Modelling of radionuclides transport in groundwater

NATIONAL CENTRE FOR NUCLEAR RESEARCH ŚWIERK

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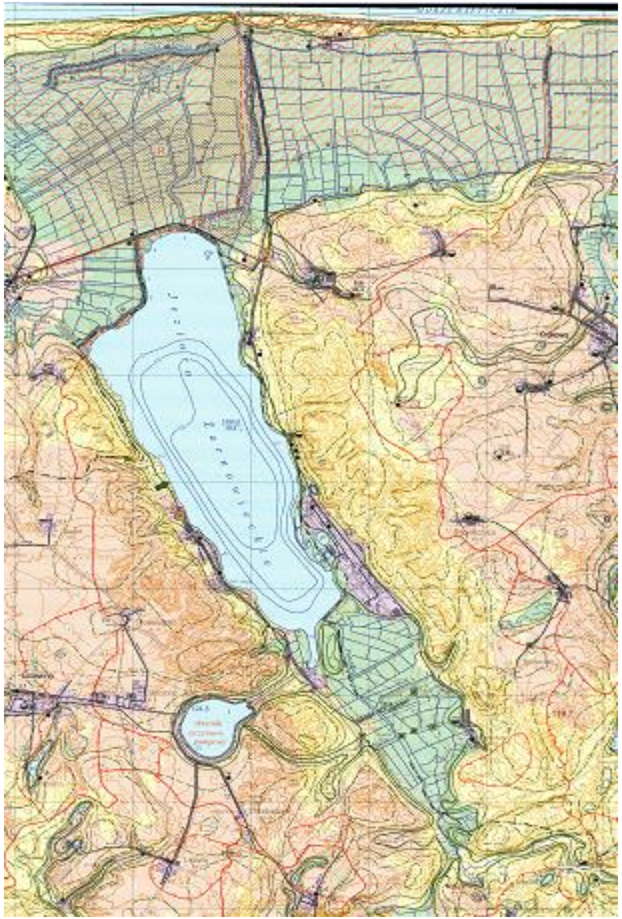
Motivation

- Long-term behavior of a high-level waste repository
- Near-surface disposal, like shallow land burial
- Uranium Mining and Milling
- Nuclear Power Plant Accidents: studies required in safety reports

Example: Dolina Kopalna Żarnowiec



Main reservoir of groundwater „Dolina Kopalna Żarnowiec”:
15 km^2, downflow region of groundwater 110 km^2, water abundance ~570 m^3/h

Modeling of radionuclides transport in groundwater: fundamentals

Transport of radionuclides through the ground can be estimated by:

- using tracers,
- groundwater dating,
- mathematical models,
- combination of all these techniques.

To obtain needed parameters chemical or radioactive tracers can be introduced to the groundwater and monitored through wells for directly determining groundwater velocity and transport.

Modeling of radionuclides transport in groundwater: fundamentals

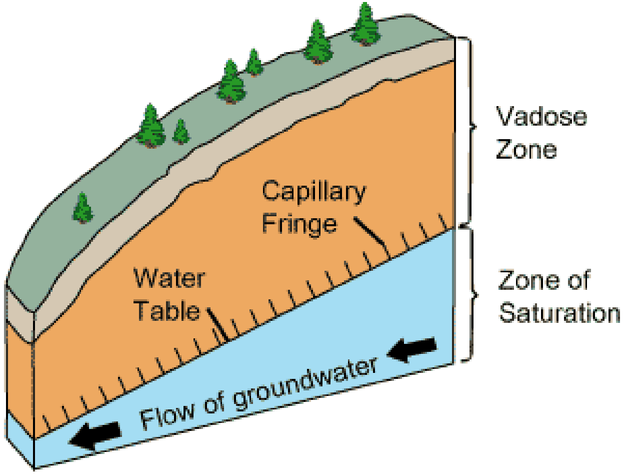
Models needed:

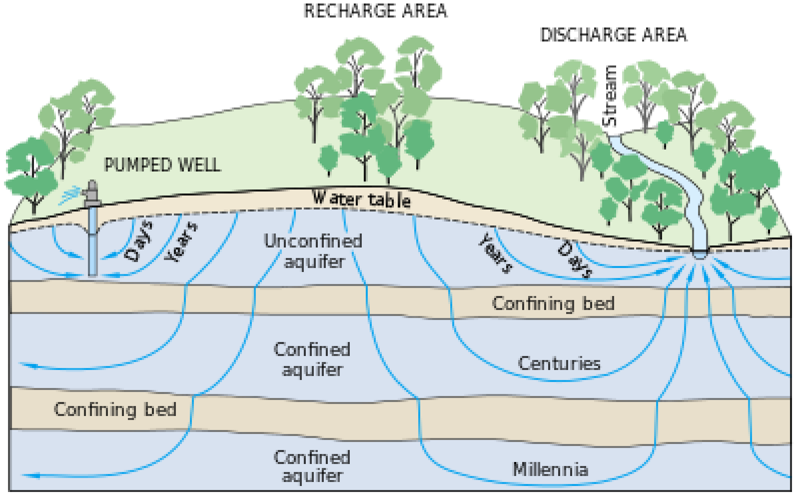
- Determination of the portion of the radioactive source released by infiltrating water containing radionuclides,
- Prediction of the migration of radionuclides from the source to locations (accessible to the public), basing on measurable hydrologic parameters,
- Determination of the potential radiation dose using the radionuclide concentrations that reach accessible locations.

