BoxModel Concept: ReacFlow3D

Modelling of the flow of mine water and groundwater, mass and heat transport

Program description

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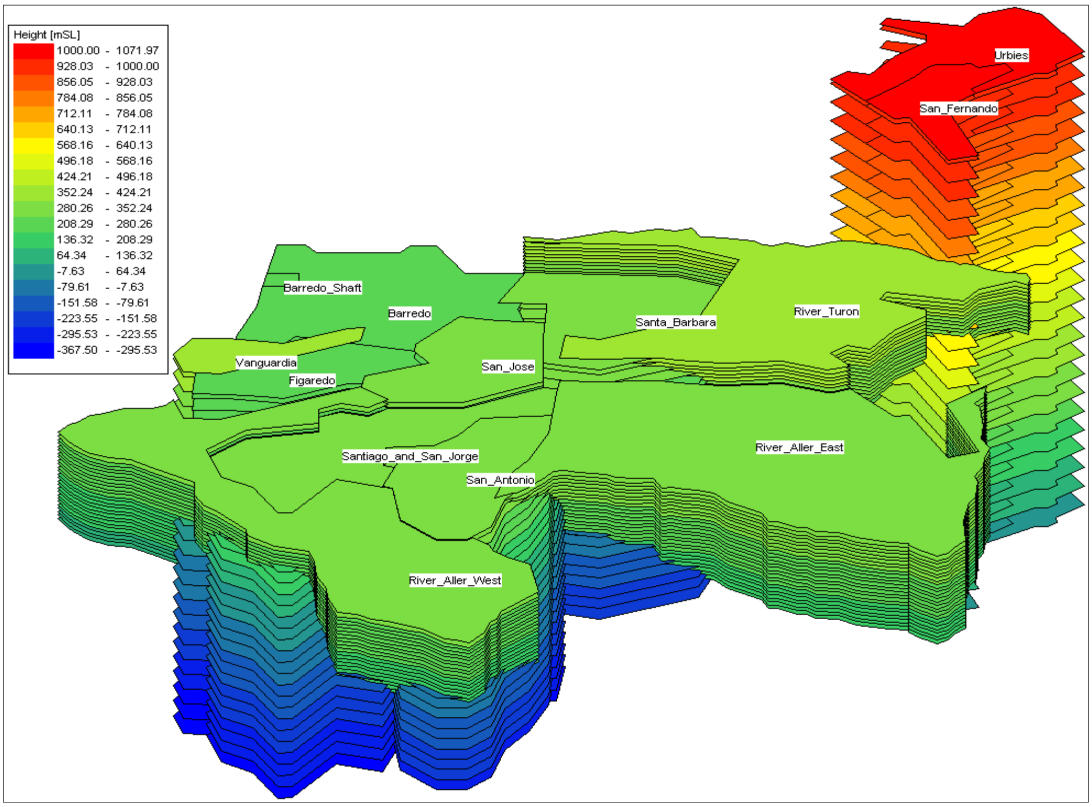
BoxModel Concept: ReacFlow3D

CAD system:	BOXCAD
Pre-processor:	PRAEBOX
Box model:	BOX3D

Rev. 2, 10/2011



BoxModel Asturias (Spain)

Contents

1 Scope of services

The BoxModel Concept: ReacFlow3D is a 3D finite volume program for modelling the flow of groundwater and mine water, heat transport and multi-component mass transport including sorption, microbial degradation and the reactions with minerals. A special feature is the highly flexible discretisation to model geological structures such as layers and faults as well as structural mining elements and mine excavations.

Water management in operating mines

- Consideration of pump performance curves, influence of pipes, etc.
- Scenarios of breaking through between operating and abandoned mine sections

Discretisation – BoxModel Concept

- Extremely flexible discretisation
- Different quantities and structures of cells (boxes) per slice
- Numerous quantities and types of connection between cells (boxes)
- Compatible with all FE/FD models
- Turbulent flow in pipes, drives and shafts
- Reduction of cell quantities using the Analytical Element Method (AEM)

Multi-component transport

- 57 pre-installed transport units
  (MKW, PAH, VOC, SO4, CO3, Fe, pH-, Eh-calculation)
- Organics and inorganics
- Pitzer coefficients
- Surface complexation
- Ion exchange

2 Application examples

The following figures give an overview of the great flexibility of the applications.

2.1 Geothermal energy from mine water

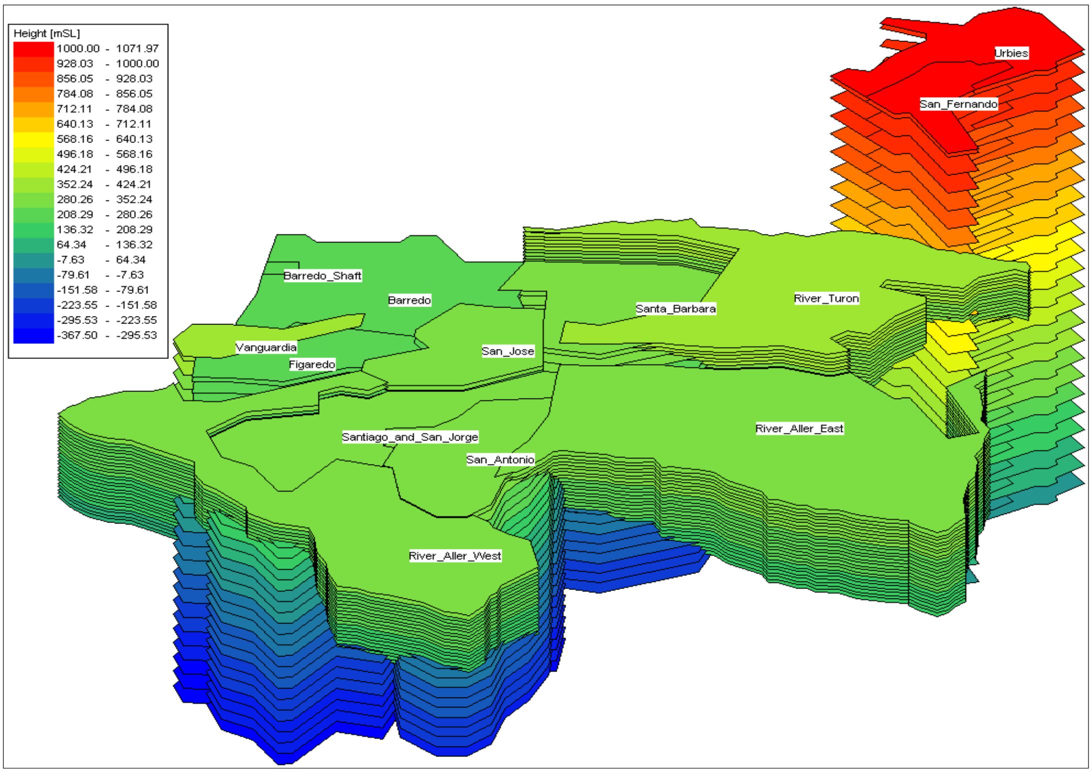


Figure 1: *BoxModel of Asturias, Spain*

- Calculation of flooding dynamics, variation of temperature, variation of sulphate and iron concentrations and distribution
- Characterised by highly textured bedrock

