Centrum voor Wiskunde en Informatica

REPORT RAPPORT

Brine Transport in Porous Media: On the use of Von Mises and Similarity Transformations

C.J. van Duijn, R.J. Schotting

Modelling, Analysis and Simulation (MAS)

MAS-R9724 September 30, 1997

Report MAS-R9724
ISSN 1386-3703

CWI
P.O. Box 94079
1090 GB Amsterdam
The Netherlands

Brine Transport in Porous Media: On the use of Von Mises and Similarity Transformations

C.J. van Duijn & R.J. Schotting[1]
CWI
P.O. Box 94079, 1090 GB Amsterdam, The Netherlands
email: hansd@cwi.nl & ruuds@cwi.nl

ABSTRACT
In this paper we use a Von Mises transformation to study brine transport in porous media. The model involves mass balance equations for fluid and salt, Darcy's law and an equation of state, relating the salt mass fraction to the fluid density. Application of the Von Mises transformation recasts the model equations into a single nonlinear diffusion equation. A further reduction is possible if the problem admits similarity. This yields a formulation in terms of a boundary value problem for an ordinary differential equation which can be treated by semi-analytical means. Three specific similarity problems are considered in detail: (i) One-dimensional, stable displacement of fresh water and brine in a porous column, (ii) Flow of fresh water along the surface of a salt rock, (iii) Mixing of parallel layers of brine and fresh water.

1991 Mathematics Subject Classification: 35K65, 58G11, 76S05
Keywords and Phrases: Brine transport, Von Mises transformation, Similarity transformation, Groundwater.
Note: Work carried out under project MAS1.3 "Partial Differential Equations in Porous Media Research".

1 Introduction

Brine transport in porous media is a process which is described by the fluid and salt mass balance equations, the fluid movement equation and an equation of state, relating the salt mass fraction to the fluid density, see e.g. Hassanizadeh & Leijnse [12]. This yields a mathematical model consisting of a system of coupled partial differential equations which has to be solved in the flow domain, subject to appropriate boundary and initial conditions.

In a heterogeneous, multi dimensional flow domain the model equations have to be solved numerically in order to determine the spreading of salt in the subsurface. However, under simplified and highly idealized conditions it is possible to reduce the partial differential equations by means of Von Mises and similarity transformations to a single ordinary differential equation, which can be solved by semi-analytical means. The purpose of this paper is to draw attention to such transformations. We shall work out three specific cases for which we give an interpretation of the results in the physical sense.

The idea behind the Von Mises transformation is to take the stream function of the flow as one of the unknowns and to reduce the partial differential equations to a single nonlinear diffusion equation. To illustrate this procedure we recall the example of a laminar, stationary and two-dimensional flow over a flat plate. Let U, V denote the velocity components in the x, y-direction and let the plate be situated along the positive $x-$-axis. Following for instance,

[1]Corresponding author

Chorin & Marsden [5] or Curle [9], one has to consider the Prandtl boundary layer equations

$$\begin{cases} \dfrac{\partial U}{\partial x} + \dfrac{\partial V}{\partial y} = 0 \\ U\dfrac{\partial U}{\partial x} + V\dfrac{\partial U}{\partial y} = \nu\dfrac{\partial^2 U}{\partial y^2} \end{cases} \tag{1.1}$$

for $(x, y) \in \mathbf{R}^+ \times \mathbf{R}^+$, subject to the boundary conditions

$$U(x, 0) = 0 \text{ for } x \in \mathbf{R}^+ \tag{1.2}$$

and

$$U(0, y) = U_0(y) \text{ for } y \in \mathbf{R}^+ \tag{1.3}$$

where U_0 is the velocity distribution at the leading edge of the plate. In (1.1), ν denotes the viscosity of the fluid. Assuming the existence of a stream function $\psi = \psi(x, y)$ satisfying

$$U = \frac{\partial \psi}{\partial y} \text{ and } V = -\frac{\partial \psi}{\partial x}, \tag{1.4}$$

one introduces the change of variables

$$x = x \text{ and } \psi = \psi(x, y) = \int_0^y U(x, s)\, ds \tag{1.5}$$

and the Von Mises transformation

$$\tilde{U}(x, \psi) = \tilde{U}(x, \psi(x, y)) = U(x, y). \tag{1.6}$$

Under this transformation we obtain for $\tilde{U}$ the nonlinear diffusion equation

$$\frac{\partial \tilde{U}}{\partial x} = \frac{\nu}{2}\frac{\partial^2 \tilde{U}^2}{\partial \psi^2} \text{ with } (x, \psi) \in \mathbf{R}^+ \times \mathbf{R}^+, \tag{1.7}$$

and the conditions

$$\tilde{U}(0, \psi) = \tilde{U}_0(\psi) := U_0(y) \text{ for } \psi \in \mathbf{R}^+, \tag{1.8}$$

and

$$\tilde{U}(x, 0) = 0 \text{ for } x \in \mathbf{R}^+. \tag{1.9}$$

Note that if U_0 is a positive constant, say $U_0(y) = U_0^* > 0$ for all $y > 0$, this initial-boundary value problem can be reduced to a boundary value problem for an ordinary differential equation in terms of the similarity variable $\psi/\sqrt{x}$. The solution of this boundary value problem describes the behavior of the solution of problem (1.7)-(1.9) for large values of x, provided $U_0(y) \to U_0^*$ as $y \to \infty$. Such convergence results are well known for nonlinear diffusion problems, see for example Van Duijn & Peletier [10], who studied the large time behavior of a uniformly parabolic version of problem (1.7)-(1.9) in terms of such a similarity solution.

Thus the combination of Von Mises and similarity transformations provides a straight forward way to establish the large time behaviour of the original system. With this in mind, we return to the transport of brine and consider as examples three time dependent problems that allow Von Mises and similarity transformations. These problems are: (i) Brine displacing fresh water in an infinitely long porous column, (ii) Flow of fresh water along a salt dome and (iii) Mixing of parallel layers of brine and fresh water. The flow geometry of (i) is one-dimensional while the flow domains of (ii) and (iii) are two dimensional. However, in all three problems the boundary conditions are chosen such that the resulting fluid and salt balance equations are one-dimensional. The unknowns are the density and the specific discharge.

Analogous to the Prandtl system one can reduce the two balance equations to a single nonlinear diffusion equation for the density. Here the fluid balance equation suggests the existence of a modified stream function which serves as the new independent Von Mises variable. Considering in addition a piecewise constant initial condition for the density a further reduction is possible in terms of a similarity variable. A boundary condition for the specific discharge is used in the (back) transformation to the original variables, yielding semi-analytical expressions in terms of the similarity solution. This is illustrated in Section 3.

Characteristic for the brine model is the nonlinear coupling between fluid density and specific discharge which is caused by gravity and salinity induced fluid volume changes. Gravity causes enhanced rotational flow in regions where horizontal density variations occur and local high density gradients induce volume changes in the fluid which in turn may cause enhanced fluid flow as well. Because the three example problems to be discussed are essentially one-dimensional, gravity will not play a role and only the second mechanism causes enhanced fluid flow.

Raats [25], [29] introduced a similar modified stream function, which he called 'parcel function', when studying one-dimensional transport of fluid and solutes in unsaturated soils. The fluid balance equation in unsaturated soils in one space dimension reads

$$\frac{\partial \theta}{\partial t} + \frac{\partial}{\partial z}(\theta v) = 0 \ \text{ for } \ (z,t) \in \mathbf{R} \times \mathbf{R}^+, \tag{1.10}$$

where θ denotes the volumetric water content and v the velocity of water. Analogous to (1.1) and (1.4) a function Ξ is introduced which satisfies

$$\theta = \frac{\partial \Xi}{\partial z} \ \text{ and } \ \theta v = -\frac{\partial \Xi}{\partial t}. \tag{1.11}$$

Integration of the total differential $d\Xi$ gives

$$\Xi(z,t) = \Xi(0,0) - \int_0^t \theta_0 v_0 \, d\tau + \int_0^z \theta \, d\xi, \tag{1.12}$$

which effectively labels all members of a collection of parcels of water. The function Ξ can be interpreted as a measure of soil water storage in a region or as the cumulative flux across a surface. Raats [26] does not consider coupling between fluid velocity and solute concentration in the solute mass balance equation. This assumption only is valid when the fluid density is not affected by of the solute concentration. In brine transport however the coupling between salt concentration and fluid density is an essential property.

This paper is organized as follows. In Section 2 we give the mathematical formulation of the brine model. In Section 3 we explain the details of the Von Mises transformation for one-dimensional problems and in Section 4 we study the application to the three examples with similarity, thus specifying the large time limit of three corresponding classes of problems. Finally, in Section 5, we present the conclusions.

2 The brine equations

A general study of the transport of brine through porous media was presented by Hassanizadeh & Leijnse [12]. Simplifying their formulation by taking Fick's law for the diffusive salt flux and the conventional form of Darcy's law for the fluid momentum equation we arrive at the following set of equations:

Mass balance equation for the fluid

$$n\frac{\partial \rho}{\partial t} + \text{div }(\rho \mathbf{q}) = 0, \tag{2.1}$$

where ρ denotes the density of the fluid, $\mathbf{q}$ the specific discharge vector and n the porosity of the porous medium.