Two equations are typically required:

- Description of the flow in the ground
- Transport and dispersion of radionuclides

Modeling of radionuclides transport in groundwater: basic notions





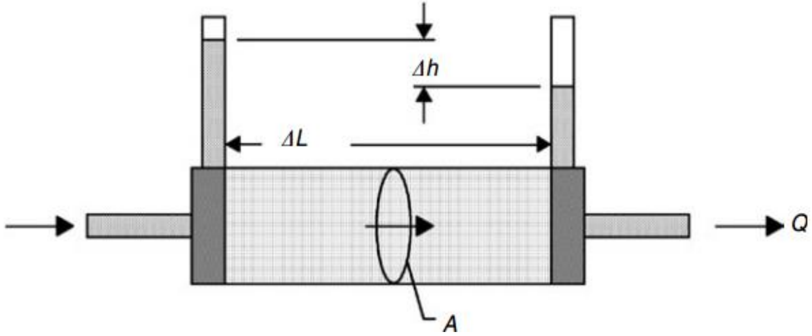
Macroscopic parameters:

Porosity: fraction of void space over total volume

Hydraulic conductivity: describes the ease with which a fluid can move through porous media (ratio of velocity to hydraulic gradient)

Permeability: ability of a porous material to allow fluids to pass through it.

Modeling of radionuclides transport in groundwater: basic notions



$$V_x = -K\frac{dh}{dx} \cong -K\frac{\Delta h}{\Delta x}$$ Darcy law (saturated zone)

$$U = \frac{V_x}{n_e}$$ pore velocity, n_e – effective porosity

Assuming that the medium is saturated, homogenous and isotropic the flow is described as: $\nabla^2 H = \frac{S_s}{K}\frac{\partial H}{\partial t}$

H = total head = *h* + *z* (cm) (i.e., the height to which a column of water would rise above the datum, z = 0)

S_s - specific storage coefficient (storage of water caused by the compressibility of water and the medium)

K - hydraulic conductivity

Modeling of radionuclides transport in groundwater: basic notions

Transport of mass:

$$R_d\theta\frac{\partial c}{\partial t}-\nabla\cdot\left(\theta\bar{\bar{D}}\cdot\nabla c\right)+\nabla\cdot\left(\bar{V}c\right)+\left[R_d\frac{\partial c}{\partial t}+\lambda\theta R_d\right]c=0$$

R_d - retardation coefficient

Θ - moisture content

c - concentration of dissolved constituent [g cm^{-3}]

$\bar{\bar{D}}$ - dispersion tensor [cm^2 s^{-1}]

$\bar{V}$ - flux vector [cm s^{-1}]

λ - radioactive decay constant [s^{-1}], $\lambda=\frac{ln2}{t_{1/2}}$

For homogenous and isotropic dispersion tensor:

$$R_d\frac{\partial c}{\partial t}-\nabla\cdot\left(\bar{\bar{D}}\cdot\nabla c\right)+\frac{\bar{V}}{n}\cdot\nabla c+\lambda R_d c=0$$

Modeling of radionuclides transport in groundwater: basic notions

For fluid flux uniform along the x-axis:

$$\frac{\partial c}{\partial t} - \frac{D_x}{R_d}\frac{\partial^2 c}{\partial x^2} - \frac{D_y}{R_d}\frac{\partial^2 c}{\partial y^2} - \frac{D_z}{R_d}\frac{\partial^2 c}{\partial z^2} + \frac{U}{R_d}\frac{\partial c}{\partial x} + \lambda c = 0$$

U - pore velocity

D_x, D_y, D_z- dispersion coefficient along the x-, y-, and z [$cm^2\ s^{-1}$].