2.2 Special discretisation considering faults

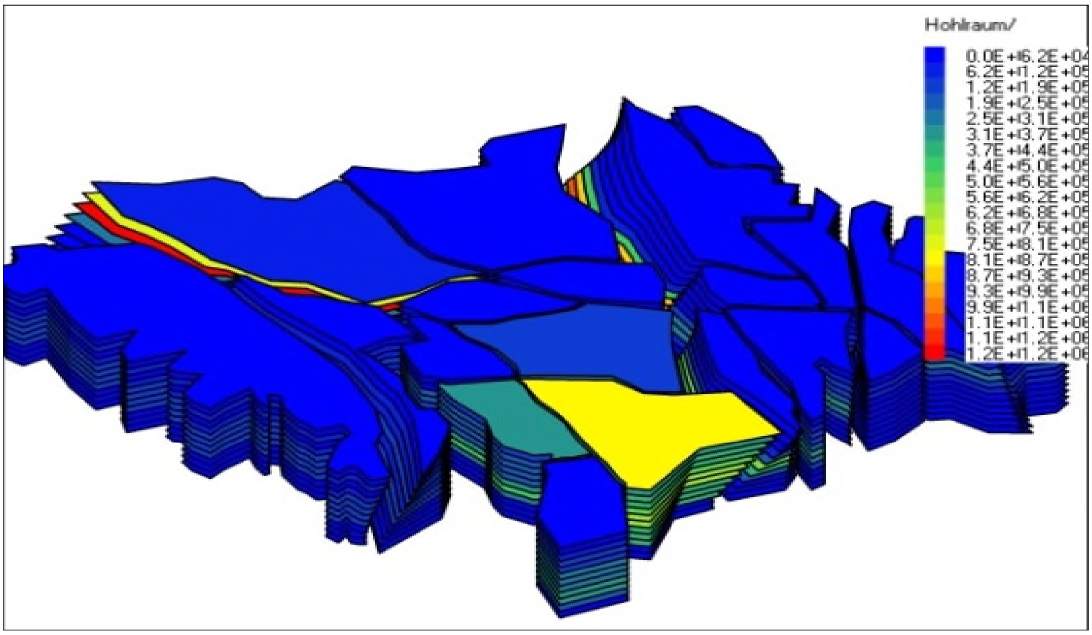


Figure 2: *BoxModel of Oelsnitz, Germany*

- Calculation of flooding dynamics
- Adaptation to fault system

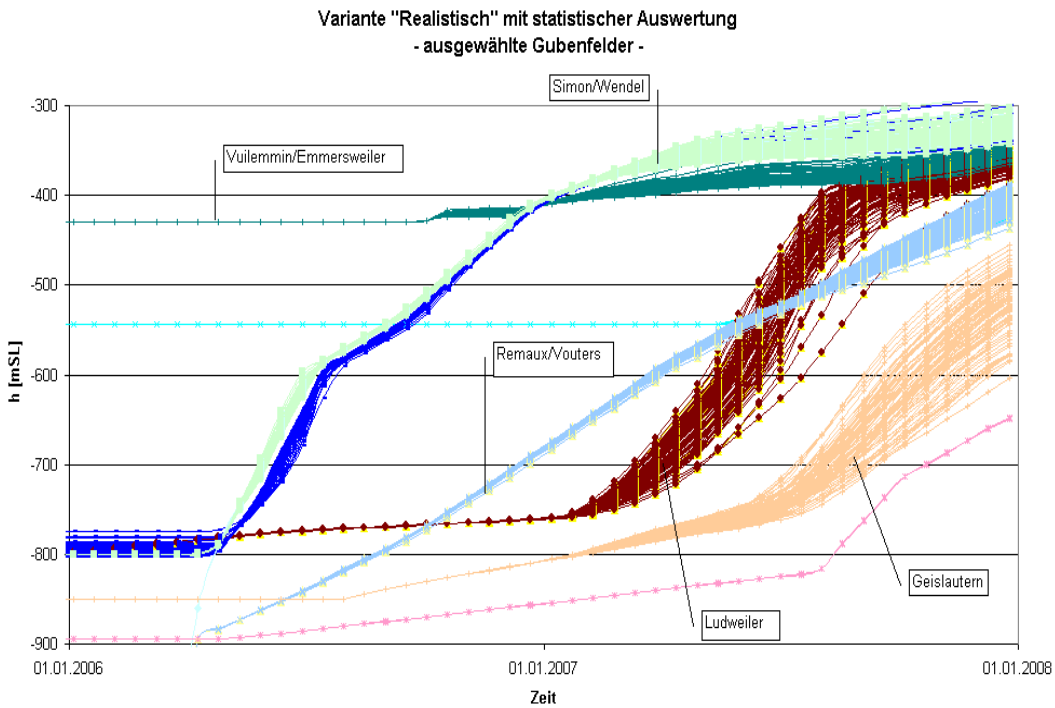


Figure 3: *Statistical evaluation of flooding scenario*

2.3 Prediction of quality of overflowing mine water

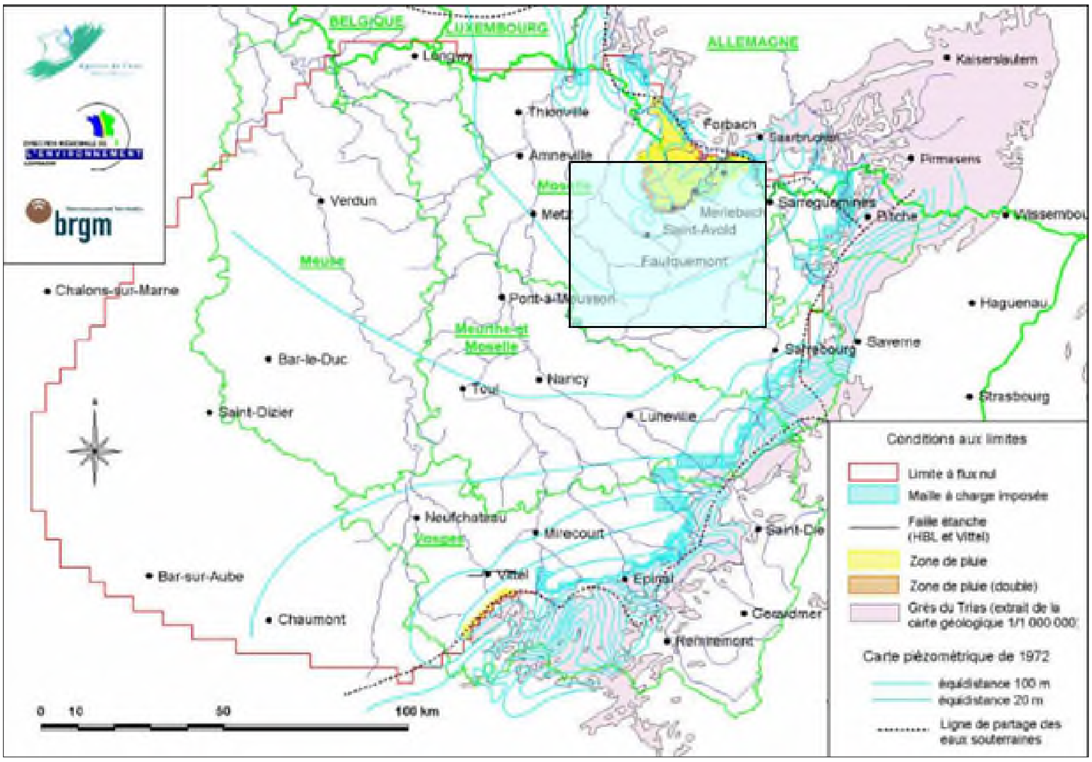


Figure 4: *Area map of Lorraine District, France*

- Calculation of flooding in the Lorraine coal mining district
- Calculation of the change in water quality
- Linking the aquifer and coal mine box model

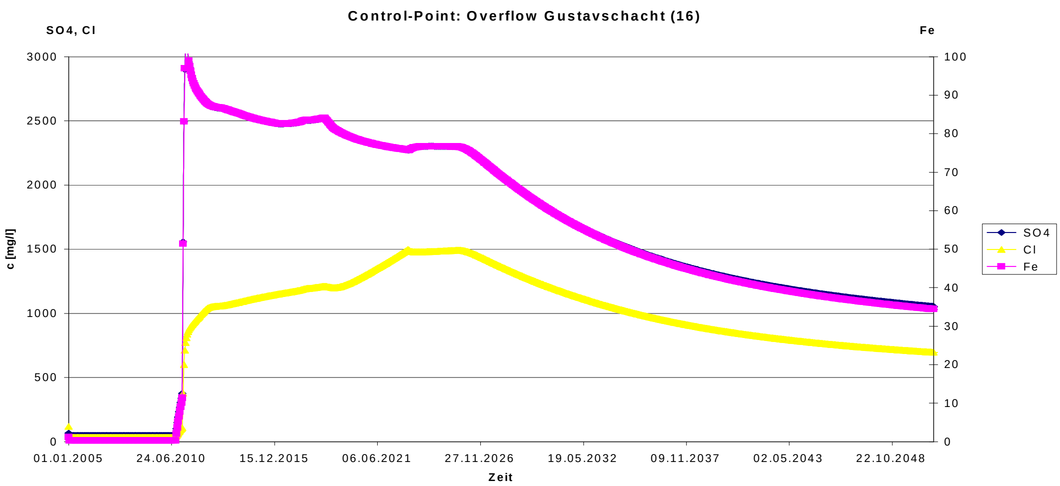


Figure 5: *Prediction of quality of overflowing mine water*

Prediction of water quality

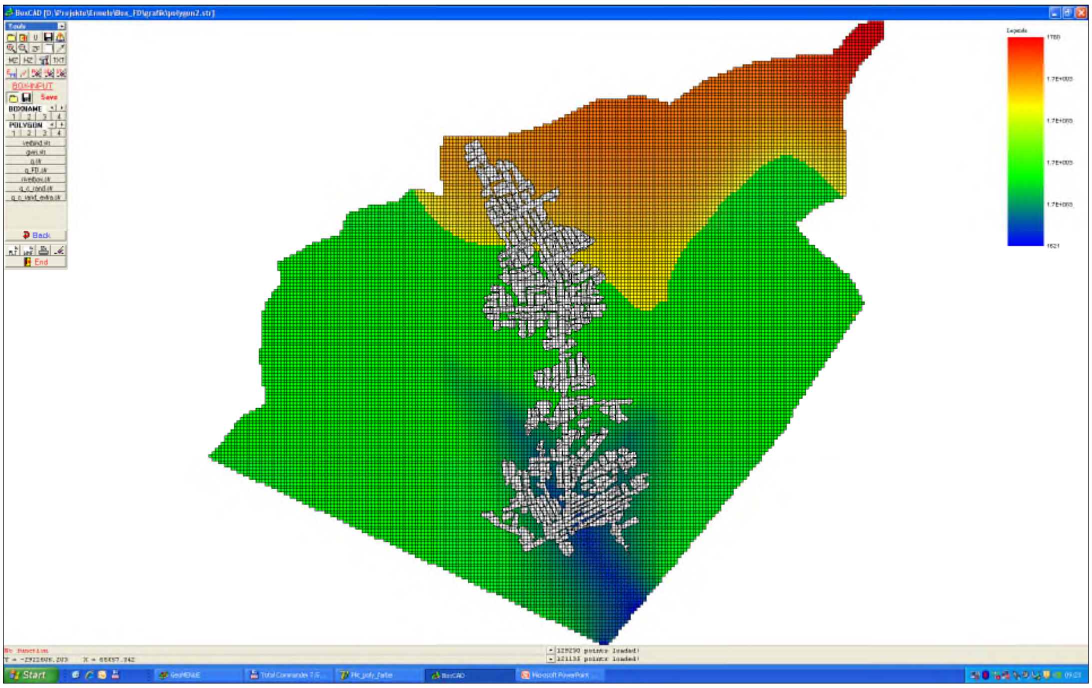


Figure 6: *Water model of Ermelo, South Africa*

- Calculation of flooding. Question: Will there be an overflow due to flooding
- Calculation of change in water quality
- Linking the aquifer and coal mine box model

