West Pomeranian University of Technology, Szczecin
Department of Sanitary Engineering
Civil Building and Architecture Faculty

Andrzej Aniszewski

Analysis of the most important processes impact on the concentration reduction values for the chosen contaminants moving in groundwater (based on computational solutions)

The basic simplified assumptions

- **Leaving out of advection terms ($u_y\ \partial C/\partial y = u_z\ \partial C/\partial z = 0$) for one – dimensional flow of groundwater in *x* direction ($u_y = u_z = 0$)**

- **Leaving out of transverse dispersion term ($D_z\ \partial^2 C / \partial z^2 = 0$) in z direction for slotted contaminant outflow and initial concentration equalization in this direction**

- **Leaving out of molecular diffusion process due to low values of molecular diffusion coefficients (D_M) in relation to values of dispersion rates (D_x and D_y)**

- **Leaving out of turbulent diffusion process (D_B) for laminar groundwa ter flow in sandy ground medium (low graining)**

The most simplified well-known 2D advection-dispersion equation without adsorption process:

$$\frac{\partial C}{\partial t} + u_x \frac{\partial C}{\partial x} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} \quad (1)$$

C **– the solute concentration in flowing groundwater in aqueous phase (in the local equilibrium conditions),**

u_x **– the component of the average (real) seepage velocity in pore space along the x axis (as pore velocity),**

D_x **– the component of the longitudinal dispersion coefficient along the x axis,**

D_y **– the component of the transverse dispersion coefficient along the y axis,**

t **– the co-ordinate of time,**

x*, *y **– the co-ordinates of the assumed reference system.**

The well-known 2D advection-dispersion equation with adsorption process:

$$\frac{\partial C}{\partial t}\left(1+\frac{\rho}{m}\frac{\partial S}{\partial C}\right)+u_x\frac{\partial C}{\partial x}=D_x\frac{\partial^2 C}{\partial x^2}+D_y\frac{\partial^2 C}{\partial y^2} \qquad (2)$$

S – the mass of the solute species adsorbed on the grounds per unit bulk dry mass of the porous medium (in the local equilibrium conditions),

ρ – the bulk density of the porous medium ,

m – the effective porosity of the porous medium,

$[1+(\rho/m)(\partial S/\partial C)]$ – the constant in time retardation factor (R) resulting from sorption process.

The general equation describing retardation factor for adsorption process (as the Freundlich non-linear isotherm) takes the form:

$$R = 1 + \frac{\rho}{m} \cdot \frac{\partial S}{\partial C} = 1 + \frac{\rho}{m} \cdot N \cdot K \cdot C^{(N-1)} \qquad (3)$$

K*, *N **– the parameters of the Freundlich non-linear isotherm accepted for mathematical description of adsorption process for all the chosen in this paper indicators.**

The well-known 2D advection-dispersion equation with biodegradation – biological denitrification and adsorption processes:

$$\frac{\partial C}{\partial t}\left(1+\frac{\rho}{m}\frac{\partial S}{\partial C}\right)+u_x\frac{\partial C}{\partial x}=D_x\frac{\partial^2 C}{\partial x^2}+D_y\frac{\partial^2 C}{\partial y^2}-k_1\left(C-\frac{\rho\, S}{m}\right) \qquad (4)$$

k_1 – the first-order reaction rate for the kinetically-controlled biodegradation – biological denitrification process (in this analysis the same k_1 parameter was assumed for both the dissolved-aqueous and the sorbed-solid phase.

The well-known 2D advection-dispersion equation with radioactive decay and adsorption processes:

$$\frac{\partial C}{\partial t} + u_x \frac{\partial C}{\partial x} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} - \frac{\rho}{m} \frac{\partial S}{\partial t} - \lambda \left(C - \frac{\rho S}{m}\right) \qquad (5)$$

λ – the first-order decay rate usually expressed as a half-life ($t_{1/2}$) (for radioactive decay we can assume that the reaction generally occur at the same rate for both the dissolved-aqueous and the sorbed-solid phase.

