Centrum voor Wiskunde en Informatica

REPORT*RAPPORT*

A note on singularities caused by the hydrodynamic dispersion tensor

R.A. Trompert

Department of Numerical Mathematics

Report NM-R9302 January 1993

CWI is the National Research Institute for Mathematics and Computer Science. CWI is part of the Stichting Mathematisch Centrum (SMC), the Dutch foundation for promotion of mathematics and computer science and their applications. SMC is sponsored by the Netherlands Organization for Scientific Research (NWO). CWI is a member of ERCIM, the European Research Consortium for Informatics and Mathematics.

P.O. Box 4079, 1009 AB Amsterdam (NL)
Kruislaan 413, 1098 SJ Amsterdam (NL)
Telephone +31 20 592 9333
Telefax +31 20 592 4199

A Note on Singularities Caused by the Hydrodynamic Dispersion Tensor

Ron Trompert
CWI
P.O. Box 4079, 1009 AB Amsterdam, The Netherlands

Abstract

In this paper we show that the equation, describing transport in a porous medium, is not uniquely defined in points of the domain where the velocity of the fluid is zero. This is due to the fact that the hydrodynamic dispersion tensor is defined as a not sufficiently differentiable function of the fluid velocity. The implications of this non-smoothness for the numerical simulation of fluid flow and transport in porous media will also be discussed.

1991 Mathematics Subject Classification: 76S05
1991 CR Categories: G.1.8.
Key words & Phrases: partial differential equations, fluid-flow/solute-transport in porous media, hydrodynamic dispersion tensor, singularities.
Note: This work was carried out as a part of contract research by order of the Laboratory for Soil and Groundwater Research of RIVM - the Dutch National Institute of Public Health and Environmental Protection - in connection with project "Locatiespecifieke Modelvalidatie" 725205. Financial support for this project was provided by the Dutch Ministry of Economic Affairs.

1. Introduction

In this paper we show that the equation, describing transport in a porous medium, is not uniquely defined in points of the domain where the velocity of the fluid is zero. This occurs only when the fluid velocity is zero at isolated points such as stagnation points or centers of vortices. It does not happen when the velocity is zero in a finite region. The fact that the hydrodynamic dispersion tensor is not differentiable when the velocity is zero, is the cause of these singularities. It can be shown that when the velocity is zero in a certain point, the transport equation will result in two different partial differential equations in one space dimension and an infinite number of partial differential equations in two and three space dimensions. Only the two dimensional case will be discussed in this paper.

In Section 2, we discuss a model of two dimensional fluid flow and transport in porous media. Section 3 deals with the singularities caused by the hydrodynamic dispersion tensor and in the final section, Section 4, we briefly discuss the consequences for the numerical simulation of fluid flow and transport in porous media.

Report NM-R9302
ISSN 0169-0388
CWI
P.O. Box 4079, 1009 AB Amsterdam, The Netherlands

2. Model of Fluid Flow and Transport in Porous Media

We consider a model for unsteady, isothermal, single-phase, two-component saturated flow in a porous medium in two space dimensions. This model contains two conservation laws, namely one for the mass of the whole fluid, i.e. water and solute and one for the mass of solute only. The mass conservation of the fluid supplemented with Darcy's law for the velocity field is given by

$$\frac{\partial}{\partial t}(n\rho) + \nabla.(\rho\mathbf{q}) = 0, \quad \mathbf{q} = -\frac{k}{\mu}(\nabla p - \rho\mathbf{g}), \quad \mathbf{q} = (q_1, q_2)^T, \quad \mathbf{g} = (g_1, g_2)^T, \tag{2.1}$$

where n is the porosity of the porous medium, ρ is the mass density and $\mathbf{q}$ the velocity vector of the total fluid. The permeability of the porous medium is denoted by k, μ is the dynamic viscosity, p the pressure and $\mathbf{g}$ the acceleration of gravity vector. The mass conservation law of solute and Fick's law for the dispersive mass fluxes are given by

$$\frac{\partial}{\partial t}(n\rho\omega) + \nabla.(\rho\omega\mathbf{q} + \mathbf{J}) = 0, \quad \mathbf{J} = -\rho n\mathbf{D}\nabla\omega, \quad \mathbf{J} = (J_1, J_2)^T, \tag{2.2}$$