2.4 Modelling of the flow in faults

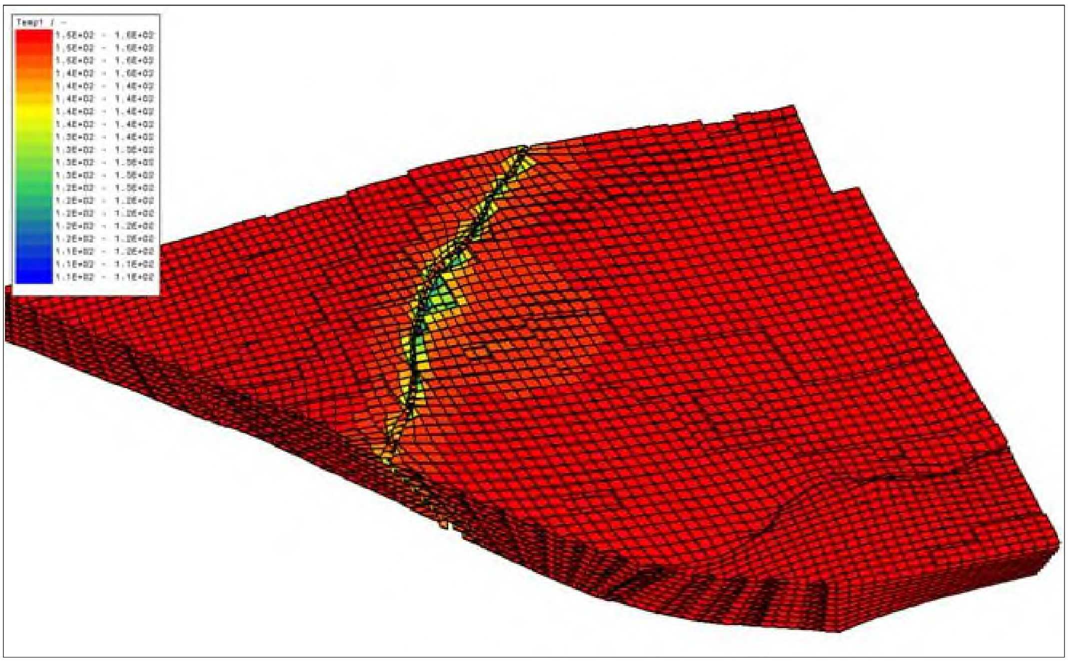
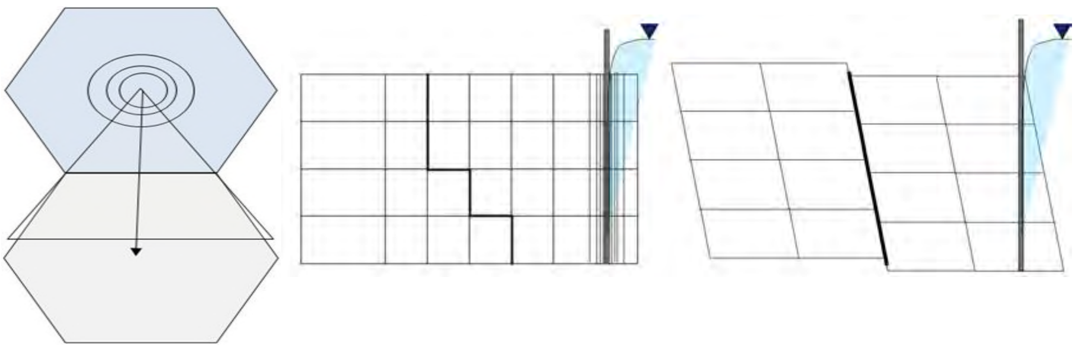


Figure 7: *Explicit modelling of the flow in faults with Petrel interface (deep geothermal aquifer, Germany) using the Analytical Element Method*

- Geothermal energy project
- Heat propagation in faults
- Functional discretisation
- Using Analytical Element Method:
  $Q = (h - h_B) \cdot 2 \cdot \pi \cdot k_f \cdot m / \ln(r / r_B) \cdot angle\_sector / 360$



2.5 Regional model including numerous mine drives

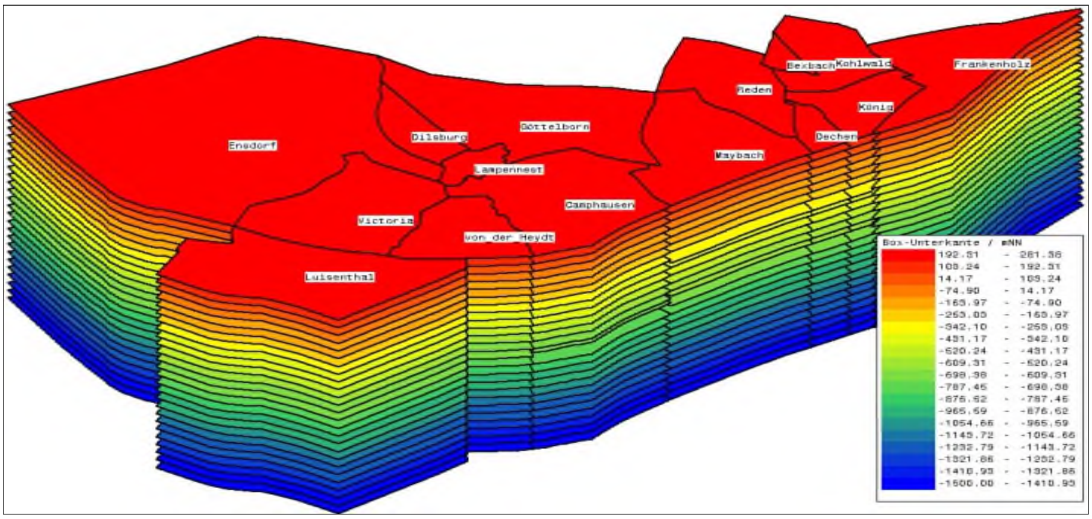


Figure 8: *BoxModel of Saar District, Germany*

- Box model of mine
- Calculation of change in water quality
- Incorporating more than 100 drives without additional refinement of the boxes

2.6 Interrelationship between complex mining system and aquifers in the overburden

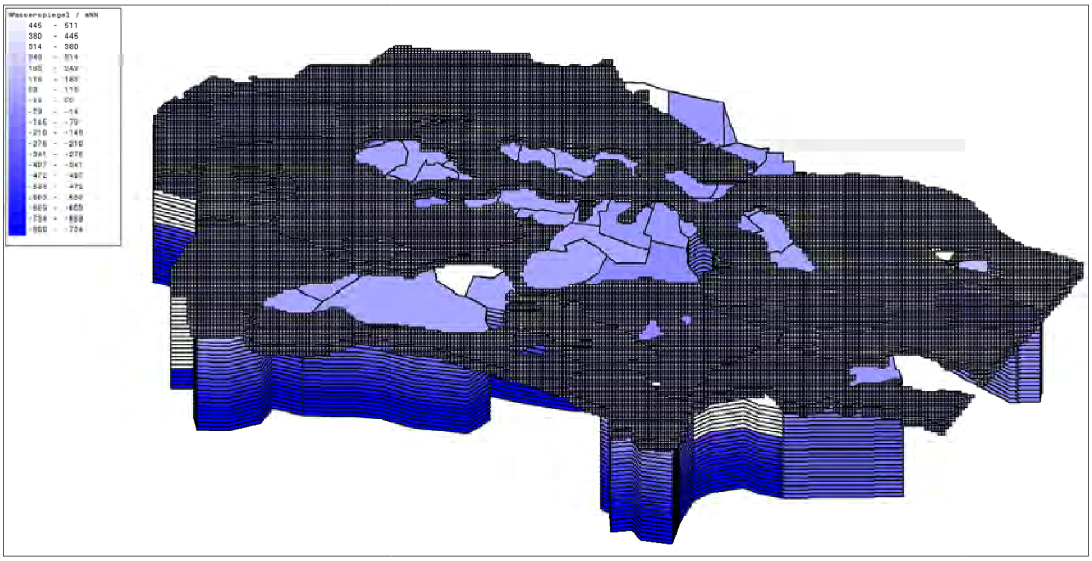


Figure 9: *Water model of Silesian Coal Basin, Poland*

- Linking up coal mine box model and three aquifers
- Calculation of flooding
- Calculation of change in of water quality

2.7 Sulphite prediction / scenarios of water breaking through between operating and abandoned areas

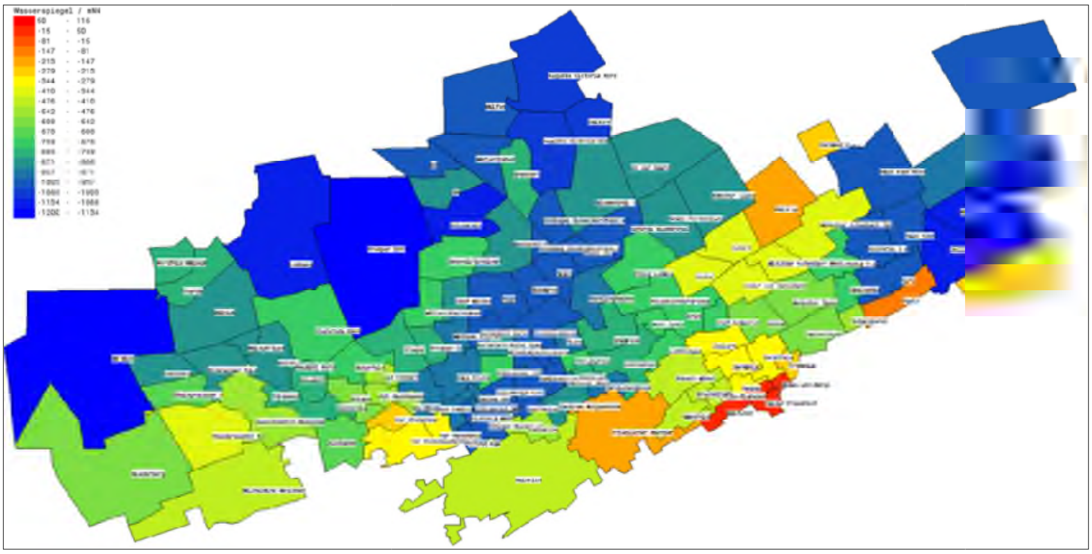


Figure 10: *Water model of Ruhr District, Germany*

- Expansive model area (120 km x 80 km)
- Calculation of flooding
- Calculation of change in of water quality (e.g. Cl-, SO42-, iron, barium)
- Safety investigations into a possible break-through of mine water between operating and abandoned mine areas
- Implementation of density layering

