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Simulation of Density Dependent Transport in Groundwater

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Abstract

A mathematical model of water flow and transport of chemical substances is presented in the paper. This model takes into account the influence of variable density and viscosity of water caused by variable solute concentration in soil. A solution of the problem of water flow and solute transport was sought using numerical methods. A finite elements method for solution of water flow equation and Monte-Carlo method to simulate solute transport were applied.

Advantages of the presented model are illustrated on the example of water flow and salt transport in two dimensional ground profile in the region of Puck Bay. The geology of this profile is taken from Jankowska et al (1994). Obtained results from the proposed model are qualitatively conformable with observations in situ.

Key words: groundwater flow, saturated and unsaturated soil, intrusion, hydrodynamic dispersion, density driven flow

1. Introduction

During simulation of ground water transport processes, in most cases one assumes that variations of water density are very small and their variations have no significant influence on ground water flow. Such an assumption is true first of all when concentrations of substance dissolved in ground water is vestigial. However, there exist such cases of ground water flow where differences of water density are of basic meaning in explaining transport mechanism. One such problem is the problem of salty sea water intrusion in fresh ground-water.

In the coastal zone of oceans and seas upper ground layers are influenced by water with variable physical properties, such as density and viscosity. Together with growth of salinity, ground water becomes heavier and stickier as compared with fresh water. These properties cause such phenomena as convection, dispersion and density driven flow to occur in ground water hydrology in the zone of influence of seas. In the paper a numerical model is presented, which enables taking into account of these phenomena in both saturated and unsaturated soils.

The presented model can be useful wherever flat and sandy beaches occur and also where sea-water frequently overflows the beaches. On the one hand, it should be useful when explaining the occurrence of fresh water in deeper ground layers in the region of Gdańsk Bay, and from the other the influence of this water on reduction of sea-water salinity in bottom layers of some regions of the bay mentioned.

The problem of water flow with variable density is described by two second order differential partial equations: the first describes water flow, whereas the second describes hydrodynamic dispersion. Change of salt concentration alters density and viscosity of water which in the result changes hydraulic conductivity of soil and soil water potential. Such a process can exist in both saturated and unsaturated zones of soil, for variable boundary conditions in time and in the space under consideration. Two numerical methods were applied for solutions of the presented problem: the finite element method for water flow and Monte-Carlo method for salt transport.

2. Theoretical Description of the Transport Phenomenon

2.1. Influence of Salinity on Density and Viscosity of Water

Changes in density and viscosity of ground water cause water characterized by greater salinity to fall towards the bottom of the ground profile and fresh water with smaller density to rise towards the surface, while changes of ground water viscosity influence the hydraulic conductivity. Dependence of density and viscosity of water on concentration for sodium chloride is disccused, for example, by (Huyakorn et al 1987, Hassanizadeh et al 1990, Thiele 1993). Concentration of salt in sea-water is considerably lower than the saturated concentration. Therefore, in case of sea-salty water intrusion to fresh ground water, one can assume linear dependences of density ρ and viscosity μ on concentration c in the following linear form:

for density ρ

$$\rho = \rho_o \left(1 + \eta_\rho \frac{c^*}{c_s}\right), \tag{1}$$

and for kinematic viscosity μ

$$\mu = \mu_o \left(1 + \eta_\mu \frac{c^*}{c_s}\right), \tag{2}$$

where:

$$\eta_\rho = \frac{\rho\,(c_s) - \rho_o}{\rho_o}, \tag{3}$$

$$\eta_\mu = \frac{\mu\,(c_s) - \mu_o}{\mu_o}, \tag{4}$$

where:

ρ_0, μ_0 – density and kinematic viscosity of the fresh water for reference pressure $p = p_o$;

c_s – maximum concentration for the considered problem.

Expressions (1–3) were used, for example, by Huyakorn et al. (1987) for modelling density driven flow in saturated ground layers.

