al.*, 1997; Hornung, 1997; David, 1998; Ingebritsen and Sanford, 1998; Charbeneau, 1999; Nield and Bejan, 1999; Selvadurai, 2000a; Zheng and Bennett, 2002). For completeness, however, a brief derivation of the basic partial differential equation governing advective–diffusive transport of a chemical species through a non-deformable porous medium will be presented (see e.g. Selvadurai, 2000a). Consider an arbitrary region V of a porous medium with surface S . The porosity of the medium, defined by the ratio of the volume of *pore space* to the *total volume*, is denoted by n^* . The concentration of the chemical species per *unit volume of the fluid* contained in the pore space is defined by $\tilde{C}(\mathbf{x}, t)$, where \mathbf{x} is a position vector and t is time. Define a concentration $C(\mathbf{x}, t)$, which is measured per *unit total volume* of the porous medium. At any given location at any time

$$C(\mathbf{x}, t) = n^* \tilde{C}(\mathbf{x}, t) \quad (1)$$

The velocity vector $\mathbf{v}(\mathbf{x}, t)$ defines the advective velocity in the pore space. Again, an averaged advective velocity $\tilde{\mathbf{v}}(\mathbf{x}, t)$, taken over the entire cross-section over which flow takes place is defined, such that

$$\tilde{\mathbf{v}}(\mathbf{x}, t) = n^* \mathbf{v}(\mathbf{x}, t) \quad (2)$$

The assumption (2) pre-supposes that the *area porosity* is identical to the *volume porosity*. This need not be the case for all porous media (Drew and Passman, 1999). For porous media that display a relatively orientation-independent internal fabric, the two measures of porosity are assumed to be approximately the same. The *flux* is defined as the mass of the chemical species either *entering* or *leaving* a unit total area in unit time. The flux vector, or mass being transported by *advection*, per unit total area per unit time is given by

$$\mathbf{F}_a = n^* \tilde{\mathbf{v}} C(\mathbf{x}, t) = \mathbf{v} C(\mathbf{x}, t) \quad (3)$$

The mass of the chemical transported by diffusion is obtained from Fick's law: that is,

$$\mathbf{F}_d = -D n^* \nabla \tilde{C}(\mathbf{x}, t) = -D \nabla C(\mathbf{x}, t) \quad (4)$$

where D is a diffusion coefficient that is positive. The rate at which total mass of the chemical species enters the volume V through the surface S is given by

$$m_i = - \iint_S \mathbf{n}[\mathbf{v}C - D\nabla C] dS = - \iiint_V \nabla \cdot [\mathbf{v}C - D\nabla C] dV \quad (5)$$

where \mathbf{n} is the outward unit normal to the elemental surface area dS .

The rate at which the chemical species accumulates within the fluid in the void space of the porous medium is given by

$$m_a = \frac{d}{dt} \iiint_V n^* \tilde{C} dV = \iiint_V \frac{\partial C}{\partial t} dV \quad (6)$$

Consideration of the effects of natural attenuation of the chemical species due to decay processes within the porous medium gives

$$m_p = - \iiint_V n^* \xi \tilde{C} dV = - \iiint_V \xi C dV \quad (7)$$

where ξ is a positive parameter and measured per unit time. The importance of the natural attenuation process in mitigating the chemical migration process is discussed at length by Werner (2003). For conservation of mass of the species, $m_a = m_i + m_p$, which, when combined with the *Dubois–Reymond Lemma* for the existence of a local equation, gives the partial differential equation governing advective–diffusive transport of a chemical species as follows:

$$D\nabla^2 C - \nabla \cdot (\mathbf{v}C) - \xi C = \frac{\partial C}{\partial t} \quad (8)$$

The representation in terms of the volume-averaged concentration becomes more convenient and appropriate when considering integral representations applicable to the entire volume and the entire surface of a control volume.