Density layering

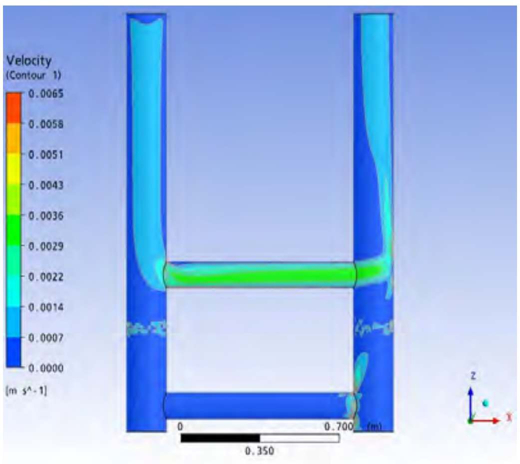


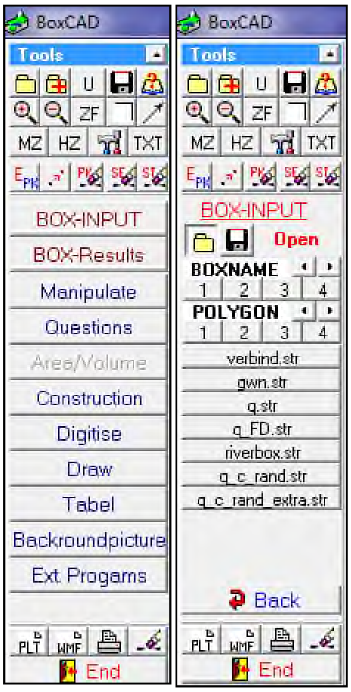
Figure 11: *Consideration of double diffusion*

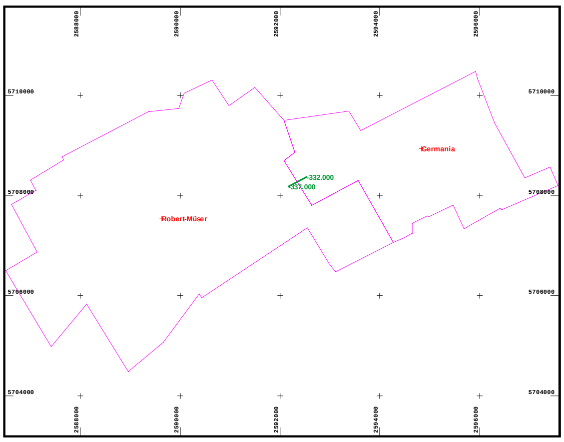
3 Program structure

BOXCAD

The program distinguishes between CAD data and model data. The former are saved in a graphics path, the model data are saved in a model path. Results of the simulation are saved in a subdirectory of the model path (<modelpath/result>).

Graphic data	Model data
- Boxes - Hydraulic connections between boxes including properties	1. Initial conditions, e.g.: - Hydraulic conductivity - Permeability - Porosity 2. Boundary conditions, e.g.: - Hydraulic head - Pumping rates - Flux - Recharge → All defined in the corresponding files (see chapter 4.2)

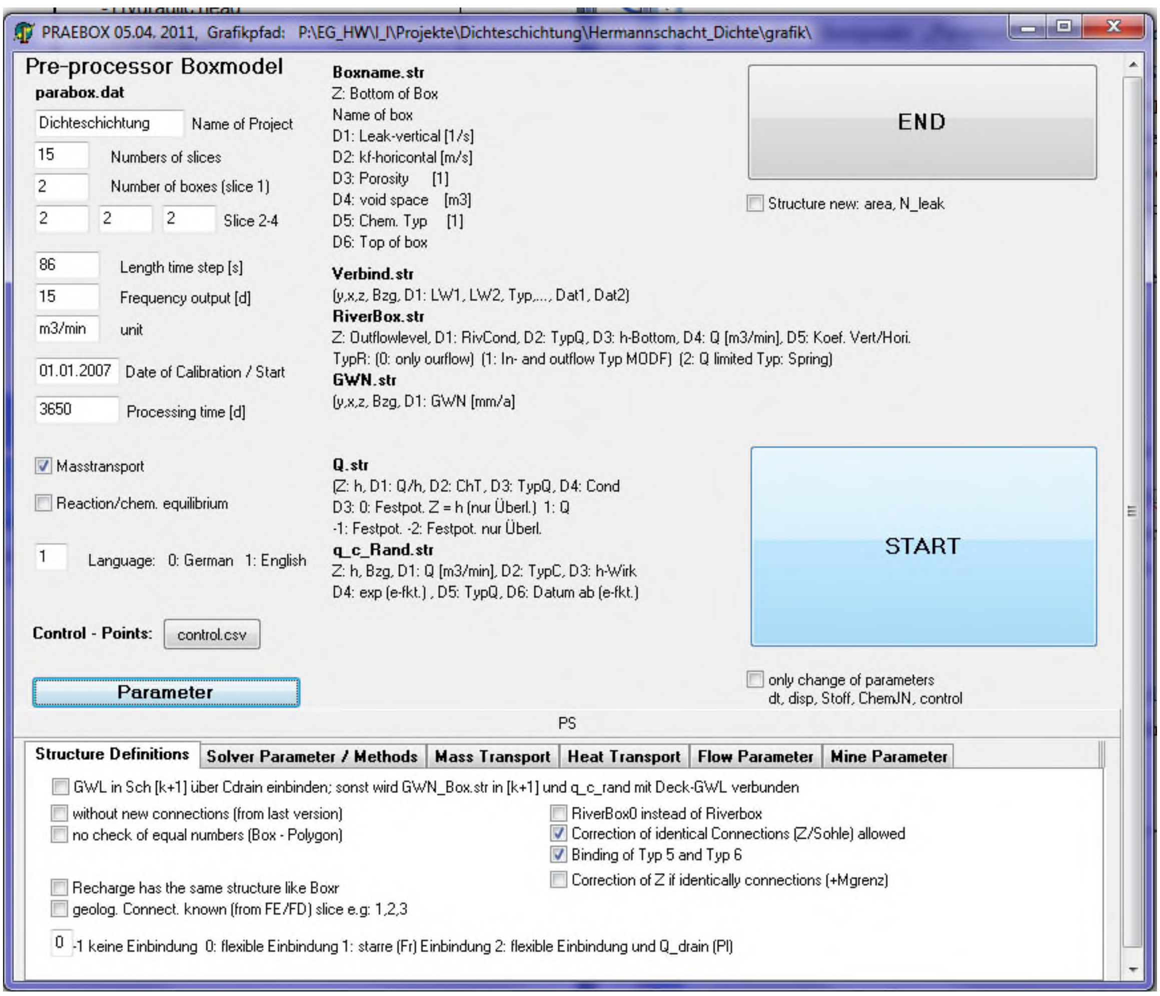




Example of a connection in CAD system

PRAEBOX

After setting the graphic and model data, the PRAEBOX is started and all the data are recreated in the preprocessor. When the preprocessor has completed the calculations and created the matrixes, the box model can be started.

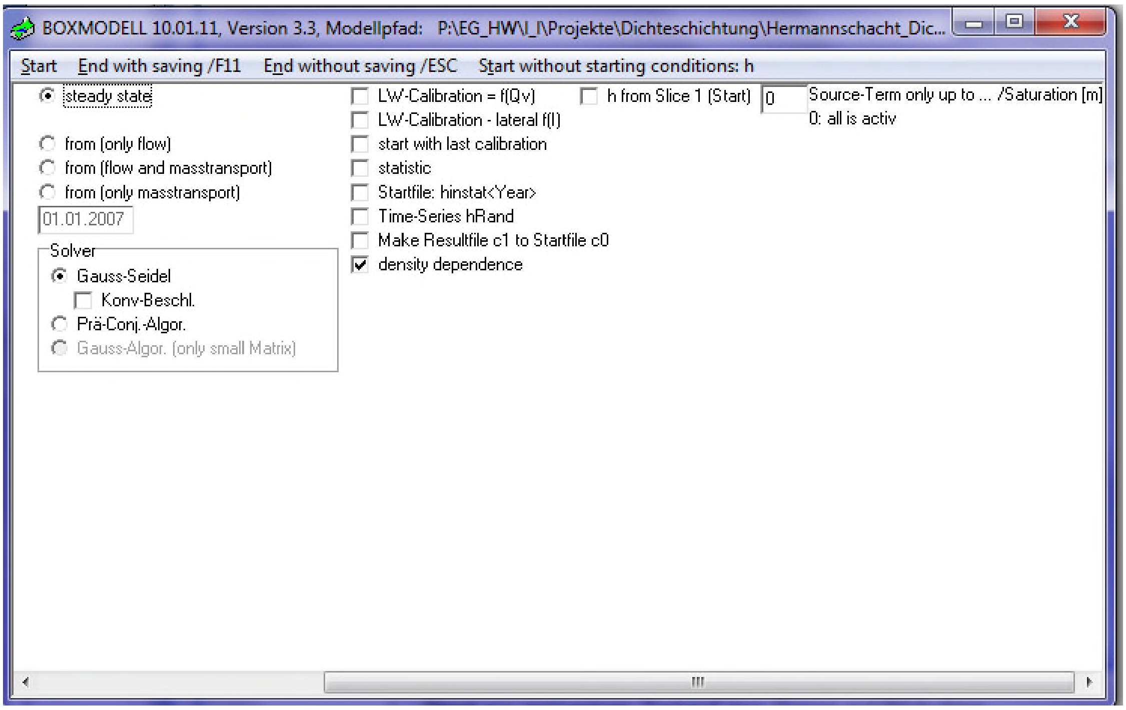


In this dialogue, the control and process parameters, solver methods as well as parameters for mass and heat transport, flow and mine parameters and so on can be defined.