$D_x = \alpha_x U$ $D_y = \alpha_y U$ $D_z = \alpha_z U$ where α_x α_y α_z are dispersivity coefficients determined by calibration versus observed groudwater solute transport

Sorption is a mechanism which makes retardation in the migration of radionuclides in groundwater, described by the retardation factor:

$R_d = \frac{n}{n_e} + \frac{\rho_b}{n_e} K_d$ K_d - distribution coefficient depending on the media and radionuclide

n - total porosity, n_e - effective porosity, ρ_b - bulk density ($g\ cm^{-3}$)

Modeling of radionuclides transport in groundwater: basic notions

For fluid flux uniform along the x-axis:

$$\frac{\partial c}{\partial t} - \frac{D_x}{R_d}\frac{\partial^2 c}{\partial x^2} - \frac{D_y}{R_d}\frac{\partial^2 c}{\partial y^2} - \frac{D_z}{R_d}\frac{\partial^2 c}{\partial z^2} + \frac{U}{R_d}\frac{\partial c}{\partial x} + \lambda c = 0$$

Solution for vadose zone based on the Green's function:

$$c = \frac{1}{n_e R_d} X_1(x,t) Y_1(y,t) Z_1(z,t)$$

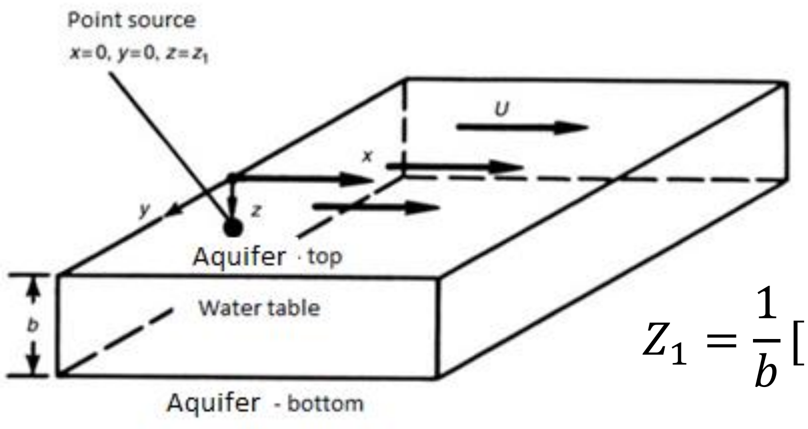
at some point (*x, y, z*) and time *t*.

Example for point source release:

$$X_1 = \frac{1}{\sqrt{4\pi D_x\, t/R_d}} \exp\left[- \frac{\left(x - \frac{Ut}{R_d}\right)^2}{\frac{4D_x t}{R_d}} - \lambda t \right]$$

$$Y_1 = \frac{1}{\sqrt{4\pi D_y t/R_d}} \exp\left[-\frac{y^2}{\frac{4D_y t}{R_d}}\right]$$

$$Z_1 = \frac{1}{b}\left[1 + 2\sum_{m=1}^{\infty} \exp\left(-\frac{m^2\pi^2 D_z t}{b^2 R_d}\right) cos m\pi \frac{z_s}{b}\, cos m\pi \frac{z}{b}\right]$$



Datasets

Typical values of hydraulic conductivity of porous materials (McWhorter and Sunada 1977)

Material	Number of analyses	Range ($cm\ s^{-1}$)	Arithmetic mean ($cm\ s^{-1}$)
Igneous rocks			
Weathered granite	7	$(3.3–52) \times 10^{-4}$	1.65×10^{-3}
Weathered gabbro	4	$(0.5–3.8) \times 10^{-4}$	1.89×10^{-4}
Basalt	93	$(0.2–4{,}250) \times 10^{-8}$	9.45×10^{-6}
Sedimentary materials			
Sandstone (fine)	20	$(0.5–2{,}270) \times 10^{-6}$	3.31×10^{-4}
Siltstone	8	$(0.1–142) \times 10^{-8}$	1.9×10^{-7}
Sand (fine)	159	$(0.2–189) \times 10^{-4}$	2.88×10^{-3}
Sand (medium)	255	$(0.9–567) \times 10^{-4}$	1.42×10^{-2}
Sand (coarse)	158	$(0.3–6{,}610) \times 10^{-4}$	5.20×10^{-2}
Gravel	40	$(0.3–31.2) \times 10^{-1}$	4.03×10^{-1}
Silt	39	$(0.09–7{,}090) \times 10^{-7}$	2.83×10^{-5}
Clay	19	$(0.1–47) \times 10^{-8}$	9×10^{-8}
Metamorphic rocks			
Schist	17	$(0.002–1{,}130) \times 10^{-6}$	1.9×10^{-4}

Typical values of effective porosity (or specific yield) of aquifer materials (McWhorter and Sunada 1977)