Mass balance equation for the salt

$$n\frac{\partial (\rho\omega)}{\partial t} + \text{div }(\omega\rho\mathbf{q} - \rho I\!D \text{ grad } \omega) = 0, \tag{2.2}$$

where ω denotes the mass fraction of the salt and $I\!D$ the hydrodynamic dispersion tensor. The mass fraction is defined as the concentration of the salt component divided by the density of the fluid.

Darcy's law

$$\frac{\mu}{\kappa}\mathbf{q} + \text{grad } p - \rho\mathbf{g} = 0, \tag{2.3}$$

where κ denotes the intrinsic permeability of the porous medium, μ the dynamic viscosity of the fluid and $\mathbf{g}$ the acceleration of gravity.

Equation of state

$$\rho = \rho_f e^{\gamma\omega}, \tag{2.4}$$

where ρ_f denotes the density of fresh water and γ a constant:$\gamma \approx 0.6923 \approx \ln(2)$. In writing (2.4) we implicitly assumed that the density is a function of ω only (no pressure or thermal effects). In the subsequent analysis we also assume that the fluid viscosity is constant.

It is common practice to use for the hydrodynamic dispersion tensor $I\!D = (D_{ij})$ in (2.2) the expression, see for instance Bear [3],

$$D_{ij} = \{\alpha_T|\mathbf{q}| + nD_{\text{mol}}\}\delta_{ij} + (\alpha_L - \alpha_T)q_iq_j/|\mathbf{q}|. \tag{2.5}$$

Here α_L and α_T are the longitudinal and transversal dispersion lengths, and D_{mol} is the effective molecular diffusivity incorporating the effect of tortuosity. Further, δ_{ij} denotes the Kronecker δ and $|\cdot|$ the Euclidian norm in $\mathbf{R}^2$. However, for mathematical convenience we use in almost all of this paper the approximation

$$D_{ij} = nD\delta_{ij}, \tag{2.6}$$

where D is a positive constant. If α_L and α_T are small (fine granular, homogeneous material), this approximation is justified for $D = D_{mol}$. However, if the influence of the heterogeneities is significant, then D in (2.6) accounts for dispersion in an averaged sense. Only when discussing the examples in Sections 4.2 and 4.3 we allow for some velocity dependence of D_{ij}, however different from (2.5).

As in Van Duijn et.al. [11] we first rewrite equations (2.1)- (2.4). Expansion of equation (2.2) gives

$$n\rho\frac{\partial \omega}{\partial t} + n\omega\frac{\partial \rho}{\partial t} + \omega\text{div }(\rho\mathbf{q}) + \rho\mathbf{q}\cdot\text{grad }\omega - \text{div }(\rho I\!D\text{grad }\omega) = 0 \tag{2.7}$$

Multiplication of equation (2.1) by ω and subtracting the result from equation (2.7) results in

$$n\rho\frac{\partial \omega}{\partial t} + \rho \mathbf{q}\cdot \text{grad } \omega - \text{div } (\rho I\!D \text{grad } \omega) = 0. \tag{2.8}$$

Next we substitute the equation of state (2.4) in (2.8) and obtain

$$n\frac{\partial \rho}{\partial t} + \mathbf{q}\cdot \text{grad } \rho - \text{div } (I\!D \text{grad } \rho) = 0, \tag{2.9}$$

as a second equation for the unknowns ρ and $\mathbf{q}$. Note that equation(2.9) is no longer in divergence form and that the constant γ has vanished from the equations. The latter is due to the exponential form of the equation of state. Hence, the resulting system of equations is

$$\begin{cases} n\dfrac{\partial \rho}{\partial t} + \text{div } (\rho \mathbf{q}) = 0 \\ \\ n\dfrac{\partial \rho}{\partial t} + \mathbf{q}\cdot \text{grad } \rho - \text{div } (I\!D \text{grad } \rho) = 0 \end{cases} \tag{2.10}$$

In view of the applications in Section 4 we confine ourselves to the analysis of (2.10) in one space dimension. After appropriate scaling, imposed by the geometry and hydrology of each individual application in Section 4 and assuming (2.6) for the moment, we obtain the dimensionless system

$$\begin{cases} \dfrac{\partial u}{\partial t} + \dfrac{\partial}{\partial z}(qu) = 0 & (z,t) \in \Omega \times \mathbf{R}^+ \\ \\ \dfrac{\partial u}{\partial t} + q\dfrac{\partial u}{\partial z} - \dfrac{\partial}{\partial z}\left(\dfrac{\partial u}{\partial z}\right) = 0 & (z,t) \in \Omega \times \mathbf{R}^+ \end{cases} \tag{2.11}$$

where Ω denotes the one-dimensional domain $\mathbf{R}$ or $\mathbf{R}^+$. Details of the scaling rules for each problem will be given in Section 4. Equations (2.11) can be combined to give

$$u\frac{\partial q}{\partial z} - \frac{\partial}{\partial z}\left(\frac{\partial u}{\partial z}\right) = 0 \quad (z,t) \in \Omega \times \mathbf{R}^+. \tag{2.12}$$

This expression shows that in order to solve (2.11) uniquely, one has to prescribe initial-boundary conditions for u and a single boundary condition for q. Specifically, if $\Omega = \mathbf{R}$ we consider (2.11) subject to the conditions

$$u(z,0) = u_0(z) \ \text{ for } \ z \in \mathbf{R} \tag{2.13}$$

and

$$q(-\infty,t) = q_0(t) \ \text{ for } \ t \in \mathbf{R}^+, \tag{2.14}$$

where u_0 and q_0 are the given, scaled initial density distribution and limiting discharge value.

If $\Omega = \mathbf{R}^+$, we consider (2.11) subject to initial condition

$$u(z,0) = u_f \ \text{ for } \ z \in \mathbf{R}^+, \tag{2.15}$$

and the boundary conditions

$$u(0,t) = u_s \ \text{ and } \ q(0,t) = q_0(t). \tag{2.16}$$

Here u_f and u_s are the scaled densities of fresh water and brine. Concerning the behavior of solutions of these problems we assume that for all $t \geq 0$:

$$u_f \leq u(z,t) \leq u_s \quad \text{for} \quad z \in \Omega, \tag{2.17}$$

and

$$\lim_{z \to -\infty} u(z,t) = u_s \quad (\text{if} \ \ \Omega = \mathbf{R}), \ \lim_{z \to +\infty} u(z,t) = u_f. \tag{2.18}$$

Remark: Introduction of the material derivative

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \frac{\mathbf{q}}{n} \cdot \text{grad} \tag{2.19}$$

in the fluid balance equation (2.1) results in

$$\frac{n}{\rho}\frac{D\rho}{Dt} + \text{div } \mathbf{q} = 0. \tag{2.20}$$

This expression shows that density variations may effect the divergence or local volume of the fluid, which in turn can cause additional movement of fluid. This effect will be investigated in the examples presented in Section 4.

3 Von Mises transformation

To reduce system (2.11) to a single, nonlinear diffusion equation we apply a coordinate transformation which is a variant of the Von Mises transformation, see e.g. Mises & Friedrichs [21]. Considering the fluid balance equation in (2.11) as the divergence operator in the (t,z)-plane, acting on the vector (u, uq), we introduce a modified stream function $\Psi = \Psi(z,t)$, which satisfies

$$u = \frac{\partial \Psi}{\partial z} \quad \text{and} \quad uq = -\frac{\partial \Psi}{\partial t}. \tag{3.1}$$

The new independent variables are

$$t = t \quad \text{and} \quad \Psi = \int_{h(t)}^{z} u(s,t)\, ds, \tag{3.2}$$

where $h(t)$ is a yet unknown function of time which will be determined later on from the boundary condition on q. It will be normalized such that $h(0) = 0$. The Von Mises transformation is

$$\hat{u} = \hat{u}(\Psi,t) = \hat{u}(\Psi(z,t),t) = u(z,t). \tag{3.3}$$

We use it to rewrite system (2.11) into the equation

$$\frac{\partial \hat{u}}{\partial t} = \hat{u}\frac{\partial}{\partial \Psi}\left(\hat{u}\frac{\partial \hat{u}}{\partial \Psi}\right) \quad \text{with} \quad \Psi \in Q, \ t \in \mathbf{R}^+. \tag{3.4}$$

Here Q denotes the range of Ψ.
First we consider the case $\Omega = \mathbf{R}$. Properties (2.17),(2.18) and definition (3.1) imply that Ψ is monotonically increasing in z with $\Psi(-\infty,t) = -\infty$ and $\Psi(+\infty,t) = +\infty$ for all $t > 0$. Hence

$Q = \mathbf{R}$ in (3.4). To find the initial condition corresponding to (3.4) we need to transform the function u_0. To this end we consider (3.2) at $t = 0$:

$$\Psi = \int_0^z u_0(s)\, ds. \tag{3.5}$$

This expression defines the function $z = z(\Psi)$ for $-\infty < \Psi < +\infty$, which we use to obtain the transformed initial condition

$$\hat{u}(\Psi, 0) = u_0(z(\Psi)) \text{ for } \Psi \in \mathbf{R}. \tag{3.6}$$

The initial value problem (3.4),(3.6) admits a similarity solution for piecewise constant initial data. If u_0 is given by

$$u_0(z) = \begin{cases} u_s & \text{for } z < 0 \\ u_f & \text{for } z > 0 \end{cases} \tag{3.7}$$

then the same is true for $\hat{u}(\Psi, 0)$: i.e.

$$\hat{u}(\Psi, 0) = \begin{cases} u_s & \text{for } \Psi < 0 \\ u_f & \text{for } \Psi > 0 \end{cases} \tag{3.8}$$

The corresponding solution is a similarity solution of the form $\hat{u}(\Psi, t) = f(\eta)$ with $\eta = \Psi/\sqrt{t}$.