where ω is the concentration of solute and $\mathbf{J}$ the dispersive mass flux vector. $\mathbf{D}$ is the hydrodynamic dispersion tensor defined by

$$n\mathbf{D} = (nd_m + \alpha_T|\mathbf{q}|)\mathbf{I} + (\alpha_L - \alpha_T)\frac{\mathbf{q}\mathbf{q}^T}{|\mathbf{q}|}, \quad |\mathbf{q}| = (\mathbf{q}^T\mathbf{q})^{1/2}, \quad \mathbf{D} = \begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix}, \tag{2.3}$$

where α_L denotes the longitudinal and α_T the transversal dispersivity and d_m the molecular diffusion. $\mathbf{I}$ is the 2×2 identity matrix. The parameters n, d_m, α_L, α_T and k in this model are assumed to be constant. Temperature and compressibility effects are neglected in this model, as well as sources, sinks and deformation of the porous medium. To complete the model we have an equation of state for the fluid mass density ρ:

$$\rho = \rho_0 \exp(\gamma\omega), \tag{2.4}$$

where ρ_0 is the reference density and γ is a coefficient obtained from laboratory experiments.

After some elementary calculations (2.1) can be written as

$$n\gamma\frac{\partial\omega}{\partial t} + \gamma\mathbf{q}.\nabla\omega + \nabla.\mathbf{q} = 0, \tag{2.5}$$

and (2.2) as

$$\rho n\frac{\partial\omega}{\partial t} + \rho\mathbf{q}.\nabla\omega + \nabla.\mathbf{J} = 0. \tag{2.6}$$

In cases of a low concentration of solute, (2.5) and (2.6) are only weakly coupled. Therefore, the flow can then be regarded as being independent from the density gradients caused by differences in the concentration of solute since these gradients prove to be negligible. The flow field is then considered to be divergence free. Hence, (2.5) reduces to $\nabla.\mathbf{q} = 0$. If this is the case then (2.5) and (2.6) can be solved separately where (2.5) has to be solved only once to compute the flow. However, when the concentration of solute is high, the flow is not independent from the density gradients and the coupling between (2.5) and (2.6) is no longer negligible. In this case, (2.5) and (2.6) have to be solved together at each time step.

With this model we have followed *Hassanizadeh* and *Leijnse* [3] in the description of solute transport, except for Darcy's law and Fick's law. In our paper these laws are used in their classical formulation, valid for low concentration cases. For the purpose of our paper, the precise form of this model is, apart from (2.3), of little importance, since the singularities can occur at all times, regardless of concentration values, compressibility effects, source terms etcetera. In the next section we will show that the mathematical definition of the hydrodynamic dispersion tensor (2.3) is the cause of the previously mentioned singularities.

3. Singularities Caused by the Hydrodynamic Dispersion Tensor

In this section we show that the mathematical definition of the hydrodynamic dispersion tensor, given by (2.3), causes singularities at the points where the velocity $\mathbf{q}$ is zero, or to be more precise, where $\nabla p - \rho \mathbf{g}$ vanishes, in case $\mathbf{q}$ is given by (2.1). When this happens, (2.6) will not denote a single partial differential equation but infinitely many partial differential equations. This singularity is caused by the fact that the elements of the dispersion tensor are not sufficiently smooth functions of the velocity vector components q_1 and q_2. We will see that this occurs only when $\nabla p - \rho \mathbf{g}$ is zero at isolated points, not when $\nabla p - \rho \mathbf{g}$ is zero in a region.

Using the definitions of the previous section we can rewrite (2.6) as

$$n\frac{\partial \omega}{\partial t} + (q_1 - \frac{\partial nD_{11}}{\partial x} - \frac{\partial nD_{12}}{\partial y})\frac{\partial \omega}{\partial x} + (q_2 - \frac{\partial nD_{12}}{\partial x} - \frac{\partial nD_{22}}{\partial y})\frac{\partial \omega}{\partial y}$$
$$- \gamma nD_{11}(\frac{\partial \omega}{\partial x})^2 - 2\gamma nD_{12}\frac{\partial \omega}{\partial x}\frac{\partial \omega}{\partial y} - \gamma nD_{22}(\frac{\partial \omega}{\partial y})^2 \tag{3.1}$$
$$- nD_{11}\frac{\partial^2 \omega}{\partial x^2} - 2nD_{12}\frac{\partial^2 \omega}{\partial x \partial y} - nD_{22}\frac{\partial^2 \omega}{\partial y^2} = 0.$$

