



Lecture Modelling of Hydro-systems

Mass Transport Process Part I

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Outline

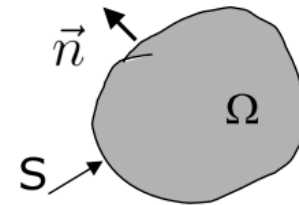
- Advection – Diff. / Disp. – Equation (ADE)
- Dispersion and Diffusion
- Sorption Isotherms and Decay
- Exercise on the mass transport simulation

Governing Equations

If you can only remember one equation, then the Reynolds Transport Theorem.

$$\frac{\partial}{\partial t} \int_{\Omega} \psi d\Omega = - \oint_{\partial\Omega} \mathbf{\Phi}^{\psi} \cdot d\mathbf{S} + \int_{\Omega} q^{\psi} d\Omega \quad (\text{Eq. 0})$$

Or, you can remember a story.



$$\left\{ \begin{array}{l} \text{Rate of} \\ \text{accumulation} \\ \text{for unknown } \Psi \\ \text{within the} \\ \text{volume } \Omega \end{array} \right\} = \left\{ \begin{array}{l} \text{Net influx of } \Psi \text{ into} \\ \text{the volume } \Omega \\ \text{through its} \\ \text{surface } S \end{array} \right\} + \left\{ \begin{array}{l} \text{Net rate of } \Psi \\ \text{production} \\ \text{within the} \\ \text{volume } \Omega \end{array} \right\}$$

Governing Equations

Because of the Gauss Divergence Theorem.

$$\oint_{\partial\Omega} \Phi^\psi \cdot dS = \int_{\Omega} \nabla \cdot \Phi^\psi d\Omega$$

So, our Eq. 0 becomes.

$$\frac{\partial}{\partial t} \int_{\Omega} \psi d\Omega = - \int_{\Omega} \nabla \cdot \Phi^\psi d\Omega + \int_{\Omega} q^\psi d\Omega \quad (\text{Eq. 1})$$

Advection Dispersion Equation (ADE)

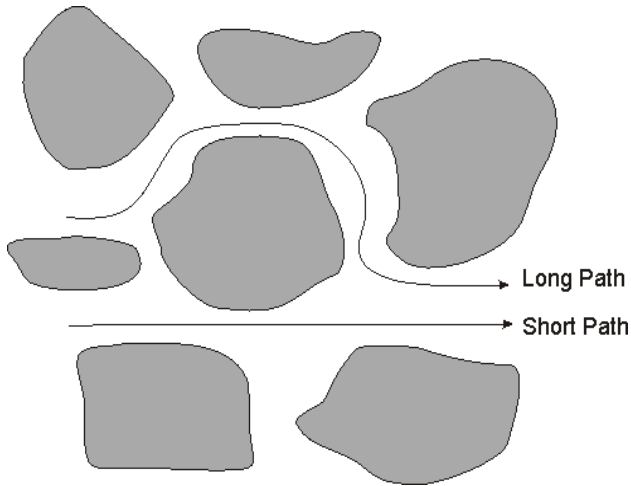
If we write Eq. 1 in derivative form,

$$\frac{\partial \psi}{\partial t} = \nabla(\Phi) + Q \quad (\text{Eq. 2})$$

Our primary unknown is Mass
 $\psi = n_e C dA$

Our flux is composed of:
 1) Advective flux
 2) Diff./ Disp. flux

Source / Sink



Advection (Mass takes a free ride)

Flux of advection $F_{adv} = v_i n_e C dA$

Average Linear Velocity $v_x = -\frac{K}{n_e} \frac{dh}{dl}$

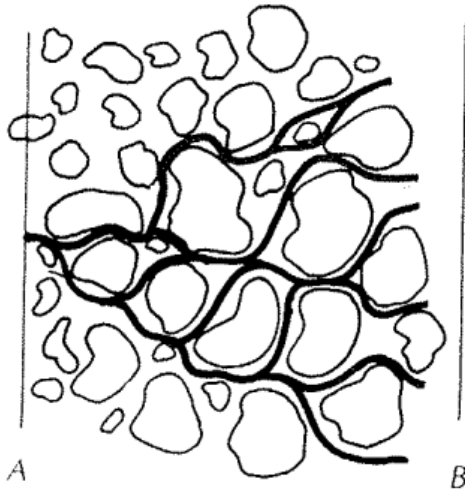
AKA, Pore Velocity $v_x = \frac{q}{n_e}$

Flux

Effective porosity

Velocity of a conservative tracer.