Aquifer material	Number of analyses	Range	Arithmetic mean
Sedimentary materials			
Sandstone (fine)	47	0.02–0.40	0.21
Sandstone (medium)	10	0.12–0.41	0.27
Siltstone	13	0.01–0.33	0.12
Sand (fine)	287	0.01–0.46	0.33
Sand (medium)	297	0.16–0.46	0.32
Sand (coarse)	143	0.18–0.43	0.30
Gravel (fine)	33	0.13–0.40	0.28
Gravel (medium)	13	0.17–0.44	0.24
Gravel (coarse)	9	0.13–0.25	0.21
Silt	299	0.01–0.39	0.20
Clay	27	0.01–0.18	0.06
Limestone	32	~0–0.36	0.14
Wind-laid materials			
Loess	5	0.14–0.22	0.18
Eolian sand	14	0.32–0.47	0.38
Tuff	90	0.02–0.47	0.21
Metamorphic rock			
Schist	11	0.22–0.33	0.26

Datasets

Distribution coefficients: strontium and cesium (Isherwood 1981)

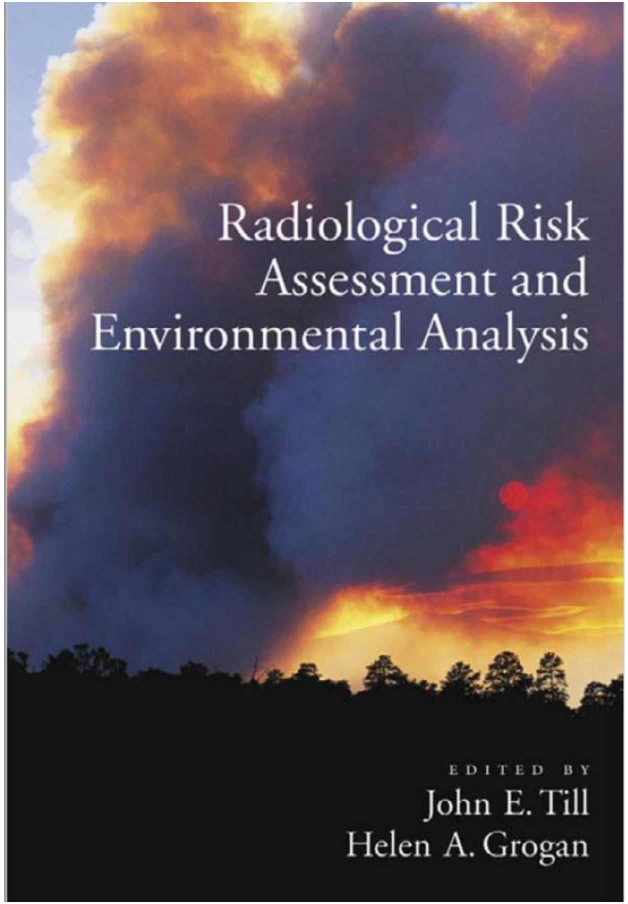
Materials	K_d (mL g^{-1})	
	Strontium	Cesium
Basalt, 32–80 mesh	16–135	792–9,520
Basalt, 0.5–4 mm, 300 ppm TDS	220–1,220	39–280
Basalt, 0.5–4 mm, seawater	1.1	6.5
Basalt, fractured in situ measurement	3	
Sand, quartz—pH 7.7	1.7–3.8	22–314
Sands	13–43	100
Carbonate, >4 mm	0.19	13.5
Dolomite, 4,000 ppm TDS	5–14	
Granite, >4 mm	1.7	34.3
Granodiorite, 100–200 mesh	4–9	8–9
Granodiorite, 0.5–1 mm	11–23	1,030–1,810
Hanford sediments	50	300
Tuff	45–4,000	800–17,800
Soils	19–282	189–1,053
Shaley siltstone < 4 mm	8	309
Shaley siltstone > 4 mm	1.4	102
Alluvium, 0.5–4 mm	48–2,454	121–3,165
Salt, > 4 mm saturated brine	0.19	0.027

Dispersivity values α_L and α_T obtained by calibration of numerical transport models against observed groundwater solute transport (Evenson and Dettinger 1980)