2.2. Water Flow

Water flow with variable density can be described using Einstein's summation convention by an equation in the following form (for example Zaradny and Maciejewski 1994a):

$$\frac{\partial}{\partial x_i}\left[k^r K_{ij}\left(\frac{\partial H}{\partial x_j} + \eta_\rho c e_j\right)\right] = \frac{\rho}{\rho_o}[C(\psi) + S_w S_s]\frac{\partial H}{\partial t} + \theta\frac{\rho}{\rho_o}\eta_\rho\frac{\partial c}{\partial t} - \frac{\rho}{\rho_o}S, \quad (5)$$

where:

$H = \psi + z$ – comparative hydraulic head related to fresh water, for which $\rho = \rho_o$,

$C(\psi) = \frac{d\theta}{d\psi}$ – so called differential water capacity of soil, $C(\psi) \neq 0$ for $\theta < \theta_s$ and $C(\psi) = 0$ for $\theta = \theta_s$,

ψ – hydraulic head of soil water ($\psi = p/(\rho_o g)$), $\psi < 0$ for $\theta < \theta_s$,

α – compressibility coefficient of ground,

c_m – maximum salt concentration – in ground water for the considered problem (concentration of salt in sea water), for which $c = c_s = 1$,

c – relative concentration of salt in ground water $c \leq c_s = 1$.

p – water pressure,

ρ – water density,

g – acceleration due to gravity,

e_j – j-th component of unit vector (for $j = 3$, $e_j = \pm 1$ and $e_j = 0$ for $j \neq 3$),

S – source or sink (volumetric),

x_i – i-th coordinate ($i = 1, 2, 3$),

$z = x_3$ – elevation of water above a reference level,

t – time,

$K_{ij} = \frac{\rho g k_{ij}}{\mu}$ – component of saturated soil conductivity tensor for water with density ρ and viscosity μ,

k_{ij} – component of soil intrinsic permeability tensor,

k^r – relative hydraulic conductivity dependent on degree of water saturation,

$S_w = \theta/\theta_s$ – where θ water content and θ_s – saturated water content,

S_s – specific retention capacity of saturated soil.

Solution of water flow equation (5) with appropriate initial and boundary conditions allow estimating distribution of hydraulic head H in soil profile. Using this solution H and hydraulic characteristics of soils, one can obtain distributions of water content and hydraulic conductivity in flow area. Component q_i of water flux vector in soil profile are calculated from Darcy's law expressed by equation (6):

$$q_i = -k^r K_{ij} \left(\frac{\partial H}{\partial x_j} + \eta_\rho c e_j \right). \tag{6}$$

This expression serves to estimate water flow velocity this being necessary for simulation of hydrodynamic dispersion.

2.3. Hydrodynamic Dispersion Equation

The equation of water movement with variable density introduced in the previous paragraph does not completely describe the behavior of fluid in the ground as this equation does not take into account phenomena of mixing of water with different solute concentration. Mixing of liquid with different concentrations is caused by molecular diffusion and mechanical dispersion. Mechanical dispersion is the phenomena of fluid mixing caused by unhomogeneities of velocity field resulting from complexity of ground pore geometry. The hydrodynamic dispersion equation with source term one can describe in the following form (for example Maciejewski 1993):

$$\frac{\partial}{\partial x_i} \left(D_{ij} \theta \frac{\partial c}{\partial x_j} \right) - \frac{\partial (c q_i)}{\partial x_i} = \frac{\partial (c\theta)}{\partial t} + S \left(c - c^{**} \right), \tag{7}$$

where:

D_{ij} – component of dispersion tensor **D**,

q_i – component of Darcy velocity vector **q**,

c^{**} – relative concentration at source or uptake.

System of two partial differential equations (5) and (7), together with initial and boundary conditions, describe density driven ground flow water in saturated and unsaturated soils. The presented theoretical description of flow was applied to simulation of the intrusion of sea-water to ground water.

