DRUtES

TUTORIAL: COUPLED CONTAMINANT AND WATER TRANSPORT – PART 1

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GOAL AND COMPLEXITY

Complexity: Medium

Prerequisites: None

The goal of this tutorial is to introduce contaminant transport. For this we couple the *DRUtES* standard Richards equation module with the ADE module. ADE stands for Advection-Dispersion-Equation. The advection will be calculated through the Richards-Equation (water flow).

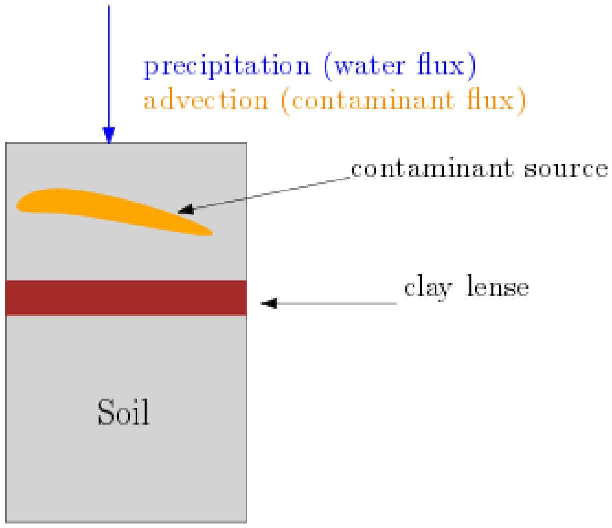

Figure 1: Simplified scheme of coupled model.

In this example we assume that the contaminant is soluble and in the water. No adsorption or desorption occurs.

In this tutorial five configuration files will be modified step by step. All configuration files are located in the folder *drutes.conf* and respective subfolders.

1. For selection of the module, dimension and time information we require *global.conf*. *global.conf* is located in *drutes.conf / global.conf*.

2. To define the mesh or spatial discretization in 1D, we require *drumesh1D.conf*. *drumesh1D.conf* is located in *drutes.conf / mesh / drumesh1D.conf*.

3. To define the precipitation, we require *matrix.conf*. *matrix.conf* is located in *drutes.conf /water.conf/ matrix.conf*.

4. To select the ADE module and link it to the water module, we require *ADE.conf*. *ADE.conf* is located in *drutes.conf /ADE/ ADE.conf*.

5. To define the contaminant transport, we require *contaminant.conf*. *contaminant.conf* is located in *drutes.conf /ADE/ contaminant.conf*.

DRUtES works with configuration input file with the file extension .conf. Blank lines and lines starting with # are ignored. The input mentioned in this tutorial therefore needs to be placed one line below the mentioned keyword, unless stated otherwise.

SOFTWARE

1. Install *DRUtES*. You can get *DRUtES* from the github repository drutes-dev or download it from the drutes.org website.

2. Follow website instructions on drutes.org for the installation.

3. Working R installation (optional, to generate plots you can execute freely distributed R script)

SCENARIOS

We are using the well-known van Genuchten-Mualem parameterization to describe the soil hydraulic properties of our soils and contaminant transport.

Table 1: Material properties needed for scenarios.

Parameter	Description	Sand	Clay	Contaminant
α [cm^{-1}]	inverse of the air entry value	0.05	0.01	
n [-]	shape parameter	2	1.4	
m [-]	shape parameter	0.5	0.2857	
θ_s [-]	saturated vol. water content	0.45	0.45	
θ_r [-]	residual vol. water content	0.05	0.05	
Ss [cm^{-1}]	specific storage	0	0	
K_s [cm d^{-1}]	saturated hydraulic conductivity	100	1	
D [cm^2 d^{-1}]	diffusion	10e-3	10e-3	
D$_v$ [cm]	dispersivity	30	100	
c_{init} [mg cm^{-3}]	initial concentration			2

The domain scheme is shown in Fig. 2. We need to define 4 boundary conditions. Our mesh requires 5 different layers to accomodate for the contaminantion, the extra soil and the layers in between.