Having obtained a solution $\hat{u} = \hat{u}(\Psi, t)$ we use (3.1) to return to the original variables. Integrating the first equation of (3.1) gives

$$z = \int_0^{\Psi(z,t)} \frac{1}{\hat{u}(s,t)}\, ds + h(t) \text{ for } (z,t) \in \mathbf{R} \times \mathbf{R}^+, \tag{3.9}$$

where $h(t)$ is an integration constant depending on t only, satisfying $h(0) = 0$ (which implies $\Psi(0,0) = 0$). If the function $h(t)$ were known, then (3.9) would define the modified stream function $\Psi = \Psi(z,t)$ and the solution in terms of the original variables would be given by

$$u(z,t) = \hat{u}(\Psi, t) \text{ for } (z,t) \in \mathbf{R} \times \mathbf{R}^+. \tag{3.10}$$

To find $h(t)$ we differentiate (3.9) with respect to t and use the second equation in (3.1). This yields an expression for q which is given by

$$q(z,t) = h'(t) - \int_0^{\Psi(z,t)} \frac{\hat{u}_t}{\hat{u}^2}(s,t)\, ds. \tag{3.11}$$

where $\hat{u}_t$ denotes the partial derivative of $\hat{u}$ with respect to t. Next we use the discharge boundary condition (2.14) to determine $h(t)$. Letting $z \to -\infty$ in (3.11) we find upon integration

$$h(t) = \int_0^t \left\{ q_0(\xi) - \int_{-\infty}^0 \frac{\hat{u}_t}{\hat{u}^2}(s,\xi)\, ds \right\} d\xi, \tag{3.12}$$

provided that this integral exists. Substituting (3.12) in (3.11) gives for the discharge the expression

$$q(z,t) = q_0(t) - \int_{-\infty}^{\Psi(z,t)} \frac{\hat{u}_t}{\hat{u}^2}(s,t)\, ds, \tag{3.13}$$

which completely determines the solution of the problem on $\mathbf{R}$.

Next we consider $\Omega = \mathbf{R}^+$. This case is more involved because the presence of the boundary at $z = 0$ which implies that the domain Q becomes time dependent. Using boundary condition (2.16) and integrating the second equation in (3.1) yields for $Q = Q(t)$

$$Q(t) = (\Psi(0,t), \infty) \quad \text{for} \quad t \geq 0, \tag{3.14}$$

where

$$\Psi(0,t) = -u_s \int_0^t q_0(\xi)\, d\xi. \tag{3.15}$$

Let $\hat{u} = \hat{u}(\Psi, t)$ denote the solution of (3.4) subject to (3.6), now with $\Psi > 0$, and the boundary condition $\hat{u}(\Psi(0,t), t) = u_s$. Similarly to (3.12) we introduce

$$h(t) = \int_0^t \left\{ q_0(\xi) + \int_0^{\Psi(0,\xi)} \frac{\hat{u}_t}{\hat{u}^2}(s,\xi)\, ds \right\} d\xi, \tag{3.16}$$

and define $\Psi = \Psi(z,t)$ for $(z,t) \in \mathbf{R}^+ \times \mathbf{R}^+$ by

$$z = \int_0^{\Psi(z,t)} \frac{1}{\hat{u}(s,t)}\, ds + \int_0^t \left\{ q_0(\xi) + \int_0^{\Psi(0,\xi)} \frac{\hat{u}_t}{\hat{u}^2}(s,\xi)\, ds \right\} d\xi. \tag{3.17}$$

Then u is given by

$$u(z,t) = \hat{u}(\Psi(z,t), t) \tag{3.18}$$

and

$$q(z,t) = q_0(t) - \int_{\Psi(0,t)}^{\Psi(z,t)} \frac{\hat{u}_t}{\hat{u}^2}(s,\xi)\, ds. \tag{3.19}$$

If q_0 is not explicitly given but, as in the salt dome problem in Section 4.2, a function of $\partial u/\partial z$ at the boundary $z = 0$, then $\Psi(0,t)$ denotes a free boundary in the (Ψ, t)-plane. The position of the free boundary is a priori unknown and is part of the solution of the problem. When, as in Section 4.2, the discharge q_0 is given by

$$q_0(t) = -C\, \frac{\partial u}{\partial z}(0,t) \quad \text{for all} \quad t > 0, \tag{3.20}$$

where C denotes a positive constant, then the following Stefan condition holds at the free boundary:

$$\frac{d\varphi(t)}{dt} = C\, \hat{u}^2(\varphi(t), t) \frac{\partial \hat{u}}{\partial \Psi}(\varphi(t), t) = C\, u_s^2 \frac{\partial \hat{u}}{\partial \Psi}(\varphi(t), t), \tag{3.21}$$

where $\varphi(t) := \Psi(0,t)$. This condition relates the speed of the free boundary in the (Ψ, t)-plane to the spatial derivative of $\hat{u}$ at the free boundary.

The nonlinear diffusion problems that arise from these transformations are well known and received much attention in the existing literature, for instance see the book of Crank [6] on the mathematics of diffusion or the book of Meirmanov [20] on the Stefan problem. Considering the role of similarity solutions as large time solutions of nonlinear diffusion problems we refer to the paper of Van Duijn & Peletier [10] and the book by Barenblatt on intermediate asymptotics [2].

The initial and boundary conditions of the flow problem discussed in the next section are chosen such that the corresponding nonlinear diffusion problems are solvable in terms of similarity solutions. With the Von Mises transformation as intermediate step such similarity solutions are natural to the problem and straight forward to find. Moreover, we know that they represent the large time behavior of the corresponding flow problem with more general (i.e. non-constant) boundary/initial data.

4 Applications

4.1 Flow in a porous column

In the first application we study brine transport in an infinitely long, one-dimensional porous column. From a practical point of view it would be more realistic to study a column with finite length. But when the phenomenon to be studied occurs at a sufficiently large distance from the inlet and outlet of the column one expects only minor differences between the results for a finite and an infinite column. The column is in vertical position, directed along the z-axis, and gravity points downwards in the negative z-direction. The porous medium is saturated with fluid. The flow is in the positive z-direction, such that brine displaces fresh water in a stable manner. Initially the region $z > 0$ is filled with fresh water ($\rho = \rho_f$), and the region $z < 0$ with brine ($\rho = \rho_s$), such that the fluids are separated by a sharp transition at $z = 0$. At $z = -\infty$ the column is infiltrated with brine, with constant density ρ_s and constant specific discharge q_s. The mathematically relevant initial-boundary conditions for this problem are

$$q(-\infty, t) = q_s, \quad \text{with} \quad t \in \mathbf{R}^+ \tag{4.1}$$

and

$$\rho(z, 0) = \begin{cases} \rho_s & \text{for} \quad z < 0 \\ \rho_f & \text{for} \quad z > 0 \end{cases} \tag{4.2}$$

Note that the initial condition implies $\rho(-\infty, t) = \rho_s$ for $t > 0$, implying that indeed brine is injected into the column. Assuming the column to be filled with homogeneous, fine granular material we consider a constant dispersivity according to (2.6). This choice is also motivated by the fact that in this application the Von Mises transformation is not applicable for a velocity dependent dispersivity.