3. Solution of Two-Phase Fluid Transport Problem

The solution to practical problems occurring in situ described by equations (5) and (7) can be obtained using only numerical methods. Analytical solutions for such problems do not exist. To solve the water flow equation, the finite element method based on the Galerkin assumption (for example Zaradny 1993) was used, while the Monte-Carlo method was applied to solve the hydrodynamic dispersion equation.

The essence of the Monte-Carlo method relies on indirect estimation of concentration distribution using numerical simulation of movement of virtual particles. These particles imitate dissolved substance. Theoretical principles of the Monte-Carlo method based on the theory of stochastic processes are given, for example, by Papoulis (1972). Change of particle position during time Δt is calculated using simple expression (for example Maciejewski, Zaradny 1992):

$$\Delta x_i = m_i \Delta t + \sigma_{ik} V_k \sqrt{\Delta t}, \tag{8}$$

where

V_k – random variable with normal distribution $N(0, 1)$,
Δt – time step

and components of matrix $\boldsymbol{\sigma}$ are calculated using equation

$$2D_{ij} = \sigma_{ik}\sigma_{jk}, \tag{9}$$

while one can evaluate components of vector $\mathbf{m}$ using equation:

$$m_i = \frac{q_i}{\theta} + \frac{\partial D_{ij}}{\partial x_j} + \frac{D_{ij}}{\theta}\frac{\partial \theta}{\partial x_j}. \tag{10}$$

Matrix $\boldsymbol{\sigma}$ is symmetrical because dispersion tensor $\mathbf{D}$ is symmetrical. For two dimensional flow expression (9) describes a set of three nonlinear algebraic equations where unknown values are σ_{11}, σ_{12} and σ_{22}. For each time step values of components m_i and σ_{ij} were calculated using equations (9) and (10) and numerical procedure for solving the set of equations (9).

The mass of dissolved substance is divided into n particles ($n = 100000, 500000$, ...), then the position of these particles for time $t + \Delta t$ is calculated from the position at time t using equation (8). The number of particles in each sub-domain of flow domain is proportional to the mass of substance in the sub-domain. Knowing density and water content one can calculate relative concentration $c(\mathbf{x},t)$. Exactitude of obtained solution depends on the estimation of ground water velocity field exactness, on the number of particles assumed in calculations, and also on assumed time step. When the number of particles assumed in calculations will tend to infinity and simultaneously time step will tend to zero then a solution strives to exact solution.

As the initial condition a known concentration of salt is assumed, due this condition virtual particles are properly distributed in the flow area (x, y, z) for time $t = 0$. Boundary conditions are assumed as a reflecting or absorbing screen. The reflecting screen describes impermeable boundaries, while the absorbing screen describes the permeable boundaries of the flow domain. The second type of these boundary conditions is used to describe ground water contact with a reservoir of water with given solute concentration.

The advantage of the Monte-Carlo method, as compared with the finite differences or finite element method, is smaller sensibility of solution of hydrodynamic dispersion equation to estimation errors of flow velocities. The next important advantage is elimination of numerical dispersion. The drawback of the presented method is the extension of calculation time caused by the greater numbers of particles. These are indispensable to obtain acceptable accuracy of calculation. Another essential matter is the number of boundary sections of the examined area. For each particle, in every time step, one should examine whether a particle does not cross the borders of the area, therefore, an increase in the number of border sections causes an increase in calculation time. In each time step, first the water flow equation is solved. This is necessary to know water velocity and water content fields. Then the hydrodynamic dispersion equation is solved using the above obtained results. The calculated concentration is used to estimate current hydraulic parameters of soil and the calculated process is repeated.

The presented mathematical model enables transport simulation of water and solute for a real system of ground layers, which may have different hydraulic properties. This model simultaneously takes into account both saturated and unsaturated zones. Boundary conditions for the problems considered can vary as regards values or type (Dirichlet, Neumann or mixed).