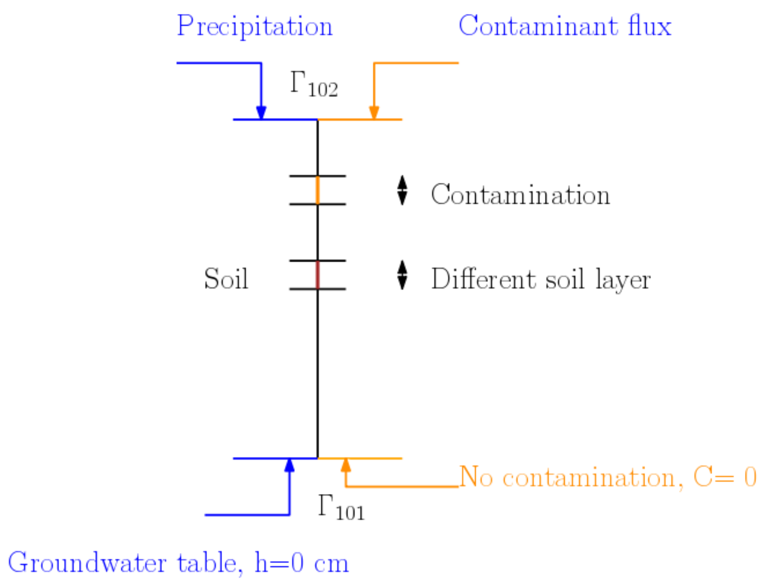

Figure 2: 1D domain set-up of coupled scenario with top and bottom boundary conditions. There are now two boundary condtions at the top and two boundary conditions at the bottom: contaminant transport and water flow. The top boundary is defined by the interactions with the atmosphere and the bottom boundary is defined by the constant groundwater table.

SCENARIO 1

We first assume that the soil is homogeneous.

global.conf: Choose correct model, dimension, time discretization and observation times.

1. Open ***global.conf*** in a text editor of your choice.

2. Model type: Your first input is the module. Input is **ADE**.
3. Initial mesh configuration
   a) The dimension of our problem is 1. Input: 1.
   b) We use the internal mesh generator. Input: 1.
4. Error criterion
   a) Maximum number of iteration of the Picard method: 20
   b) h tolerance: 1e-3.
5. Time information
   a) Time units are in hours: input d
   b) Initial time: 1e-4.
   c) End time: 10.
   d) Minimum time step: 1e-12.
   e) Maximum time step: 0.005.
6. Observation time settings
   a) Observation time method: 2
   b) Set file format of observation: pure. Output in 1D is always in raw data. Different options will not impact output in 1D.
   c) Make sequence of observation time: n
   d) Number of observation times: 9
   e) Observation time values: 1, 2, 3,4,5,6,7,8,9. Use a new line for each input. *DRUtES* will generate 11 output files for each modeled component, e.g.*RE_matrix_press_head-x.dat*, where x is the ID of the observation point. The initial and final time value will be automatically be printed.
7. Observation point settings
   a) Number of observation points: 6
   b) Observation point coordinates: 200, 195,187.5,182.5,175, 150. Use a new line for each input. *DRUtES* will generate 6 output files for each modeled component, e.g. *obspt_RE_matrix-1.out*, where x is the ID of the observation point.
8. Ignore other settings for now.
9. Save *global.conf*

drumesh1D.conf: Mesh definition, i.e. number of materials and spatial discretization

1. Open ***drumesh1D.conf*** in a text editor of your choice.
2. Geometry information: 200 cm - domain length
3. Amount of intervals: 1
4.

density	bottom	top
4	0	200

5. number of materials: 5

6.

id	bottom	top
1	0	170
2	170	180
3	180	185
4	185	190
5	190	200

7. Save *drumesh1D.conf*

matrix.conf: Configuration file for water flow

1. Open *matrix.conf* in a text editor of your choice.
2. How-to use constitutive relations? [integer]: 1
3. Length of interval for precalculating the constitutive functions: 200
4. Discretization step for constituitive function precalculation: 0.1
5. number of soil layers [integer]: 5
6.

alpha	n	m	theta_r	theta_s	specific storage
0.05	2	0.5	0.05	0.45	0
0.05	2	0.5	0.05	0.45	0
0.05	2	0.5	0.05	0.45	0
0.05	2	0.5	0.05	0.45	0
0.05	2	0.5	0.05	0.45	0