Next we introduce the dimensionless variables

$$u = \frac{1}{\varepsilon} + \frac{\rho - \rho_f}{\rho_s - \rho_f} \left(= \frac{\rho}{\rho_s - \rho_f} = \frac{1}{\varepsilon} \frac{\rho}{\rho_f} \right), \quad q^* = \frac{q}{q_s}, \quad t^* = t \frac{q_s^2}{nD}, \quad z^* = z \frac{q_s}{D}. \tag{4.3}$$

where ε is the relative density difference

$$\varepsilon = \frac{\rho_s - \rho_f}{\rho_f}. \tag{4.4}$$

Typical values of the relative density difference are: $\varepsilon \approx 0.025$ for sea water and $\varepsilon \approx 0.2$ for saturated brine; hence $(0 \leq) \varepsilon \leq 0.2$. Applying this scaling to (2.10) (in one space dimension), (4.1) and (4.2), and dropping the asterisks again in the notation, we obtain the mixed initial-boundary value problem

$$\begin{cases} \dfrac{\partial u}{\partial t} + \dfrac{\partial}{\partial z}(qu) = 0 \\ \dfrac{\partial u}{\partial t} + q \dfrac{\partial u}{\partial z} = \dfrac{\partial^2 u}{\partial z^2} \end{cases} \tag{4.5}$$

for $(z, t) \in \mathbf{R} \times \mathbf{R}^+$, with

$$q(-\infty, t) = 1 \qquad \text{for} \quad t \in \mathbf{R}^+, \tag{4.6}$$

$$\tag{4.7}$$

and

$$u(z, 0) = \begin{cases} 1 + \frac{1}{\varepsilon} & \text{for} \quad z < 0, \\ \frac{1}{\varepsilon} & \text{for} \quad z > 0. \end{cases} \tag{4.8}$$

The Von Mises transformation (3.1)-(3.3) now gives the initial value problem

$$\begin{cases} \dfrac{\partial \hat{u}}{\partial t} = \hat{u}\dfrac{\partial}{\partial \Psi}\left(\hat{u}\dfrac{\partial \hat{u}}{\partial \Psi}\right) & \text{for } (\Psi, t) \in \mathbf{R} \times \mathbf{R}^+, \\ \tilde{u}(\Psi, 0) = \begin{cases} 1 + \frac{1}{\varepsilon} & \text{for } \Psi < 0, \\ \frac{1}{\varepsilon} & \text{for } \Psi > 0. \end{cases} \end{cases} \tag{4.9}$$

The special form of the initial condition implies similarity. Let

$$\eta = \frac{\Psi}{\sqrt{t}} \text{ and } \hat{u}(\Psi, t) = f(\eta), \tag{4.10}$$

then $f(\eta)$ should satisfy the boundary value problem

$$\frac{1}{2}\eta f' + f\{ff'\}' = 0 \text{ for } \eta \in \mathbf{R} \tag{4.11}$$

with

$$f(-\infty) = 1 + \frac{1}{\varepsilon} \text{ and } f(+\infty) = \frac{1}{\varepsilon}. \tag{4.12}$$

Here the primes denote differentiation with respect to η. No explicit solution to this boundary value problem is known. However, qualitatively the picture is quite complete: we know that there exists a unique C^∞ solution, strictly decreasing on $\mathbf{R}$, and much is known about the asymptotic behavior of $f(\eta)$ as $\eta \to \pm\infty$, see Van Duijn & Peletier [10], Atkinson & Peletier [1].

We will solve problem (4.11), (4.12) numerically. For this purpose it is convenient to transform the problem to one on a bounded domain, by considering a equation for the flux with f as independent variable. This transformation and the resulting flux equation have been studied in detail by Atkinson & Peletier [1], Van Duijn et.al [11] and Bouillet & Gomez [4]. Since f is strictly decreasing on $\mathbf{R}$ we can define the inverse

$$\eta = \sigma(f), \text{ with } \sigma = f^{-1}, \tag{4.13}$$

and the flux function

$$w(f) := -ff'(\sigma(f)) \text{ for } \frac{1}{\varepsilon} \le f \le 1 + \frac{1}{\varepsilon}. \tag{4.14}$$

For w we find the boundary value problem

$$\begin{cases} -w\{fw'\}' = \dfrac{f}{2} \\ w(f) > 0 \\ w(\frac{1}{\varepsilon}) = w(1 + \frac{1}{\varepsilon}) = 0 \end{cases} \tag{4.15}$$

for $1/\varepsilon < f < 1 + 1/\varepsilon$, where now primes denote differentiation with respect to f. The sign of w implies that fw' is decreasing. We use this observation to determine $f = f(\eta)$ from the identity

$$\eta = 2fw'(f), \tag{4.16}$$

which also shows that w' changes sign at $f(0) = f_0 \in (1/\varepsilon, 1+1/\varepsilon)$ and that $\lim_{f \downarrow 1/\varepsilon} w'(f) = +\infty$ and $\lim_{f \uparrow 1+1/\varepsilon} w'(f) = -\infty$.

We solve (4.15) numerically by discretizing the derivatives central in f on a equidistant grid. The discretization of (4.15) leads to a set of nonlinear algebraic equations which we solve iteratively using a standard multi-dimensional Newton method. Once accurate numerical approximations of $w(f)$ and thereby of $w'(f)$ are obtained we compute $\sigma(f)$ directly using (4.16) and $f = f(\eta)$ by inverting the result. Figure 1 shows $w(f)$ and $f(\eta$ for $\varepsilon = 0.2$. The singular nature of w' at the boundary points is not visible in Figure 1. This is due to the asymptotic behavior of w', which is proportional to $\sqrt{\ln(1/w(f))}$ for $f \downarrow 1/\varepsilon$ and $f \uparrow 1 + 1/\varepsilon$, i.e. for $w(f) \downarrow 0$.

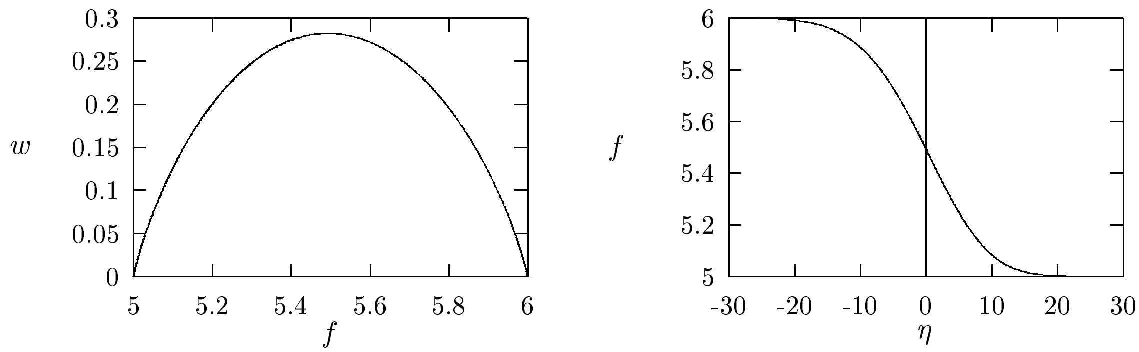

Figure 1. The functions $w(f)$ and $f(\eta)$ for $\varepsilon = 0.2$

Introduction of the similarity variables (4.10) in (3.13),(3.9) and (3.12) yields

$$q = q(\Psi, t) = 1 + \frac{1}{2\sqrt{t}} \int_{-\infty}^{\frac{\Psi}{\sqrt{t}}} \frac{sf'}{f^2}\, ds \text{ for all } -\infty < \Psi < +\infty, t > 0, \tag{4.17}$$

and

$$z = z(\Psi, t) = \sqrt{t} \int_0^{\frac{\Psi}{\sqrt{t}}} \frac{1}{f(s)} ds + t + \sqrt{t} \int_{-\infty}^0 \frac{sf'}{f^2}\, ds \text{ for all } -\infty < \Psi < +\infty, t > 0. \tag{4.18}$$

This completes the construction of the solution of the column problem with piecewise constant initial data. The solution is given as parametric pairs $(z(\Psi,t), u(\Psi,t))$ and $(z(\Psi,t), q(\Psi,t))$. Figure 2 shows the results of $u = u(z,t)$ and $q = q(z,t)$ as function of z at fixed time levels, for $\varepsilon = 0.2$.

When using $v := (\rho - \rho_f)/(\rho_s - \rho_f)$ in the scaling (4.3), we arrive at the dimensionless system

$$\left\{ \begin{array}{l} \dfrac{\partial v}{\partial t} + \dfrac{\partial}{\partial z}(qv) + \dfrac{1}{\varepsilon}\dfrac{\partial q}{\partial z} = 0 \\ \dfrac{\partial v}{\partial t} + q\dfrac{\partial v}{\partial z} - \dfrac{\partial}{\partial z}\left(\dfrac{\partial v}{\partial z}\right) = 0 \end{array} \right. \tag{4.19}$$

for $(z,t) \in \mathbf{R} \times \mathbf{R}^+$. Note that the same result can be achieved by setting $u = v + 1/\varepsilon$ in (2.11). When passing to the limit $\varepsilon \to 0$ (4.19) reduces to

$$\left\{ \begin{array}{l} \dfrac{\partial q}{\partial z} = 0 \\ \dfrac{\partial v}{\partial t} + q\dfrac{\partial v}{\partial z} - \dfrac{\partial}{\partial z}\left(\dfrac{\partial v}{\partial z}\right) = 0 \end{array} \right. \tag{4.20}$$

for $(z,t) \in \mathbf{R} \times \mathbf{R}^+$, implying upon integration $q(z,t) = q_s$ and

$$v(z,t) = \frac{1}{2}\left(1 - \text{erf}\left(\frac{z-t}{2\sqrt{t}}\right)\right). \tag{4.21}$$

A formal justification of this limit is given in Van Duijn et.al. [11]. We refer to (4.21) as the Boussinesq solution of the column problem.