Here, the identity $nD_{21} = nD_{12}$ was used, since the dispersion tensor is symmetric. In order to investigate (3.1) when the velocity components q_1 and q_2 are both approaching zero, we first examine the behavior of the dispersion tensor elements and their partial derivatives with respect to the spatial co-ordinates. The definition (2.3) can be rewritten as

$$nD_{11} = nd_m + \frac{1}{|\mathbf{q}|}(\alpha_L q_1^2 + \alpha_T q_2^2), \tag{3.2}$$

$$nD_{12} = \frac{1}{|\mathbf{q}|}(\alpha_L - \alpha_T) q_1 q_2, \tag{3.3}$$

$$nD_{22} = nd_m + \frac{1}{|\mathbf{q}|}(\alpha_T q_1^2 + \alpha_L q_2^2). \tag{3.4}$$

Using (3.2)-(3.4) and applying the chain rule we obtain

$$\frac{\partial nD_{11}}{\partial x} = |\mathbf{q}|^{-3}\{[(2\alpha_L - \alpha_T)q_1 q_2^2 + \alpha_L q_1^3]\frac{\partial q_1}{\partial x} + [(2\alpha_T - \alpha_L)q_1^2 q_2 + \alpha_T q_2^3]\frac{\partial q_2}{\partial x}\}, \tag{3.5}$$

$$\frac{\partial nD_{12}}{\partial x} = |\mathbf{q}|^{-3}(\alpha_L - \alpha_T)\{q_2^3\frac{\partial q_1}{\partial x} + q_1^3\frac{\partial q_2}{\partial x}\}, \tag{3.6}$$

$$\frac{\partial nD_{12}}{\partial y} = |\mathbf{q}|^{-3}(\alpha_L - \alpha_T)\{q_2^3\frac{\partial q_1}{\partial y} + q_1^3\frac{\partial q_2}{\partial y}\}, \tag{3.7}$$

$$\frac{\partial nD_{22}}{\partial y} = |\mathbf{q}|^{-3}\{[(2\alpha_T - \alpha_L)q_1q_2^2 + \alpha_T q_1^3]\frac{\partial q_1}{\partial y} + [(2\alpha_L - \alpha_T)q_1^2q_2 + \alpha_L q_2^3]\frac{\partial q_2}{\partial y}\}. \tag{3.8}$$

It is easy to see that in case $q_1, q_2 \to 0$, the velocity-dependent parts of the dispersion tensor will vanish. The elements of the dispersion tensor are then given by

$$nD_{11} = nd_m, \quad nD_{12} = 0, \quad nD_{22} = nd_m. \tag{3.9}$$

The behavior of the partial derivatives of the dispersion tensor elements for $q_1, q_2 \to 0$, depends on the behavior of functions like, for example, $|\mathbf{q}|^{-3}[(2\alpha_L - \alpha_T)q_1q_2^2 + \alpha_L q_1^3]$ which are present in (3.5)-(3.8). If we substitute $|\mathbf{q}|\cos(\phi)$, $|\mathbf{q}|\sin(\phi)$, for q_1, q_2 respectively, then we will have

$$|\mathbf{q}|^{-3}[(2\alpha_L - \alpha_T)q_1q_2^2 + \alpha_L q_1^3] = (2\alpha_L - \alpha_T)\cos(\phi)\sin^2(\phi) + \alpha_L\cos^3(\phi), \tag{3.10}$$

where $\phi = \tan^{-1}(q_2/q_1)$. We can conclude from (3.10) that the values of these functions when $q_1, q_2 \to 0$ depends on how q_1 and q_2 tend to zero relative to one another. In other words, this value at the point where $q_1, q_2 = 0$ depends on ϕ. Since ϕ can take any value, this means that these functions can have infinitely many different values, so they are not uniquely defined. Assuming that the partial derivatives of the velocity components, $\partial q_1/\partial x$, $\partial q_1/\partial y$, $\partial q_2/\partial x$ and $\partial q_2/\partial y$, are continuous functions at a point where $q_1, q_2 = 0$, then it is clear that the partial derivatives of the dispersion tensor elements, given by (3.5)-(3.8), are also not uniquely defined at this point, unless $\partial q_1/\partial x$, $\partial q_1/\partial y$, $\partial q_2/\partial x$ and $\partial q_2/\partial y$ are all equal to zero. The latter will occur when the velocity is zero in a region, but not necessarily when the velocity is zero at isolated points. This means that the transport equation (3.1) results in infinitely many different partial differential equations at a point where $q_1, q_2 = 0$.

