Demo — Adsorption and transport of elements in the GWB

Instructions are provided for calculating a speciation diagram using **React** and tracing a model of mass transport using **X1t**. A complete list of input files for the remaining examples follows. Double-click on a .rea, .x1t, or .x2t file to run that example. The .tdat and .sdat files are special thermodynamic or surface reaction datasets loaded in some of the examples. The As_reduction_scatter.gss contains scatter data which can be overlain on the results of the Arsenate_reduction.rea example in **Gtplot**.

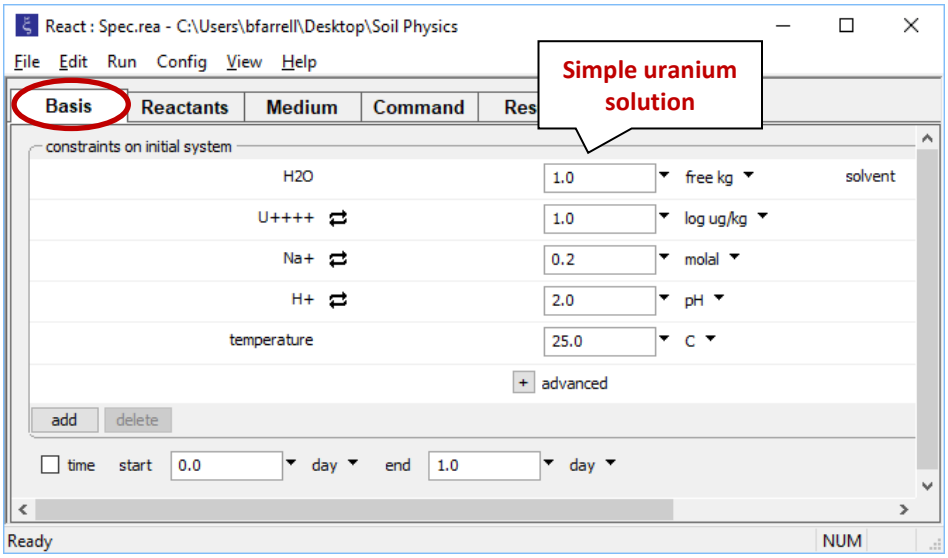
Examples		*Files needed*
1	Speciation diagram	Spec.rea*
2	Surface Complexation	Complexation.rea
3	Microbial Arsenate reduction	Arsenate_reduction.rea thermo+Lactate.tdat As_reduction_scatter.gss
4	Mass transport	Pulse.x1t* Dispersion.x2t
5	Dual Porosity	DualPorosity.x1t DualPorosity.x2t
6	Sorption	Sorbing.x1t Pb-Kd.sdat Pb-Freundlich.sdat Sorbing.x2t
7	Surface Complexation	3metals.x1t 3Metals.x2t
8	Biodegradation	Benzene.x1t thermo+benzene.tdat Benzene_Kd.sdat Benzene.x2t
9	Dissolution and Precipitation	
	**Instructions provided below*	

Speciation diagram — Uranium speciation

React is a flexible program that models equilibrium states and geochemical processes in systems that contain an aqueous fluid. Like **SpecE8**, **React** can calculate the equilibrium distribution of aqueous species in a fluid, a fluid's saturation state with respect to minerals, and the fugacities of gases dissolved in a fluid.

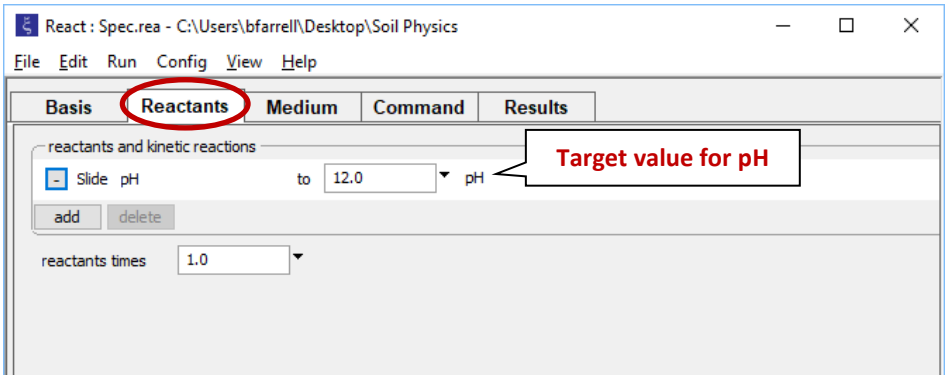
The program can also trace the evolution of a system as it undergoes reversible or irreversible reaction in an open or closed system, either at a given temperature or polythermally. **React** can integrate kinetic rate laws and simulate the fractionation of stable isotopes in a reacting system.

As an example, you can use it to see how the speciation of uranium changes with pH. Double-click on file "Spec.rea" and when **React** opens, look at the **Basis** pane



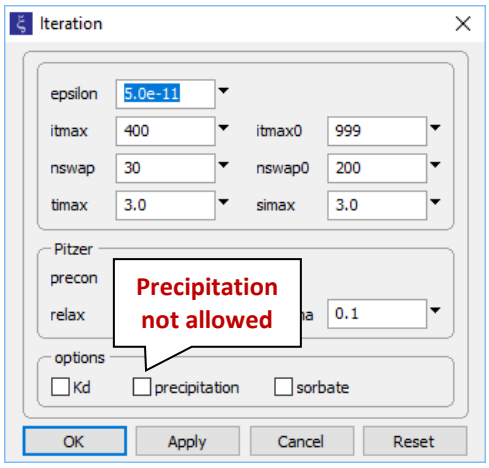
The pane shows the concentration of the dissolved uranium component in the fluid and the initial pH. In this simple example we've turned off the requirement for maintaining charge balance.