Advection Dispersion Equation (ADE)



Dispersion

Diff./ Disp. Flux (Fick's 1st Law)

$$F_{dis/diff} = -D \frac{dC}{dx} \quad 1D$$

$$F_{dis/diff} = -D \nabla (C) \quad 3D$$

Think about:

Why negative sign?

Hydrodynamic Dispersion (Mechanical spreading)

$$D_L = \alpha_L v_i + D^*$$

$$D_T = \alpha_T v_i + D^*$$

Diffusion coefficient

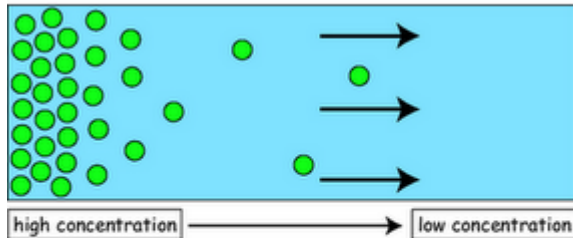
Longitudinal / transverse dispersivity

Note: Dispersivity values are often scale dependent!

$$\alpha_L = 0.83(\log L)^{2.414} \quad \text{Xu and Eckstein (1995)}$$

Advection Dispersion Equation (ADE)

Diffusion



● solute

Solute transport is from the left to the right; movement of the solutes is due to the concentration gradient (dC/dx).

Diffusion (Molecular spreading)

- It is orders magnitudes lower than dispersion effect.
- Does not dependent on the flow process.
- It is largely temperature dependent.

Putting advection and dispersion into Eq. (2).

We get the governing equation for the mass transport process:

$$\frac{\partial C}{\partial t} + v_x \frac{\partial C}{\partial x} - D \frac{\partial^2 C}{\partial x^2} = Q$$

Diffusion of ions in sea water and in deep-sea sediments

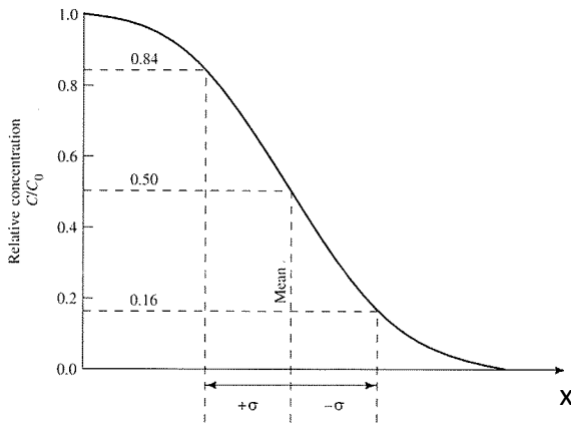
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Table 1. Tracer and self-diffusion coefficients of ions at infinite dilution

Cation	D_j^0 (10^{-6} cm ² /sec)			Anion	D_j^0 (10^{-6} cm ² /sec)		
	0°C	18°C	25°C		0°C	18°C	25°C
H ⁺	56.1	81.7	93.1	OH ⁻	25.6	44.9	52.7
Li ⁺	4.72	8.69	10.3	F ⁻	—	12.1	14.6
Na ⁺	6.27	11.3	13.3	Cl ⁻	10.1	17.1	20.3
K ⁺	9.86	16.7	19.6	Br ⁻	10.5	17.6	20.1
Rb ⁺	10.6	17.6	20.6	I ⁻	10.3	17.2	20.0
Cs ⁺	10.6	17.7	20.7	IO ₃ ⁻	5.05	8.79	10.6
NH ₄ ⁺	9.80	16.8	19.8	HS ⁻	9.75	14.8	17.3
Ag ⁺	8.50	14.0	16.6	S ²⁻	—	6.95	—
Tl ⁺	10.6	17.0	20.1	HSO ₄ ⁻	—	—	13.3
Cu(OH) ⁺	—	—	8.30	SO ₄ ²⁻	5.00	8.90	10.7
Zn(OH) ⁺	—	—	8.54	SeO ₄ ²⁻	4.14	8.45	9.46
Be ²⁺	—	3.64	5.85	NO ₂ ⁻	—	15.3	19.1
Mg ²⁺	3.56	5.94	7.05	NO ₃ ⁻	9.78	16.1	19.0
Ca ²⁺	3.73	6.73	7.93	HCO ₃ ⁻	—	—	11.8
Sr ²⁺	3.72	6.70	7.94	CO ₃ ²⁻	4.39	7.80	9.55
Ba ²⁺	4.04	7.13	8.48	H ₂ PO ₄ ⁻	—	7.15	8.46
Ra ²⁺	4.02	7.45	8.89	HPO ₄ ²⁻	—	—	7.34