7. The angle of the anisotropy determines the angle of the reference coordinate system. 0 means vertical flow. Anisotropy description. Anisotpropy description and hydraulic conductivity

angle [degrees]	K_11
0	100
0	100
0	100
0	100
0	100

8. sink(-) /source (+) term per layer:
0
0
0
0
0

9. Initial condition is a constant pressure head of -200 cm across the soil.

init. cond [real]	type of init. cond	RCZA method [y/n]	RCZA method val.
0.0	H_tot	n	0
0.0	H_tot	n	0
0.0	H_tot	n	0
0.0	H_tot	n	0
0.0	H_tot	n	0

10. number of boundaries: 2
11.

boundary ID	boundary type	use rain.dat [y/n]	value
101	1	n	0.0
102	2	n	0.5

12. Save matrix.conf.

Contaminant transport *ADE.conf*

1. Open *ADE.conf* in a text editor of your choice.
2. specify coupling with Richards equation [y/n]: y
3. use sorption: n
4. Save ADE.conf.

contaminant.conf

1. Open *contaminant.conf* in a text editor of your choice.
2. number of layers: 5
3. molecular diffusion:
   10e-3
   10e-3
   10e-3
   10e-3
   10e-3
4. dispersivity:

angle [degrees]	D_11
0	30
0	30
0	30
0	30
0	30

5. initial condition:

value	type
0	ca
0	ca
0	ca
2	ca
0	ca

6. number of different orders of reactions: 1
7. orders of reaction:
   1
   1
   1
   1
   1
8. reaction coefficients:
   0
   0
   0
   0
   0
9. number of boundaries: 2
10.

boundary ID	boundary type	use rain.dat [y/n]	value
101	1	n	0.0
102	2	n	0.0

11. save *contaminant.conf*

RUN SCENARIO 1

Run the simulation in the terminal console.

1. Make sure you are in the right directory.
2. To execute *DRUtES*:
   $ bin/drutes
3. After the simulation finishes, to generate png plots execute provided R script:
   $ Rscript drutes.conf/makeplot.R -name coupled_samesoil
4. The output of the simulation can be found in the folder out

SCENARIO 2

In scenario 2 we introduce a clay layer in depth 170-180 cm. For this, we need to change matrix.conf and contaminant.conf.

Changes in matrix.conf

1. Change the 2nd van Genuchten parameter set:

alpha	n	m	theta_r	theta_s	specific storage
0.05	2	0.5	0.05	0.45	0
0.01	1.4	0.2857	0.05	0.45	0
0.05	2	0.5	0.05	0.45	0
0.05	2	0.5	0.05	0.45	0
0.05	2	0.5	0.05	0.45	0

2. Change the 2nd hydraulic conductivity. The angle of the anisotropy determines the angle of the reference coordinate system. 0 means vertical flow. Anisotropy description. Anisotpropy description and hydraulic conductivity

angle [degrees]	K_11
0	100
0	1
0	100
0	100
0	100

3. save *matrix.conf*

Changes in contaminant.conf

1. Change the second dispersivity value to 100. dispersivity:

angle [degrees]	D_11
0	30
0	100
0	30
0	30
0	30

2. save contaminant.conf

RUN SCENARIO 2

Run the simulation in the terminal console.

1. Make sure you are in the right directory.
2. To execute *DRUtES*:
   $ bin/drutes
3. After the simulation finishes, to generate png plots execute provided R script:
   $ Rscript drutes.conf/makeplot.R -name coupled_claylense
4. The output of the simulation can be found in the folder out

TASKS

1. Describe the distribution of the contaminant without and with the clay layer.
2. Investigate how the simulation differs: (i) With a different soil material (ii) when you include a reaction in contaminant.confS

SIMULATION SRESULTS

The simulation nicely shows how the contamination moves downwards into the soil and disperses to compensate for concentration differences. The clay layer hinders the water flow into deeper layers and therefore also the advection. Due to the high dispersion in the clay layer the contaminant concentration becomes more evenly distributed in that layer.