Move to the **Reactants** pane.



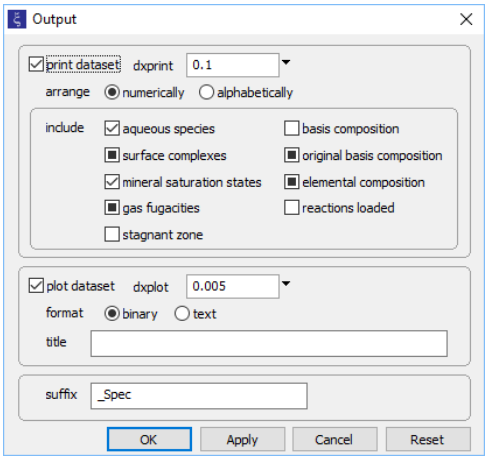
The input causes **React** to scan over a range of pH values, starting with the value of 2.0 and ending at 12. If the slide command was not already set, you would do so by clicking **add → Sliding → pH** and setting the target value.

On the **Config → Iteration…** dialog

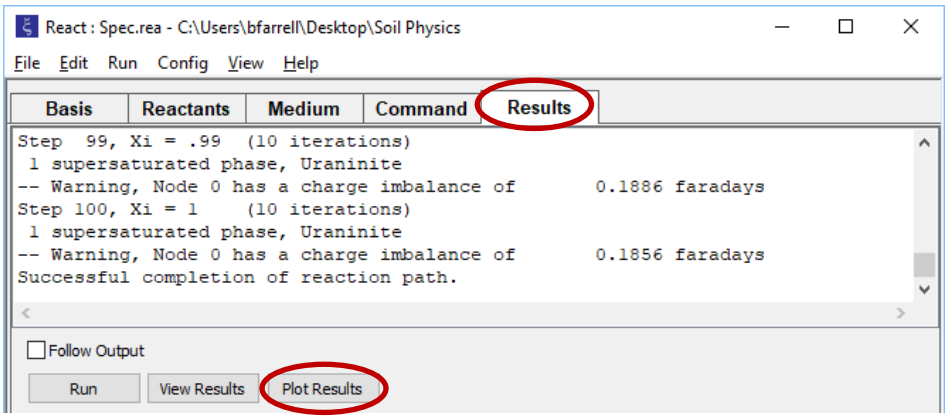


we see the precipitation option has been deselected. This setting will prevent supersaturated minerals from forming in our simulation (since we assume a fixed solution composition). Click **OK**

On **Config → Output…** set a suffix "_Spec".

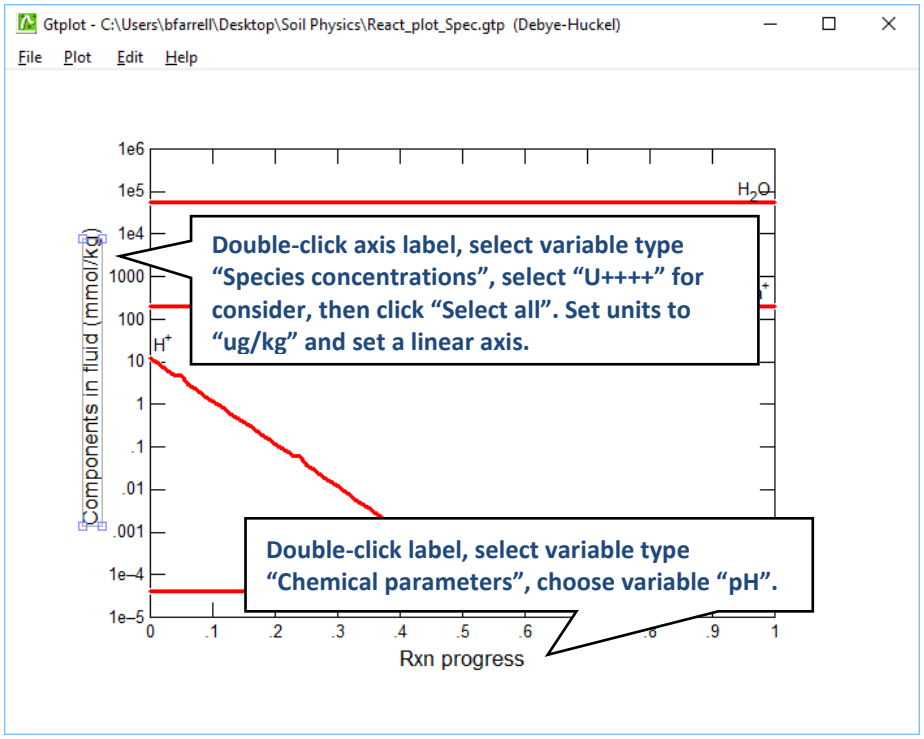


Click **OK**, then on the main window select **Run → Go** (or touch ctrl+g). **React** will move to the **Results** pane and trace the simulation.