Setting	α_L(m)	α_T (m)	Δx^a (m)	$\overline{U}^b$ (m day^{-1})	Method[c]
Rocky Mountain Arsenal alluvial sediments	30.5	30.5	305		Areal (moc)
Arkansas River Valley coalluvial sediments	30.5	9.1	660 × 1,320		Areal (moc)
California alluvial sediments	30.5	9.1	305		Areal
Long Island glacial deposits	21.3	4.3	Variable (50–300)	0.4	Areal (fe)
Brunswick, Georgia, limestone	61	20	Variable		Areal (moc)
Snake River, Idaho, factured basalt	91	136.5	640		Areal
Idaho, fractured basalt	91	91	640		Areal (fe)
Hanford site, Washington fractured basalt	30.5	18			Areal (rw)
Barstow, California, alluvial deposits	61	18	305		Areal (fe)
Roswell Basin, New Mexico, limestone	21.3				Areal
Idaho Falls, lava flows and sediments	91	137	Variable		Areal
Barstow, California, alluvial sediments	61	0.18	3 × 152		Profile (fe)
Alsace, France, alluvial sediments	15	1			Profile
Florida (SE) limestone	6.7	0.7	Variable		Profile
Sutter Basin, California, alluvial sediments	80–200	8–20	(2–20 km)		3-D (fe)

[a] Δx = grid size in program.
[b] $\overline{U}$ = groundwater seepage velocity.
[c] (fe), use of a finite element model; (moc); method of characteristics; (rw), random walk model.

Where to find information ?



United States Department of Agriculture

Agricultural Research Service

Technical Bulletin Number 1661

Analytical Solutions of the One-Dimensional Convective-Dispersive Solute Transport Equation

More advanced models

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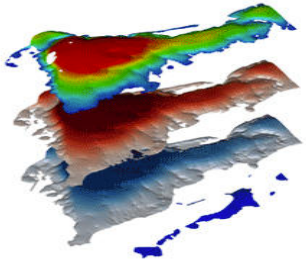
Water Resources

MODFLOW and Related Programs

Overview | Publications | Software

MODFLOW is the USGS's modular hydrologic model. MODFLOW is considered an international standard for simulating and predicting groundwater conditions and groundwater/surface-water interactions. MODFLOW 6 is presently the core MODFLOW version distributed by the USGS. The previous core version, MODFLOW-2005, is actively maintained and supported as well.

Originally developed and released solely as a groundwater-flow simulation code when first published in 1984, MODFLOW's modular structure has provided a robust framework for integration of additional simulation capabilities that build on and enhance its original scope. The family of MODFLOW-related programs now includes capabilities to simulate coupled groundwater/surface-water systems, solute transport, variable-density flow (including saltwater), aquifer-system compaction and land subsidence, parameter estimation, and groundwater management.



MODFLOW Development Plans, July 20, 2020

The USGS Water Mission Area actively develops and supports the MODFLOW suite of programs. Ongoing efforts include providing maintenance and support for existing versions of MODFLOW such as MODFLOW 6, MODFLOW-2005, MODFLOW-NWT, MODFLOW-USG, MODPATH, MT3D-USGS, and related and supporting programs such as FloPy and PEST++. Current development efforts are focused on adding new capabilities to MODFLOW 6. These development efforts include:

- A Basic Model Interface (BMI) for MODFLOW 6 to support easier coupling with other models such as those that simulate groundwater recharge, geochemical mixing, and optimization and management, as well as models that would benefit from tight coupling.
- A Groundwater Transport (GWT) Model that works with structured or unstructured grids, the Newton formulation, and the advanced stress packages available in MODFLOW 6.
- A new Buoyancy (BUY) Package that extends the Groundwater Flow (GWF) Model of MODFLOW 6 to represent variable-density groundwater flow. This new BUY Package makes it possible to simulate problems related to saltwater intrusion, deep-well injection, aquifer storage and recovery, and brine migration.
- Extension of MODPATH to track particles in MODFLOW 6 models that use Discretization by Vertices (DISV) and fully unstructured (DISU) grids.
- Parallelization of the MODFLOW 6 multi-model framework for High-Performance Computing (HPC) using the Message Passing Interface (MPI). Preliminary versions of MODFLOW 6 with this new capability have been used to solve groundwater models with billions of model cells. This new parallelization capability is being developed in a general manner that can be easily extended for future MODFLOW model types (for example GWT); applied at local, regional, and continental scales; and can be used on desktops and HPC systems.

Status - Active

Contacts

USGS MODFLOW Team

Email: modflow@usgs.gov

Explore More Science:

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More advanced models

Core Versions

- MODFLOW 6: current core version
- MODFLOW-2005: previous core version

MODFLOW Variants: Newer, specialized, or advanced versions of MODFLOW for use by experienced modelers

- MODFLOW-NWT: MODFLOW-NWT uses a Newton-Raphson formulation to improve solution of unconfined groundwater-flow problems.
- MODFLOW-USG: MODFLOW-USG uses an unstructured-grid approach to simulate groundwater flow and tightly coupled processes using a control volume finite-difference formulation.
- GSFLOW: GSFLOW is a coupled groundwater and surface-water flow model based on the USGS Precipitation-Runoff Modeling System (PRMS), MODFLOW-2005, and MODFLOW-NWT.
- GWM: The Groundwater Management (GWM) Process for MODFLOW-2000 and MODFLOW-2005 is used to simulate groundwater management

MODFLOW-Based Particle Tracking and Solute Transport

- MODPATH: MODPATH is a particle-tracking post-processing model that computes flow paths using output from MODFLOW.
- MT3D-USGS: MT3D-USGS is a groundwater solute transport simulator for MODFLOW.
- SEAWAT: SEAWAT is a combined version of MODFLOW and MT3DMS for simulation of variable-density groundwater flow and transport.