Li Yuan-Hui, Sandra Gregory (1974) Diffusion of ions in sea water and in deep-sea sediments. *Geochimica et Cosmochimica Acta*, Volume 38, Issue 5, 703-714

Advection Dispersion Equation (ADE) – Analytical Solutions



Complementary Error function

For the governing Equation with only dispersion / diffusion,

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

Analytical solution (Crank 1956)

$$C(x, t) = C_0 \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)$$

$$\operatorname{erfc}(B) = 1 - \operatorname{erf}(B)$$

$$\operatorname{erf}(B) = \frac{2}{\sqrt{\pi}} \int_0^B e^{-t^2} dt$$

Use a checking table,
Or in Excel and other soft., it is provided.

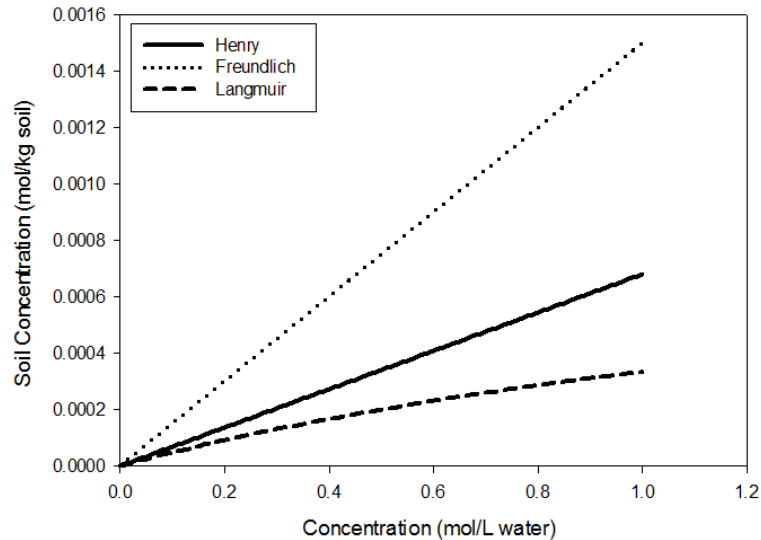
For the Advection - Dispersion / Diffusion equation,

$$\frac{\partial C}{\partial t} + v_x \frac{\partial C}{\partial x} - D \frac{\partial^2 C}{\partial x^2} = Q$$

Analytical solution (Ogata 1970)

$$C(x, t) = \frac{C_0}{2} \left[\operatorname{erfc}\left(\frac{L - v_x t}{2\sqrt{D_L t}}\right) + \exp\left(\frac{v_x L}{D_L}\right) \operatorname{erfc}\left(\frac{L + v_x t}{2\sqrt{D_L t}}\right) \right]$$

Sorption and Decay



- Sorption isotherm describes the distribution of a particular chemical component in the aqueous and solid phase.
- It is called as isotherm because it is measured at a constant temperature.
- Because of different property of the solid phase and sorption component, the isotherm behaves differently and can be described by different mathematical equations.
- Another important behavior of the chemical component is the decay process. Simplest decay process can be described as the first-order decay.
- The radioactive decay exactly follows this decay process.