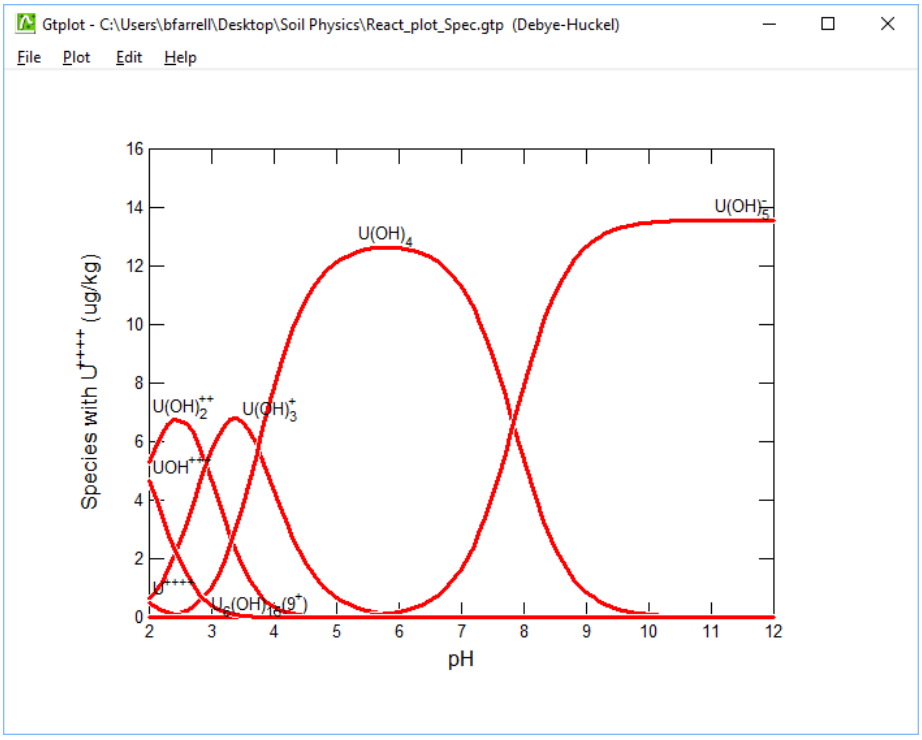


Click on the **Plot Results** button to launch **Gtplot**.

To make a plot of uranium species concentration vs. pH, configure the plot as indicated:



Your diagram should look like this:

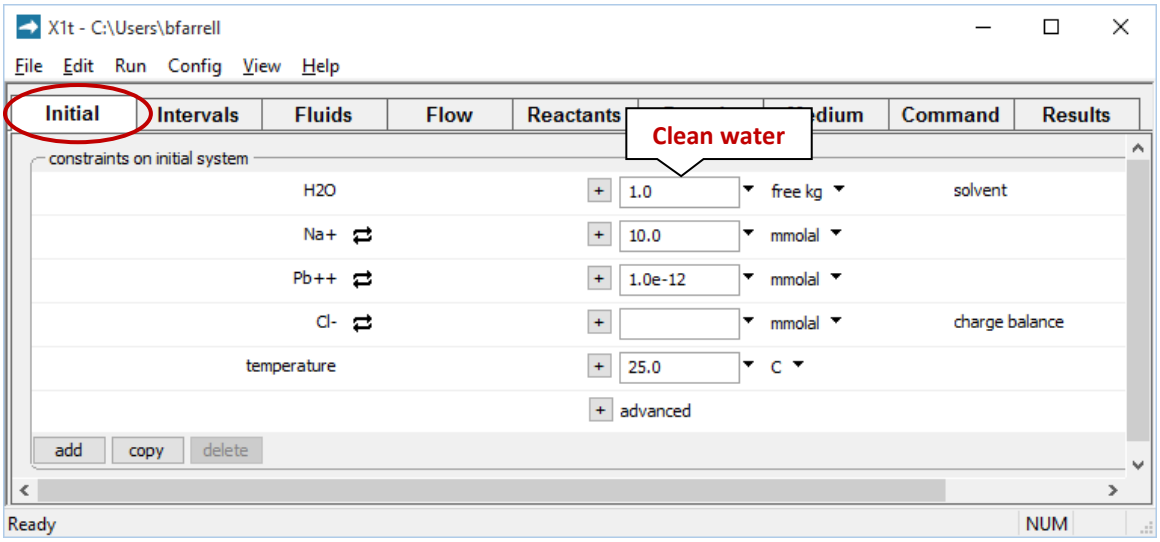


Mass transport — Migration of a non-reacting contaminant

Let's construct a model of how a contaminant might migrate in flowing groundwater, neglecting for the moment the possibility of chemical reaction.

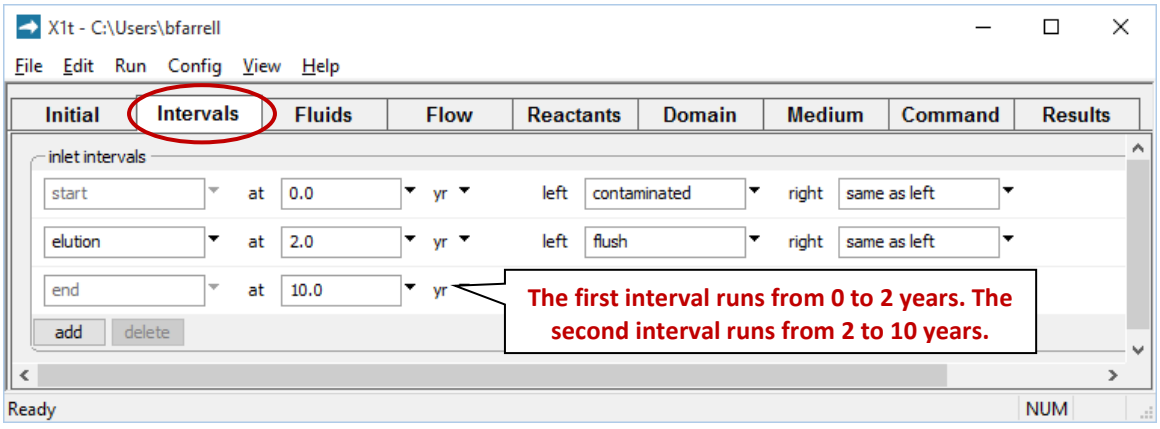
In our model, inorganic Pb contamination passes into an aquifer. After 2 years, the source is removed and the aquifer is flushed with ambient water.