The dashed line in the u-plot in Figure 2 corresponds to the Boussinesq solution (4.21) at $t = 1$. The difference between $(u(z,1)$ and $v(z,1)$ is small but noticeable, e.g. up to $\approx 5\%$ in this example. The results in Figure 2 clearly demonstrate the effect of a high concentration (or density) gradient on the fluid flow. At the short time scale of the problem, the deviation from the background flow ($q_s = 1$) is significant. As time proceeds, diffusion flattens the density profile, which in turn causes decay of the specific discharge distribution towards its limiting value $q(z,\infty) = q_s = 1$.

At the short time scale of the problem $q(\infty,t)$ is negative which means that fluid enters the column at $z = +\infty$. After $t = \hat{t}$, defined by

$$\hat{t} = \frac{1}{4q_s^2}\left(\int_{-\infty}^{+\infty} \frac{sf'}{f^2}\, ds\right)^2, \tag{4.22}$$

$q(\infty,t)$ changes sign and outflow will occur at $z = +\infty$.

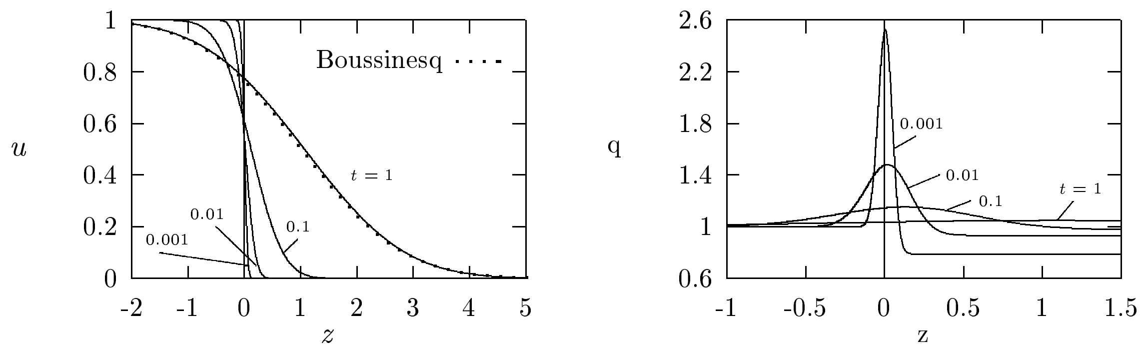

Figure 2. Scaled density and velocity profiles for column problem at $t = 0.001, 0.01, 0.1$ and 1.

Remark:

In his study of the laminar boundary layer equations, Crocco [7] introduced a transformation, in literature referred to as the Crocco transformation, which is related to the Von Mises transformation. Crocco takes the velocity in the x-direction and the x-coordinate as new independent variables and the viscous stress and enthalpy as dependent variables. For the case of zero pressure gradient, Crocco [8] proposed a solution procedure which resembles the solution procedure given in this paper. He also derives an equation which is similar to the differential equation in (4.15). For details we refer to Crocco's original paper [8] or to the book by Curle [9]

4.2 The salt dome problem

The salt dome problem models the flow of fresh groundwater along the surface of a salt rock; see Van Duijn et.al. [11] for a detailed description. A sketch of the flow geometry is given in Figure 3.

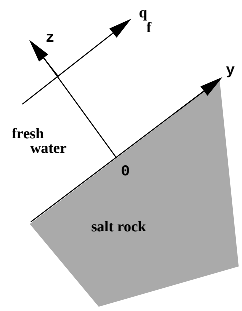

Figure 3. Flow geometry of the salt dome problem.

The flow domain consists of the upper half space $\{z > 0\}$ and is bounded below by an impermeable salt rock (= the salt dome) which has the inclination β with the horizontal plane.

Initially fresh water, $\rho = \rho_f$, is present in the flow domain which is maintained at a constant flow, $q_y = q_f$, far above and parallel to the salt rock boundary. Further, the presence of the salt rock ensures that $\rho = \rho_s$ along the boundary $\{z = 0\}$. Because ρ_f, ρ_s and q_f are constant and because the $y-$coordinate ranges from $-\infty$ to $+\infty$, we look for solutions with the dependence

$$\rho = \rho(z,t) \quad \text{and} \quad \mathbf{q} = \mathbf{q}(z,t), \tag{4.23}$$

satisfying

$$\rho(z,0) = \rho_f \ \text{ for } \ z \in \mathbf{R}^+, \tag{4.24}$$

$$\rho(0,t) = \rho_s \ \text{ for } \ t \in \mathbf{R}^+, \tag{4.25}$$

and

$$q_y(\infty,t) = q_f \ \text{ for } \ t \in \mathbf{R}^+. \tag{4.26}$$

Under assumption (4.23) we obtain a linear relation between the y-component of the specific discharge and the fluid density, see e.g. De Josseling De Jong & Van Duijn [16]. It is found by eliminating the pressure from Darcy's law. Taking the curl yields

$$\frac{\partial}{\partial z}\{q_y - \frac{\kappa}{\mu}\rho g_y\} - \frac{\partial}{\partial y}\{q_z - \frac{\kappa}{\mu}\rho g_z\} = 0, \tag{4.27}$$

which implies after integration

$$q_y + \frac{\kappa}{\mu}\rho g \,\sin\beta = \ \mathrm{C}, \tag{4.28}$$

where C is a constant. Initial condition (4.24) implies

$$\rho(+\infty,t) = \rho_f \ \text{ for } \ t \in \mathbf{R}^+, \tag{4.29}$$

which we use, together with (4.26), to determine the constant C in (4.28). This yields in the linear relation

$$q_y = q_f - \frac{\kappa}{\mu}(\rho - \rho_f)g \ \sin\beta. \tag{4.30}$$

In this example we consider $I\!\!D$ to be velocity dependent. However, we cannot treat the full dispersion matrix, but we have to make the assumption that the flow in the $y-$direction dominates the induced flow (q_z): i.e. $|q_z| << |q_y|$. Then the dispersion tensor only has non-trivial diagonal elements, given by

$$\begin{cases} D_{zz} = \alpha_T|q_y| + nD_{\text{mol}} \\ D_{yy} = \alpha_L|q_y| + nD_{\text{mol}} \end{cases} \tag{4.31}$$

Because ρ satisfies (4.23), only D_{zz} appears in the model description. Note that D_{zz} combined with (4.30) gives

$$D_{zz} = \alpha_T|q_f - \frac{\kappa}{\mu}(\rho - \rho_f)g\sin\beta| + nD_{\text{mol}} := D(\rho). \tag{4.32}$$

The object is now to solve the balance equations (2.10) (in one space dimension, the $z-$direction), with the dispersivity given by (4.32) and subject to conditions (4.24),(4.25). As in the example treated in Section 4.1, we need an additional boundary condition forq_z, here along the salt rock boundary. Following Hassanizadeh & Leijnse [12] we require for the specific discharge along the salt rock boundary

$$q_z(0,t) = -\frac{D(\rho_s)}{\gamma\rho_s\{1-\omega_s\}}\frac{\partial\rho}{\partial z}(0,t) \ \text{ for } \ t \in \mathbf{R}^+. \tag{4.33}$$

Here ω_s denotes the salt mass fraction of saturated brine, i.e. $\rho_s = \rho_f e^{\gamma\omega_s}$. To put the equations in dimensionless form we introduce the variables

$$\mathbf{q}^* = \frac{\mathbf{q}}{\hat{q}},\ z^* = \frac{z}{\alpha_T},\ t^* = t\frac{\hat{q}}{n\alpha_T},\ \ D^* = \frac{D}{\alpha_T\hat{q}},\ \ \varepsilon = \frac{\rho_s - \rho_f}{\rho_f} \ \text{ and } \ u = \frac{1}{\varepsilon} + \frac{\rho - \rho_f}{\rho_s - \rho_f}, \tag{4.34}$$

where $\hat{q} = \frac{\kappa}{\mu}(\rho_s - \rho_f)g\ \sin\beta$. Dropping the asterisk notation, the dimensionless dispersivity is expressed as

$$D(u) = \lambda + |U - u|, \tag{4.35}$$

with

$$\lambda = \frac{nD_{\text{mol}}}{\alpha_T\hat{q}} \quad \text{and} \quad U = \frac{q_f}{\hat{q}} + \frac{1}{\varepsilon}, \tag{4.36}$$

and the scaled specific discharge component in the y-direction is given by

$$q_y = U - u. \tag{4.37}$$

The scaling proposed here differs from the one used in Section 4.1. It allows us to consider the limit of small molecular diffusion with respect to transversal dispersion, i.e. $\lambda = 0$, a mathematically interesting limit because it leads to degenerate diffusion at points where $u = U$. As a result we obtain the initial-boundary value problem

$$\begin{cases} \dfrac{\partial u}{\partial t} + \dfrac{\partial}{\partial z}(q_z u) = 0 \\ \dfrac{\partial u}{\partial t} + q_z\dfrac{\partial u}{\partial z} = \dfrac{\partial}{\partial z}\left\{(\lambda + |U - u|)\,\dfrac{\partial u}{\partial z}\right\} \end{cases} \tag{4.38}$$

for $(z,t) \in \mathbf{R}^+ \times \mathbf{R}^+$, subject to

$$\begin{aligned} &u(0,t) = 1 + \frac{1}{\varepsilon} \ \text{ for } \ t \in \mathbf{R}^+, \\ &q_z(0,t) = -\varepsilon K(\varepsilon)\{\lambda + |U - u(0,t)|\}\frac{\partial u}{\partial z}(0,t) \ \text{ for } \ t \in \mathbf{R}^+, \\ &u(z,0) = \frac{1}{\varepsilon} \ \text{ for } \ z \in \mathbf{R}^+, \end{aligned} \tag{4.39}$$

where, through ρ_s and ω_s, K is a function of ε given by

$$K(\varepsilon) = \frac{1}{(1+\varepsilon)(\gamma - \log(1+\varepsilon))} \quad \text{for} \quad 0 < \varepsilon < e^{\gamma} - 1. \tag{4.40}$$