Henry

$$C^* = K_D C$$

Freundlich

$$C^* = K_1 C^{K_2}$$

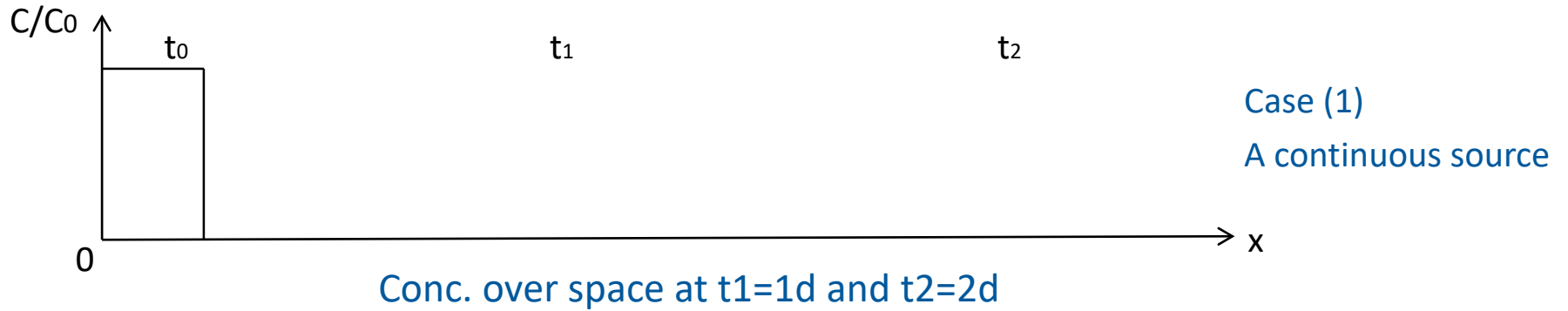
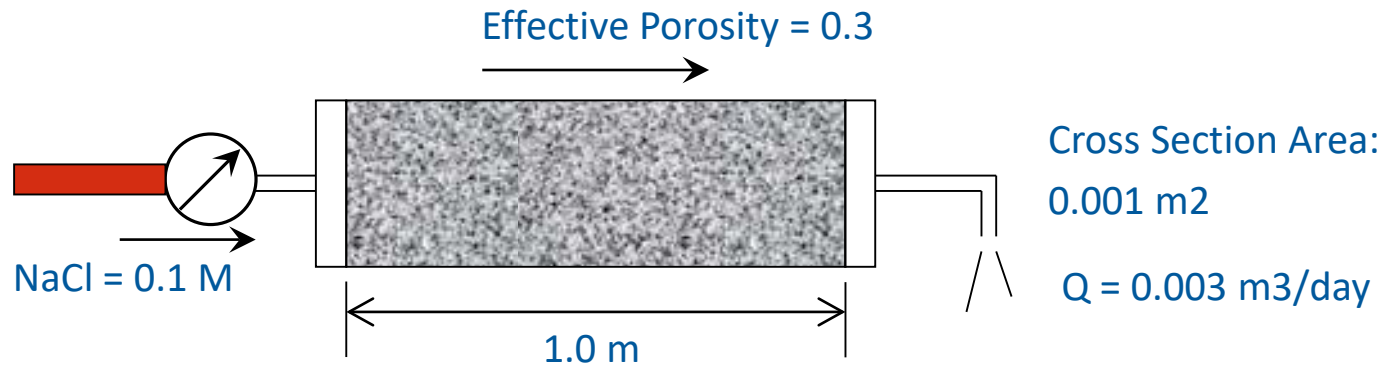
Langmuir