Double-click on file "Pulse.x1t" and look at the **Initial** pane in **X1t**



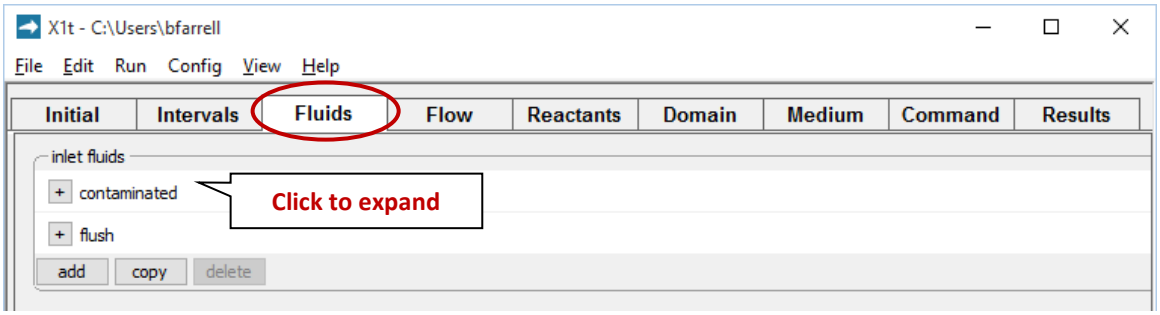
We've specified here that the aquifer be filled initially with clean water.

Moving to the **Intervals** pane

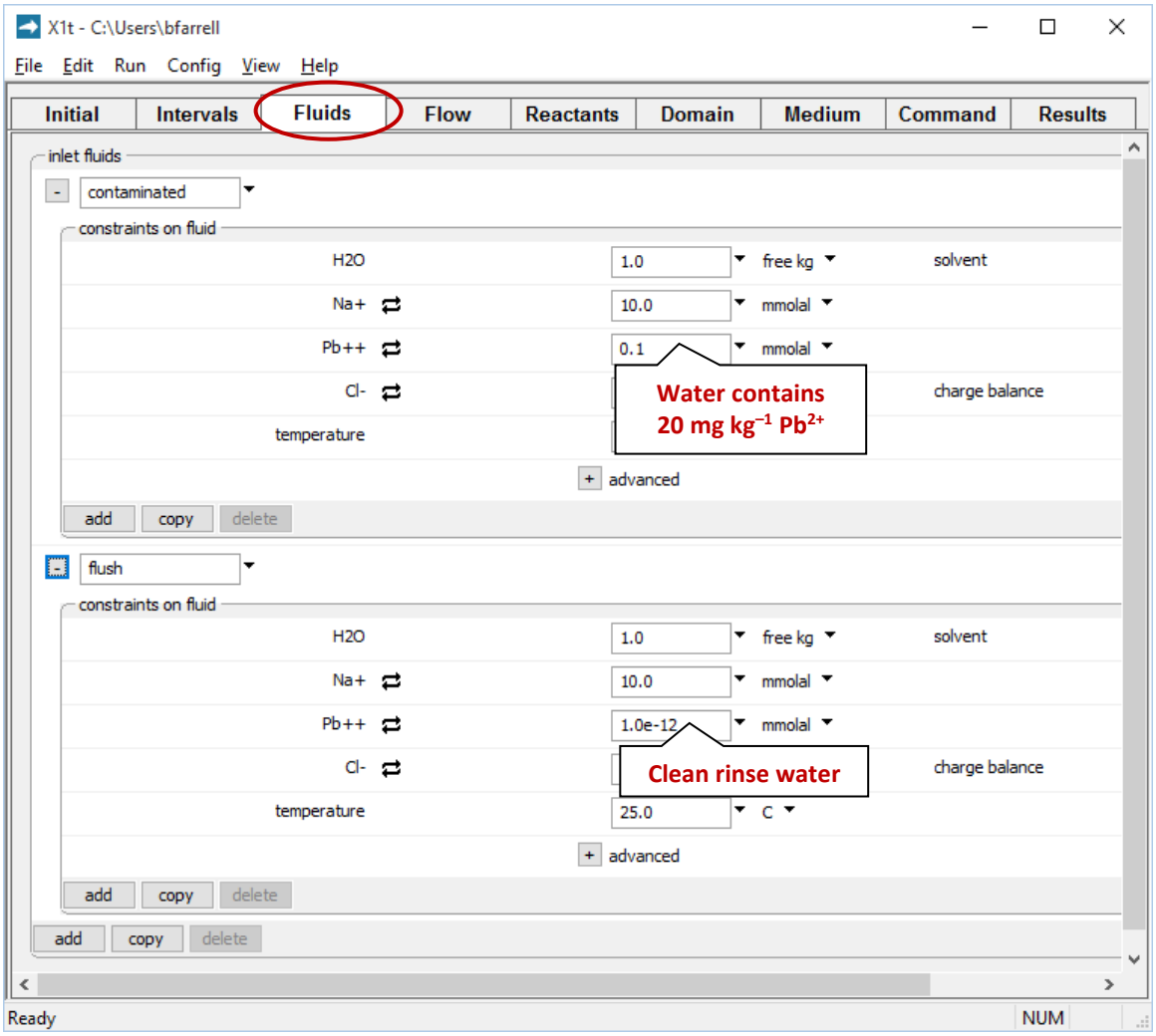


we've set start and end times for two reaction intervals, the imbibition and elution legs of the simulation. We've additionally designated two fluids, "contaminated" and "flush", to flow into the left side of the domain during the imbibition (start) and elution intervals, respectively.