The complete solution of the salt dome problem involves q_y, q_z and u. The pair (q_z, u) solves (4.38),(4.39), while q_y follows directly from (4.37), once u is known. To solve (4.38),(4.39) we apply the Von Mises transformation and obtain in the (Ψ, t)-plane the problem

$$\begin{cases} \dfrac{\partial \hat{u}}{\partial t} = \hat{u}\dfrac{\partial}{\partial \Psi}\left\{(\lambda + |U - \hat{u}|)\hat{u}\dfrac{\partial \hat{u}}{\partial \Psi}\right\} & \text{for} \quad \{(\Psi, t) : \varphi(t) < \Psi < +\infty, t > 0\} \\ \hat{u}(\Psi, 0) = \dfrac{1}{\varepsilon} & \text{for} \quad \Psi > \varphi(0) \\ \hat{u}(\varphi(t), t) = 1 + \dfrac{1}{\varepsilon} & \text{for} \quad t > 0 \end{cases} \tag{4.41}$$

Here the function $\varphi(t)$ denotes a free boundary in the (Ψ, t)-plane for which we need an additional condition. This condition is obtained by applying the Von Mises transformation to (4.39). It takes the from of a Stefan condition:

$$\frac{d\varphi}{dt}(0, t) = \frac{(1+\varepsilon)^2}{\varepsilon} K(\varepsilon)\{\lambda + |U - 1 - \frac{1}{\varepsilon}|\}\frac{\partial \hat{u}}{\partial \Psi}(\varphi(t), t) \quad \text{for} \quad t \in \mathbf{R}^+. \tag{4.42}$$

This expression relates the salt mass flux at the salt rock boundary to the speed of the free boundary in the (Ψ, t)-plane. It is interesting to observe that the Von Mises transformation in the salt dome problem reduces to a nonlinear Stefan problem.

The free boundary problem (4.41), (4.42) too allows similarity of the form (4.10), with the free boundary given by

$$a = \frac{\varphi(t)}{\sqrt{t}} \quad \text{for} \quad t \in \mathbf{R}^+. \tag{4.43}$$

The similarity solution $f = f(\eta)$, $\eta \geq a$, and the free boundary $\eta = a$ are found from the transformed ordinary differential equation problem:

$$\begin{aligned} &\tfrac{1}{2}\eta f' + f(\{\lambda + |U - f|\}ff')' = 0 \quad \text{for} \quad \eta > a, \\ &f(a) = 1 + \frac{1}{\varepsilon}, \quad f(+\infty) = \frac{1}{\varepsilon} \end{aligned} \tag{4.44}$$

and

$$f'(a) = \frac{a}{2\varepsilon K(\varepsilon)\{\lambda + |U - f(a)|\}f^2(a)} \tag{4.45}$$

One can show that a solution of (4.44), (4.45) is strictly decreasing with respect to η. Consequently, from (4.45), we find $a < 0$.

As in Section 4.1 we solve the similarity problem by considering the corresponding flux equation. Setting, again,

$$w = \sigma(f) \quad \text{and} \quad w = w(f) = -2\{\lambda + |U - f|\}ff'(\sigma(f)), \quad \frac{1}{\varepsilon} < f < 1 + \frac{1}{\varepsilon}, \tag{4.46}$$

we obtain for w the boundary value problem

$$w\{fw'\}' = -2\{\lambda + |U - f|\}f \quad \text{in} \quad f \in (1/\varepsilon, 1 + 1/\varepsilon), \tag{4.47}$$

with

$$w(1+\frac{1}{\varepsilon}) = -\frac{a}{(1+\varepsilon)K(\varepsilon)}, \quad w'(1+\frac{1}{\varepsilon}) = \frac{\varepsilon a}{1+\varepsilon} < 0 \tag{4.48}$$

and

$$w(\frac{1}{\varepsilon}) = 0. \tag{4.49}$$

To solve this transformed w-problem we apply a shooting procedure: First, for a given $a < 0$, we solve the initial value problem (4.47), (4.48) for $f \in (1/\varepsilon, 1+1/\varepsilon)$ and then adjust a such that (4.49) is satisfied.

For two reasons it is more convenient to solve the w-problem in stead of the f-problem directly: (i) the domain is fixed and finite and (ii) the formulation allows to pass to the limit $\lambda \to 0$ without (numerical) difficulty. To solve the initial value problem (4.47), (4.48) we apply a Runge-Kutta method with w and w' as primary unknowns.

Once the solution $f(\eta)$ is obtained we return to the original variables in the (z,t)-plane, using expressions (3.18), (3.17), (3.19) combined with the boundary condition (4.39) on q_z. Application of the Von Mises transformation in (4.39) yields

$$q_z(0,t) = q_0(t) = -\varepsilon K(\varepsilon)\{\lambda + |U - \hat{u}(\varphi(t),t)|\}\hat{u}(\varphi(t),t)\frac{\partial \hat{u}}{\partial \Psi}(\varphi(t),t). \tag{4.50}$$

Introduction of the similarity variables in (4.50) and using (4.45) in the result gives

$$q_0 = -\frac{a}{2f(a)}. \tag{4.51}$$

After rewriting (3.17) in terms of the similarity variables and substitution of (4.51), we obtain

$$z = \sqrt{t}\int_0^\eta \frac{1}{f(s)}\,ds + \int_0^t \frac{1}{2\sqrt{t}}\left\{-\frac{a}{f(a)} - \int_0^a \frac{\eta f'}{f^2}\,d\eta\right\}\,dt, \tag{4.52}$$

implying

$$\xi := \frac{z}{\sqrt{t}} = \int_a^\eta \frac{1}{f(s)}\,ds \;\text{ for }\; \eta > a,\; t \in \mathbf{R}^+. \tag{4.53}$$

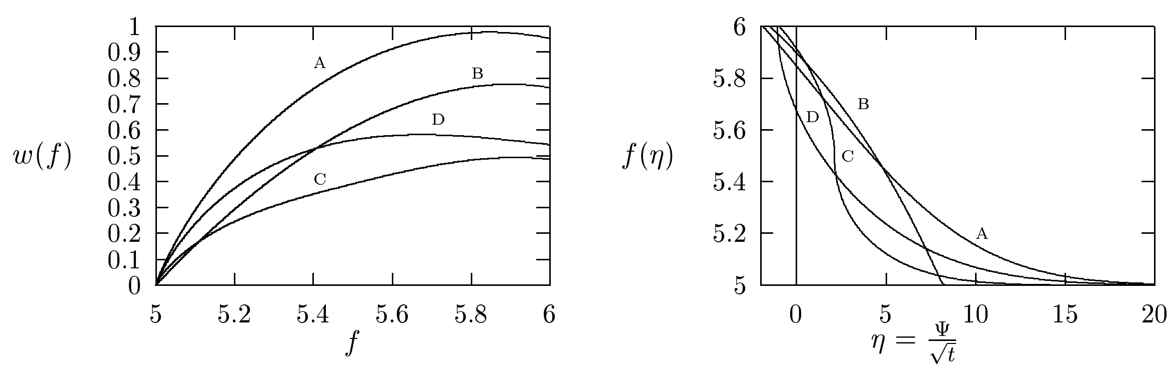

Figure 4. The solutions $w(f)$ and $f(\eta)$ for different λ and U values and $\varepsilon = 0.2$, see Table 1.

In a similar fashion, i.e. after combining (3.19), (4.10) and (4.51), we obtain

$$q_z = \frac{1}{2\sqrt{t}}\left\{-\frac{a}{f(a)} + \int_a^\eta \frac{sf'}{f^2}\,ds\right\} \;\text{ for }\; \eta > a,\; t \in \mathbf{R}^+. \tag{4.54}$$

Note that equation (4.53) implies that η $(= \Psi/\sqrt{t})$ only depends on ξ, which we write as $\eta = \phi(\xi)$. Consequently

$$u(z,t) = \hat{u}(\Psi(z,t),t) = f(\eta) = f(\phi(\xi)) := r(\xi), \tag{4.55}$$

and from (4.54)

$$q_z(z,t) = \frac{1}{2\sqrt{t}}\left\{-\frac{a}{f(a)} + \int_a^{\phi(\xi)} \frac{sf'}{f^2}\, ds\right\} := \frac{1}{\sqrt{t}} s(\xi). \tag{4.56}$$

The identities (4.55) and (4.56) show the relation between solutions obtained with the Von Mises transformation and solutions that result from direct similarity transformation of the one-dimensional balance equations. Properties of the functions $r(\xi)$ and $s(\xi)$ have been extensively studied in Van Duijn et.al. [11]. Parameter values for λ, U and computed values of a are given in Table 1. The labels A-D refer to the corresponding curves in Figures 4 and 5. Case A is computed with $D = \lambda = 1.0$, i.e. omiting the density dependent dispersivity term. The other three degenerate cases B-D are computed with $\lambda = 0$.

