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LIE GROUP ANALYSIS OF TWO DIMENSIONAL ADSORPTION-DIFFUSION EQUATIONS

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Abstract

We consider two dimensional adsorption-diffusion equations in both Cartesian and stream function coordinates. Symmetry classification of the arbitrary functions that appear as coefficients in these equations seems impossible. However, using the elements of the one dimensional optimal systems of admitted Lie algebras and two dimensional Abelian Lie subalgebras, we perform some reductions to fewer independent variables for the special cases of the realistic water flows backgrounds and choices of physical dispersion coefficient. Some invariant solutions are constructed.

1. Introduction

The quest for analytical solutions of equations for water flow and solute transport equations has continued unabated. Among other reasons, these exact solutions are needed to give insight into transport processes and also to be used as bench marks for the numerical schemes.

Solute dispersion is complicated even at the macroscopic level because the dispersion coefficient increases with fluid velocity, which in

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general is varying in space and time. The fluid velocity vector cannot be an arbitrary smooth function of space and time; it must conform to the established laws of fluid flow in porous media [4]. Although passive scalar transport in solvent-conducting porous media has been extensively studied by many people for many years, realistic exactly solvable models with spatially varying dispersion coefficient are very rare. Most existing solutions are for solute transport under point source water flow [6, 13]). Zoppou and Knight [15] constructed exact solutions for dispersion in a background of hyperbolic water streamline bounded by a wedge. Furthermore, some exotic solutions, which satisfy some physical boundary conditions, have been obtained for the linear two dimensional solute transport under realistic water flow background [4, 9]).

Here, we analyse the two dimensional transport equation for adsorbing solutes. The equations for transport of such solutes have an added complication of being nonlinear. Moitsheki et al. [8], considered the one dimensional adsorbing solute transport problem. To this end, we consider two dimensional equation in Cartesian coordinates and select a form of the solute transport in stream function coordinates.

This paper is divided as follows: In Section 2, we discuss the derivation of the adsorption-diffusion equation for solute transport. In Sections 3 and 4, we analyse the solute transport equations in Cartesian and stream function coordinates, respectively. Special cases of dispersion coefficient and realistic water flow backgrounds are selected. We employ Lie point symmetries in our analysis; the reader is referred to text such as those of, e.g., [2, 10], for further details. Lastly, we provide conclusions.

2. Nonlinear Adsorption-diffusion Equations

Combining the equation for continuity, for mass conservation

$$\frac{\partial(c\theta)}{\partial t} + \nabla \cdot \mathbf{J} = 0,$$

together with the form of total flux density

$$\mathbf{J} = -\theta D_0 \nabla c_f - \theta D_e(v) \nabla c_f + c_f \mathbf{V},$$

which is due to molecular diffusion, dispersion and convection, we obtain the adsorption-diffusion equation (ADE)

$$\frac{\partial(c\theta)}{\partial t} = \nabla \cdot (\theta D_0 \nabla c_f + \theta D_e(v) \nabla c_f) - \nabla \cdot (c_f \mathbf{V}). \tag{1}$$

Here, $\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right)$, t is time, $c = c_a + c_f$ is total solute concentration, c_a is the concentration of the adsorbed component, and c_f is the concentration within the liquid. D_0 is the diffusion coefficient. The dispersion coefficient D_e is found to be an increasing function of pore water, the velocity is modelled by the power law $D_e = D_1 v^m$, with $1 \leq m \leq 2$ and D_1 being the proportionality constant. Since, D_0 and D_e are microscopically similar (see, e.g., [1], these terms are usually combined, i.e., $D(v) = D_0 + D_e(v)$. Here, molecular diffusion is negligible compared to dispersion, hence $D(v)$ is approximated by $D_e(v)$, i.e., $D(v) = v^p$ with p experimentally observed to be $1 \leq p \leq 2$. If the adsorption process is bimolecular and the desorption process is monomolecular [12], then the equilibrium condition is

$$\frac{c_f c}{c_a} = \kappa.$$

Since, $c = c_a + c_f$, the locally free concentration is given by

$$c_f = \frac{c}{1 - \kappa^{-1} c},$$

where κ is the equilibrium constant. Equation (1) takes the form

$$\frac{1}{(1 - \kappa^{-1} c_f)^2} \frac{\partial(c_f \theta)}{\partial t} = \nabla \cdot (\theta D(v) \nabla c_f) - \nabla \cdot (c_f \mathbf{V}). \tag{2}$$

