Applied Hydrogeology
Introduction to Modflow

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Modflow – introduction

The most widespread computer code for groundwater flow - **MODFLOW**

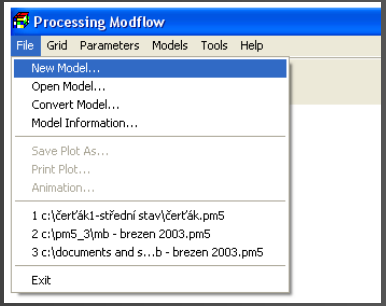
Modflow versions: 88, 96, 2000 and 2005

Software packages with modflow code: PMWIN (version 96), Processing modflow Pro (version 96), Visual Modflow (version 2000), GMS (version 2000)

PMWIN:

Finite differences, saturated flow, steady-state and transient flow, water budget, inverse modelling (PEST, UCODE), transport advective modelling (MT3D, MT3DMS, MOC3D), advective modelling (PMPATH)

New model – crate new folder - choose simple path (e.g. C: Document: My model folder)

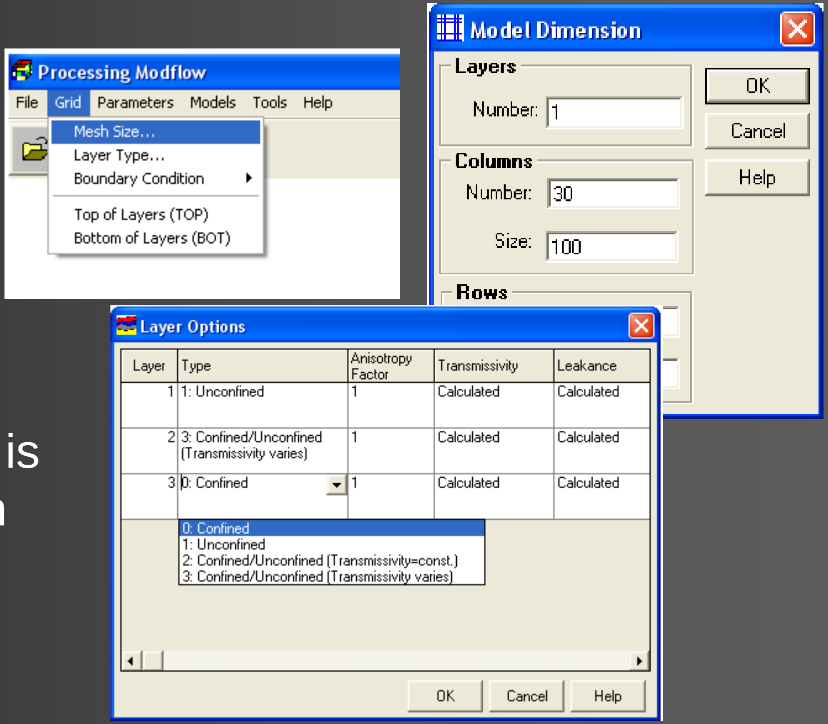


Modeled area discretization

Keep the mine basical principles and rules in the grid preaparation! (see previous presentation)

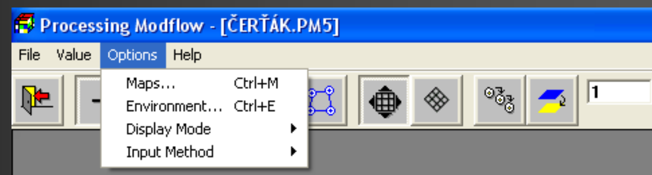
Grid creation – define modeled area extent and consequently define number and size of rows, columns and layers

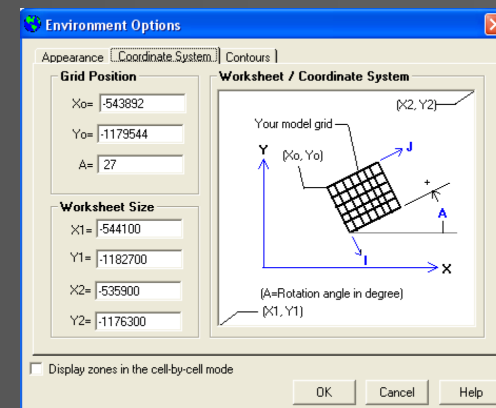
Define the layer type – preferable is the confined/unconfined layer with transmissivity varies



PMWIN – Grid

Environment and Maps

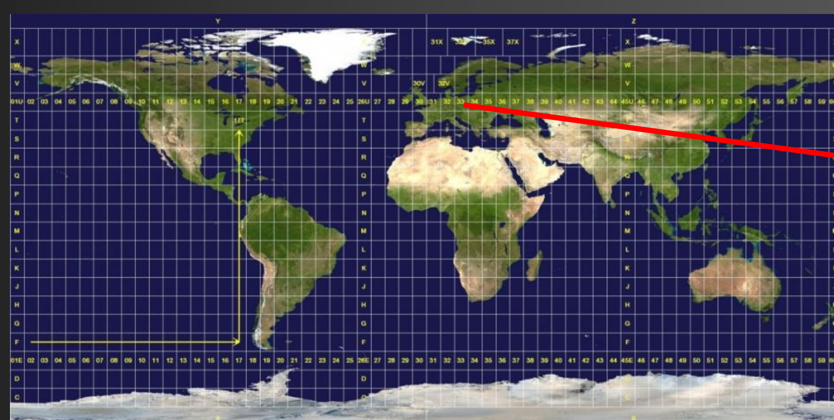


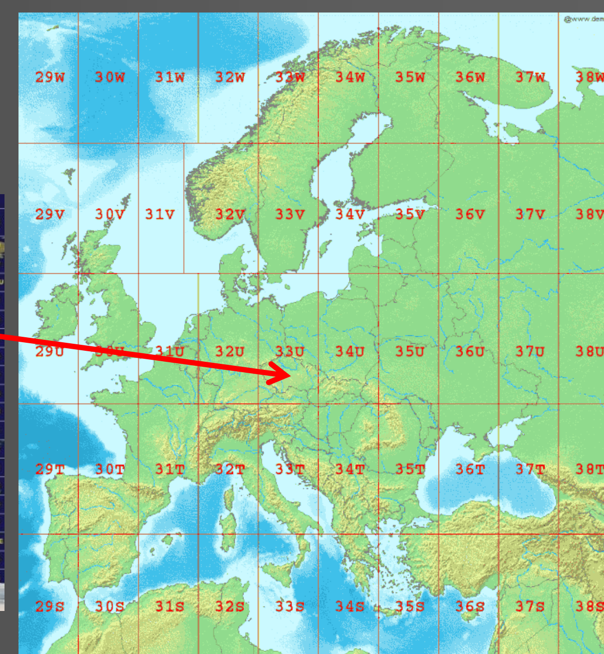


Environment

Find out:

- Extent of modeled area discretized by grid
- Extent of the underlying map - set up the same size for the worksheet
- Define X and Y coordinates – Universal Trasnverse mercator – **UTM** – depiction of elipsoid's parts in plan





Latitude – 60 zones marked by numbers

Longitude – 20 zones marked by letter of the alphabet

Environment and Maps

Maps

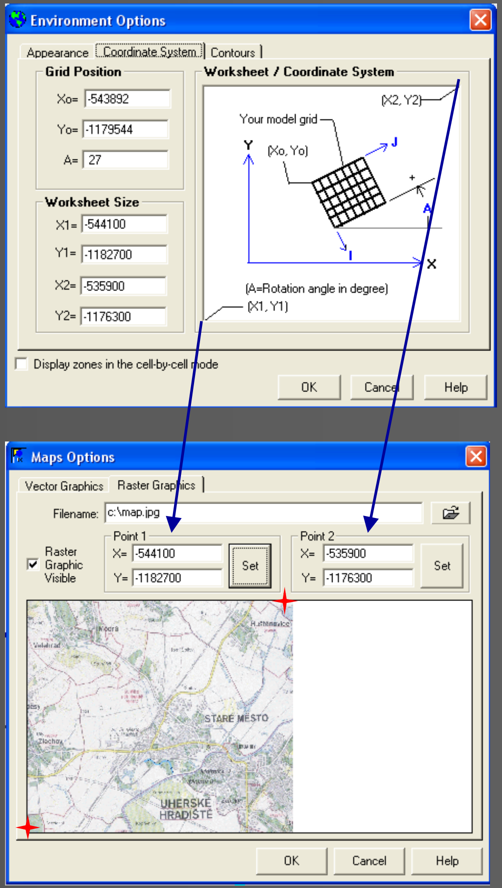
- Underlying map – vector map (DXF) or raster map (bmp, jpg)

- Define the left-lower and right-upper edge of the map

(Ctrl + left mouse button - decrease the map view, Shift + left mouse button – increase the map view)

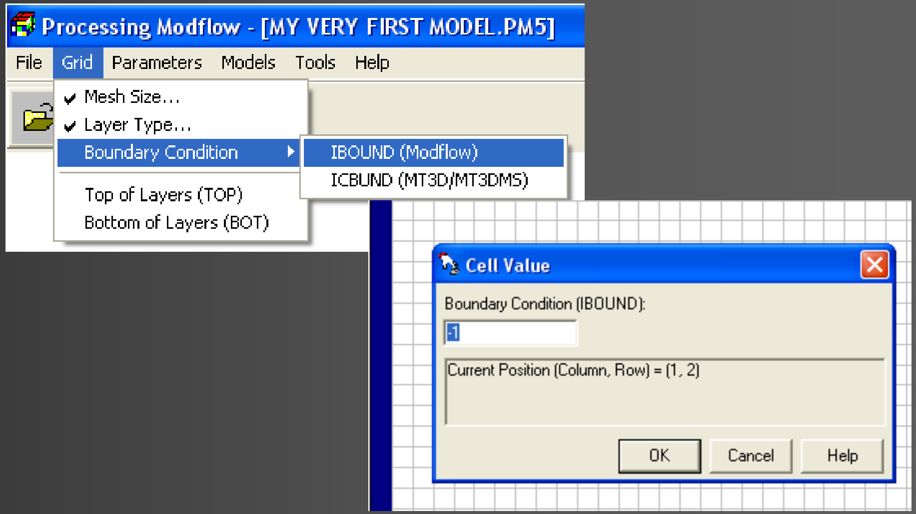
Environment

move and rotate the model grid to desired position according to underlaid map



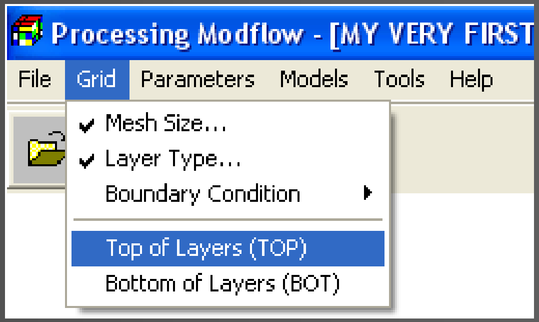
Define the boundary conditions – assign number:

- Active cell = 1
- Inactive cell = 0 (II. type)
- Constant cell = -1 (I. type)

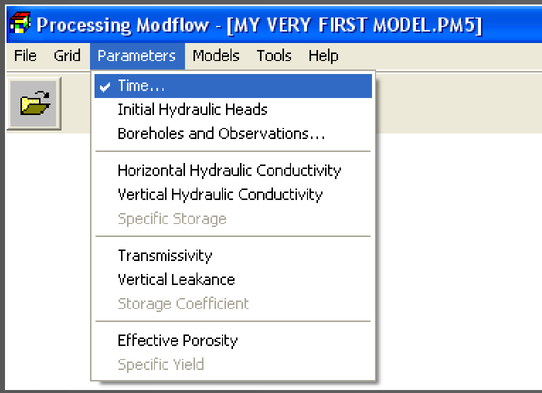


Define the top and bottom of layers:

- Manual – cell by cell or zonal input method
- Interpolation – Digitizer, Field interpolator



Input parameters – time, observations, starting heads and hydraulic parameters

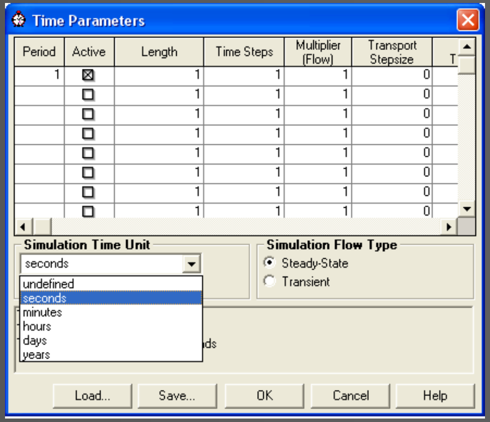


Time:

Steady state flow type - steady-state flow even for several Stress periods

Transient flow type – time is discretizated to Time steps in Stress periods

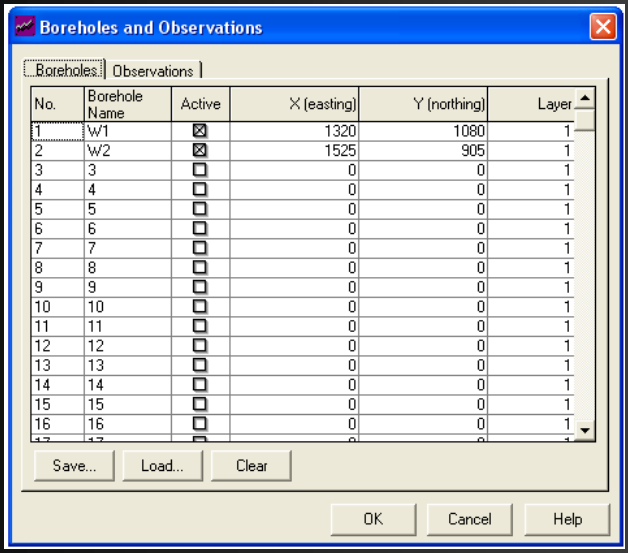
Choose time unit

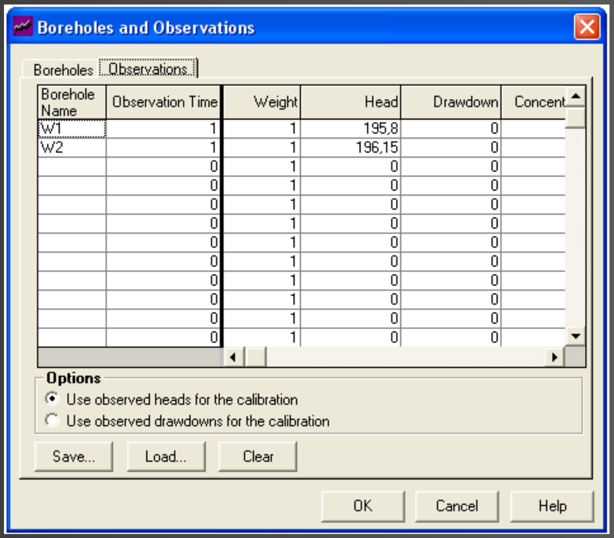


Initial starting heads:

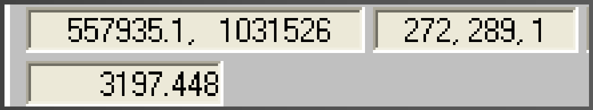
- Steady–state flow – require exactly determined heads only in boundary conditions
- Transient flow – require exactly determined heads in the whole model

Boreholes and Observations - insert name, coordinate system and observed hydraulic head





- Real-world coordinate system – UTM *(The Universal Transverse Mercator)*

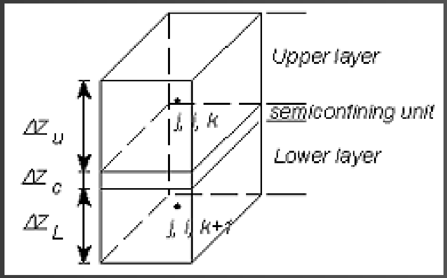


- Relative coordinate system – relative position of modeled grid in the status bar

Hydraulic parameters:

- Horizontal hydraulic conductivity – one or more values
- Vertical hydraulic conductivity – in the multi-layer model, the ratio of horizotnal to vertical conductivity is vertical conductivity ranging from 3:1 to 10:1
- Anisotropy factor – the ratio of horizontal conductivity (or transmissivity) along the x and y direction
- Vertical leakance – *quasi-three dimensional models* – replace the modeled layer and represent semiconfining unit - resistance to the vertical flow

$$VCONT = \frac{2}{\frac{\Delta Z_u}{(K_z)_u} + \frac{2\Delta Z_c}{(K_z)_c} + \frac{\Delta Z_L}{(K_z)_L}}$$



- Transmissivity – define in Layer Type → User specified or Calculated

PMWIN – Parameters

Storage parameters - transient simulation – water is released from or taken into storage within the porous material

- Specific storage (S_s) – volume of water released from storage within a unit volume of porous material per unit decline in head

- Storage coefficient (S) – in the 2-D areal simulations, vertically averaged parameter equal to the volume of water released per unit area of aquifer per unit decline in head

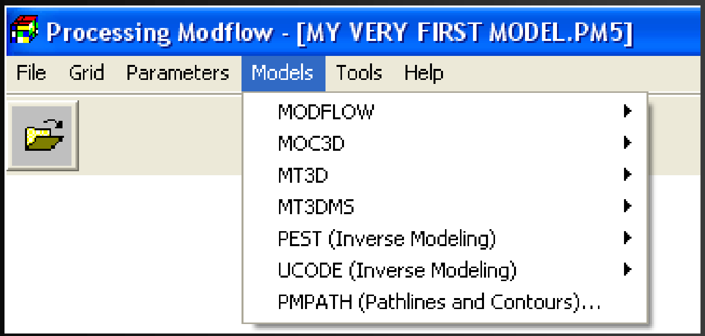
$$S = bS_s$$

b = aquifer thickness

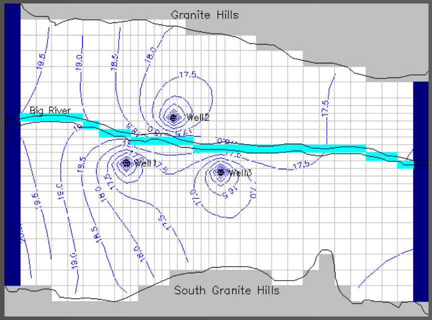
- Specific yield – storage parameter of the unconfined aquifer, volume of gravity drainaged water per volume of porous material

Effective porosity – advective modelling, from 1 % (fractured rocks) to 35 % (coarse grained sand or gravel)