λ	U	a	Curve label
1.0	-	-1.866	A
0.0	5.0	-1.494	B
0.0	5.5	-0.952	C
0.0	6.0	-1.064	D

Table 1. Parameters and computed a-values.

Parameter	Value	Unit
κ	$1.0\ 10^{-12}$	m^2
μ	$1.0\ 10^{-3}$	kg/ms
ρ_s	1200	kg/m^3
ρ_f	1000	kg/m^3
ε	0.2	–
β	$\pi/4$	45^0
g	10.0	m/s^2
n	0.4	–
D_{mol}	$1.5\ 10^{-9}$	m^2/s
α_T	0.5	m

(4.57)

Table 2. Parameter values.

In most practical situations, λ is small compared to the magnitude of the other dimensionless parameters. Table 2 lists a set of feasible geohydrological parameters in the vicinity of a salt dome, mainly adopted from Herbert et.al. [14]. Using the numbers from Table 1 we obtain $\hat{q} = 1.414\ 10^{-6}$m/s ≈ 45 m/y and thereby $\lambda = 8.485\ 10^{-4} \approx 10^{-3} (<< 1!)$.

Figure 4 shows numerical approximations of the solutions $w(f)$ and $f(\eta)$ for the parameter values listed in Table 1. Figure 5 shows the corresponding similarity solution $r(z/\sqrt{t})$ and the scaled specific discharge, plotted as $s(z/\sqrt{t}) = q_z\sqrt{t}$. We omit the plots of $u(z,t)$ and $q(z,t)$ for these cases.

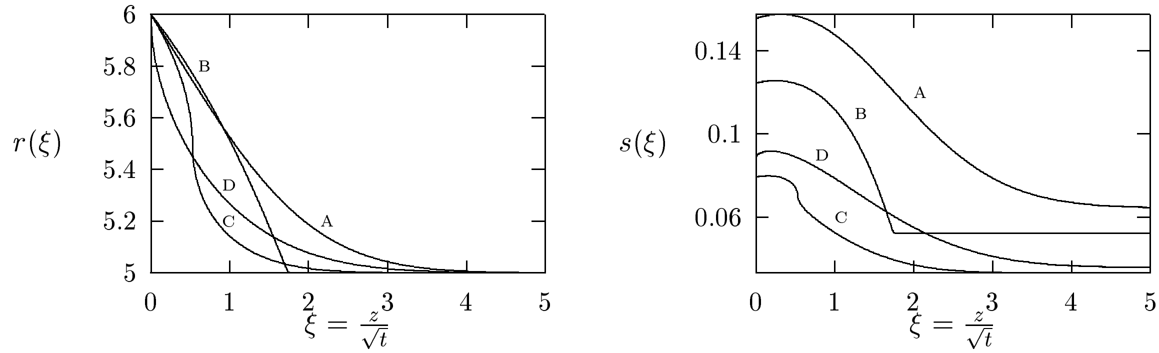

Figure 5. The similarity solutions $r(z/\sqrt{t})$ and $s(z/\sqrt{t})$ for different λ and U values and $\varepsilon = 0.2$, see Table 1.

In case of the non-degenerate example (A), both r and s are smooth, continuously differentiable functions. The degeneracy, i.e. $\lambda = 0$ and $u \to U$ in (4.35), causes singular behavior of the derivative r' (and thereby of u'). In case of the examples D and C, r' becomes infinite if $r(\xi) \to U$, where respectively $U = 6.0$ and $U = 5.5$. The corresponding scaled discharges s converge towards their limiting value as $\xi \to \infty$. The degenerate behavior of case B is different: at some point, say $\xi = \xi_0$, the function r attains the value of the (fresh water) boundary/initial condition $1/\varepsilon = 5.0 (= U)$ and remains constant for all $\xi > \xi_0$. Moreover, at $\xi = \xi_0$ r' exhibits a discontinuity, while $r' = 0$ for $\xi > \xi_0$. This point corresponds to an interface in the $(z,t)-$plane which moves with a finite speed of propagation. At the left hand side of the interface we have $u > 1/\varepsilon$, $u' < 0$, and on the right hand side $u = 1/\varepsilon$, $u' = 0$. The scaled discharge s (curve B) has a constant value for $\xi \geq \xi_0$. The discharges depicted in Figure 5 only result from the volume changes of the fluid due to the presense of (high) density gradients. Moreover, the induced flow is perpendicular to the main (or back ground) flow q_f.

4.3 Mixing of parallel fluid layers

Minor changes to the boundary and initial conditions in the salt dome problem lead to the problem of mixing of parallel flowing layers of fresh and salt water. De Josselin De Jong & Van Duijn [16] studied this problem for the incompressible case, i.e. $\mathrm{div}(\mathbf{q}) = 0$ and Van Duijn et.al. [11] extended the analyses to the compressible case, when volume changes in the fluid occur. We consider the same flow geometry as is the salt dome problem, but replace the salt rock below the plane $\{z = 0\}$ by porous medium initially saturated with brine with density $\rho = \rho_s$. Equations (4.23)-(4.37) hold and the boundary conditions are

$$u(-\infty, t) = 1 + \frac{1}{\varepsilon}, \ \ u(+\infty, t) = \frac{1}{\varepsilon} \ \text{ and } \ q_z(-\infty, t) = 0 \tag{4.58}$$

for $t \in \mathbf{R}^+$, while the initial conditions are given by

$$u(z,0) = \begin{cases} 1 + \frac{1}{\varepsilon} & \text{for} \quad z < 0 \\ \frac{1}{\varepsilon} & \text{for} \quad z > 0 \end{cases} \tag{4.59}$$

The choice of of the boundary condition $q_z(-\infty, t) = 0$ is arbitrary. When solving (2.11) subject to (4.58),(4.59) using Von Mises and similarity transformations we obtain (skipping all details)

$$\frac{z}{\sqrt{t}} = \int_0^\eta \frac{1}{f(\xi)} \, d\xi + \int_{-\infty}^0 \frac{\xi f'}{f^2} \, d\xi \tag{4.60}$$

and

$$q_z = \frac{1}{2\sqrt{t}} \int_{-\infty}^{\eta} \frac{\xi f'}{f^2}\, d\xi, \tag{4.61}$$

where f is the solution of the boundary value problem

$$\begin{cases} \frac{1}{2}\eta f' + f(\{\lambda + |U - f|\} f f')' = 0 \ \text{ for } \ \eta \in \mathbf{R} \\ f(-\infty) = 1 + \frac{1}{\varepsilon} \\ f(+\infty) = \frac{1}{\varepsilon} \end{cases} \tag{4.62}$$

Notice again the dependence of η on $z/\sqrt{t}$ in this example, which is due to the choice of the boundary condition $q_z(-\infty, t) = 0$. This implies that the problem also allows a transformation of type (5.1).

5 Discussion and conclusions

The Von Mises transformation provides a reduction of the governing balance equations to a single second-order nonlinear diffusion equation, which has been studied extensively in the mathematics literature. Much is known about the large time behavior of this equation for fairly general initial functions. In particular, sharp estimates were obtained for the rate at which the solutions converge to the self-similar profile, see e.g. Van Duijn & Peletier [10]. The examples given in Section 4 are special because they allow similarity transformation. The result is a second-order ordinary differential equation which makes the mathematical analysis more tractable.

When discussing the salt dome problem in Section 4, we observed that the similarity variable η $(= \Psi/\sqrt{t})$ only depends on ξ $(= z/\sqrt{t})$ (see (4.2)), which implies

$$\Psi(z,t) = \sqrt{t}\ \phi(\xi). \tag{5.1}$$

This is a well known transformation in the theory of boundary layers, usually derived through scaling arguments, see e.g. Chorin & Marsden [5]. Considering (3.1) and introducing (5.1) directly, we obtain

$$u = \frac{d\phi}{d\xi} := \phi' \ \text{ and } \ q_z = \frac{1}{2\sqrt{t}} \left(\frac{\xi\phi' - \phi}{\phi'} \right) \tag{5.2}$$

After substitution of (5.2) in (2.11) and using the boundary conditions, we obtain a third-order initial value problem:

$$\begin{cases} \frac{1}{2}\frac{\phi''\phi}{\phi'} + (\{\lambda + |U - \phi'|\}\phi'')' = 0 \ \text{ for } \ \xi > 0 \\ \phi(0) = \alpha \\ \phi'(0) = 1 + \frac{1}{\varepsilon} \\ \phi''(0) = \dfrac{1}{2(1+\varepsilon)K(\varepsilon)\{\lambda + |U - \phi'(0)|\}}\ \alpha \end{cases} \tag{5.3}$$

which reads: find α such that the boundary condition $\phi'(+\infty) = 1/\varepsilon$ is satisfied.