In most transport problems, water flow is adequately modelled by steady state flows rather than transient flows. The one dimensional version of the adsorption-diffusion equation was considered in [8]. For two dimensional steady saturated water flows, where $\theta = \theta_s$, along with Darcy's law $\mathbf{V} = -K_s \nabla \Phi$, equation (2) reduces to

$$\frac{1}{(1-\kappa^{-1}c)^2} \frac{\partial c}{\partial t} = \nabla \cdot (D(v)\nabla c) + k\nabla\Phi \cdot \nabla c, \tag{3}$$

wherein we have, without loss of generality, dropped the subscript *f*. Here, $k = K_s/\theta_s$, $v = |k\nabla\Phi|$, θ_s is the volumetric water content at saturation, Φ is the total hydraulic pressure head and K_s is hydraulic conductivity at saturation. Note that, for flow in saturated soils the equation of continuity is given by $\nabla \cdot \mathbf{V} = 0$ together with Darcy's law implies Laplace equation $\nabla^2\Phi = 0$. The problem is difficult, when v must be the modulus of the potential flow velocity field for incompressible fluid. However, the Laplace preserving transformations or the conformal mappings from the Cartesian to streamline coordinates result in an easier to handle equation [3, 4, 7]. In our case equation (3) reduces to

$$\frac{1}{(1-\kappa^{-1}c)^2} \frac{\partial c}{\partial t} = v^2\overline{\nabla} \cdot [D(v)\overline{\nabla} c] + v^2 \frac{\partial c}{\partial \phi}. \tag{4}$$

Here, $\overline{\nabla} = \left(\frac{\partial}{\partial\phi}, \frac{\partial}{\partial\psi}\right)$. Equating κ to unity and introducing normalised concentration and time, $C = c/c_s$ and $T = t/t_s$, with c_s and t_s being the suitable concentration and time, we rewrite equation (4) as

$$\frac{1}{(1-C)^2} \frac{\partial C}{\partial T} = v^2\overline{\nabla} \cdot [D(v)\overline{\nabla} C] + v^2 \frac{\partial C}{\partial \phi}. \tag{5}$$

3. Lie Point Symmetry Reduction for Equation (3)

In the ADE (3), we assume that $D(v)$ is a constant, say $D(v) = 1$. Since, one may choose a length scale l_s and a time scale t_s so that, $l_s^2/t_s = D$. Introducing dimensionless variables $T = t/t_s$, $C = c/c_s$ and $x_* = x/l_s$ and $y_* = y/l_s$ and taking $\kappa = 1$, we then, consider a system of equations

$$\frac{1}{(1-C)^2}\frac{\partial C}{\partial T} = \nabla^2 C + k\nabla\Phi\cdot\nabla C, \tag{6}$$

$$\nabla^2\Phi = 0. \tag{7}$$

With no confusion arising, we may drop the subscript $*$ of the spatial variables, so that, $\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right)$. k may be interpreted as the Pèclet number [3]. Very few solutions for this system are known, even for the case of non-reactive, non-adsorbing solutes (see, e.g., [3]), except for the one dimensional steady water flow (see, e.g., [11]). Point symmetry analysis for this system reveals finite six Lie algebra plus an infinite symmetry being admitted, namely

$$\Gamma_1 = (C-1)\frac{\partial}{\partial C} + y\frac{\partial}{\partial y} + x\frac{\partial}{\partial x},\ \Gamma_2 = \frac{\partial}{\partial T},\ \Gamma_3 = \frac{\partial}{\partial y},\ \Gamma_4 = \frac{\partial}{\partial x},$$

$$\Gamma_5 = y\frac{\partial}{\partial y} + x\frac{\partial}{\partial x} + 2T\frac{\partial}{\partial T},\ \Gamma_6 = x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \text{ and } \Gamma_7 = g(T)\frac{\partial}{\partial \Phi}, \tag{8}$$

where g is an arbitrary function of T. Using the methods in [10], we obtain the one dimensional optimal system

$$\{\Gamma_1 + a\Gamma_5 + b\Gamma_6,\ \Gamma_6 + a\Gamma_5,\ \Gamma_5 \pm \Gamma_2,\ \Gamma_2 \pm \Gamma_4,\ \Gamma_3,\ \Gamma_4\},$$