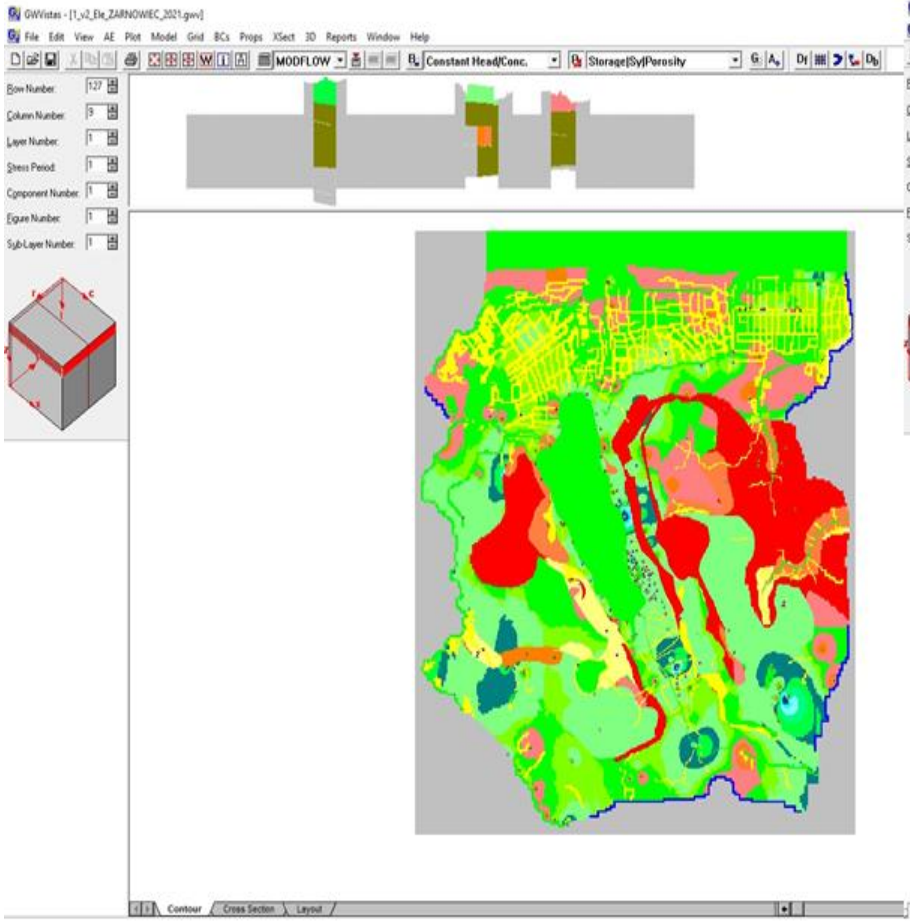
Parameter Estimation and Uncertainty Analysis