BOX3D

After creating the matrixes, the box model BOX3D is started.

Several options can now be selected.



Options:

1. **Start**ing from a steady state, the date can be defined.
2. **End with saving**.
3. **End without saving**.
4. **Start without starting conditions: h** (“cold boot”)

When a new project is started for the first time, there is no initial water table information set for the calculation. In this case only, option 4 is required. The program starts by setting the water table at 1 m above the level of the bottom of each box.

Each simulation run must be completed by option 2 or 3 (End with or End without saving). If a steady state simulation is carried out, the result of the water table calculation is saved by option 2 in a data file (e.g <h2007.dat>). This data file can then define the starting conditions for further unsteady state calculations. Follow-up work on the model (calibration, increasing water table calculation) usually employs option 1. Option 4 is required only if a structural change such as “addition of boxes” or “increasing number of slices” is made.

Results

The strategy for further processing is to utilize the spatial data results of the simulations with GeoCAD (creation of the 3D string format) and outsource various files to a format that can be read by Excel™ (.csv) for further processing. Specifically this concerns the following data:

<u>CAD (string) data</u>	
Flow vectors	VEK1.str
Water table	h-nz.str
<u>Time series</u>	
Water table (hydraulic potential) development	h1(t).csv
Flow rate, outflow	Q-(t).csv
Flow rate, inflow	Q+(t).csv
Concentrations	c1(t).csv...cn(t).csv
<u>Tables</u>	
Water table	h1.csv
Flow rate, outflow	Qbound(-).csv
Flow rate, inflow	Qbound(+).csv
Void volume	BergHV.csv
Porosity	Po.csv
Box balance	Bilanz.csv
Vertical flow rate	Vz.csv
<u>Text data</u>	
Individual balance sheet	Bilanz.txt
Balance of the boxes with the same name	Summe-2d.dat

The csv.-format can now be imported into Excel™, where the axes labels should have already been assigned.

The most detailed balance is given in the results file <BILANZ.txt>. An example is shown below. Each partial stream is listed separately for each mining claim.

In the data file all positive values define an inflow into the balance area, all negative values define an outflow.

Example for Bilanz.txt:

Balance for mining claims:

Current state	04.03.2011 09:12:08
Calculating time d, a	18.00

Total void volume (pores + mine)	[m³]	6.59E+08
Total water volume (leakage + flooding)	[m³]	6.59E+08
Water volume (leakage)	[m³]	0.00E+00
Total mining void volume	[m³]	6.59E+08
Discharge	[m³/min]	138.277
Total precipitation	[m³/min]	134.339
Total precipitation (maximum)	[m³/min]	134.339
Total pump volume	[m³/min]	0.000
Balance	[m³/min]	-3.937
Balance	[%]	-2.9309

Slice 1

Mine field name, i, k	An_der_Haard 1 1		
Catchment area ÜT	[km²]	17.983	
Percolation rate	[mm/a]	15.000	
Water table	[msL]	-637.562	
Bottom of slice	[mSL]	-637.610	
Q with cell i, k	[m³/min] 3, 8 =	0.00000	Blumenthal_C -638.14779 type: 10
Q total	[m³/min]	0.00000	
Q(k-)	[m³/min]	0.51320	
Q(k+)	[m³/min]	0.51320	
Pumping rate	[m³/min]	0.00000	
Q boundary(-)	[m³/min]	0.00000	
Q boundary(+)	[m³/min]	0.00000	
Balance	[m³/min]	0.00000	
Balance	[%]	0.00000	

4 Details of program units

4.1 Introduction to program units

BOX3D has been developed to calculate stationary and transient state three-dimensional flow and reactive mass as well as the heat transport in unsaturated and saturated porous media with a special adaptation to the conditions found in mines. The mathematical base of the software is a freely definable volume balance method, which is able to consider irregular geometries (boxes). The flow model is directly coupled to a reactive mass transport model. Both models are solved simultaneously.BOX3D can take into account several hydraulic elements such as groundwater layers, mine drives, faults and fractures, drainage systems and so on.

Besides the great variety of hydraulic elements the model considers several hydraulic laws such as laminar and turbulent flow and the time dependence of conductance. The **PRAEBOX** pre-processor accepts the prepared CAD datasets into the world of model data.

The data are input as CAD datasets and all changes within the model are effected by changing these datasets. The basic data format is Surpac™. The Box Model has its own CAD tool integrated; this is named **BOXCAD** and is a simplified Surpac™ with the original Surpac™ format. Alternatively it is possible to use the original Surpac™ software.

4.2 Model data

CAD datasets

The principles of modelling with BOX3D are given in the following CAD datasets and text files. Everything is implemented by means of these. The format of the CAD datasets is identical to those of the mining planning tool Surpac™ from the company GEMCOM Software International Inc.:

CAD data (northing, easting, altitude):

BoxnameX.str (1)	**Point**: 3D coordinates of each central point of a box
	name, leak coefficient, permeability, porosity, void, chemical type (X: generated per model slice)
PolygonX.str	**Boundary polygons** for each box
	(X: generated per model slice)
Verbind.str	**Line**: hydraulic connection between boxes
	Coefficient 1 , coefficient 2, type, length, from, to (date)
GWN.str (2)	**Point**: recharge rate per box in slice 1
Q.str (3)	**Point:** pumping rate / boundary conditions (type 1, 2)
Q_c_Rand.str (4)	**Point:** external boundary (type 3)
RiverBox.str 5)	**Point:** river package per box
Linie1.str	**Points, lines: background while model is running**

Text files:

Control.csv	Control points for time series
Parabox	environmental parameters
ZusatzHV.csv	additionally estimated void space if detailed information is not available

For mass transport:

Chemieaktiv.csv	pH/Eh value – identification of those boxes for calculation with chemical equilibrium: if box is not mentioned, default is no
Stoffinaktiv.csv	Identification of those boxes for calculation of mass transport: if box is not mentioned, default is yes

Fakliq.dat, Faksol.dat, Fakgas.dat

	Conversion factors [mg/l] to [mol/l] in liquid, solid and gaseous phase
LiquidX.dat	Field of concentration set for chemical type X, liquid
LiquidRX.dat	Field of concentration set for chemical type X, stagnant
EfakBoxX.dat	Kinetic constants for chemical reactions

The first piece of information of a Surpac™ dataset is the number of the string. The string number is responsible for the colour on the screen and/or for the grouping of themes. The next columns contain the X-(RW), Y-(HW), and Z-(ZW) values and seven additional blanks for description, each separated by a comma.

Example:

Str, Y-, X-, Z-, D1, D2, D3, D4, D5, D6, D7

1, 56700.123, 45300.543, 541.243, XYZ, 53.7, Meyer, Gold, 1E-8, 01.01.2000, 31.12.2009

The accuracy of the X-, Y-, Z- coordinates is one mm [0.001 m].

The simplest dataset is a **point**.

A **segment** is a row of points. A row filled with zeros separates points. Points without a "zero row" are connected to a line.

4.2.1 Boxname.X.str

- Graphic element: point in 3D-space

- Related to the central point of a box (storage parameters and chemical data)

- X means that this dataset has to be generated for each slice X

The same applies for the following file <Polygon..X.str>.

Str	HW	RW	ZWUK	Boxname	Leak	k_f	Po	HV	ChTyp	ZWOK
[1]	[m]	[m]	[mSL]	text	[1/s]	[m/s]	[1]	[m^3]	[1]	[mSL]

Text line

Text line

1, 5714522.908, 2588111.219, -170.000, FriedrichderGrosse, 1.00E-08, 1.00E-08, 0.00030, 0, 8, ,

0, 0.000, 0.000, 0.000,

1, 5715893.882, 2576352.516, -250.000, Bismarck, 1.00E-08, 1.00E-08, 0.00030, 185286.735, 1, ,

0, 0.000, 0.000, 0.000,

0, 0.000, 0.000, 0.000, End

ZWUK - bottom of a box

LEAK - leakage coefficient

k_f - permeability

Po - porosity

HV - void space

ChTyp - geochemical type of water in the box

ZWOK - top of a box

<u>Ch-Typ:</u>

Ch-Typ defines the geochemical type of the inflowing water. In this context, the preprocessor reads the file <LiquidRandX.dat> with the concentrations of the individual chemical ingredients.

4.2.2 Polygon.X.str

- Graphic element: closed polygon in 3D-space (last point = first point)

- Boundary polygon of boxes

The pre-processor compares each point of <BoxnameX.str> with all polygons of all slices and assigns points and polygons.