The **Fluids** pane contains the two boundary fluids

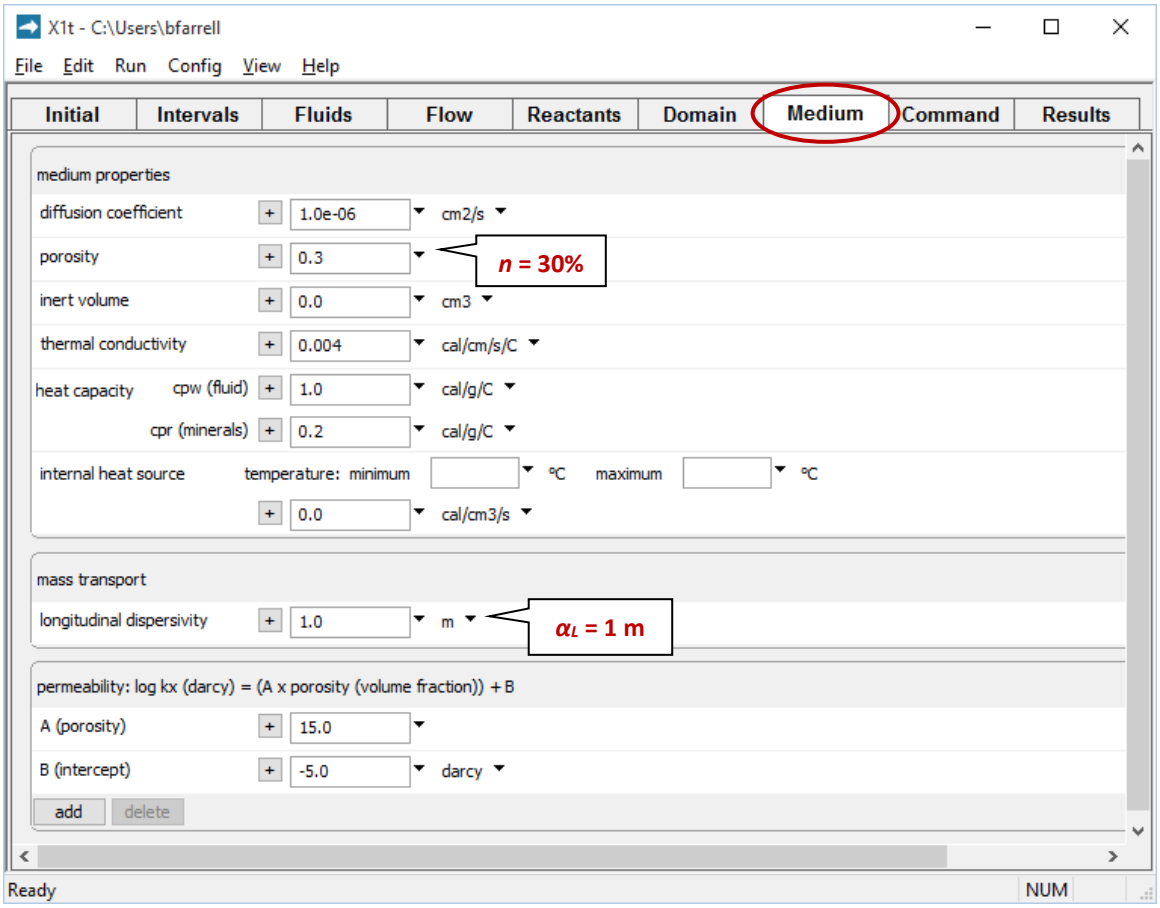


By expanding the "+" signs, we can view the "contaminated" fluid, which will be introduced in the imbibition leg