To illustrate this, we consider the case of steady flow in a confined aquifer in which a well is operating. The total flow is then determined by the superposition of the natural flow in the aquifer and the flow produced by the well. We assume that the well is placed at $x=0$, $y=0$ and that the natural flow in the aquifer is in x-direction and with a constant speed q_{01}. Further, we assume that the density variations are negligible in (2.5), meaning that the flow field is assumed to be divergence free. According to *Bear* and *Verruijt* [2], the velocity field is then given by

$$q_1 = q_{01} - \frac{Q}{2\pi nB}\frac{x}{x^2+y^2}, \quad q_2 = -\frac{Q}{2\pi nB}\frac{y}{x^2+y^2}, \tag{3.11}$$

where Q is the production of the well, n is the porosity and B is the thickness of the aquifer. In this case, there will be a stagnation point at $x=Q/(2\pi nBq_{01})$, $y=0$. The partial derivatives of the velocity components at the stagnation point are continuous and given by

$$\frac{\partial q_1}{\partial x} = \frac{2\pi nB}{Q}q_{01}^2, \quad \frac{\partial q_1}{\partial y} = 0, \quad \frac{\partial q_2}{\partial x} = 0, \quad \frac{\partial q_2}{\partial y} = -\frac{2\pi nB}{Q}q_{01}^2. \tag{3.12}$$

In the vicinity of this point, the velocity components are approximated as

$$q_1 \approx \frac{2\pi nB}{Q}q_{01}^2(x - \frac{Q}{2\pi nBq_{01}}), \quad q_2 \approx -\frac{2\pi nB}{Q}q_{01}^2 y. \tag{3.13}$$

Using (3.5)-(3.9) and (3.12) and substituting once more $|\mathbf{q}|\cos(\phi)$, $|\mathbf{q}|\sin(\phi)$ for q_1, q_2 in (3.5)-(3.8), the transport equation (3.1) at the stagnation point will then be given by

$$n\frac{\partial\omega}{\partial t} - [(2\alpha_L - \alpha_T)\cos(\phi)\sin^2(\phi) + \alpha_T\cos^3(\phi)]\frac{2\pi nB}{Q}q_{01}^2\frac{\partial\omega}{\partial x}$$

$$+ [(2\alpha_L - \alpha_T)\cos^2(\phi)\sin(\phi) + \alpha_T\sin^3(\phi)]\frac{2\pi nB}{Q}q_{01}^2\frac{\partial\omega}{\partial y} \qquad (3.14)$$

$$- \gamma nd_m(\frac{\partial\omega}{\partial x})^2 - \gamma nd_m(\frac{\partial\omega}{\partial y})^2 - nd_m\frac{\partial^2\omega}{\partial x^2} - nd_m\frac{\partial^2\omega}{\partial y^2} = 0,$$

$$\phi = \tan^{-1}(\frac{q_2}{q_1}) \approx \tan^{-1}(\frac{-y}{x - \frac{Q}{2\pi nBq_{01}}}).$$

From this equation we conclude that ϕ determines how q_2 tends to zero relative to q_1, or from which direction in the domain the stagnation point is approached. Since ϕ can take any possible value, (3.14) denotes infinitely many different partial differential equations for ω at the stagnation point.

4. The Consequences for the Numerical Simulation of Flow and Transport in Porous Media

We have showed that the mathematical definition of the dispersion tensor (2.3) can cause singularities in the domain. This happens when the velocity is zero at isolated points such as stagnation points or centers of vortices. At such points the partial differential equation, describing transport in porous media given by (3.1), is not uniquely defined. This is due to the fact that the partial derivatives of the dispersion tensor elements are depending on the direction of the flow field and need not necessarily tend to zero when the velocity tends to zero. In the vicinity of a point where the velocity is zero the direction of flow can vary considerably. Hence, $\partial nD_{11}/\partial x$, $\partial nD_{12}/\partial x$, $\partial nD_{12}/\partial y$ and $\partial nD_{22}/\partial y$ exhibit strong variations in this region if this is the case.