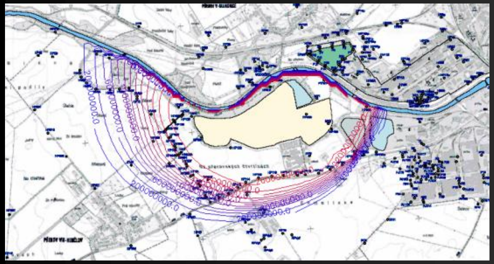
PMWIN – Models

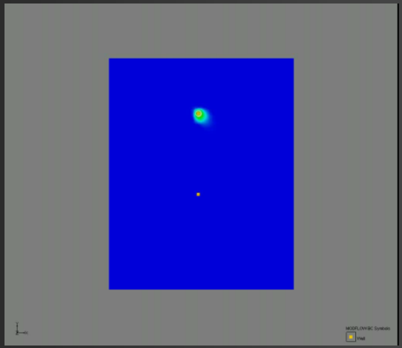


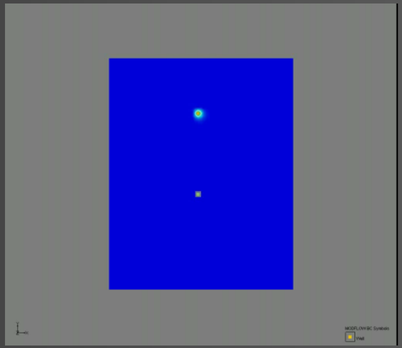
MODFLOW – flow field



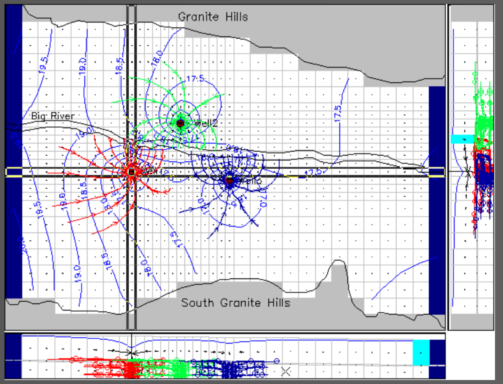
MOC3D, MT3D, MT3DMS – transport modeling







PMPATH – advective modeling



PEST, UCODE – automated parameter estimation

```
                              OPTIMISATION RESULTS

Parameters ----->

Parameter          Estimated          95% percent confidence limits
                   value              lower limit        upper limit
 rch_1            4.000760E-09        3.275596E-09       4.886464E-09

Note: confidence limits provide only an indication of parameter uncertainty.
      They rely on a linearity assumption which  may not extend as far in
      parameter space as the confidence limits themselves - see PEST manual.

See file PESTCTL.SEN for parameter sensitivities.
```

PMWIN – Models

Flow packages - inflow and outflow to/from model and within the model

III. Type of boundary condition

Drain, GHB, Evapotranspiration, Reservoir, River, Streamflow-Routing

Sources and Sinks

Recharge, Well

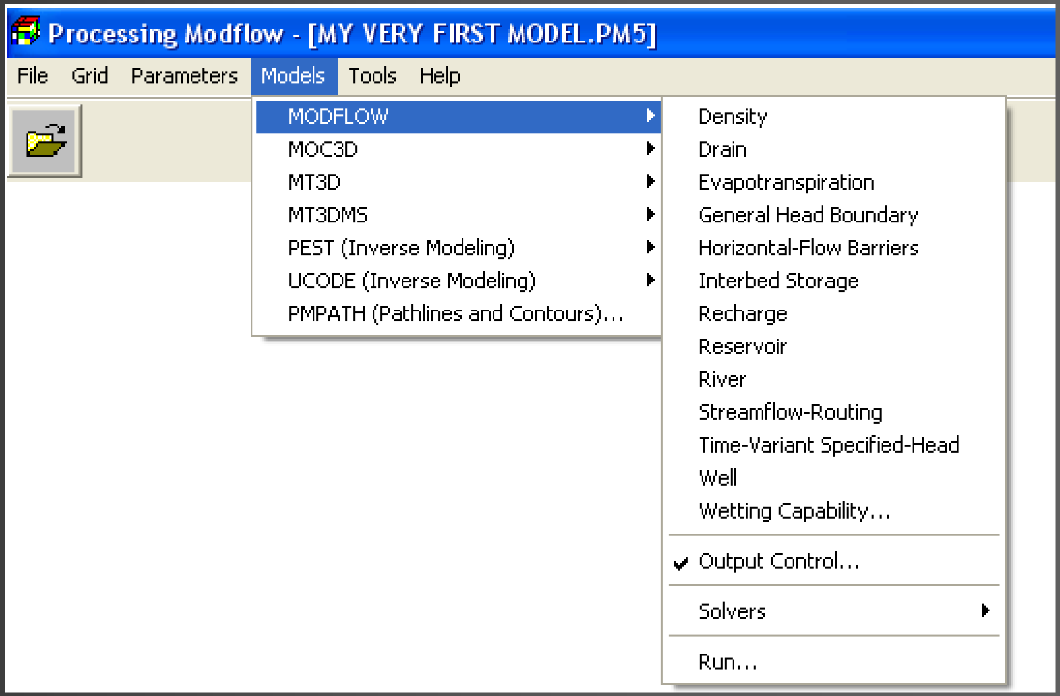
Additional

Horizontal-Flow barriers

Density

Interbed Storage

Wetting Capability



III. Type of boundary condition: flux across is dependent on the difference between a user-supplied specified head on one side of the boundary and the model-calculated head on the other side

$$L = Q_L / A = K_z^{\prime} / b^{\prime} (h_{source} - h)$$

L = leakage rate
Q_L = volumetric flux
A = area of the cell
$K_z^{\prime}$ = vertical hydraulic conductivity of the interface
$b^{\prime}$ = thickness of the interface
h_{source} = head in the source reservoir
h = head in the aquifer

- **Drain** – water releases model
- **GHB** – simulation of the distant constant head boundary condition
- **Evapotranspiration** – water releases model in accordance with extinction depth
- **River** – upper limit for water inflow
- **Streamflow Routing** – allow hyraulic parameters of the stream channel flow
- **Reservoir** – similar to River package, allow simulate more reservoirs