where a and b are constants. Upon attempting to classify single equation (6), to choose only that function Φ satisfying equation (7), we obtained some long linear combination of the function Φ together with its derivatives with respect to the spatial variables. We herein, omit this linear combination. Full symmetry classification of this equation appears to be a major task. However, we obtain reductions listed in Table 1 using the elements of the optimal systems of the Lie algebras admitted by the system of equations (6) and (7). Wherever, they appear c_1, c_2 and c_3 are constants. Since, among others, Γ_1 and Γ_6 span a two dimensional Abelian Lie subalgebra, a complete reduction of the system to O.D.E.s is possible. The reduction by a group of rotations leads to the functional form

$$\Phi = H(R), \quad \text{where } R = \sqrt{x^2 + y^2},$$

with H satisfying the ODE

$$H'' + \frac{1}{R} H' = 0.$$

Hence,

$$\Phi = c_1 + c_2 \ln\left|\sqrt{x^2 + y^2}\right|.$$

Also, $C = G(R, t)$, where G satisfies

$$\frac{G_t}{(1 - G)^2} = \frac{(kc_2 + 1)}{R} G_R + G_{RR}. \tag{9}$$

Now, equation (9) admits Γ_1, which in new variables may be written as:

$$\Gamma_1 = (G - 1)\frac{\partial}{\partial G} + R\frac{\partial}{\partial R}$$

and leads to the functional form

$$G = 1 + Rf(t),$$

where f satisfies the O.D.E.

$$f' = (kc_2 + 1)f^3.$$

Thus, in original variables we obtain

$$C = 1 \pm \sqrt{\frac{x^2 + y^2}{c_3 - 2(c_2 k + 1)t}}.$$

Table 1. Reductions for the system (6) and (7)

Symmetry	Functional form and reduced equations
$\Gamma_1 + a\Gamma_5 + b\Gamma_6$	$\Phi = H(\rho)$, where $\rho = \frac{a+1}{b}\tan^{-1}(y/x) - \ln\lvert\sqrt{b(x^2+y^2)}\rvert$ and $H'' = 0 \Rightarrow \Phi = c_1\rho + c_2$. Equation (6) is impossible to be reduced, since the second invariant cannot be determined.
$\Gamma_6 + a\Gamma_5$	$\Phi = H(\rho)$, where $\rho = a\tan^{-1}(y/x) - \ln\lvert\sqrt{x^2+y^2}\rvert$ and $H'' = 0 \Rightarrow \Phi = c_1\rho + c_2$. Equation (6) is impossible to be reduced, since the second invariant cannot be determined.
$\Gamma_5 + \Gamma_2$	$\Phi = H(\rho)$, $C = G(\rho, \gamma)$, where $\rho = \frac{y}{x}$, $\gamma = \frac{x}{\sqrt{T+1}}$, where H and G satisfy $(\rho^2+1)H_{\rho\rho} + 2\rho H_\rho = 0$, i.e., $\Phi = c_1 + c_2\tan^{-1}\left(\frac{y}{x}\right)$, and $\left[\frac{1}{(1-G)^2} + kc_2\rho\gamma\right]G_\gamma$ $= \left[2\rho + \frac{kc_2}{1+\rho^2}(\rho^2+1)\right]G_\rho + \rho^2 G_{\rho\rho} + \gamma^2 G_{\gamma\gamma}$.
$\Gamma_2 + \Gamma_4$	$\Phi = H(y)$, $C = G(\rho, y)$ with $\rho = T - x$ so that $\Phi = c_1 y + c_2$ and G satisfies the PDE $\frac{G_\rho}{(1-G)^2} = G_{\rho\rho}$ $+ G_{yy} + kc_2 G_\rho$.

4. Lie Point Symmetry Reduction for Equation (5)

In the analysis of equation (5), we consider three cases for dispersion coefficient $D(v)$, with both radial and point vortex water flow. For saturated radial water flows from a line source of strength $\boldsymbol{Q}$, in terms of the radial coordinate r, the Darcian flux is $\mathbf{V} = Q/r$ and the pore velocity is $\mathbf{v} = \mathbf{V}/\theta_s$. The velocity potential is $\phi = -(Q/\theta_s)\log r$ and the stream function is $\psi = -(Q/\theta_s)\arctan(y/x)$. For the relevant normalised point water source, $\phi = -\log R$, ψ is simply the clockwise polar angle coordinate–$\arctan(Y/X)$ and $v = e^{\phi}$. Point vortex water flow is conjugate to the point source flow. For relevant normalised point vortex water flow, $\psi = \log R$, $\phi = -\arctan(Y/X)$ and $v = e^{-\psi}$. We consider three cases:

Case (a). Point source water flow, $D(v) = 1$, $v = e^{\phi}$

The case $D(v) = 1$, $v = e^{\phi}$, corresponds to the solute transport with constant dispersion coefficient under radial water flow. In this case, equation (5) admits a four dimensional Lie algebra spanned by the vectors

$$\Gamma_1 = (1 - C)\frac{\partial}{\partial C} + 2T\frac{\partial}{\partial T}, \; \Gamma_2 = \frac{\partial}{\partial T}$$

$$\Gamma_3 = (1 - C)\frac{\partial}{\partial C} + \frac{\partial}{\partial \phi}, \text{ and } \Gamma_4 = \frac{\partial}{\partial \psi}.$$

The one dimensional optimal system is given by

$$\{\Gamma_2, \Gamma_3 \pm \Gamma_2, \Gamma_4 + \alpha\Gamma_3 \pm \Gamma_2, \Gamma_1 + \alpha\Gamma_3 + \beta\Gamma_4\},$$

where α and β are arbitrary constants. The reductions by elements of the optimal system are given in Table 2. Transport with constant dispersion coefficient of non-reactive solutes has been extensively studied in [9]. Since, Γ_1 and Γ_3 span a two dimensional Abelian Lie subalgebra, then reduction of the governing equation to an O.D.E. using these symmetries is possible. Γ_1 leads to a functional form

$$C = 1 - T^{-1/2}F(\phi, \psi),$$

where F satisfies the reduced P.D.E.

$$\frac{\partial^2 F}{\partial \phi^2} + \frac{\partial^2 F}{\partial \psi^2} + \frac{\partial F}{\partial \phi} + \frac{1}{2e^{2\phi}F} = 0. \tag{10}$$

The reduced equation (10) inherits the symmetry Γ_3, which now takes the form

$$\Gamma_3 = \frac{\partial}{\partial \phi} - F\frac{\partial}{\partial F}$$

and leads to the reduction

$$F = e^{-\phi} g(\psi),$$

with

$$2gg'' + 1 = 0. \tag{11}$$

Table 2. Reduced partial differential equations: $D(v) = 1$.

Symmetry	Functional form and reduced equations
$\Gamma_2 + \Gamma_3$	$\gamma = \phi - T,\ C = e^{-t}F(\psi, \gamma) + 1$ with F satisfying $F_{\gamma\gamma} + F_{\psi\psi} + \left[\frac{1}{e^{2\gamma}} + 1\right]F_{\gamma} + \frac{1}{e^{2\gamma}F} = 0$
$\Gamma_4 + \alpha\Gamma_3 + \Gamma_2$	$\rho = T - \psi,\ \gamma = T - \frac{1}{\alpha}\phi,\ C = e^{\alpha T}F(\rho, \gamma) + 1,$ with F satisfying $\frac{1}{F^2}\left[F_{\rho} + F_{\gamma} - \alpha F\right] = e^{-2\gamma}\left[\frac{1}{\alpha^2}F\gamma\gamma + F_{\rho\rho} - F\rho\right]$
$\Gamma_1 + \alpha\Gamma_3 + \beta\Gamma_4$	$\rho = te^{-2/\alpha}\phi,\ \gamma = te^{-2/\beta\psi},\quad C = t^{-(1+\alpha)/2}F(\rho, \gamma) + 1$ with F satisfying $\left[\frac{\rho}{F^2} + \frac{4}{\alpha^2}\rho^{1-\alpha} + \frac{2}{\alpha}\rho^{1-\alpha}\right]F_{\rho} + \left[\frac{\gamma}{F^2} - \frac{4}{\beta^2\rho^{\alpha}}\right]F_{\gamma} - \frac{1+\alpha}{2F} = \frac{4}{\alpha^2}\rho^{2-\alpha}F_{\rho\rho} + \frac{4}{\beta^2\rho^2}\gamma^2 F_{\gamma\gamma}$

Equation (11) is a form of Newton's second law with potential energy function $\frac{\log(g)}{2}$, and integrates to the first order energy function

$$\frac{(g')^2}{2} + \frac{\log(g)}{2} = E, \tag{12}$$

where E is a constant. The trivial solution to equation (12) is $g = e^{2E}$, however, this is not necessarily the solution to equation (11) (this is because upon integrating, we first multiplied equation (11), by the first derivative of (g). Hence, it may be erroneous to write the solution of the original PDE (5) in terms of this trivial solution. The nontrivial solution which satisfies both equations (12) and (11) is given by

$$\psi + c_1 = \pm \int^{g(\psi)} \frac{ds}{\sqrt{2E - \log|s|}},$$

where c_1 is a constant.