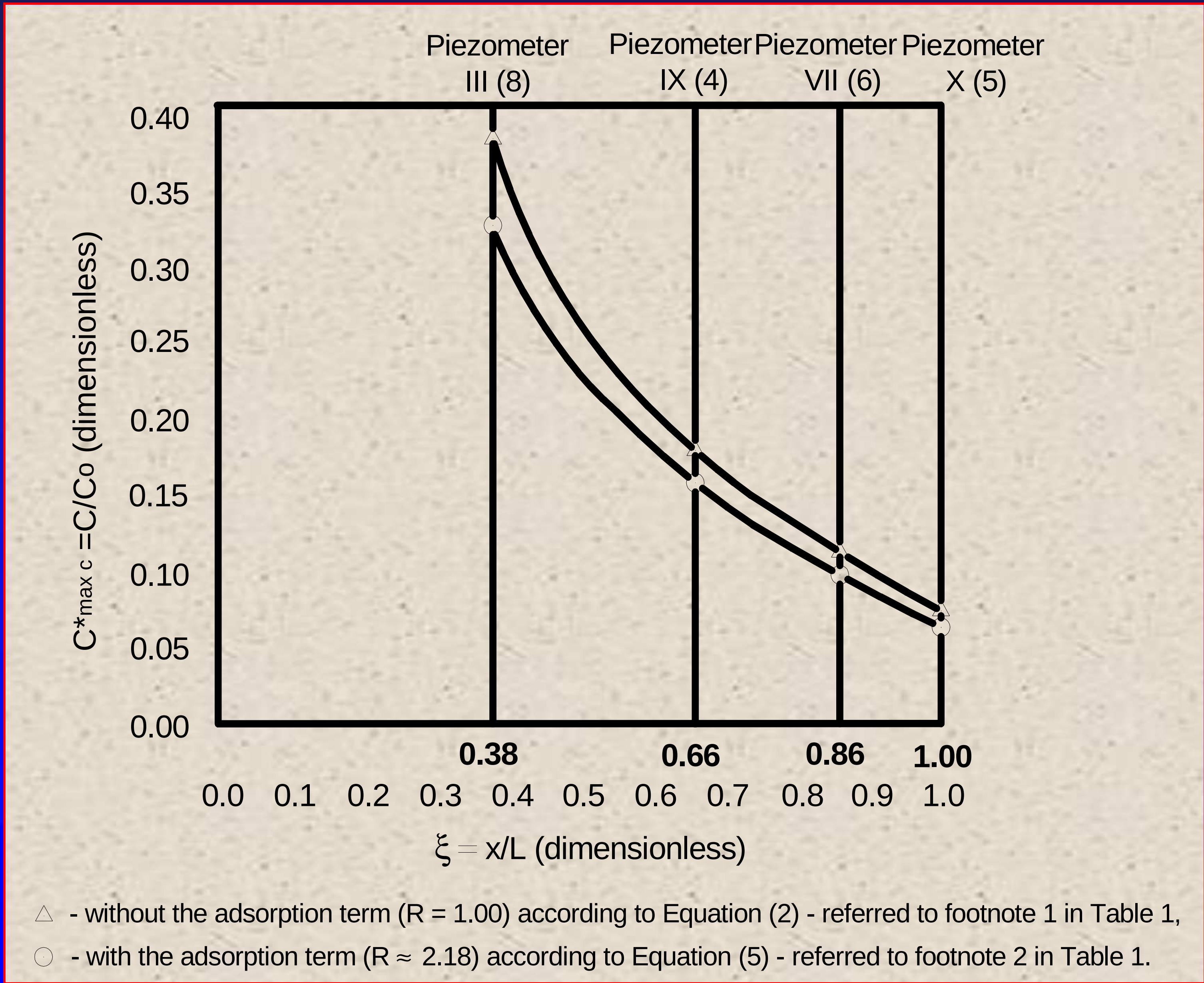
Maximal dimensionless values of the chosen contaminant concentrations (C^*_{maxc}) calculated in relation to appropriate equations:

Chosen contamination in relation to considered processes	Numbers of chosen piezometers with dimensionless and dimensional distances the leakage source in lagoon 4 [total distance L to piezometer X (5)			
	III (8) 0.38 x ≈ 40.0 m	IX (4) 0.66 x ≈ 70.0 m	VII (6) 0.86 x ≈ 90.0 m	X (5) 1.00 x (L) ≈ 105.0 m
Chlorides (NaCl) [adsorption process]	0.4394[1)] 0.4035[2)] 1.00[a)]	0.2536[1)] 0.2383[2)] 1.00[a)]	0.1837[1)] 0.1758[2)] 1.00[a)]	0.0939[1)] 0.0910[2)] 1.00[a)]
Sulfates (Na_2SO4) [adsorption process]	0.3846[1)] 0.3276[2)] 1.00[a)]	0.1795[1)] 0.1584[2)] 1.00[a)]	0.1129[1)] 0.0978[2)] 1.00[a)]	0.0743[1)] 0.0634[2)] 1.00[a)]
Nitrates (NO_3^-) [biodegradation process]	0.4983[2)] 0.4979[3)] 1.00[a)]	0.2171[2)] 0.2145[3)] 1.00[a)]	0.1040[2)] 0.1031[3)] 1.00[a)]	0.0335[2)] 0.0333[3)] 1.00[a)]
BOD indicator [biodegradation process]	0.6524[2)] 0.6504[3)] 1.00[a)]	0.5252[2)] 0.5242[3)] 1.00[a)]	0.3534[2)] 0.3524[3)] 1.00[a)]	0.2126[2)] 0.2116[3)] 1.00[a)]
Chosen radionuclide [radioactive decay]	0.4035[2)] 0.3879[4)] 1.00[a)]	0.2383[2)] 0.2308[4)] 1.00[a)]	0.1758[2)] 0.1708[4)] 1.00[a)]	0.0910[2)] 0.0895[4)] 1.00[a)]