$$C^* = \frac{K_1 C}{1 + K_2 C}$$

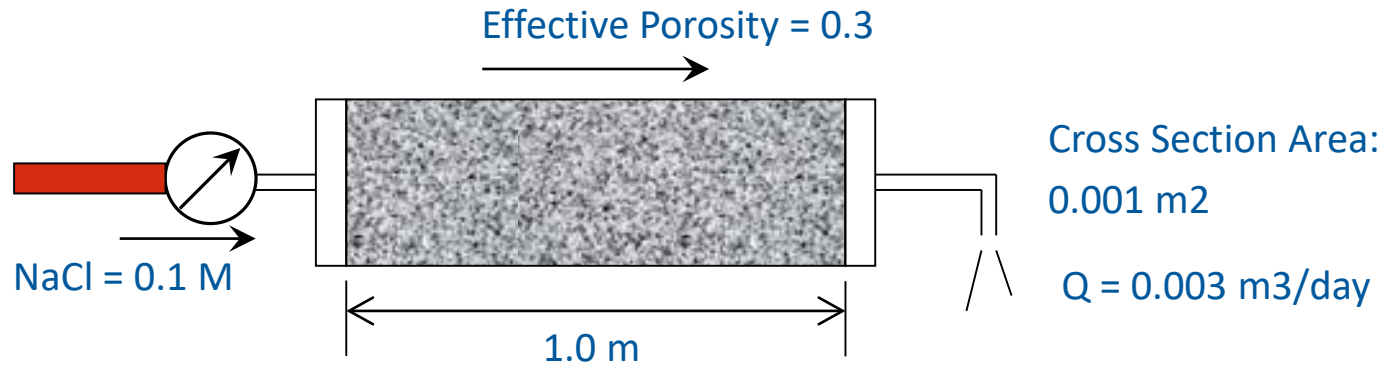
1st-order decay

$$\frac{\partial C}{\partial t} = -\lambda C$$

Exercise

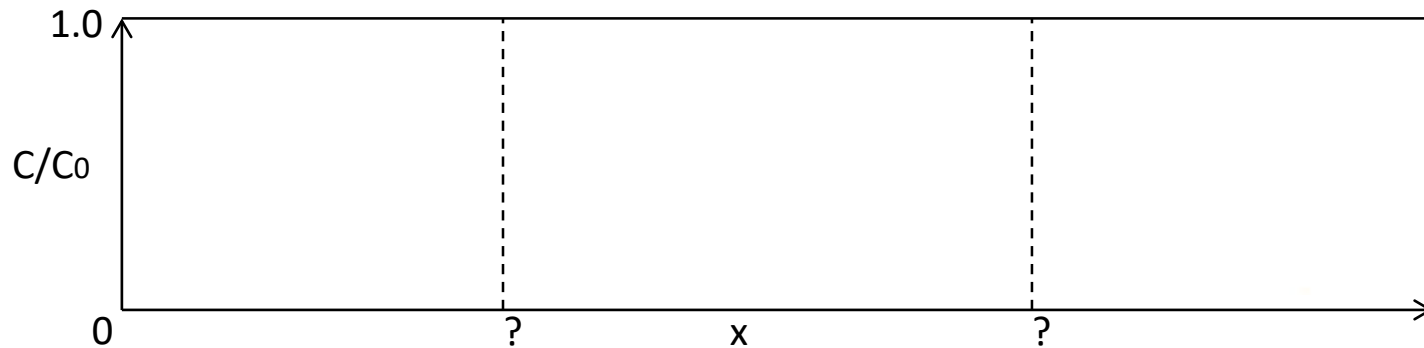


Exercise



Case (3): Assuming soil grain density is 2000 kg/m³, $K_d = 2.0$ mL/g, how much is the retardation factor R ? How does this retardation effect influence the concentration profile?