In this paper attention is restricted to steady flow fields characterized by Darcy's law and the pore space flow velocities \mathbf{v} , which, for a hydraulically isotropic medium are given by

$$\mathbf{v} = -k\nabla\phi \quad (9)$$

where k is the Dupuit-Forchheimer hydraulic conductivity ($= \tilde{k}/n^*$, where \tilde{k} is the Darcy hydraulic conductivity) and $\phi(\mathbf{x})$ is the reduced Bernoulli potential governing fluid flow through the porous medium, which includes only the datum potential and the pressure potential. For incompressible flow of the pore fluid and for non-deformability of the porous solid

$$\nabla \cdot \mathbf{v} = 0 \quad (10)$$

and the partial differential equation governing the flow potential is Laplace's equation

$$\nabla^2 \phi(\mathbf{x}) = 0 \quad (11)$$

The partial differential equations governing the advective transport problem are therefore (8) and (11), respectively, for the time-dependent chemical concentration $C(\mathbf{x}, t)$ and the flow potential $\phi(\mathbf{x})$.

These partial differential equations represent a *weakly coupled system*, which has a second-order elliptic equation for $\phi(\mathbf{x})$ and a second-order parabolic–hyperbolic equation for $C(\mathbf{x}, t)$. The weak coupling stems from the fact that the potential problem governing $\phi(\mathbf{x})$ can be solved independently of the advective–diffusive transport problem. The boundary conditions associated with $\phi(\mathbf{x})$ are relatively standard. The inhomogeneous Dirichlet boundary conditions correspond to surfaces S_D^ϕ on which total hydraulic potential is prescribed and the Neumann boundary conditions refer to S_N^ϕ surfaces through which the normal flow rates are prescribed, such that $S_D^\phi \cup S_N^\phi = S$ and $S_D^\phi \cap S_N^\phi = 0$ (Figure 1). Both sets of boundary conditions are necessary and sufficient for well-posedness of the potential problem in a Hadamard sense and the uniqueness of solution to the potential problem is well established (see e.g. Courant and Hilbert, 1962; Weinberger, 1965; Selvadurai, 2000a). The surfaces S_D^ϕ and S_N^ϕ may themselves be composed of subsets, such that $S_D^\phi = S_{D1}^\phi \cup S_{D2}^\phi \cup \dots \cup S_{Dn}^\phi$ and $S_N^\phi = S_{N1}^\phi \cup S_{N2}^\phi \cup \dots \cup S_{Nn}^\phi$. The homogeneous Neumann boundary condition corresponds to the conventional impervious boundary through which no flow occurs. The Robin-type boundary conditions applicable to $\phi(\mathbf{x})$ are mathematically consistent but not readily realizable in a practical context. The initial boundary value problem governing $C(\mathbf{x}, t)$ is subject to both an initial condition and Dirichlet and Neumann type boundary

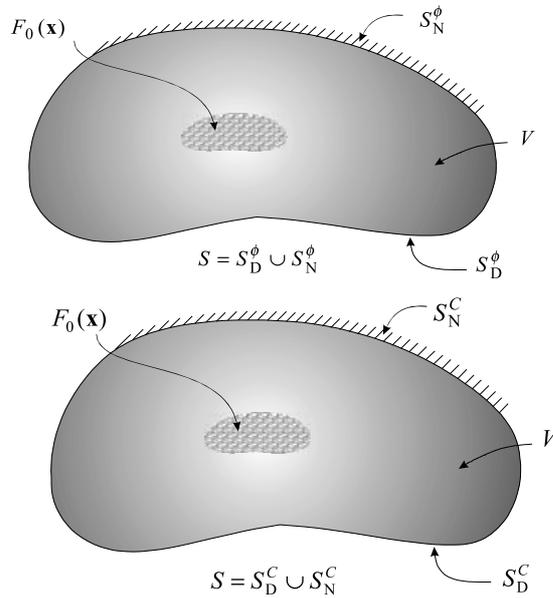


Figure 1. The domain and the relevant boundary conditions applicable to the flow potential and the concentration.