Dimensionless standard error values (Δ / C^*_{maxc}) in relation both to chosen contaminant and to appropriate equations:

Chosen contamination in relation to considered processes	Numbers of chosen piezometers with dimensionless and dimensional distances the leakage source in lagoon 4 [total distance L to piezometer X (5)			
	III (8) 0.38 x ≈ 40.0 m	IX (4) 0.66 x ≈ 70.0 m	VII (6) 0.86 x ≈ 90.0 m	X (5) 1.00 x (L) ≈ 105.0m
Chlorides (NaCl) [adsorption process]: Δ / C^*_{maxc} eq. (2) × 100% $\Delta = \mid C^*_{maxc}$ [eqs. (1) – (2)] $\mid$	6.5[1)]	5.3[1)]	3.9[1)]	2.7[1)]
Sulfates (Na_2SO_4) [adsorption process]: Δ / C^*_{maxc} eq. (2) × 100% $\Delta = \mid C^*_{maxc}$ [eqs. (1) – (2)] $\mid$	14.4[1)]	10.7[1)]	7.8[1)]	6.0[1)]
Nitrates (NO_3^-) [biodegradation process]: Δ / C^*_{maxc} eq. (4) × 1000 $^o/_{oo}$ $\Delta = \mid C^*_{maxc}$ [eqs. (2) – (4)] $\mid$	9.8[2)]	8.7[2)]	6.2[2)]	0.8[2)]
BOD indicator [biodegradation process]: Δ / C^*_{maxc} eq. (4) × 1000 $^o/_{oo}$ $\Delta = \mid C^*_{maxc}$ [eqs. (2) – (4)] $\mid$	4.7[2)]	3.3[2)]	2.5[2)]	2.0[2)]
Chosen radionuclide [radioactive decay]: Δ / C^*_{maxc} eq. (5) × 100% $\Delta = \mid C^*_{maxc}$ [eqs. (2) – (5)]	4.0[3)]	3.2[3)]	2.9[3)]	1.8[3)]

Maximal values of dimensionless calculated sulfate concentrations (Na_2SO_4) in the chosen piezometers



Final results of numerical calculations:

- **the standard errors between the maximum dimensionless concentrations based on eqs. (2) and (1) (with and without adsorption process) are: from 2.7 to 6.5 for chlorides and from 6.0 to 14.4 for sulfates (as the maximal errors) (values referred to footnote 1 in Table 2, in %),**

- **the standard errors between the maximum dimensionless concentrations based on eqs. (4) and (2) (with and without biodegradation process and with adsorption in both cases) are: from 0.8 to 9.8 for nitrates and from 2.0 to 4.7 for the BOD indicator (as the minimal errors) (values referred to footnote 2 in Table 2, in $^{o}/_{oo}$),**

- **the standard errors between the maximum dimensionless concentrations based on eqs. (5) and (2) (with and without radioactive decay and with adsorption in both cases) are: from 1.8 to 4.0 for the chosen radionuclide (values referred to footnote 3 in Table 2, in %).**

General conclusions

1) Basing on the numerical calculations, one can say that the non-linear adsorption process is of a very great importance in terms of the concentration reduction, especially for the sulfates and in less range for the chlorides moving in a natural aquifer,

2) Basing on the numerical calculations, one can say that the biodegradation of the chosen compounds (as nitrates and the BOD indicator) moving in a natural groundwater is of a very small importance in terms of the concentration reductions,

3) Basing on the numerical calculations, one can say that the radioactive decay is of a small importance in terms of the concentration reductions.

Thank you for your attention