Str	HW	RW	ZW							
[1]	[m]	[m]	[mSL]							

Text line

Text line

4, 5717203.470, 2574302.410, 50.000, , , , , , , ,

4, 5717580.128, 2575104.704, 50.000, , , , , , , ,

4, 5714929.000, 2578022.103, 50.000, , , , , , , ,

4, 5713642.634, 2576307.169, 50.000, , , , , , , ,

4, 5717203.470, 2574302.410, 50.000, , , , , , , ,

0, 0.000, 0.000, 0.000,

0, 0.000, 0.000, 0.000, End

4.2.3 Verbind.str

- Graphic element: line (drive/connection with start and end point) in 3D-space

- File for all connections (horizontal, vertical and diagonal)

The pre-processor compares all the lines with all the polygons of all slices and detects which boxes are hydraulically connected.

Str	HW	RW	ZW	Text	Conductance1	Coeff2	Type	I	Date1	Date2
[1]	[m]	[m]	[mSL]	text	[m²/s]	[1]	[1]	[m]	01.03.89	01.03.02

Text line
Text line
1, 5706789.443, 2590188.855, -566.000, Strecke A, 1, 0, 1, 200, 01.01.1959, 01.01.2030,
1, 5705205.565, 2590291.952, -566.000, Strecke A, 1, 0, 1, 200, 01.01.1959, 01.01.2030,
0, 0.000, 0.000, 0.000,
1, 5708789.443, 2590688.855, -566.000, Strecke B, 1, 0, 1, 100, 01.01.1959, 01.01.2030,
1, 5703205.565, 2590867.952, -566.000, Strecke B, 1, 0, 1, 100, 01.01.1959, 01.01.2030,
0, 0.000, 0.000, 0.000,
0, 0.000, 0.000, 0.000, END

Date1 - date of installing a drive or connection

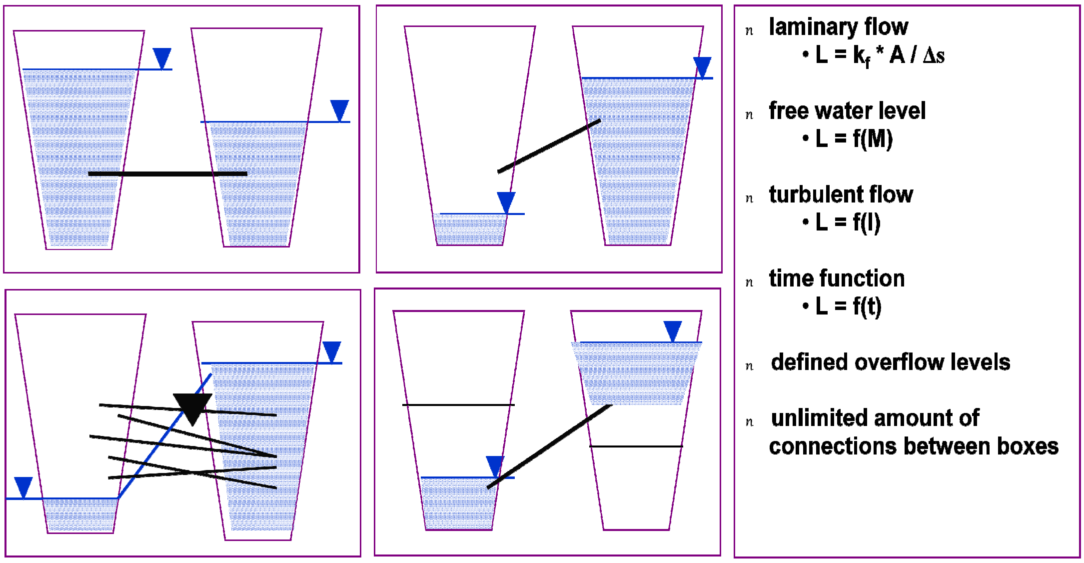


Figure 12: *Hydraulic connection types between boxes*

3	pipe (or drive)	turbulent flow	D, L
4	drillhole	turbulent flow	D, L
5	workings with defined point of overflow	laminar flow, L constant, information for calculation of L: scheme type 6 (without time function)	SW, L, M, A, B
6	multiplicity of connections (relatively undefined) or workings	laminar flow, flow starts at lowest level, independent of direction of flow; L increases linearly with water thickness, up to the highest level	SW, L, M, A, B
7	sinking from groundwater layer	replacement of q_c_rand.str	

Types of hydraulic connection

Type no.	Object	Description	Parameter
1	drive	laminar flow, conductance constant over time, precisely defined point of overflow	L
2	workings or convergence dependent on drive	laminar flow, L dependent on convergence **always time dependent**	*Coef1, Coef2, Date1 (based on calibrations)*
8	vertical connection	laminar flow; at very high permeability, the level of the bottom of the box has to be adjusted to the point of overflow	
9	drive	as 1) time independent L, but mostly in seam	L
10	geological connection	laminar flow, L constant or L proportional to thickness of water table in cell	
11	dam in drive	L constant, limited pressure altitude	
12	fault		

4.2.4 GWN.str

- Graphic element: points in 3D-space

- Recharge; implemented on top model slice

Str	HW	RW	ZW	Text	GWN					
[1]	[m]	[m]	[0]	text	[mm/a]					

Text line

Text line

1, 5715893.882, 2576352.516, 0.000, Bismarck, 7.000, 0, 0, 0, , ,

0, 0.000, 0.000, 0.000,

0, 0.000, 0.000, 0.000, End

4.2.5 Q.Str

- Graphic element: points in 3D-space

- Pumping rates from, to (sources and sinks)

Str	HW	RW	ZW	Text	Q or h or Qmax	TypCPump	TypQ	C	from	to
[1]	[m]	[m]	[mNN]	text	[m^3/min] [mNN]	[1]	[1]		date	date

In case of TypQ = 0 or -2: Text can contain a keyword; keywords are separated in the text by semicolons; Qmax-20 or CharCurv1

Text line

Text line

1, 5456474.468, 2563975.880, -845.000, Luisenthal, -1, 0, , , 20.03.1903, 01.10.2006,

0, 0.000, 0.000, 0.000,

1, 5456474.468, 2563975.880, -945.000, Luisenthal, 7.5, 1, , , 12.03.2007, 1.10.2030,

0, 0.000, 0.000, 0.000,

0, 0.000, 0.000, 0.000, End

C - conductance [m2/s]; to specify for type ‘0’, ‘-1’ and ‘-2’ (see below)

TypQ:

Positive pumping rates are always implemented as sources (as a flow into a balance cell (box)), regardless of type.

'1': source/sink

'-1': fixed potential (analogous to MODFLOW)

'0': fixed potential in case of overflow: ZW determines altitude of filter und potential h; it is also possible to include characteristic pump curves

'-2': fixed potential in case of overflow: ZW and D1 separately determine altitude of filter and potential h

'-3': fixed pressure in altitude of ZW; on D1: pressure for gas production

ZW sets the level of the pump or filter and does not define a water table or potential! Exception: Type '0'.

Consideration of time-dependent pumping (cyclic):

In case of TypQ(-2;-1;0;1)+10 = TypQ(8;9;10;11) the model considers the convention of the file:

<pumpfreqDay.dat>

Header

0

0

0

0

0

1

1

In this example the pump operates only on Saturdays and Sundays.

In the case of type '0' and type '10' or type '-2' or '8' it is possible to add a maximum pumping rate or a characteristic pump curve. In this case the text field has to be used as a keyword: Qmax or CharCurve:

Example: Qmax-20; CharCurve1

If an additional information text is used, it has to be separated by a semicolon.

The values of the characteristic pump curve are written in the folder <Pump_charact_Curve.dat>.

<u>TypCPump:</u>

The geochemical type of this boundary condition is only active if the flow is directed into a box. The concentration set has to be written in file <LiquidPumpX.dat>.

4.2.6 Q_c_Rand.str

- Graphic element: points in 3D-space

- Boundary condition such as inflows at low levels (reduction of inflow with flooding level)

Str	HW	RW	ZW	Text	Q	Typ-CRand	h-$_{Rand}$	expo-nent	TypQ	Date
[1]	[m]	[m]	[mSL]	text	[m^3/min]	[1]	[mSL]	[1]	[1]	

Text line

1, 5731768.222, 2581538.210, -1200.000, Haltern, 0.40, 8, 0, -0.0128, 1 ,01.01.1940 ,

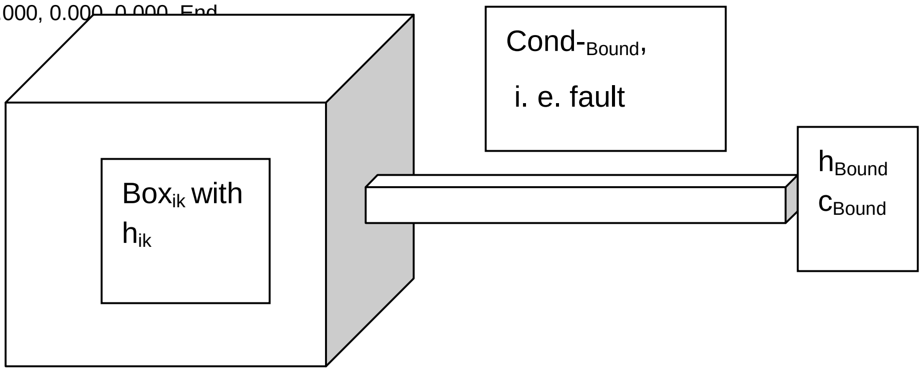
0, 0.000, 0.000, 0.000,

1, 5728517.056, 2569735.065, -860, Fürst_Leopold, 1.600, 8, 0, 0, 0 01.01.1974,

0, 0.000, 0.000, 0.000,

0, 0.000, 0.000, 0.000,

0, 0.000, 0.000, 0.000, End



TypQ_rand = 0: hydraulic gradient-dependent inflow

$Q = (h_{rand} – h_{ik}) \text{ x } C_{rand}$

TypQ_rand = 0: reduction of inflow with h-box

TypQ_rand = 1: reduction of inflow with h-box and time function for h-rand

TypQ_rand = 2: constant flow

If TypQ = 1 is used (reduction of flow by f(h, t), an exponent for an e-function is necessary.