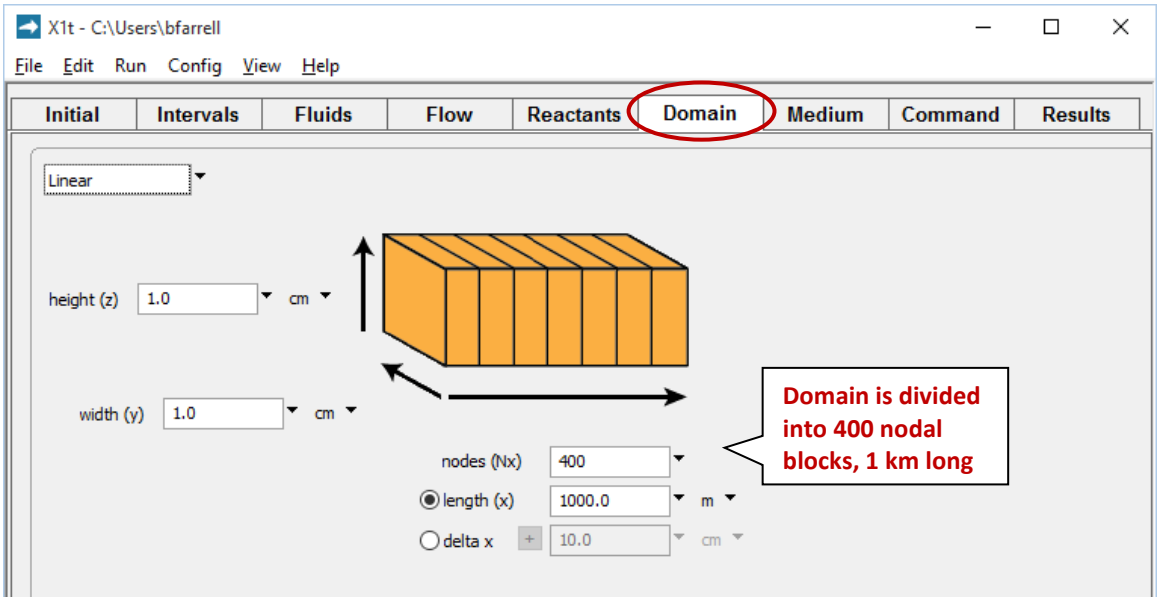


as well as the "flush" fluid: clean rinse water that will flow in during elution.

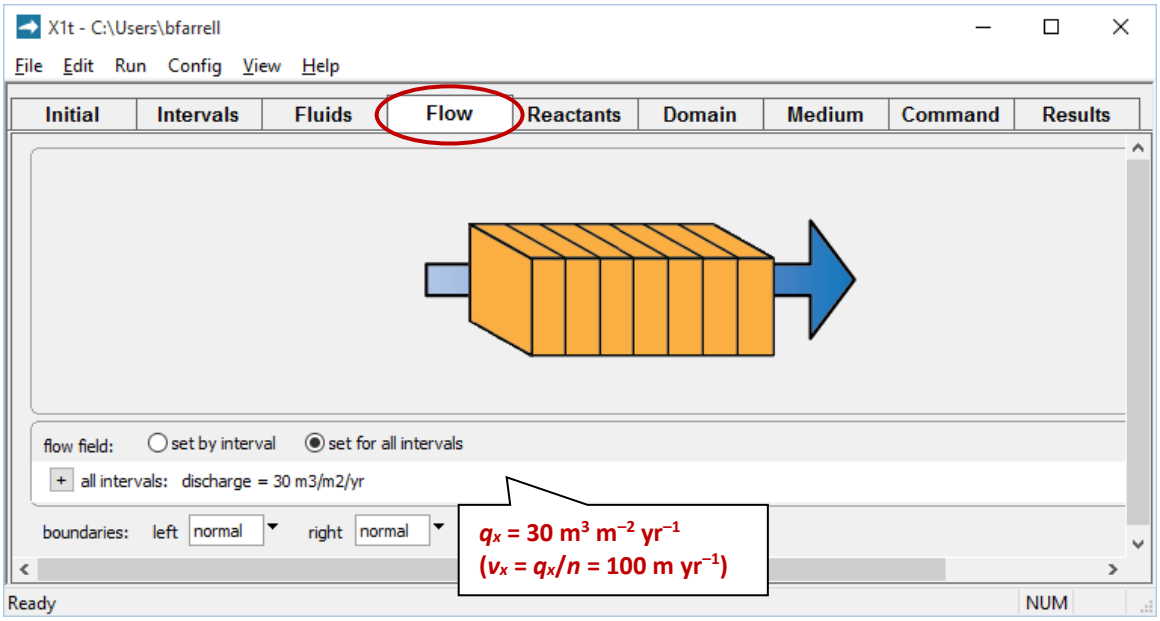
On the **Medium** pane you can see the values set for porosity and dispersivity



Check the domain size and gridding by moving to the **Domain** pane

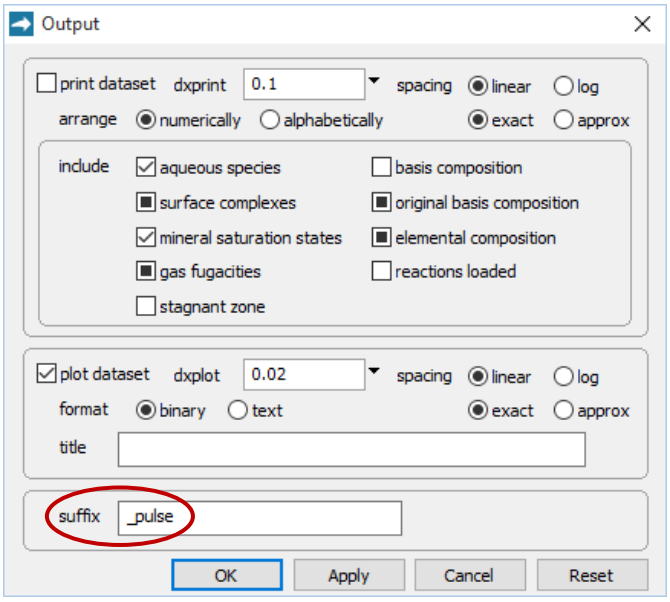


We set the rate at which fluid passes into the domain by moving to the **Flow** pane



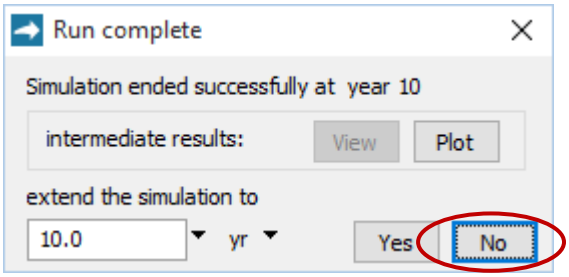
A positive specific discharge indicates that fluid will flow from left to right. The simulation spans 10 years, so given the porosity and discharge values we've set, the fluid in the aquifer will be displaced once over the course of the simulation.