A similar transformation is possible in the column problem. From expression (4.18) we deduce that the similarity variable only depends on $(z-t)/\sqrt{t}$, implying

$$\Psi(z,t) = \sqrt{t}\,\theta(\zeta) \text{ with } \zeta = \left(\frac{z-t}{\sqrt{t}}\right). \tag{5.4}$$

The function θ satisfies the third order equation

$$2\theta'''\theta' + \theta\theta'' = 0. \tag{5.5}$$

However, the combination of Von Mises and similarity transformations as proposed in Sections 3 and 4 leads to a second-order ordinary differential equation, which is preferable to the third-order equation that results from the direct transformation (5.1).

Van Duijn et. al. [11] studied the one-dimensional balance equations by looking for self-similar solutions of the form

$$\rho(z,t) = u(\eta) \text{ and } q_z(z,t) = \frac{1}{\sqrt{t}}v(\eta), \tag{5.6}$$

where $\eta = z/\sqrt{t}$. This transformation also yields a third-order ordinary differential equation. The latter can be reduced to a second-order equation of the form

$$-pp'' = \frac{1}{2}e^{2cx}, \quad p > 0, \tag{5.7}$$

where $c = \log(1+\varepsilon)$. Note that, if we divide equation (4.11) by f, introduce $x = \log(f)$ and define a flux function according to $p(x) := -e^{2x}dx/d\eta(\sigma(x))$, where $\sigma(x) = x^{-1}$, we obtain an equation which is identical to (5.7), but now with $c = 1$.

Due to the piecewise constant initial density functions, the examples discussed in Section 4 may be regarded as upper limits of the compressibility effect for a given value of ε. The induced specific discharge q_z is infinite at $t = 0$ and decays as $1/\sqrt{t}$ for $t > 0$ (see expressions (4.17), (4.54) and (4.61)). However, in most practical situations, the initial density data will be smooth, which implies that the enhanced discharge remains finite for all $t \geq 0$. Hence, in practice, the difference between Boussinesq solutions ($\text{div}(\mathbf{q}) = 0$) and solutions of the balance equations for fluid and salt will be even smaller than predicted by the corresponding similarity solutions. The compressibility effect is noticeable only at the short time scale of the problems studied in Section 4 and has little impact on the density distributions. The fact that flow is induced in a direction perpendicular to the main groundwater flow direction might be of some practical importance, in particular in connection with transport of radionuclides, leaking from a salt dome repository.

The problem of brine transport is of utmost interest in the safety and risk assessment studies of high-level radioactive waste disposal in subsurface salt formations. With this practical application in mind, many (dedicated) numerical codes have been developed, see e.g. Pinder & Cooper [24], Voss & Souza [30], Kröhn & Zielke [18], Oldenburg & Pruess [22] and Kolditz et.al. [17]. The intricate character of the problem, i.e. nonlinear coupling between the velocity field and the fluid density distribution due to both gravity (free convection) and compressibility effects, implies that the availability of exact or semi-exact solutions of test problems is rather poor. In fact, only Henry's [13] semi-explicit solution of dispersive salt water intrusion in a confined aquifer, initially filled with fresh water, is frequently used as two-dimensional test problem for code verification. In order to test numerical simulators, a particular series of benchmark problems has been proposed by the international HYDROCOIN [15] project. These benchmarks are used for cross-verification of numerical models. Whereas the compressibility effect concerned, our semi-explicit results provide both accurate quantitative and qualitative information about solutions and therefor may contribute to numerical code verification.

Acknowledgement
We acknowledge S.M. Hassanizadeh and T. Leijnse for bringing the subject of brine transport to our attention.

References

[1] Atkinson, F.V. & Peletier, L.A., Similarity solutions of the nonlinear diffusion equation, Archs. Ration. Mech. Analysis **54** (1974), p.p. 373-392.

[2] Barenblatt, G.I., Scaling, self-similarity and intermediate asymptotics, Cambridge Univ. Press (1996).

[3] Bear, J., Dynamics of fluids in porous media, Elsevier, New York, 1972

[4] Bouillet, J.E. & S.M. Gomes, An equation with a singular nonlinearity related to diffusion problems in one dimension, Quart. Appl. Math. (1985), 395-402

[5] Chorin, A.J. & J.E. Marsden, A mathematical introduction to fluid mechanics, Springer-Verlag New York Inc, 3rd edition, 1992

[6] Crank,J, Free and moving boundary problems, Oxford University Press New York (1987)

[7] Crocco,L, Atti di Giudonia, **7** (1939)

[8] Crocco, L, Monografie Scientifiche di Aeronautica, **3** (1946)

[9] Curle, N., The laminar boundary layer equations, Oxford University Press, 1962

[10] Van Duijn, C.J. & Peletier, L.A., Asymptotic behaviour of solutions of nonlinear diffusion equations, Arch. Rational Mech. Anal. **65** (1977), p.p. 363-377

[11] Van Duijn, C.J, L.A. Peletier & R.J. Schotting, On the analysis of brine transport in porous media, Europ. Journ. of Appl. Math. Vol **4** (1993), 271-302

[12] Hassanizadeh, S.M. & T. Leijnse, On the modelling of brine transport in porous media, Water Res. Research **24** (1988), 321-330

[13] Henry, H.R., Interfaces between salt water and fresh water in coastal aquifers, US Geol. Surv. Water-Supply Paper 1613-C, Sea water in coastal aquifers (1964), p.p. 35-70

[14] Herbert, A.W., C.P. Jackson & D.A. Lever, Coupled groundwater flow and solute transport with fluid density strongly dependent upon concentration, Water Res. Research **24** (1988), 1781-1795

[15] HYDROCOIN, Swedish Nuclear Inspectorate, An international project for studying groundwater hydrology modeling strategies, Level 1 Final Report: Verification of groundwater flow ,odels, Case 5. Swedish Nucl. Insp., Stockholm (1986)

[16] Josselin de Jong, G. de & C.J. Van Duijn, Transverse dispersion from an originally sharp fresh-salt interface caused by shear flow, J. Hydrology **84** (1986), 55-79

[17] Kolditz, O., Ratke, R., Diersch, H.G. and Zielke, W., Coupled groundwater flow and transport: 1. Verification of variable density flow and transport models, Adv. Water Resour. **21**(1) (1998), p.p. 27-46

[18] Kröhn, K.P., & Zielke, W, FE-Simulation von Transportvorgängen im klüftigen Gestein., Deutsche Gewässerkundliche Mitteilungen **35**(3-4) (1991), p.p. 82-88

[19] Landau, H.G., Heat conduction in a melting solid, Q. Appl. Math. **7** (1950), 81-94

[20] Meirmanov, A.M., The stefan problem, De Gruyter expositions in mathematics, Berlin-New York (1992).

[21] Mises, R. Von & K.O. Friedrichs, Fluid dynamics, Applied mathematics series 5, Springer, New York (1977), 171

[22] Oldenburg, C.M. & Pruess, K., Dispersive transport dynamics in a strongly coupled groundwater-brine flow system, Wat. Resour. Res. **31**(2) (1995), p.p. 289-302

[23] Peletier, L.A. & C.J. van Duijn, A class of similarity solutions of the nonlinear diffusion equation, Nonl. Analysis, Theory, Methods and Applications, Vol. 1 **3**, 223-233

[24] Pinder, G.F. & Cooper, H.H., A numerical technique for c alculating the transient position of the salt water front, Water Resour. Res. bf 6 (1970), p.p. 875-882

[25] Raats, P.A.C., Convective transport of ideal tracers in unsaturated soils, in: Arnold, E.M., G.W. Gee and R.W. Nelson (eds.), Proceedings of the symposium on unsaturated flow and transport modelling, Seattle, Washington, (1982), 249-265

[26] Raats, P.A.C., Tracing parcels of water and solutes in unsaturated zones, in: Yaron, B, G. Dagan and J. Goldschmid (eds.), Pollutants in porous media: The unsaturated zone between soil surface and groundwater, Berlin, Springer (1984), 4-16

[27] Raats, P.A.C., Applications of the theory of mixtures in soil science, Math. Modelling **9** (1987), 849-856

[28] Roxburgh, I.S., Geology of high-level radioactive waste disposal, An Introduction,Chapman and Hall London New York (1987).

[29] Valk, C.F. de & P.A.C. Raats, Lumped models of convective solute transport in heterogeneous porous media: One-dimensional media, Water Res. Res, Vol. **31** (1995), 883-892

[30] Voss, C.I. & Souza, W.R., Variable density flow and solute transport simulation of regional aquifers containing a narrow freshwater-saltwater transition zone. Water Resour. Res. **23**(10) (1987), p.p. 1851-1866