$Q = (h_{rand} – h_{ik}) \text{ x } C_{rand} \text{ x } \exp(-Ex \text{ x } t \text{ [a]})$

4.2.7 RiverBox.str

The hydraulic communication between rivers and boxes/groundwater layers is realized by the river package.

- Graphic element: points in 3D-space

- Boundary condition for surface dewatering (rivers) in first model slice

Str	HW	RW	ZW	text	C_{riv}-R	TypR	h-Bottom	Q_{max}
[1]	[m]	[m]	[mSL]	Text	[m^2/s]	[1]	[mSL]	[m^3/min]

Text line

Text line

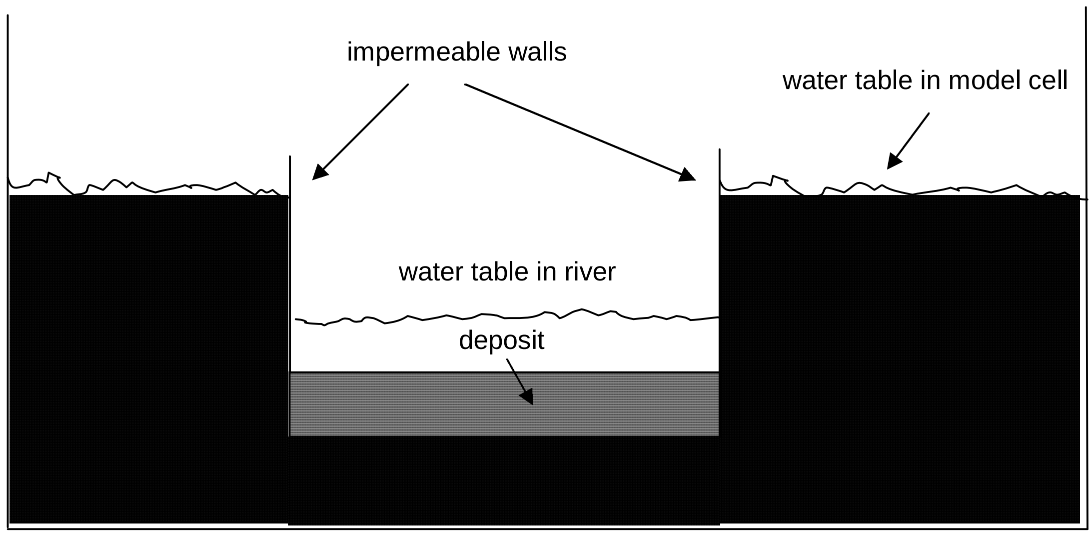
1, 5466714.984, 2568066.095, 200.000, Dilsburg, 1e-2, , , , , ,

0, 0.000, 0.000, 0.000,

0, 0.000, 0.000, 0.000, End

Q_{max} - maximum flow in the case of sinking

There are two fundamentally different types of rivers which are related to how they interact with the groundwater system: effluent and influent rivers:



Case A: Effluent stream, the groundwater table is higher than the river bed.

The volume flow is calculated by the following formula:

Equation: $\mathbf{Q = C_{riv} \times (h_{riv} - h_{i,k})}$

Q - flow [m^3/s]

C_{riv} - river bed conductance [m^2/s]

h_{riv} - water table in river [mSL]

$h_{i,k}$- water table in box [mSL]

Case B: Influent stream, the groundwater table is lower than the river bed.

The volume flow is calculated by the following formula:

Equation: $\mathbf{Q = C_{riv} \times (h_{riv} - h_{bottom})}$

Q - flow [m^3/s]

C_{riv} - river bed conductance [m^2/s]

h_{bottom} - level of bottom of deposit [mSL]

<u>TypR:</u>

-1: exfiltration and infiltration dependent on potential difference

0: only discharge

1: inflow and outflow (inflow to box is limited, related to h_{bottom}) = MODFLOW

2: inflow and outflow (inflow to box is limited, related to Q_{max}) = SPRING

(3:) solution France/Lorrain (limited by Q_{max})

If the water table in a box is lower than the bottom of the river bed, sinking starts from river into the groundwater. In this case the driving force for flow is the difference between the water table in the river and the bottom of sealing river bed.

4.3 Text files Control, ParaBox and Transfer

4.3.1 Control

To set control points for writing time series while simulating, <Control.csv> has to be used:

Control;element;	k;	h-vergl;	Qvergl;	GFname
B5;	10;	0;	0;	Box:B5;
B15;	10;	0;	0;	Box:B15;
B20;	10;	0;	0;	Box:B20;

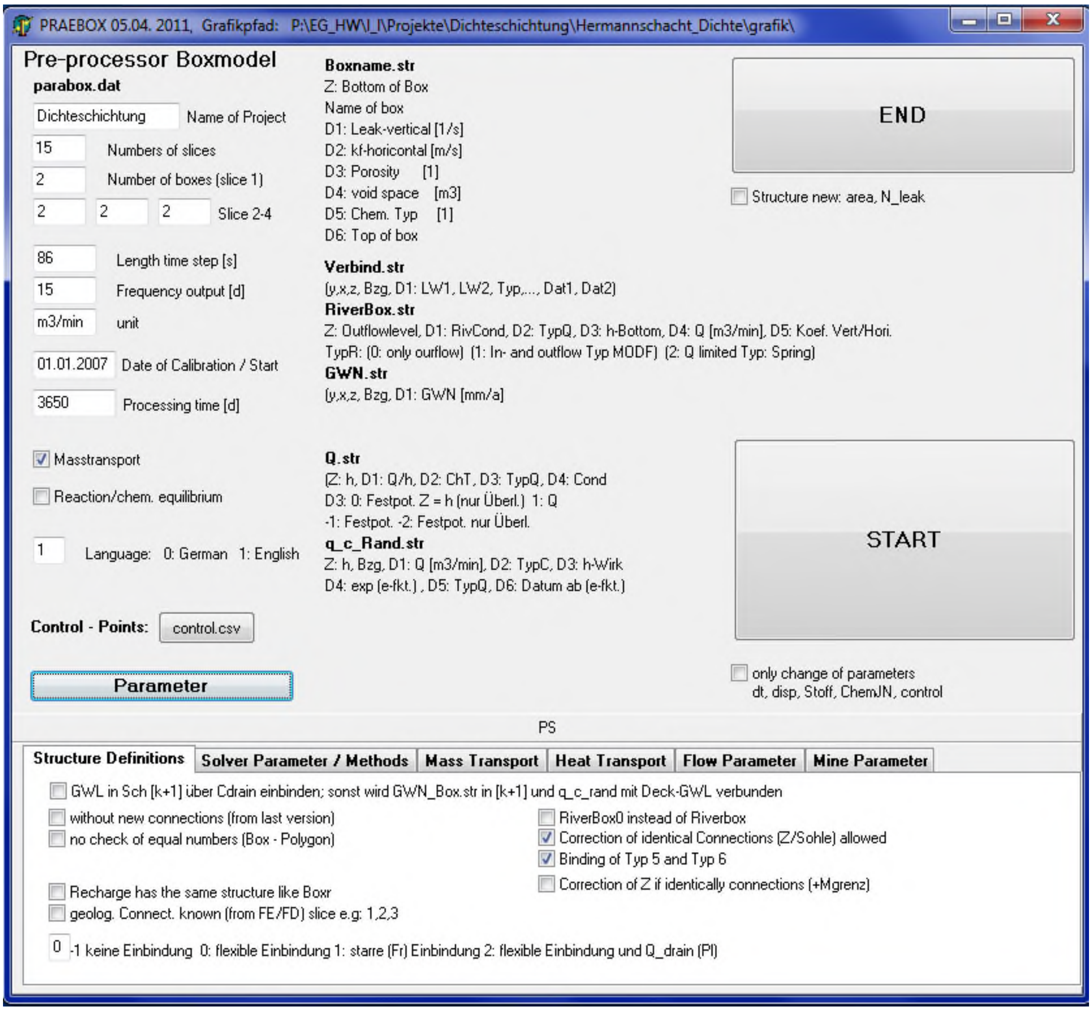
Based on this file, the preprocessor creates the file <Control.dat>. This file defines the boxes and heights for which time series have to be written in the Boxmodel.

4.3.2 ParaBox

With <Parabox.dat>, the environment parameters are set:

```
Carolinenglück
2        slices
17       Boxen Scheibe: 1
17       Boxen Scheibe: 2
0        Language:  0: German  1: English  2: France  3: Polish  4: Spanish
3600     dt [s]
0.0001   output frequency [d] (< 1: each dt, INT
0        0: without masstransport  1: with masstransport
28       ItMaxStoff
0        Time delay
m3/min
100.000  Prozess time [d]
10000    Itmaxflow
0   0:   without chem. equ. 1: with chem. equ.
1.0E+00  Condbound
1.000E-03 Poro0 [1], if Poro < Poroh and Volume < 100 m3
31.12.2011
1.000E-09 eps flow [m]
0        switch_GasJ/N
0        0: no Reakt(no Org)/no Phase Solid  1: with Solids (aktivSol.dat)  2: only precipitation (no solid-balance
0        switch_OrgJ/N  0: no organics  1: yes  2: 1+react_O2_SO4
0        switch_without_ConnectJ/N
0        switch_just_connected
0        switch_interpol_kf 0: harm  1: lowest kf  2: arithmetic
1        dt_control 0: yes   1: no
0        recharge=Box_Structur  1: yes   0: no
0        Geol_known  0: no   1: yes
0        Automash  0: no   >=1: yes to slice
0        CentrlDiff 1   Upwind 0
0.80     share of_1 of Po_stagnant (<= 0.001: not available)
0        Dispersion/Diff  1: yes   0: no   2: only vertical over Leak
10.00    Disp_longitudinal
0.00     Disp_transversal
0        write results masstrnsport 1: yes  0: no
0        special function Wismut (recharge ...)
0        q_c_rand.str only for Connection with GWL; not in Box3D directly
0        1: GWL fix in 2. Slice
0        1: All slices activ (ignore Chemieaktiv.csv: but use of Chemaktiv.3d) 0: Chemieaktiv activ
0.000    log10 of partial pressure (degasing of free water table: Expl. -2.5); 0 : ever closed system
0        Sorption with  -1: kd-R-concept(Redardation)  0: no  1: kd-concept  2: surface complexation 3: Ionen-exchange 4: (2+3) only
         if kd = -1
1        1: no heat exchange with rock (adiabat) 0: exchagne with rock -1: exchange and change of heat in rock
```

This file can be edited from the surface of Parabox (see below) or directly using the text editor:



4.3.3 Transfer

The file <Transfer.csv> defines the altitude for hydraulic communication between mining claims and the appendant pumping rates.