Accuracy of the presented method was widely tested by authors (Zaradny and Maciejewski 1994a, b).

4. Ground Water Flow in the Coastal Zone

The presented model was used to simulate ground water flow in a coastal zone. The vertical soil profile in the region of Puck Bay was selected for analyses. The supply of seawater by fresh ground water has been observed in the deeper part of this bay and was discussed by Jankowska et al (1994). The position of the analysed cross section (II–II') is presented in Fig. 1, while a hydrogeological profile of the selected section is presented in Fig. 2. Both these figures are taken from Jankowska et al (1994).

A five layeral ground system was assumed, basing on accessible geological structure materials. Distribution of soils and scheme of the flow area are shown in

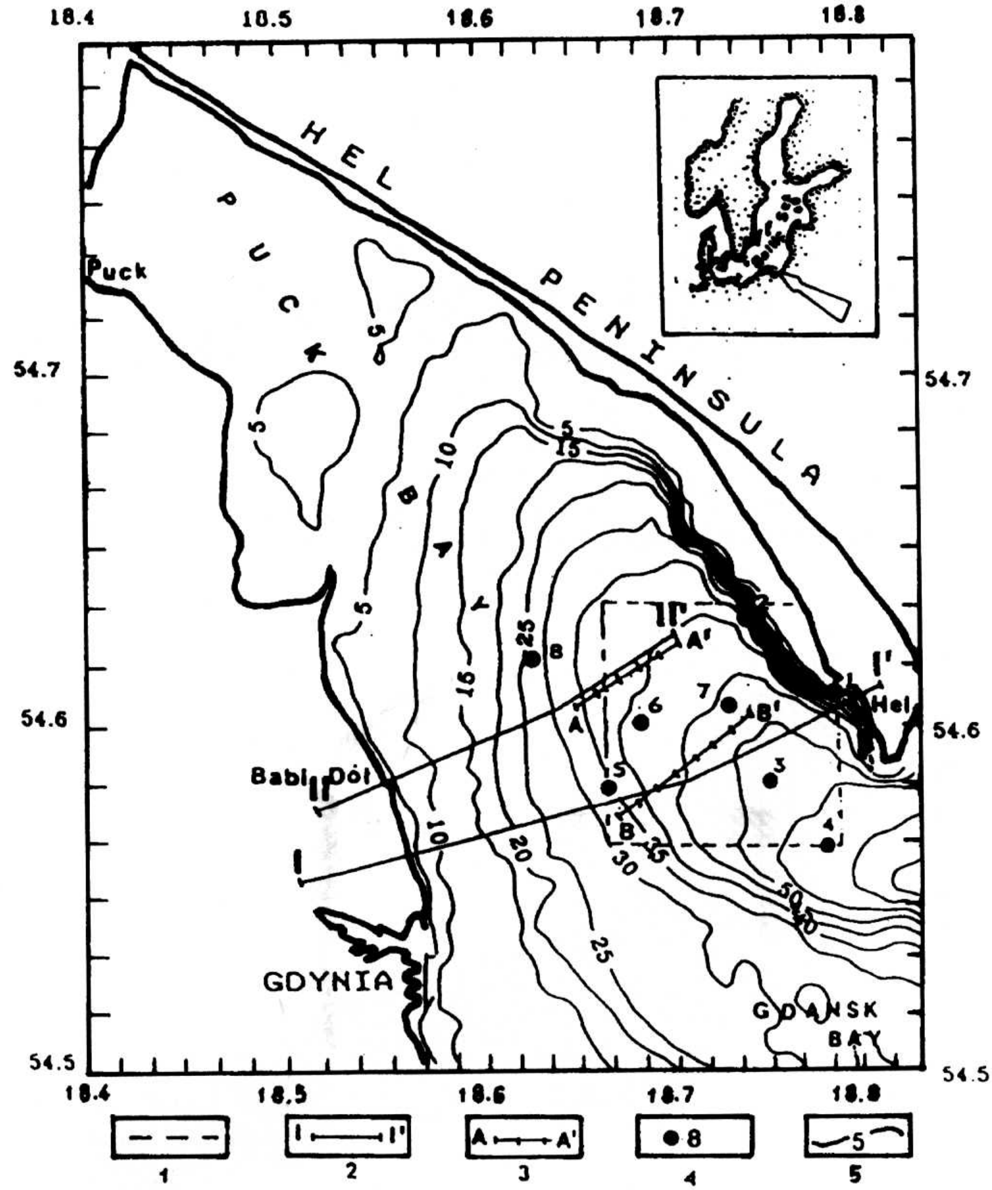

Fig. 1. Position of analysed cross section in the region of Puck Bay (Jankowska et al 1994)

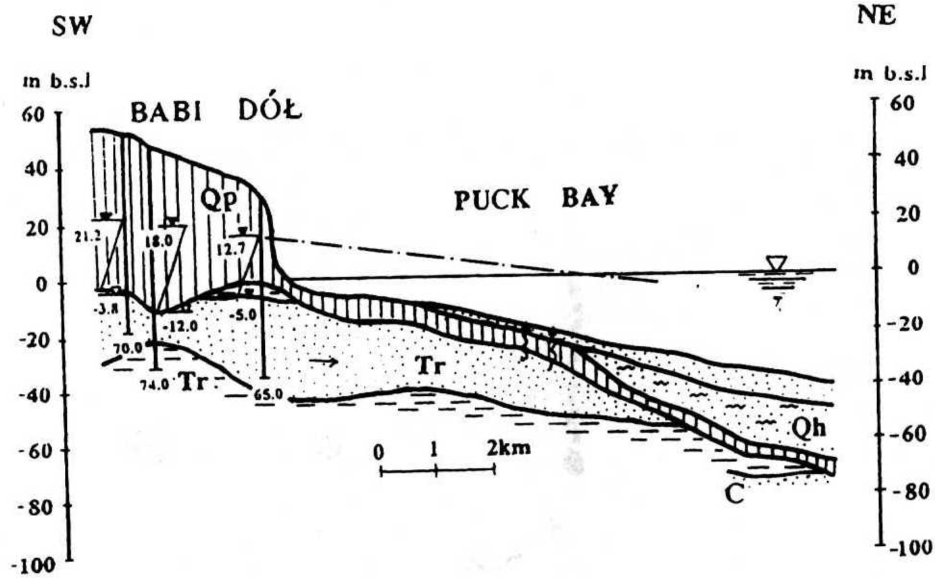

Fig. 2. Hydrogeogical profile of Babi Dół (Jankowska et al 1994)