General Head Boundary - III. Type of boundary condition

$$Q_b = C_b - (h_b - h) \qquad C_b = K.A / L$$

High C_b represents equivalent of constant head

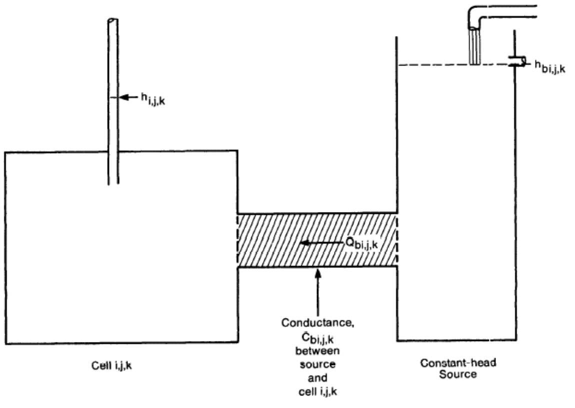


Figure 44.—Schematic diagram illustrating principle of general-head boundary package.

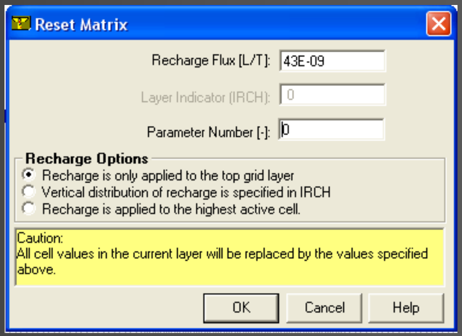
River - III. Type of boundary condition

$$C_{riv,str} = \frac{KLW}{W} \qquad Q_{riv,str} = \frac{KLW}{M}(h_s - h_a)$$

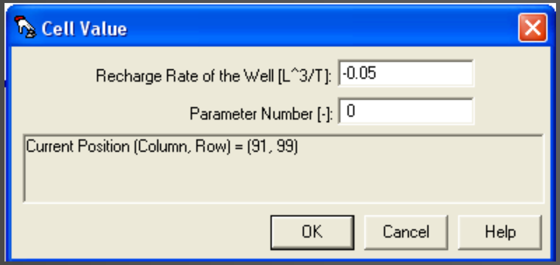
K is vertical hydraulic conductivity of riverbed sediments, *L* is lenght of the river in the cell, *W* is wide of the river and *M* is thickness of the rvierbed sediments

Sources and Sinks:

- Recharge – upper boundary condition



- Well - injection well + injected rate
  - pumping well – pumped rate



Well in multi-layer model:

- **Confined layer** - divide of pumped/injected rate in model in accordance with transmissivity of each layer

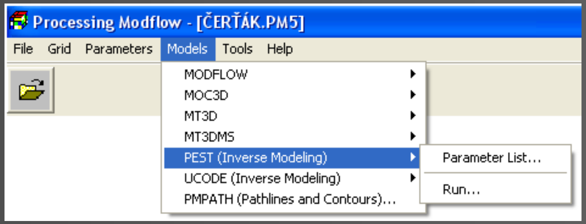
$$Q_k = Q_{total} \frac{T_k}{\sum T}$$

- **Unconfined layer** – to set a very large vertical hydraulic conductivity (e.g. 1 m/s) to all cells of the well
- **Exact extraction rate** from each penetrated layer – to set a minimal pumped rate to the each layer (e.g. 1.10^{-10}) and than use the water budget calculator

Next flow packages:

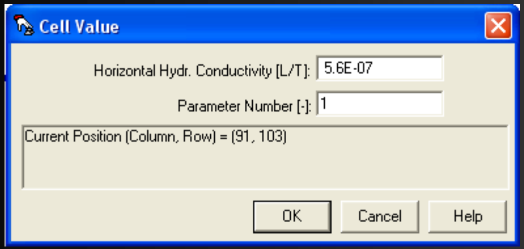
- Horizontal-Flow barrier – thin impermeable geologic feature (fault, slurry wall), impede the horizontal flow
- Density – approximation of density flow model without considering the salinity distribution
- Interbed Storage – water volume released from storage by elastic adn inelastic compaction of compressible fine-grained beds in a aquifer due to groundwater extraction
- Wetting capability – the simulation of a rising water table into dry model cells

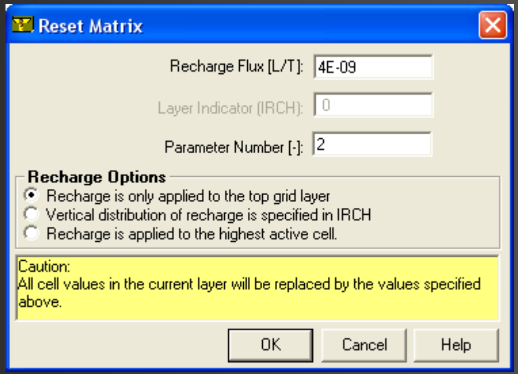
PMWIN – PEST, UCODE

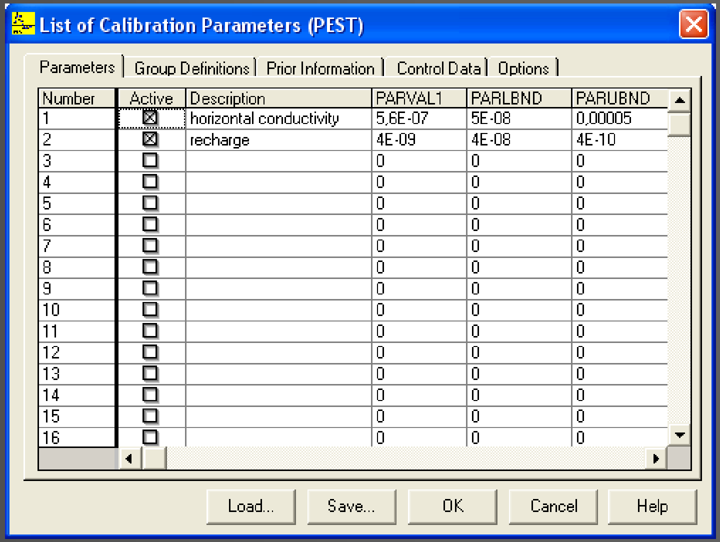


Automated parameter calibration:

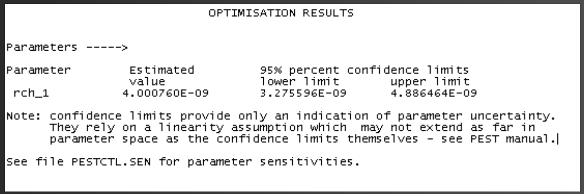
- Assign parameter number to calibrated value
- Calibrated value : hydraulic parameters, storage parameters, recharge and boundary conditions III. type







- Output file PESTCTL.REC includes optimized results



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                         OPTIMISATION RESULTS


Parameters ----->

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See file PESTCTL.SEN for parameter sensitivities.
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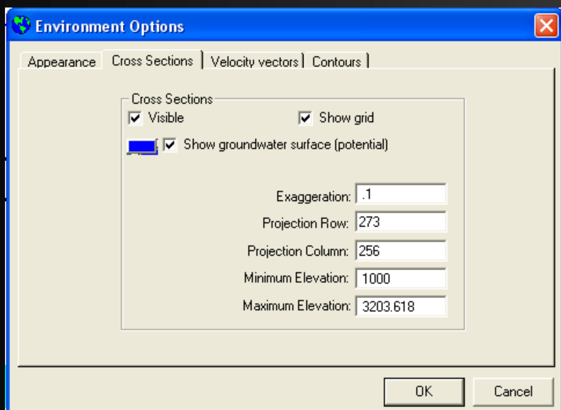
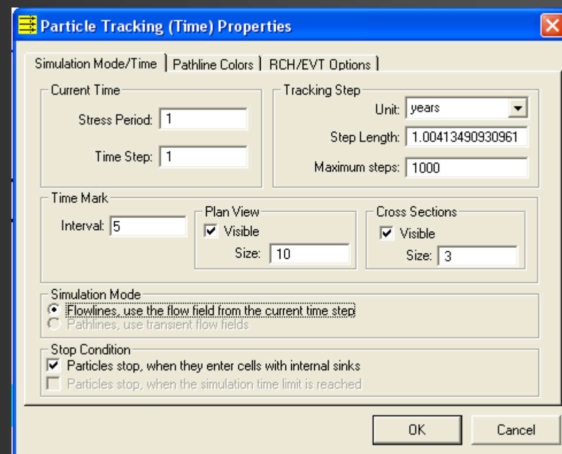
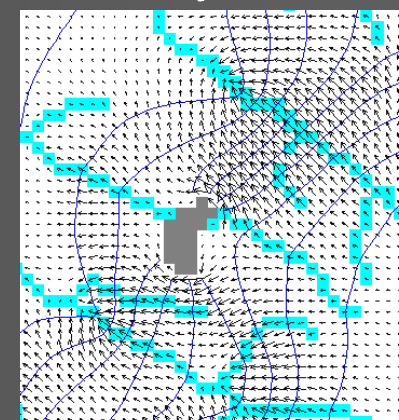
Advective modeling - based on flow field from Modflow, 3-D demonstration of the flow

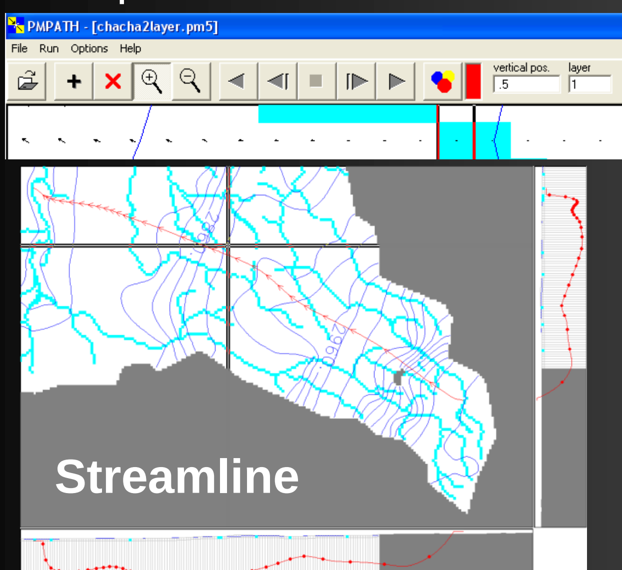




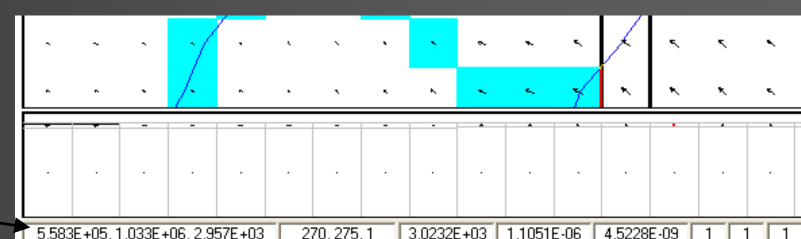
Velocity Vectors



Control panel



Information board



Position of the mouse pointer – real coordinates

Number of particles

Position of the mouse pointer – cell indices

Head at the cell

Horizontal pore velocity at the cell

Vertical pore velocity

Current stress period

Current time step

PMWIN – MOC3D, MT3D, MT3DMS

Transport models:

- based on the flow field from modflow
- solute transport - advection, affected by disperzion, diffusion and retardation

MOC3D – define the subrid for solute-transport equations

MT3D, MT3DMS – similar, solute-transport within Modflow grid with own boundary conditions

Input parameters

- Initial Concentration and Source/Sink Concentration
- Advection (from Modflow)
- Disperzion:

Horizontal transverse dispersivity

Vertical transverse dispersivity

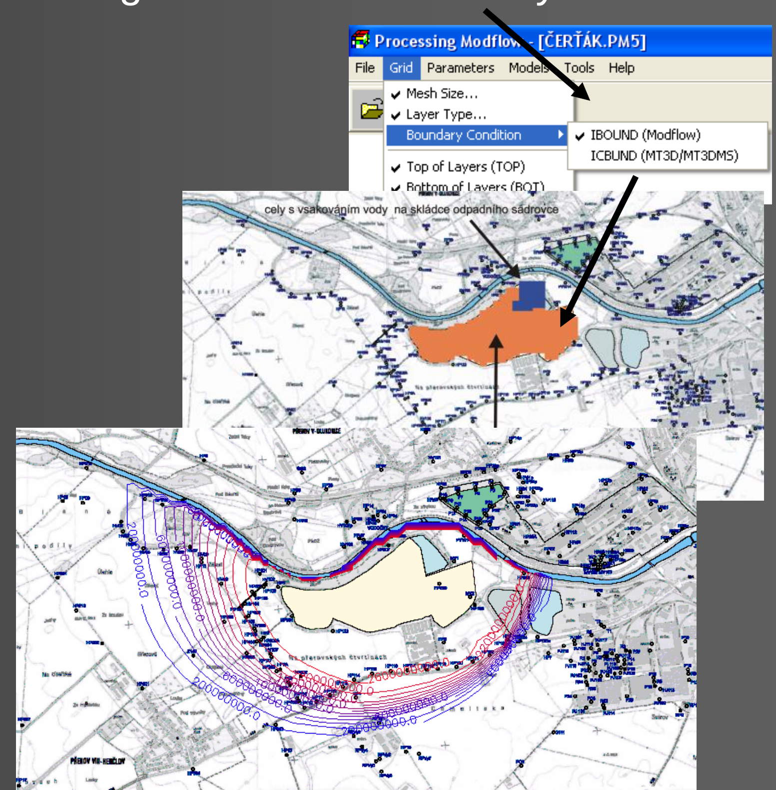
Longitudinal dispersivity

- Chemical reaction

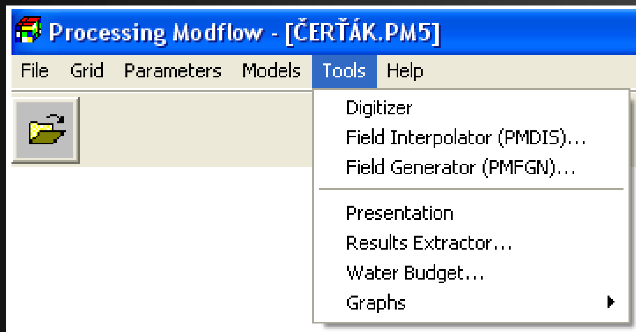
The effective molecular diffusion coefficient

Sorption - Linear and unlinear Freundlich and Langmuir equilibrium isotherm

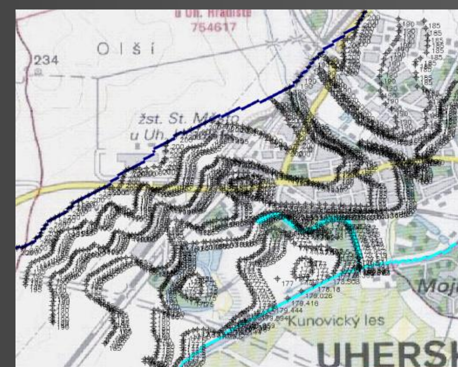
Rdioactive decay or biodegradation - First order decay rate and First order sorbed rate



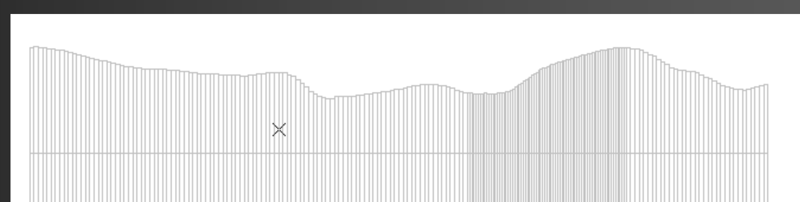
PMWIN – Tools



- Digitizer – digitized points



- Field Interpolator – interpolation of digitized points to the 3-D surface



- Field Generator – stochastic modeling – generate field with heterogeneously-distributed hydraulic conducitivity values

PMWIN – Tools

Results Extractor:

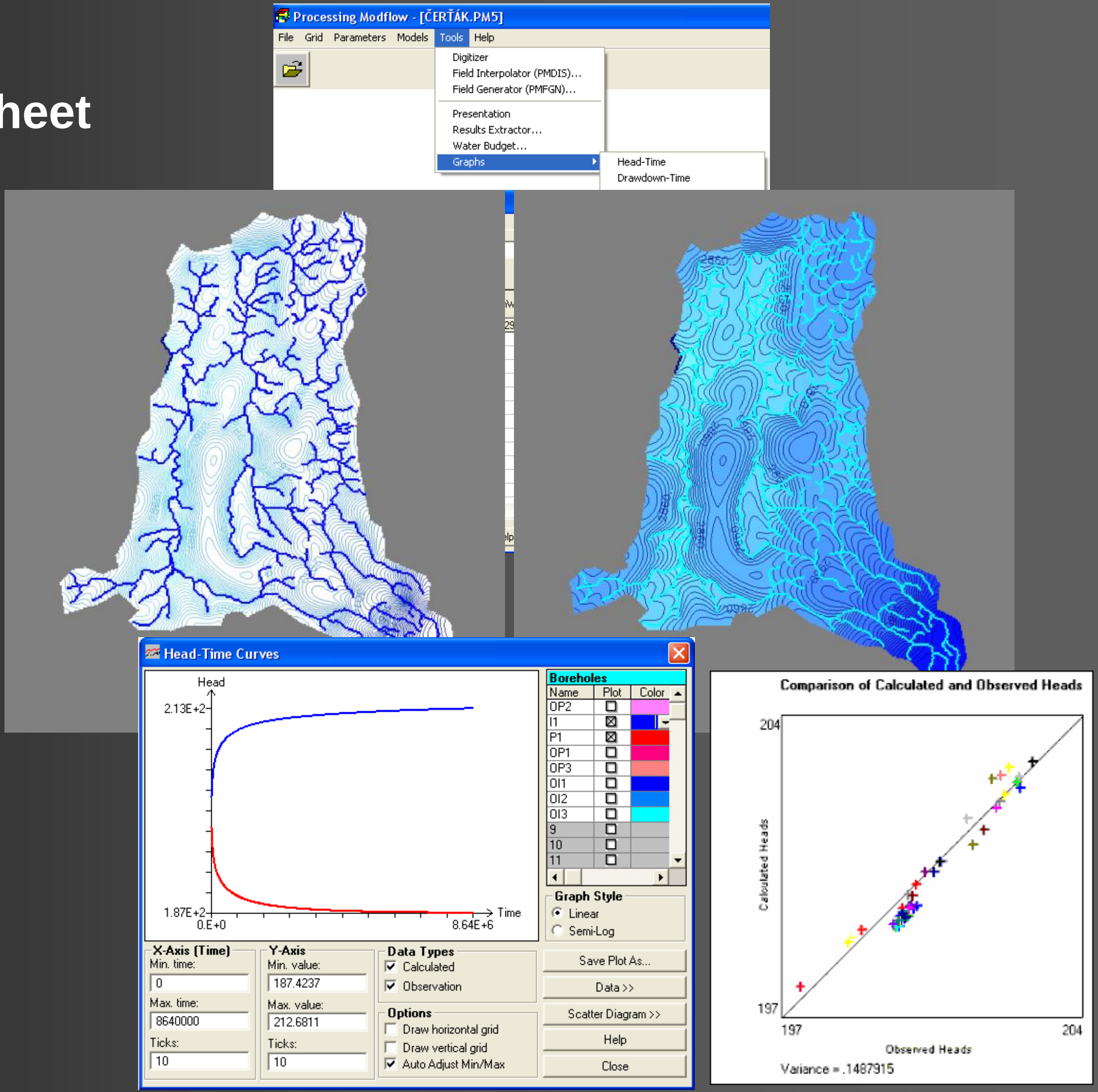
Resultant data sets in the sheet

Presentation:

Load resultant data sets

Graphs:

- Time dependent results
- Scatter diagram



Water Budget

- Check the quality of the simulation results
- Allow flow rates between all faces of model cell

- Zone – flow rate exchange across the cell
- Whole model – compare the discrepancy

Water balance Discrepancy:

- Recommended discrepancy < 1%
- Discrepancy > 1% denotes coarse grid, high closure (convergence) criterium, too long time step
- Discrepancy > 10% denotes incorrect conceptual model

```
WATER BUDGET OF ZONES WITHIN EACH INDIVIDUAL LAYER

 ZONE    1   IN LAYER    1
 ----------------------------------------------
        FLOW TERM            IN              OUT            IN-OUT
          STORAGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
    CONSTANT HEAD  0.0000000E+00  0.0000000E+00  0.0000000E+00
  HORIZ. EXCHANGE  7.8715780E-04  3.2653283E-05  7.5450452E-04
EXCHANGE (UPPER)   0.0000000E+00  0.0000000E+00  0.0000000E+00
EXCHANGE (LOWER)   1.6763251E-02  1.3197104E-03  1.5443541E-02
            WELLS  0.0000000E+00  0.0000000E+00  0.0000000E+00
           DRAINS  0.0000000E+00  0.0000000E+00  0.0000000E+00
         RECHARGE  1.5850021E-03  0.0000000E+00  1.5850021E-03
               ET  0.0000000E+00  0.0000000E+00  0.0000000E+00
    RIVER LEAKAGE  0.0000000E+00  1.7783154E-02 -1.7783154E-02
  HEAD DEP BOUNDS  0.0000000E+00  0.0000000E+00  0.0000000E+00
   STREAM LEAKAGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
INTERBED STORAGE   0.0000000E+00  0.0000000E+00  0.0000000E+00
MULTI-AQIFR WELL   0.0000000E+00  0.0000000E+00  0.0000000E+00
SUM OF THE LAYER   1.9135412E-02  1.9135518E-02 -1.0617077E-07
 DISCREPANCY [%]   0.00

 ZONE    1   DOES NOT EXIST IN LAYER    2
-------------------------------------------------------------------

WATER BUDGET OF ZONES OVER THE ENTIRE MODEL

ZONE: 1
----------------------------------------------
                             IN              OUT            IN-OUT
          STORAGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
    CONSTANT HEAD  0.0000000E+00  0.0000000E+00  0.0000000E+00
  HORIZ. EXCHANGE  7.8715780E-04  3.2653283E-05  7.5450446E-04
EXCHANGE (UPPER)   0.0000000E+00  0.0000000E+00  0.0000000E+00
EXCHANGE (LOWER)   1.6763251E-02  1.3197104E-03  1.5443541E-02
            WELLS  0.0000000E+00  0.0000000E+00  0.0000000E+00
           DRAINS  0.0000000E+00  0.0000000E+00  0.0000000E+00
         RECHARGE  1.5850021E-03  0.0000000E+00  1.5850021E-03
               ET  0.0000000E+00  0.0000000E+00  0.0000000E+00
    RIVER LEAKAGE  0.0000000E+00  1.7783154E-02 -1.7783154E-02
  HEAD DEP BOUNDS  0.0000000E+00  0.0000000E+00  0.0000000E+00
   STREAM LEAKAGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
INTERBED STORAGE   0.0000000E+00  0.0000000E+00  0.0000000E+00
MULTI-AQIFR WELL   0.0000000E+00  0.0000000E+00  0.0000000E+00
SUM OF ZONE(  1)   1.9135412E-02  1.9135518E-02 -1.0617077E-07
 DISCREPANCY [%]   0.00

WATER BUDGET OF THE WHOLE MODEL DOMAIN:

        FLOW TERM            IN              OUT            IN-OUT
          STORAGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
    CONSTANT HEAD  7.1051237E-03  2.0705394E-02 -1.3600271E-02
            WELLS  0.0000000E+00  0.0000000E+00  0.0000000E+00
           DRAINS  0.0000000E+00  0.0000000E+00  0.0000000E+00
         RECHARGE  5.6796219E-02  0.0000000E+00  5.6796219E-02
               ET  0.0000000E+00  0.0000000E+00  0.0000000E+00
    RIVER LEAKAGE  0.0000000E+00  4.3201953E-02 -4.3201953E-02
  HEAD DEP BOUNDS  0.0000000E+00  0.0000000E+00  0.0000000E+00
   STREAM LEAKAGE  0.0000000E+00  0.0000000E+00  0.0000000E+00
INTERBED STORAGE   0.0000000E+00  0.0000000E+00  0.0000000E+00
MULTI-AQIFR WELL   0.0000000E+00  0.0000000E+00  0.0000000E+00
-------------------------------------------------------------------
              SUM  6.3901342E-02  6.3907348E-02 -6.0051680E-06
 DISCREPANCY [%]  -0.01
```

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