conditions specified on S_D^C and S_N^C , respectively, such that $S_D^C \cup S_N^C = S$ and $S_D^C \cap S_N^C = 0$ (Figure 1). At this stage there are no constraints imposed on the choice of these surfaces in relation to the surfaces S_D^ϕ and S_N^ϕ on which the boundary conditions for the potential problem are prescribed. As before, the surfaces S_D^C and S_N^C may themselves be composed of subsets such that $S_D^C = S_{D1}^C \cup S_{D2}^C \cup \dots \cup S_{Dn}^C$ and $S_N^C = S_{N1}^C \cup S_{N2}^C \cup \dots \cup S_{Nn}^C$. Other mixed boundary conditions of the Robin-type could be prescribed on separate sub-sets of S , but in this paper attention is confined to the conventional Dirichlet and Neumann boundary conditions that can be readily identified in relation to recognizable physical attributes of the transport problem. For example, the inhomogeneous Dirichlet boundary condition for $C(\mathbf{x}, t)$ can be readily identified with surfaces on which the chemical or contaminant concentration is prescribed as a time-dependent function. The chemical concentration at the base of a tailings pond is one such example. In most practical situations, the Neumann boundary condition is homogeneous ensuring that there is no migration of the chemical or contaminant across the boundary. There are, of course, inhomogeneous Neumann boundary conditions that correspond to either fixed or time-dependent extraction of the chemical from a boundary; these, however, are a rarity in a practical context. The same comments apply to the Robin-type boundary conditions that are mathematically consistent but are not readily realizable in a practical context.

3. The Uniqueness Theorem

The advective–diffusion equation defined by (8) applicable to a domain of finite extent V with surface S is considered (Figure 1). The solution to the initial boundary value problem is governed by the partial differential equation

$$D\nabla^2 C - \nabla \cdot (\mathbf{v}C) - \xi C = \frac{\partial C}{\partial t} \quad \forall \mathbf{x} \in V \quad (12)$$

subject to the boundary conditions

$$C(\mathbf{x}, t) = F_D(\mathbf{x}, t) \quad \forall \mathbf{x} \in S_D^C \quad (13)$$

$$\frac{\partial C(\mathbf{x}, t)}{\partial n} = F_N(\mathbf{x}, t) \quad \forall \mathbf{x} \in S_N^C \quad (14)$$

and the initial condition

$$C(\mathbf{x}, 0) = F_0(\mathbf{x}) \quad \forall \mathbf{x} \in V \quad (15)$$

where $F_D(\mathbf{x}, t)$, $F_N(\mathbf{x}, t)$ and $F_0(\mathbf{x})$ are arbitrary functions. In (12), $\mathbf{v}(\mathbf{x})$ is a velocity field, which is derived from the potential $\phi(\mathbf{x})$ that satisfies

$$\nabla^2 \phi(\mathbf{x}) = 0 \quad \forall \mathbf{x} \in V \quad (16)$$

and subject to the boundary conditions

$$\phi(\mathbf{x}) = f_D(\mathbf{x}) \quad \forall \mathbf{x} \in S_D^\phi \quad (17)$$

$$\frac{\partial \phi(\mathbf{x})}{\partial n} = f_N(\mathbf{x}) \quad \forall \mathbf{x} \in S_N^\phi \quad (18)$$

where $f_N(\mathbf{x})$ and $f_D(\mathbf{x})$ are arbitrary functions. From the uniqueness theorem applicable to the potential problem, the boundary value problem defined by (16)–(18) yields a unique potential function and by virtue of (9), gives a unique velocity field $\mathbf{v}(\mathbf{x})$ for $\forall \mathbf{x} \in V$. Implicit in the formulation of the initial boundary value problem for the advection–diffusion equation and the boundary conditions for the potential problem is the assertion that, although the Dirichlet and Neumann boundary conditions are prescribed on separate subsets of S , these regions are distinctly separate.

Assume that the initial boundary value problem defined by (12)–(15) admits two solutions $C^{(1)}(\mathbf{x}, t)$ and $C^{(2)}(\mathbf{x}, t)$. Then the solution $C^*(\mathbf{x}, t)$, defined by

$$C^*(\mathbf{x}, t) = C^{(1)}(\mathbf{x}, t) - C^{(2)}(\mathbf{x}, t) \quad (19)$$

satisfies

$$D\nabla^2 C^* - \nabla \cdot (\mathbf{v}C) - \xi C^* = \frac{\partial C^*}{\partial t} \quad \forall \mathbf{x} \in V \quad (20)$$

subject to the boundary conditions

$$C^*(\mathbf{x}, t) = 0 \quad \forall \mathbf{x} \in S_D^C \quad (21)$$

$$\frac{\partial C^*(\mathbf{x}, t)}{\partial n} = 0 \quad \forall \mathbf{x} \in S_N^C \quad (22)$$

and the initial condition

$$C^*(\mathbf{x}, 0) = 0 \quad \forall \mathbf{x} \in V \quad (23)$$

Now consider what could be defined as the *Energy Balance* associated with the set (20)–(23), obtained by multiplying Equation (20) by $C^*(\mathbf{x}, t)$ and integrating the result over the region V :

$$\iiint_V C^* \left[\frac{\partial C^*}{\partial t} + \nabla \cdot (C^* \mathbf{v}) + \xi C^* - D\nabla^2 C^* \right] dV = 0 \quad (24)$$