Before launching the run, go to **Config → Output…** and enter "_pulse" in the suffix field



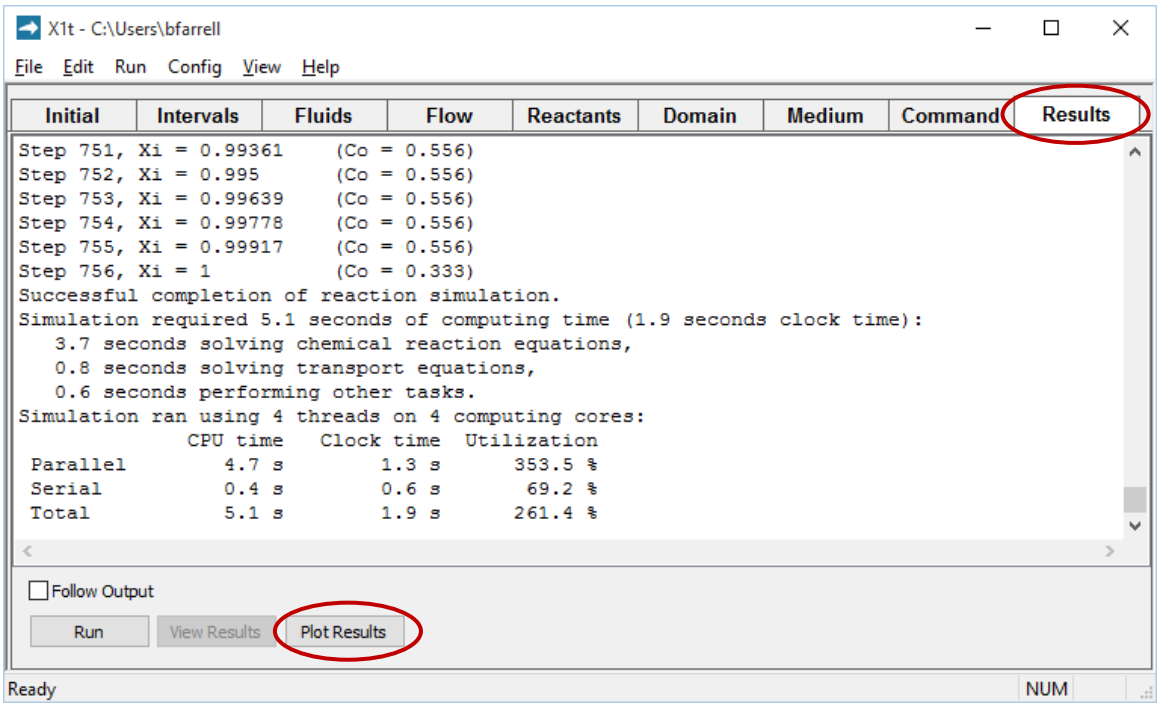
The suffix will be appended to the names of your output datasets, so you can go back to examine the results without rerunning the model. Click **OK**.

Trigger the calculation by selecting **Run → Go**. **X1t** will move to the **Results** pane, trace the simulation, and when it's done, offer to extend the run