With respect to the consequences of this to the numerical simulation of fluid flow and transport in porous media, we note the following. When the concentration of solute is high and the flow field depends on the concentration gradients, then the equation for the flow field (2.5) and the transport equation (3.1) need to be solved together at each time step. After the spatial discretization of these equations and using an implicit time stepping scheme, we have to solve a system of nonlinear algebraic equations at each time step. The situation can then arise that the numerically computed velocity becomes relatively small in a part of the domain or at an isolated point. In practice, it will rarely occur in such a case that the velocity becomes exactly zero. The velocity will usually retain some small nonzero value. Hence, the transport equation will then be uniquely defined and formally there will be no mathematical complications. However, when the velocities are small, then the direction of the flow is prone to large changes, leading to strong variations in the derivatives of the dispersion tensor elements. The transport equation (3.1) will then possess strongly varying coefficients. To which extend this affects the convergence of the iteration process when this occurs while solving the system (2.5), (3.1) depends on the magnitude of the remaining terms of (3.1), such as the terms containing the molecular diffusion. Nevertheless, when the direction of the flow changes while iteratively solving the nonlinear system of equations, one can encounter serious convergence problems. We have come across problems of this kind, solving brine transport problems in porous media containing inhomogeneities [4] and solving the HYDROCOIN, case 5 test problem [1]. In inhomogeneous porous media stagnation points or points where the velocity becomes very small can easily occur near interfaces. Convergence problems can also arise when vortices are developing. This happens in the HYDROCOIN, case 5 test problem where salt is released to the overlying groundwater system from a part of the lower boundary of the domain. In time the salt forms a plume flowing upwards and to the right and two vortices develop along the lower boundary of the domain. The convergence problems may be overcome by solving (2.5) implicitly for the pressure and after that solving (3.1) explicitly for the concentration values. This is a so-called IMPES scheme. Nevertheless, when the velocity becomes relatively small in a part of the domain, then numerical factors like the space discretization scheme of the PDE as well as the boundary conditions, the time stepping scheme and the errors caused by iteratively solving (2.5), can have a considerable effect on the numerically computed direction of the flow in that region. Since the direction of the flow is very important to the transport equation, this means that in this case, the numerical factors determine which partial differential equation (3.1) is solved. This makes the numerical result highly sensitive to the applied spatial and temporal discretization schemes etc. which implies that an accurate numerical simulation of transport in a porous medium is unlikely in such a case.

As far as low concentration cases are concerned, we note that the flow field is known a priori and only (3.1) needs to be solved. Serious convergence problems are not to be expected here, because the velocity is known at each grid point and has a fixed direction, meaning that (3.5)-(3.8) and therefore also the transport equation (3.1) are uniquely determined, unless of course a grid point is positioned exactly at a point where the velocity is zero. However, when a grid point lies very close to such a point, then which transport equation we have to solve depends very much on the position of a grid point relative to the zero-velocity point (cf. 3.14). So, even though there will be no numerical difficulties solving (3.1) in this case, the validity and accuracy of the numerical simulation of transport in the vicinity of such a point is questionable.

REFERENCES

1. SWEDISH NUCLEAR POWER INSPECTORATE (SKI), EDITOR. (1988). *The International HYDROCOIN Project. Levell: Code Verification*, NEA, OECD.
2. JACOB BEAR and ARNOLD VERRUIJT (1987). *Modeling Groundwater Flow and Pollution*, D. Reidel Publishing Company, Dordrecht-Boston-Lancaster-Tokyo.
3. S.M. HASSANIZADEH and T. LEIJNSE (1988). On the Modeling of Brine Transport in Porous Media, *Water Resources Research*, 24, 321-330.
4. R.A. TROMPERT (1992). *Local Uniform Grid Refinement and Brine Transport in Porous Media with Inhomogeneities*, NM-R9224, Centre for Mathematics and Computer Science, Amsterdam.