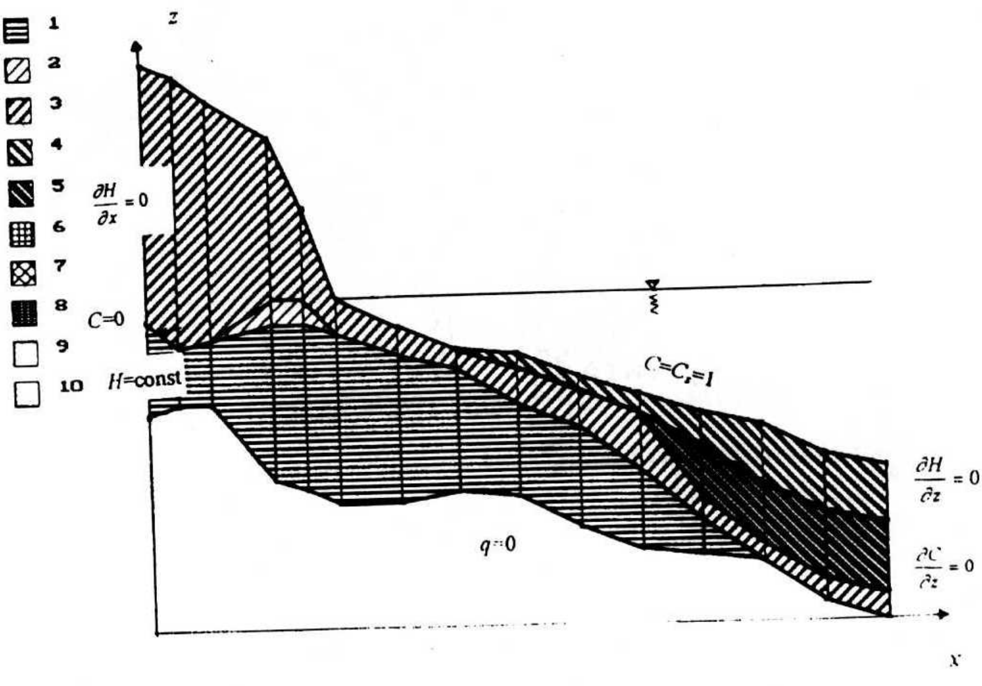

Fig. 3. Schematic diagram of the analyzed ground profile with distribution of soil layers

Fig. 3. The numerical model presented takes into account the complex geological structure which enables simulation of the properties of the medium. Characterization of the soil hydraulic property in the whole range of water content variability is necessary, as the presented model simulates transport for both saturated and unsaturated zones. The position of the unsaturated zone is shown in Fig. 4. This zone generally occurs above sea level, the saturated zone being below sea level. In Fig. 4 the saturated zone is presented as fresh water.

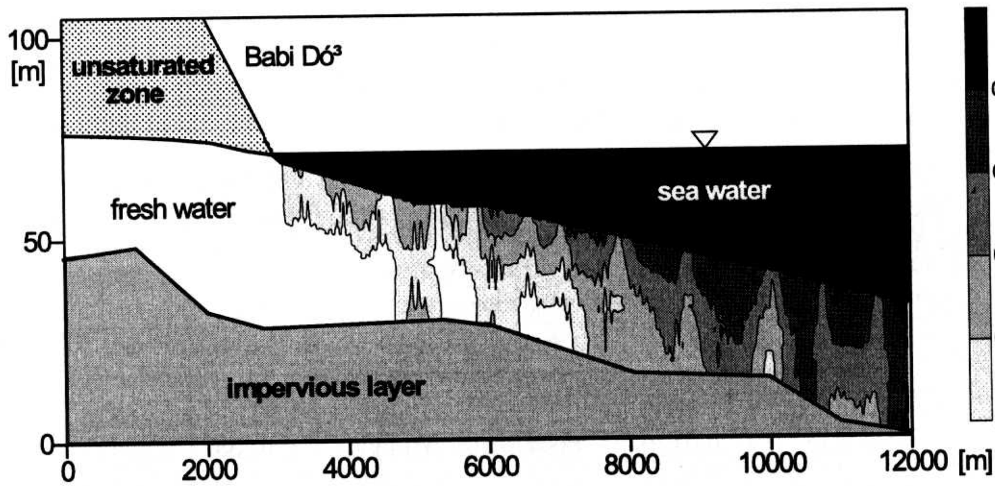

Fig. 4. Calculated relative distribution of salt concentration in ground

It was assumed that hydraulic properties of soils are described by the Mualem and van Genuchten models. The Mualem model describes the relationship between water content and pressure suction in soil, while the van Genuchten model describes the dependence of hydraulic conductivity on pressure suction. In general, these models afford good conformity of experimental results with measuring results and are very often used to describe hydraulic properties of soils in unsaturated zone.