Example: Water transfer from GF Grillo to Haus Aden (eastern mine), semicolon is used as separator.

Transfer from Grillo (6) to Haus Aden (13), from slice 26 to slice 19 (-1.320 m),
Q = 1,4 m³/min = 0,02333 m^3/s:

Haus_Aden; 19; 1.4; Grillo; 26; -1320; 01.01.1960; 31.12.2005;

4.4 Mass transport

Multi-component mass transport

In order to consider chemical reactions through modelling it is necessary to know the concentrations of the substances (specifically ions / species) involved in the chemical reaction. Therefore these substances must be transported in the numerical flow model at the same time, so that in each flow element and at each step in time, the required ion concentrations are known. Thes concentrations are needed for the reaction equations. However, for many reaction equations it is not sufficient knowing the total concentration, which is considered in the mass transport equation (e.g. ΣSO_4^{2-} (= SO_4^{2-}+ HSO_4^-+ $CaSO_4$ + ...)), but further information about the specific ion or species distribution is required. Consequently, the geochemical system of total concentrations for the equilibrium of the liquid species is solved. Afterwards it is checked whether the geochemical equilibrium system of the liquid phase is in equilibrium for the solid phase. In the case of imbalance, so-called kinetic interaction terms (such as response rates and phase exchange) are formulated to move the system toward a geochemical balance.

At present in the box model 28 inorganic chemical total concentrations can be transported when two characteristics occur. The transport unit “24” takes account of a conserved quantity for the calculation of the redox state (OPV in mol/l); the transport unit “28” has the temperature in °C. There is also the possibility of transporting several organic concentrations. Generally, the list of implemented chemical elements or compounds can be expanded as required.

Liquids:

Inorganic:

1. ∑SO_4	2 ∑CO_3	3. ∑Ca	4. ∑Fe	5. ∑Mg
6. ∑Zn	7. ∑Na	8. ∑K	9. ∑Cl	10. ∑Mn
11. ∑NO_3	12. ∑U	13. ∑As	14. ∑Ra	15. ∑Ba
16. ∑Pb	17. ∑Cr	18. ∑Co	19. ∑Cd	20. ∑Ni
21. ∑Cu	22. ∑Sr	23. ∑Al	24. OPV	25. O_2 (solute)
26. ∑Si	27. ∑Br	28. T	29. Hg	30. Imbalance
31. ∑NH_4	32. Hfo-w	33. Hfo_s		

Organic:

1. Petroleum-derived hydrocarbon
2. BTEX
3. PAH
4. Methane
5. Slightly volatile halogenated hydrocarbons
6. Sulphate-, nitrate-, iron(III)-reducing bacteria

Gaseous phase:

1. O_2 2. CO_2

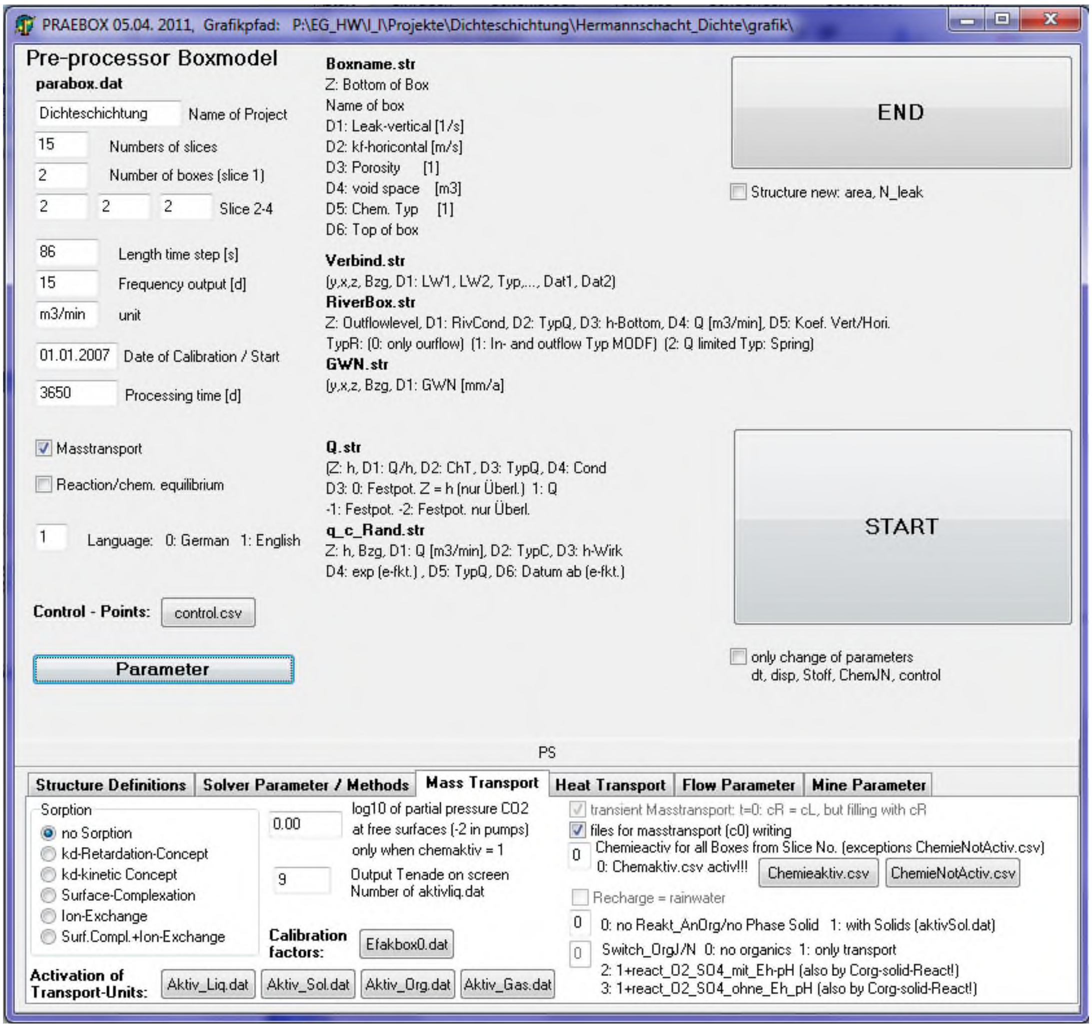
Solid phase:

Because of the large number of solids implemented in the BoxModel (current 92), only an extract of these is shown below.

1. FeS_2	2. $CaSO_4$	3. U (UO_2)	4. FeAsS	5. Ra
6. $BaSO_4$	7. PbS	8. ZnS	9. CdS	10. $NiCO_3$
11. Cr_2O_3	12. $SrCO_3$	13. MnO_2	14. $CoCO_3$	15. AlOOH
16. SiO_2	17. $NaFe_3(OH)_6(SO_4)_2$			

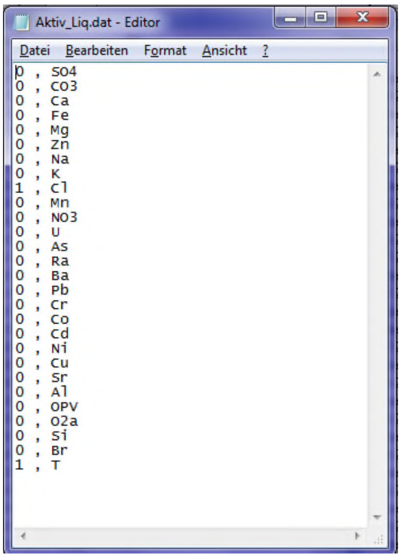
The solid phase is considered only if the switch “SchalterSol = 1” is set. Otherwise, precipitation reactions and no dissolutions are calculated.

Settings for mass transport can be made in the following dialog box:



In the files <Aktiv_Liq.dat>, <Aktiv_Org.dat>, <Aktiv_Sol.dat> and <Aktiv_Gas.dat>, all components involved in the corresponding state of aggregation can be defined.

Example for <Aktiv_Liq.dat> (0: inactive, 1: active):


Aktiv_Liq.dat - Editor

Datei Bearbeiten Format Ansicht ?

```
0 , SO4
0 , CO3
0 , Ca
0 , Fe
0 , Mg
0 , Zn
0 , Na
0 , K
1 , Cl
0 , Mn
0 , NO3
0 , U
0 , As
0 , Ra
0 , Ba
0 , Pb
0 , Cr
0 , Co
0 , Cd
0 , Ni
0 , Cu
0 , Sr
0 , Al
0 , OPV
0 , O2a
0 , Si
0 , Br
1 , T
```

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