Case (b). Point source water flow, $D(v) = v^2 = e^{2\phi}$

For a radial flow with the power law velocity dependent dispersion coefficient $D(v) = v^p$, the case, $p = 2$ is in accord with Taylor's theory [14] of dispersion and has been used as a reasonable model for dispersion in porous media [5, 11]. In this case, the admitted Lie algebra is three dimensional and spanned by base vectors

$$\Gamma_1 = (1 - C)\frac{\partial}{\partial C} + 2T\frac{\partial}{\partial T}, \; \Gamma_2 = \frac{\partial}{\partial T}, \text{ and } \Gamma_3 = \frac{\partial}{\partial \psi}.$$

The one-dimensional optimal system is

$$\{\Gamma_2, \Gamma_1 + \alpha\Gamma_3, \Gamma_3 \pm \Gamma_2\},$$

and reductions are given in Table 3.

Table 3. Reduced partial differential equations: $D(v) = e^{2\phi}$

Symmetry	Functional form and reduced equations
$\Gamma_1 + \alpha\Gamma_3$	$\rho^2 F_{\rho\rho} + F_{\phi\phi} + \left(2 + \frac{1}{e^{2\phi}}\right)F_\phi = \frac{1}{2e^{4\phi}F^2}(F + \rho F_\rho)$
$\Gamma_3 + \Gamma_2$	$F_{\phi\phi} + F_{\rho\rho} + \left(\frac{1}{2e^{2\phi}} + 2\right)F_\phi - \left(\frac{1}{1 - F}\right)F_\rho = 0$

Following reductions by Γ_1, and the elements listed in Table 2, the reduced equations admit only translation in ψ. The problem appears to be enormously difficult for this case.

Case (c). Point vortex flow, $D(v) = v^p = e^{-p\psi}$

For arbitrary constant p, we obtain three symmetry generators

$$\Gamma_1 = (1 - C)\frac{\partial}{\partial C} + 2T\frac{\partial}{\partial T}, \ \Gamma_2 = \frac{\partial}{\partial T}, \text{ and } \Gamma_3 = \frac{\partial}{\partial \phi}.$$

The Lie algebra extends for the case, $p = 0$. This case represents contaminant transport with a constant dispersion coefficient. For $p = 0$, we obtain an extra point symmetry:

$$\Gamma_4 = 2(C - 1)\frac{\partial}{\partial C} + 2\frac{\partial}{\partial \psi} + \frac{\partial}{\partial \phi}.$$

We observe here, that the symmetry Γ_1 and Γ_4 span a two dimensional Abelian Lie subalgebra. Hence, reduction of the governing P.D.E. to an O.D.E, which may or may not be solvable, is possible using these two point symmetries. Reduction by Γ_1 leads to a functional form

$$C = 1 - T^{-1/2}F(\phi, \psi),$$

with F satisfying the P.D.E.

$$F_{\phi\phi} + F_{\psi\psi} + F_{\phi} + \frac{e^{2\psi}}{2F} = 0. \tag{13}$$

Equation (13) admits Γ_4 which now takes the form

$$\Gamma_4 = 2F\frac{\partial}{\partial F} + 2\frac{\partial}{\partial \psi} + \frac{\partial}{\partial \phi}$$

and leads to the reduction

$$F = e^{\psi}g(\rho), \ \rho = \frac{\psi}{2} - \phi$$

with g satisfying the O.D.E.

$$5g'' + 2g' + 4g + \frac{2}{g} = 0. \tag{14}$$

The reduced O.D.E. (14) admits only a translation in ρ, and integrates once to Abel's equation of first kind

$$5ff' + 2f - 4g - \frac{2}{g} = 0,$$

where f depends on g.

5. Conclusion

The nonlinear adsorption-diffusion equations describing transport of adsorbing solute have proved to be harder to solve than their linear counterparts. However, Lie point symmetry reductions have been performed and some invariant solutions are constructed.

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