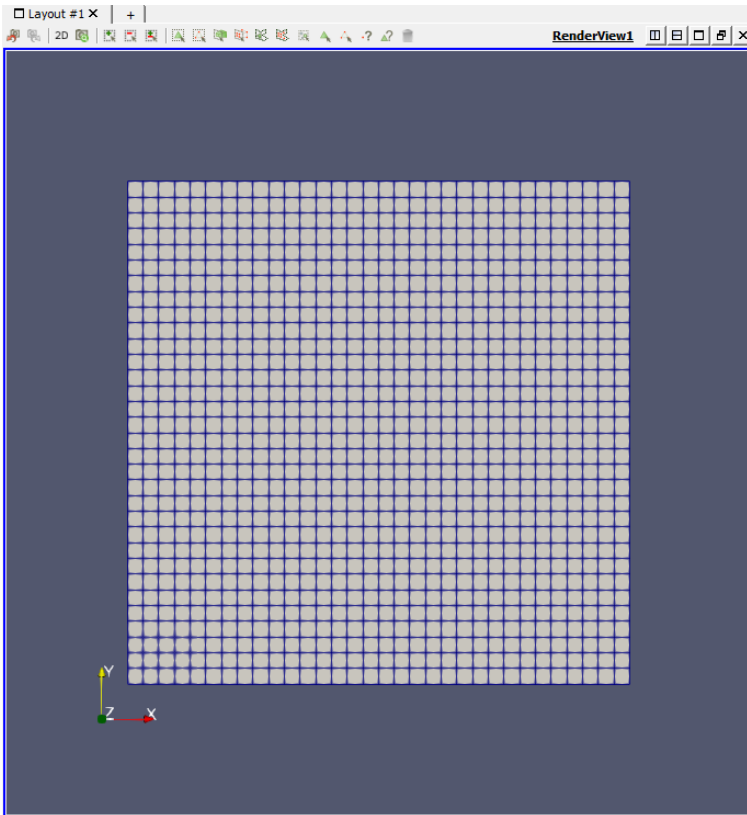
Case (4): What if there is a 1st order decay on the transported contaminant with ($\lambda = 0.7$ 1/day)



The 2D domain and geometry

- The geometry of the domain is very simple. A 1x1 m 2D domain with rectangular shape.
- The mesh was composed of 1089 nodes and 1024 quad elements connecting with each other. The mesh can be generated by a spreadsheet program or gmesh.

```
component_transport.prj
1 <?xml version="1.0" encoding="ISO-8859-1"?>
2 <OpenGeoSysProject>
3   <mesh>square_1x1_quad_1e3.vtu</mesh>
4   <geometry>square_1x1.gml</geometry>
5   <processes>
6     <process>
7       <name>hc</name>
8       <type>ComponentTransport</type>
9       <integration_order>2</integration_order>
10      <process_variables>
11        <concentration>Si</concentration>
12        <pressure>pressure</pressure>
13      </process_variables>
14      <specific_body_force>0 0</specific_body_force>
15      <secondary_variables>
16        <secondary_variable internal_name=
17          "darcy_velocity" output_name="darcy_velocity"/>
18      </secondary_variables>
19    </process>
20  </processes>
```



```
component_transport.prj | square_1x1.gml
1 <?xml version="1.0" encoding="ISO-8859-1"?>
2 <?xml-stylesheet type="text/xsl" href="OpenGeoSysGLI.xsl"?>
3
4 <OpenGeoSysGLI xmlns:xsi=
5   "http://www.w3.org/2001/XMLSchema-instance" xmlns:ogs=
6   "http://www.opengeosys.org">
7   <name>geometry</name>
8   <points>
9     <point id="0" x="0" y="0" z="0"/>
10    <point id="1" x="0" y="1" z="0" name="p1"/>
11    <point id="2" x="1" y="0" z="0"/>
12    <point id="3" x="1" y="1" z="0" name="p3"/>
13    <point id="4" x="0" y="0.5" z="0" name="p01"/>
14  </points>
15  <polylines>
16    <polyline id="0" name="left">
17      <pnt>0</pnt>
18      <pnt>1</pnt>
19    </polyline>
20    <polyline id="1" name="right">
21      <pnt>2</pnt>
22      <pnt>3</pnt>
23    </polyline>
24    <polyline id="2" name="bottom">
25      <pnt>0</pnt>
26      <pnt>2</pnt>
27    </polyline>
28    <polyline id="3" name="top">
29      <pnt>1</pnt>
30      <pnt>3</pnt>
31    </polyline>
32    <polyline id="4" name="left_half">
33      <pnt>0</pnt>
34      <pnt>4</pnt>
35    </polyline>
36  </polylines>
37 </OpenGeoSysGLI>
```