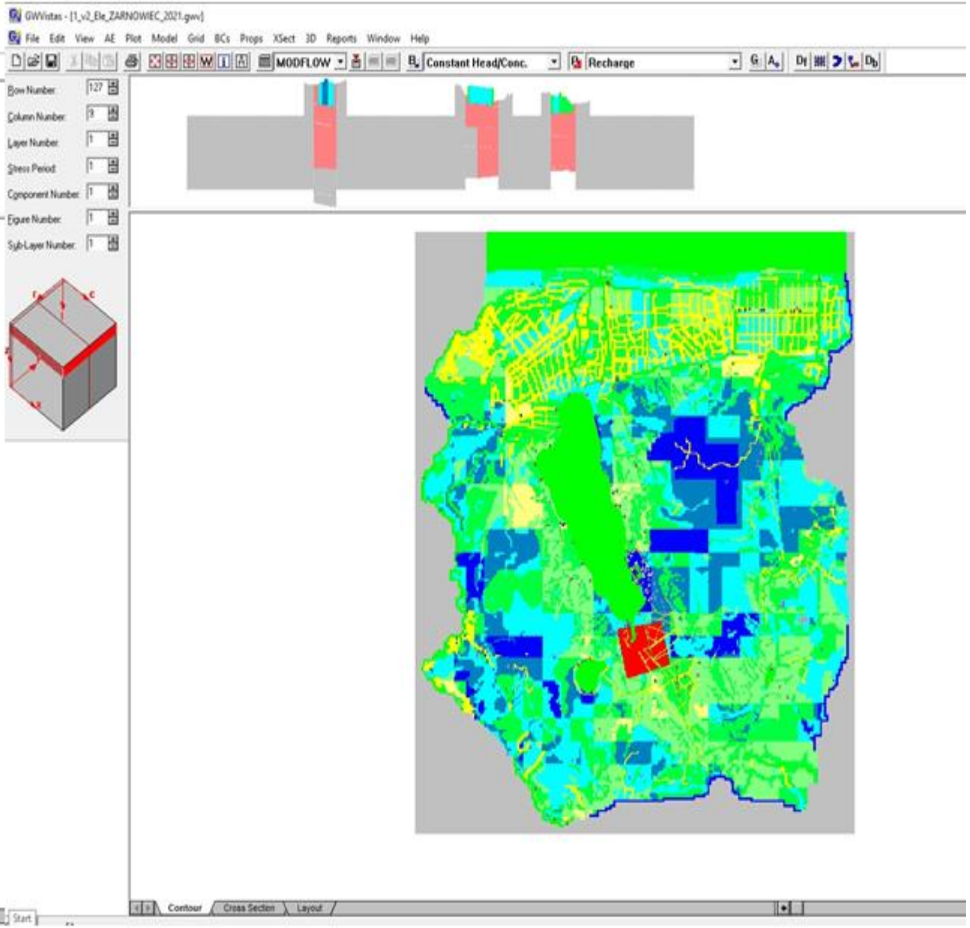
- PEST++: PEST++ is an objected-oriented universal parameter estimation code written in C++ that can be used to calibrate MODFLOW models.

MODFLOW Utilities, Post Processors, and Graphical User Interfaces (GUIs)

- FloPy: FloPy is a Python package for creating, running, and post-processing MODFLOW-based models.
- GRIDGEN: GRIDGEN is a program for generating layered quadtree grids for MODFLOW-USG.
- GW Chart: GW_Chart is a graphing application for MODFLOW, Zonebudget, and other codes. GW_Chart also converts binary cell-by-cell flow files to text files.
- ModelMuse: ModelMuse is a GUI for MODFLOW-2005, MODFLOW-LGR, MODFLOW-NWT, MT3DMS, PHAST, MODPATH, and ZONEBUDGET.
- ModelViewer: Model Viewer is a program for 3D visualization of groundwater-model results.
- ZONEBUDGET: ZONEBUDGET is a program for computing subregional water budgets for MODFLOW.

Groundwater Vistas – GUI for Modflow package





Implementation for Dolina Kopalna Żarnowiec

Basic data:

- Model in GroundwaterVistas prepared for water budget consists of 7 layers: 4 aquifers and 3 separating layers
- Dolina Kopalna Żarnowiec in the first aquifer: water table is from 1m to 5-10 below ground level.
- Thickness from 1 m to 35 m, average hydraulic conductivity 17,32 m^2/h, total porosity 0,4, effective porosity 0,25.
- Second layer consits mostly of clays and mud; thickness from 1 m to 77 m - at average 20 m, porosity 0,06
- Distributions coefficient for Cs: from 22 ml/g to 100 ml/g; for Sr: from 1,7 ml/g to 43 ml/g
- Conservative assumptions for retardation factors give the values for the first aquifer: for Cs: 145, for Sr: 14

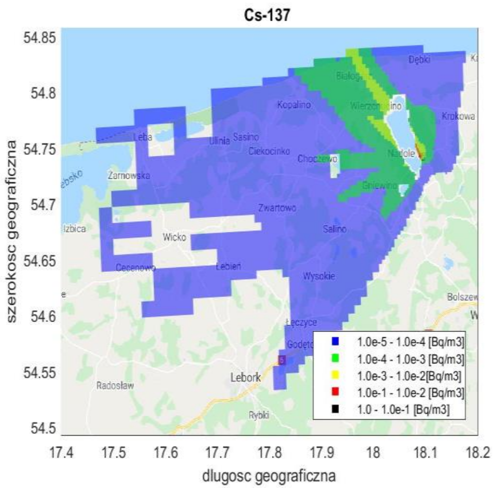
Reminder: travel time can be estimated as $t = \frac{U}{x} R_d$

U – pore velocity, x –distance, R_d – retardation factor

Implementation for Dolina Kopalna Żarnowiec

Basic question: in case of severe accident, what will be the impact of the contamination of Dolina Kopalna Żarnowiec on the Żarnowiecki Lake ?