According to Mualem, one can write the relationship between water content θ and suction head h in the following form (Mualem 1976):

$$\theta(h) = \theta_r + (\theta_r - \theta_s)\left[\frac{1}{1+(\alpha h)^n}\right]^{\beta}, \tag{11}$$

where:

θ_r – residual water content,

θ_s – saturated water content,

α, n – coefficients experimentally evaluated depending on the soil type,

$$\beta = 1 - \frac{1}{n}. \tag{12}$$

Dependence of hydraulic conductivity on suction head according to van Genuchten has the following form (van Genuchten 1979):

$$k(h) = k_s \left[\frac{1}{1 + (\alpha h)^n} \right]^{\beta/2} \left\{ 1 - \left[\frac{(\alpha h)^n}{1 + (\alpha h)^n} \right]^{\beta} \right\}^2, \tag{13}$$

where:

k_s – saturated hydraulic conductivity of soil,

α, n – coefficients described above.

Assumed values of parameters of the Mualem and van Genuchten models, calculated for each soil using the PAGLEB programme worked out by Zaradny (2003) are presented in Table 1.

Table 1. Soil parameters

soil	k_s	θ_s	θ_r	n	α
	[cm/d]	[cm^3/cm^3]	[cm^3/cm^3]	–	–
1. coarse sand	11.2000	0.395	0.00817	1.87264	0.16826
2. silty clay	0.0130	0.507	0.00000	1.19589	0.00335
3. heavy clay	0.0022	0.540	0.00000	1.17006	0.00226
4. fine sand	0.5000	0.364	0.02148	1.51958	0.02621
5. loamy sand	0.2650	0.439	0.02912	1.47659	0.06131

The parameters n, α (Table 1) were calculated for the hydraulic characteristics of soils according to Rijtema (1969).

Assumed boundary conditions for equations describing water flow and hydrodynamic dispersion are presented in Fig. 3.

Boundary conditions for equation describing water flow were assumed as:

- horizontal water flux equal to zero in the upper left part of the border, and constant value of comparative hydraulic head H in bottom border,
- vertical water flux is equal to zero on the right-hand part of border,
- infiltration is equal to zero on the upper part of the border which is placed above sea level, and constant water pressure corresponding to height of column of salty water on the upper part of the border which is placed below sea level,
- impermeable edge on bottom border of flow area.

For the hydrodynamic dispersion equation, the following boundary conditions were assumed:

- flux of salt equals to zero on the left and bottom part of the border (reflecting screen),
- absorbing screen on the right-hand side of the border,
- flux of salt equal to zero in upper part of the border which is placed above sea level, and constant relative salt concentration $c = 1$ (sea water concentration) on the upper part of the border which is placed below sea level.

Salt concentration in ground water equal to zero was assumed as an initial condition for the hydrodynamic dispersion equation. In the calculations longitudinal dispersivity equal to $\alpha_L = 1$ m, and transversal dispersivity equal to $\alpha_T = 0.5$ m were taken. Calculations were realised until the distribution of salt concentration in flow area did not change. This condition was assumed as a condition of equilibrium in the area of motion. Such solution may be assumed as the stationary for the investigated problem.

In Fig. 4. calculated relative distribution of salt concentration in ground water is presented. Fresh water is absorbed deeply into the salty-waters of Puck Bay. Calculations showed that differences of density between fresh and salt water resulted in the creation of zones of advection density driven flow. Obtained results are consistent with the qualitative view of phenomena observed in situ.

5. Summary

The presented model of density driven flow can serve to simulate transport processes in saturated and unsaturated porous media. Verification of this model was carried out previously by analysing Henry's problem described in the literature on the subject (Henry 1959, 1964).

Estimated distribution of salt concentrtation in ground water below the bed of Puck Bay are qualitatively conformable with observations. Therefore calculation for Puck Bay presented in the paper confirms the usefulness of the simulation model of the phenomenon of intrusion of salt water in sea coast zones and in flowing fresh water in the bottom layers of the bay mentioned.

One can use the model discussed for many other practical problems related, for example, to contaminant or fertilizer transport in saturated and unsaturated soils for cases in which the density convection effect plays an essential role in the mechanism of transport.

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