Process definition HC – coupled hydro-component transport

- We have one process defined in the simulation project. It is coupled HT process. It simulates the liquid flow coupled with mass transport.
- There are (at least) two primary variables required, one is pressure and the other is concentration.

```
1 <?xml version="1.0" encoding="ISO-8859-1"?>
2 <OpenGeoSysProject>
3   <mesh>square_1x1_quad_1e3.vtu</mesh>
4   <geometry>square_1x1.gml</geometry>
5   <processes>
6     <process>
7       <name>hc</name>
8       <type>ComponentTransport</type>
9       <integration_order>2</integration_order>
10      <process_variables>
11        <concentration>Si</concentration>
12        <pressure>pressure</pressure>
13      </process_variables>
14      <specific_body_force>0 0</specific_body_force>
15      <secondary_variables>
16        <secondary_variable internal_name=
17          "darcy_velocity" output_name="darcy_velocity"/>
18      </secondary_variables>
19    </process>
20  </processes>
  </media>
```

```
<parameter>
  <name>p_Dirichlet_left</name>
  <type>Constant</type>
  <value>1</value>
</parameter>
<parameter>
  <name>p_Dirichlet_right</name>
  <type>Constant</type>
  <value>0</value>
</parameter>
<parameter>
  <name>c_Dirichlet_left</name>
  <type>Constant</type>
  <value>1</value>
</parameter>
<parameter>
  <name>c_Dirichlet_right</name>
  <type>Constant</type>
  <value>0</value>
</parameter>
```

Initial and Boundary Conditions

- The boundary condition is set in a way that, pressure on the left is 1, while pressure on the right is 0.
- Similarly the concentration on the left is set to 1, and right side set to 0.

Specify the output of component concentrations

```
152 <output>
153   <type>VTK</type>
154   <prefix>CompTrans</prefix>
155   <timesteps>
156     <pair>
157       <repeat>1</repeat>
158       <each_steps>100</each_steps>
159     </pair>
160   </timesteps>
161   <variables>
162     <variable>Si</variable>
163     <variable>pressure</variable>
164     <variable>darcy_velocity</variable>
165   </variables>
166   <suffix>_ts_{:timestep}_t_{:time}</suffix>
167 </output>
```

- For the time settings, we simulate the experiment for half a day and using 1 min (60 seconds) as the time step size.

- The concentration values were given on each node. In order to print them out, the name of each component needs to be given.

- The output concentrations were defined under the each component.
- If there are more than one chemical component, multiple component names can be specified.
- The output file names can also be defined to follow the same format.

Media properties (MMP) and fluid properties (MFP)