- Calculations for the scenario representative for emergency planning (AP-1000 reactor): atmospheric dispersion models in RODOS
- Deposition calculated in RODOS system: input to other models (hydrological path, groundwater model, dose model)
- Selection of the scenarios with high deposition in the considered area
- In parallel calculations in hydrological module chain of RODOS to find concentration at the lake
- Assumption: the level of groundwater will increase such that, it will reach the bottom of the lake



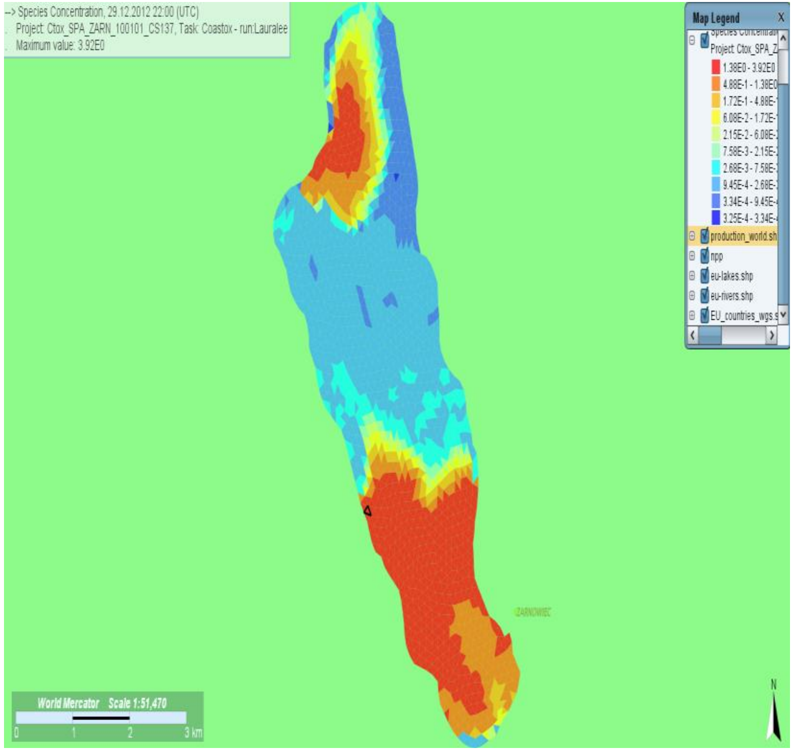
Some results of groundwater calculations

- Estimation of travel time:
  - for Cs, for the distances 5 m - 10 m (to the shore of the lake) it will be from 59 years to 110 years,
  - for Sr, for the distances 5 m, 10 m, 50 m respectively: 5 years, 10 years, 52 years.
- Estimation of concentration for Cs:
  - 5 m: 567 Bq/m^3 in 6 months
  - 10 m: 198 Bq/m^3 in 1 year
  - 50 m: 14 Bq/m^3 in 3 years
  - 100 m: 3 Bq/m^3 in 5 years
- Estimation of concentration for Sr:
  - 5 m: 1110 Bq/m^3 in 6 months
  - 10 m: 387 Bq/m^3 in 1 year
  - 50 m: 28 Bq/m^3 in 3 years
  - 100 m: 6,2 Bq/m^3 in 3 years

Comparison to the results from HDM-RODOS

Concentrations in the bottom layer of the Żarnowiecki Lake

	Cs-137	Sr-90	I-131
Ranges of maximal concentration, bottom layer initial values	10^5-10^7 Bq/m^3	10^2-10^4 Bq/m^3	10^4-10^6 Bq/m^3
Maximal initial concentration, bottom layer	1,22x10^7 Bq/m^3	8,4 x10^4 Bq/m^3	3,292 x10^6 Bq/m^3
Ranges of maximal concentration, bottom layer after 6 months	10^4-10^5 Bq/m^3	10^2-10^4 Bq/m^3	Below 10^{-3} Bq/m^3
Maximal concentration, bottom layer after 6 months	2,7 x10^5 Bq/m^3	2,4 x10^4 Bq/m^3	Below 10^{-3} Bq/m^3



Summary

- In the worst case one can expect that after 6 months due to additional inflow of Sr-90 to the Żarnowiecki Lake the activity in the bottom layer of the lake can be increased by about 4,6 % - this is conservative estimation.
- In the other cases (other radionuclides like Cs or other meteo conditions) maximal contribution will be below 1%.
- However, in case of severe accident, due to the long travel time of radionuclides in porous media the program for long-term groundwater monitoring should be established
- In general the models for the transport of radionuclides in groundwater need good calibration, which means there is a need for observation data
- Due to non-uniform composition of porous media the results can be burdened with high uncertainties