The purpose of this operation is to arrive at integrands of $C^*(\mathbf{x}, t)$ in a quadratic form, for which *positive definiteness* is assured. Considering vector operations

$$\nabla \cdot (C^* \mathbf{v}) = \nabla C^* \cdot \mathbf{v} + C^* (\nabla \cdot \mathbf{v}) \quad (25)$$

$$\nabla \cdot [(C^*)^2 \mathbf{v}] = 2C^* (\nabla C^*) \cdot \mathbf{v} + (C^*)^2 \nabla \cdot \mathbf{v} \quad (26)$$

and noting that, for incompressible potential flow, $\nabla \cdot \mathbf{v} = 0$

$$\begin{aligned} \iiint_V C^* \nabla \cdot (C^* \mathbf{v}) \, dV &= \iiint_V C^* \nabla C^* \cdot \mathbf{v} \, dV \\ &= \iiint_V \frac{1}{2} \nabla \cdot [(C^*)^2 \mathbf{v}] \, dV \end{aligned} \quad (27)$$

Using Green's theorem, the last integral of (27) gives

$$\iiint_V \frac{1}{2} \nabla \cdot [(C^*)^2 \mathbf{v}] \, dV = \frac{1}{2} \iint_S (C^*)^2 \mathbf{v} \cdot \mathbf{n} \, dS \quad (28)$$

Also, *without loss of generality*, the area integral in (28) can be rewritten as

$$\iint_S (C^*)^2 \mathbf{v} \cdot \mathbf{n} \, dS = \iint_{S_D^C} (C^*)^2 \mathbf{v} \cdot \mathbf{n} \, dS - k \iint_{S_N^C} (C^*)^2 \left(\frac{\partial \phi}{\partial n} \right) \, dS \quad (29)$$

From Green's first identity, for non-singular $C^*(\mathbf{x}, t)$

$$\iiint_V C^* \nabla^2 C^* \, dV + \iiint_V |\nabla C^*|^2 \, dV = \iint_S C^* \frac{\partial C^*}{\partial n} \, dS \quad (30)$$

The integral on the right side of (30) will always vanish in view of the conditions (21) and (22). Combining (29) and (30), Equation (24) can be written in the form

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \iiint_V [C^*]^2 \, dV &= -\frac{1}{2} \iint_{S_D^C} (C^*)^2 \mathbf{v} \cdot \mathbf{n} \, dS + \frac{k}{2} \iint_{S_N^C} (C^*)^2 \left(\frac{\partial \phi}{\partial n} \right) \, dS - \\ &\quad - D \iiint_V |\nabla C^*|^2 \, dV - \xi \iiint_V [C^*]^2 \, dV \end{aligned} \quad (31)$$

The *first surface integral* on the right side of (31) will vanish in view of (21). The *second surface integral* will vanish trivially if $S = S_D^C$. The specification of complete Dirichlet boundary conditions for $C(\mathbf{x}, t)$ is not altogether an unreasonable constraint. As an example, consider either a simply connected or a multiply connected porous domain where potential flow can be established solely by specifying $f_D(\mathbf{x})$ on the boundaries of the domain. Except for situations where $f_D(\mathbf{x}) = \text{const.}$ and the domain is simply connected, non-trivial solutions for $\mathbf{v}(\mathbf{x})$ exist. The Dirichlet boundary condition for $C(\mathbf{x}, t)$ can now be defined by specifying $F_D(\mathbf{x})$ on any part of the boundary S and the appropriate Dirichlet condition applicable to $C^*(\mathbf{x}, t)$ is exactly (21). As a further possibility, the *second surface integral* in (31) will vanish if, and only if, the Neumann boundary condition applicable to $\phi(\mathbf{x})$ is *homogeneous* and $S_N^C \in S_N^\phi$. Therefore, in general, for the second surface integral on the right side of (31) to vanish requires

$$\frac{\partial \phi}{\partial n} \equiv 0 \quad \forall \mathbf{x} \in S_N^C \in S_N^\phi \quad (32)$$