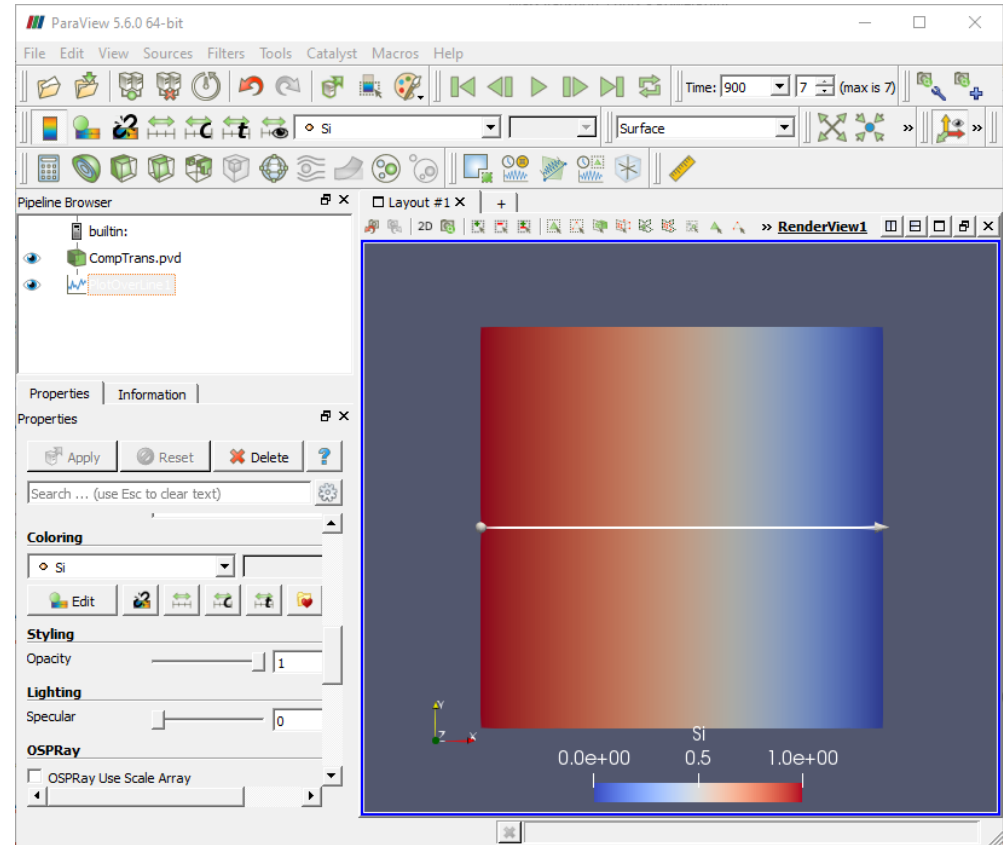
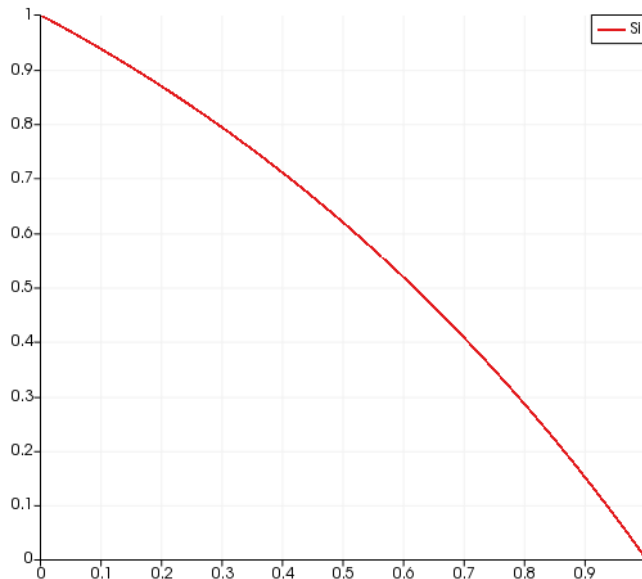
```
20 <media>
21   <medium id="0">
22     <phases>
23       <phase>
24         <type>AqueousLiquid</type>
25         <components>
26           <component>
27             <name>Si</name>
28             <properties>
29               <property>
30                 <name>pore_diffusion</name>
31                 <type>Constant</type>
32                 <value>1e-5</value>
33               </property>
34               <property>
35                 <name>retardation_factor</name>
36                 <type>Constant</type>
37                 <value>1</value>
38               </property>
39               <property>
40                 <name>decay_rate</name>
41                 <type>Parameter</type>
42                 <parameter_name>decay</parameter_name>
43               </property>
44             </properties>
45           </component>
46         </components>
47         <properties>
48           <property>
49             <name>density</name>
50             <type>Linear</type>
51             <reference_value>1</reference_value>
52             <independent_variable>
53               <variable_name>concentration</variable_name>
54               <reference_condition>0</reference_condition>
55               <slope>0.026</slope>
56             </independent_variable>
57             <independent_variable>
58               <variable_name>phase_pressure</variable_name>
59               <reference_condition>0.5</reference_condition>
60               <slope>2e-5</slope>

```

- Porosity of the sand column was defined with a value of 0.3.
- The pore diffusion coefficient is set to $1e-5$ m². So which one is bigger now, the advection or the diffusion?
- For the fluid property, we give the property of water here.
- For coupled problems, the liquid property can be dependent on temperature or concentration (following a linear slope).

Using Paraview to visualize the result

- The 2D domain can also be loaded into Paraview.
- To visualize the profile, the “Plot over Line” feature.
- Here we can also choose to show the concentrations of multiple components.
- Can you get the same concentration curve as follows?



Questions to answer at home:

- Now the model is diffusion dominant. How can I change the model to become advection dominant?
- Which part of the model is not realistic? How can I change it?
- What difference will it be if concentration is not fixed at the right boundary?