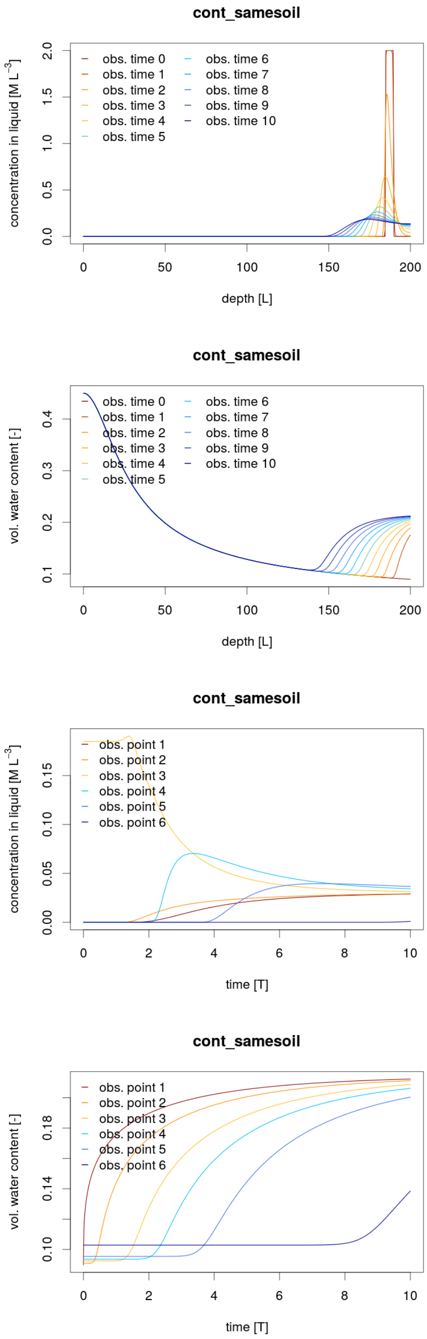

Figure 3: Water content and contaminant concentration at the observation points and observation times the homogeneous soil.

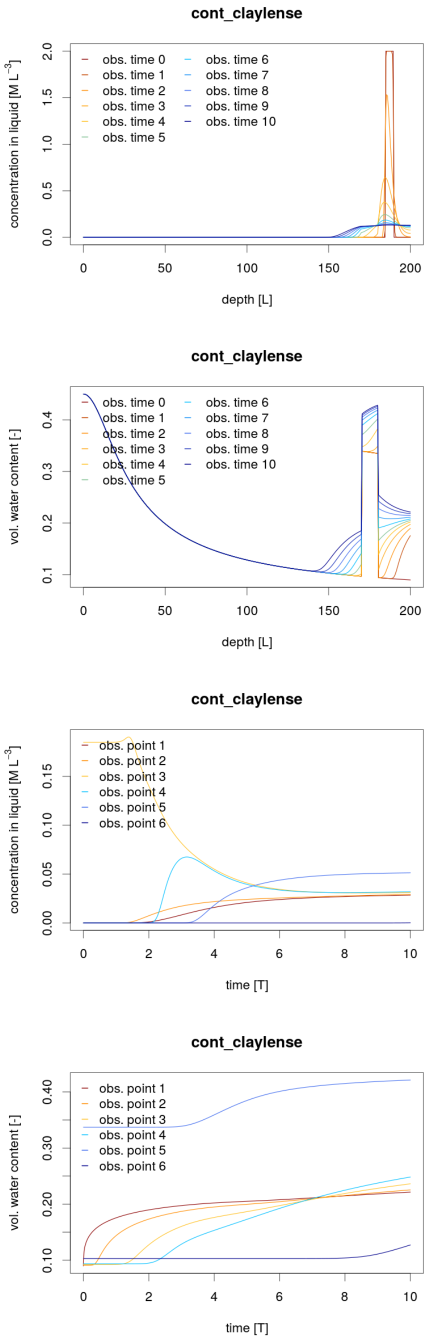

Figure 4: Water content and contaminant concentration at the observation points and observation times with a clay layer.

OUTCOME

1. You got familiar with simple contaminant transport.
2. You simulated coupled water flow and contamination transport.
3. You understand the difference between advection and dispersion.