Invoking this requirement, (31) now gives

$$\frac{1}{2} \frac{d}{dt} \iiint_V [C^*]^2 dV = -D \iiint_V |\nabla C^*|^2 dV - \xi \iiint_V [C^*]^2 dV \quad (33)$$

By defining

$$\Omega(t) = \frac{1}{2} \iiint_V [C^*]^2 dV \quad (34)$$

and considering (33), (34) and (23), it is noted that if $D > 0$ and $\xi > 0$

$$(i) \Omega(t) \geq 0, \quad (ii) \frac{d\Omega}{dt} \leq 0, \quad (iii) \Omega(0) \equiv 0 \quad (35)$$

These constraints can be satisfied, simultaneously, if and only if

$$\Omega(t) \equiv 0, \quad t \in (0, T) \quad (36)$$

where T is any finite time. Alternatively, from the Dubois–Reymond Lemma, Equation (36) implies that

$$C^*(\mathbf{x}, t) \equiv 0 \quad \forall \mathbf{x} \in V, \quad t \in (0, T) \quad (37)$$

which proves uniqueness.

The procedures for establishing uniqueness of solutions for partial differential equations, both linear and non-linear, are, in general, quite diverse and in a strict mathematical setting they invariably require detailed applications of procedures based on advanced concepts in functional analysis. For example, (24) can be interpreted in the sense of a ‘*weak form*’, only if a Hilbert space H with its inner product can be defined, such that $C^*(\mathbf{x}, t)$ can be interpreted as any element H . Examples of such mathematical techniques, *although not specifically addressing the issue of the uniqueness of solution of the classical advection–diffusion equation*, are given in a number of studies including those by Friedman (1966, 1990), Lieberstein (1972), Aris (1975), Bennet and Kloeden (1980, 1981), Hornung and Jaeger (1991), Fitzgibbon and Martin (1993), Zheng (1995) and Stakgold (1998). In addition to these presentations of a more advanced mathematical nature, there is the need to consider simpler expositions that are complemented by physical interpretations of the constraints required to arrive at a proof of a uniqueness theorem. This latter approach is of considerable pedagogical benefit, particularly in terms of presenting the concepts associated with proofs of uniqueness of solutions to partial differential equations to the engineering community (Selvadurai, 2000a, b).

4. Concluding Remarks

The uniqueness of solution to the classical advection–diffusion equation governing the movement of a chemical species in a fluid saturated porous medium can be

readily established for situations where the advective flow velocities are governed by steady potential flow and chemical transport and decay can occur as a result of diffusive phenomena and attenuation effects. In developing the proof of uniqueness, it is assumed that the entire surface S on which generalized Dirichlet and Neumann boundary conditions for the concentration $C(\mathbf{x}, t)$ are prescribed on its subsets *also* corresponds to the surface on which Dirichlet and Neumann boundary conditions are prescribed for the potential $\phi(\mathbf{x})$. Uniqueness is assured, *unconditionally*, if Dirichlet boundary conditions are prescribed for the concentration $C(\mathbf{x}, t)$ over the entire surface of the region. It is shown that in the event both Dirichlet and Neumann boundary conditions are prescribed for $\phi(\mathbf{x})$ on the surface of the region, for uniqueness to be established for the advective–diffusive transport problem, the Neumann boundary conditions for the potential problem must be *homogeneous* and the surface S_N^C on which the homogeneous Neumann boundary conditions are prescribed for $C(\mathbf{x}, t)$ must be a subset of the surface S_N^ϕ on which homogeneous boundary conditions are prescribed for the potential. From the point of view of engineering applications, either a requirement concerning coincidence of surfaces on which Dirichlet and Neumann boundary conditions are prescribed for both the concentration $C(\mathbf{x}, t)$ and the potential $\phi(\mathbf{x})$, and the requirement of *homogeneous* Neumann boundary conditions for the potential problem with $S_N^C \in S_N^\phi$, are not overly restrictive. These boundary domains are usually coincident in most plausible situations involving advective–diffusive transport in finite domains and the constraint concerning *homogeneous* Neumann boundary conditions applicable to the potential flow problem is invariably realized at boundaries of the flow domain that are considered to be impermeable.

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