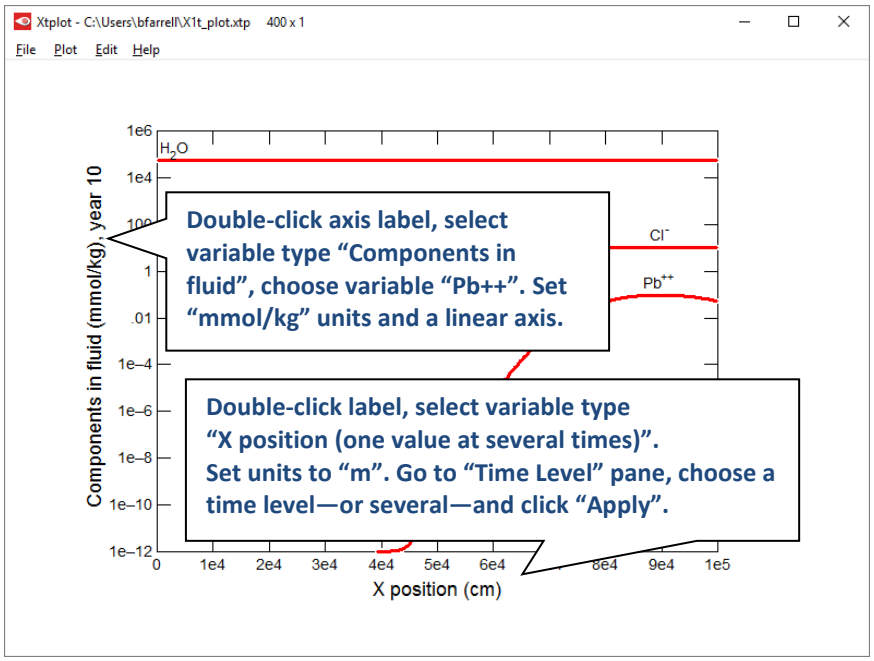
Click **No.**

Now, look at the bottom of the **Results** pane

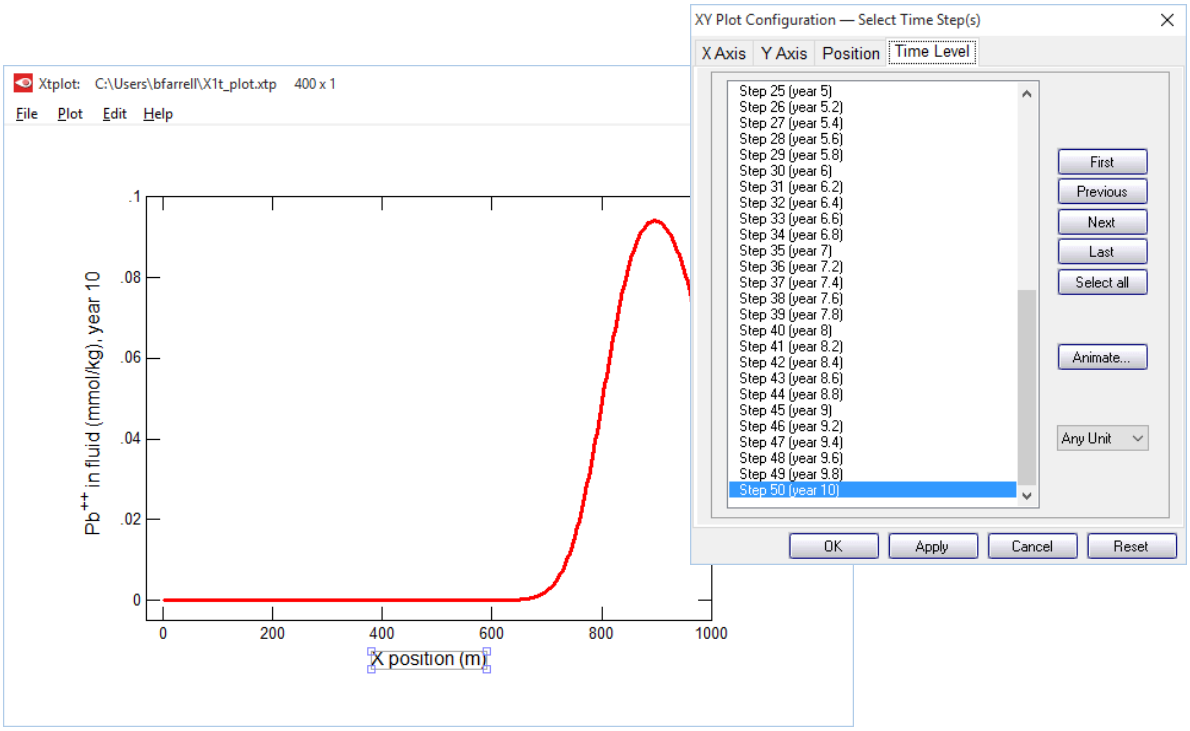


and click on the **Plot Results** button to launch **Xtplot**.

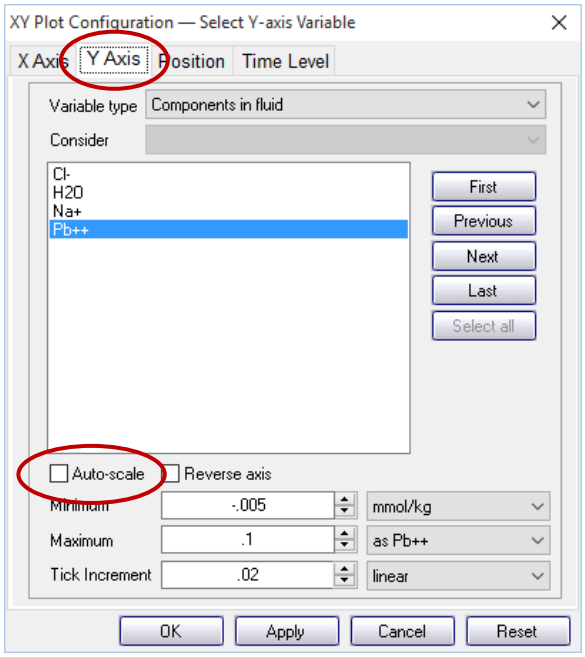
Configure the plot as indicated below



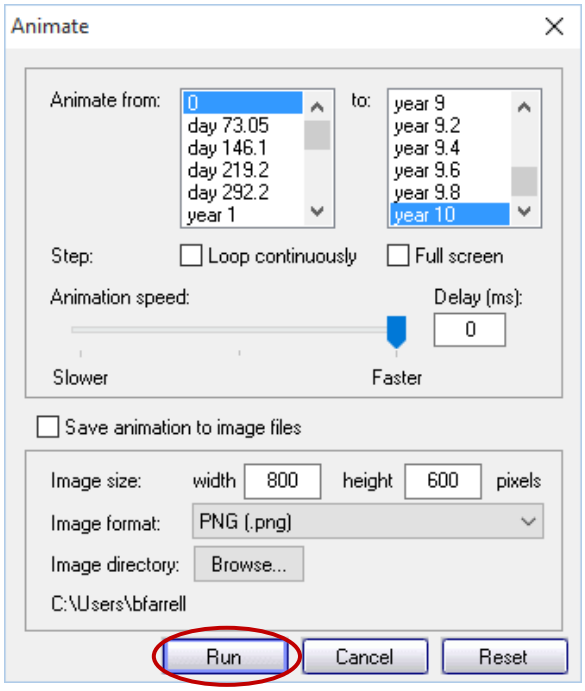
Your diagram should look like this:



Now, let's animate the plot. On the **XY Plot** dialog, go to the **Y Axis** pane and uncheck the "Auto-scale" option



In this way, you hold steady the *y*-axis range over the animation. Then, on the main window, choose **Edit → Animate…**

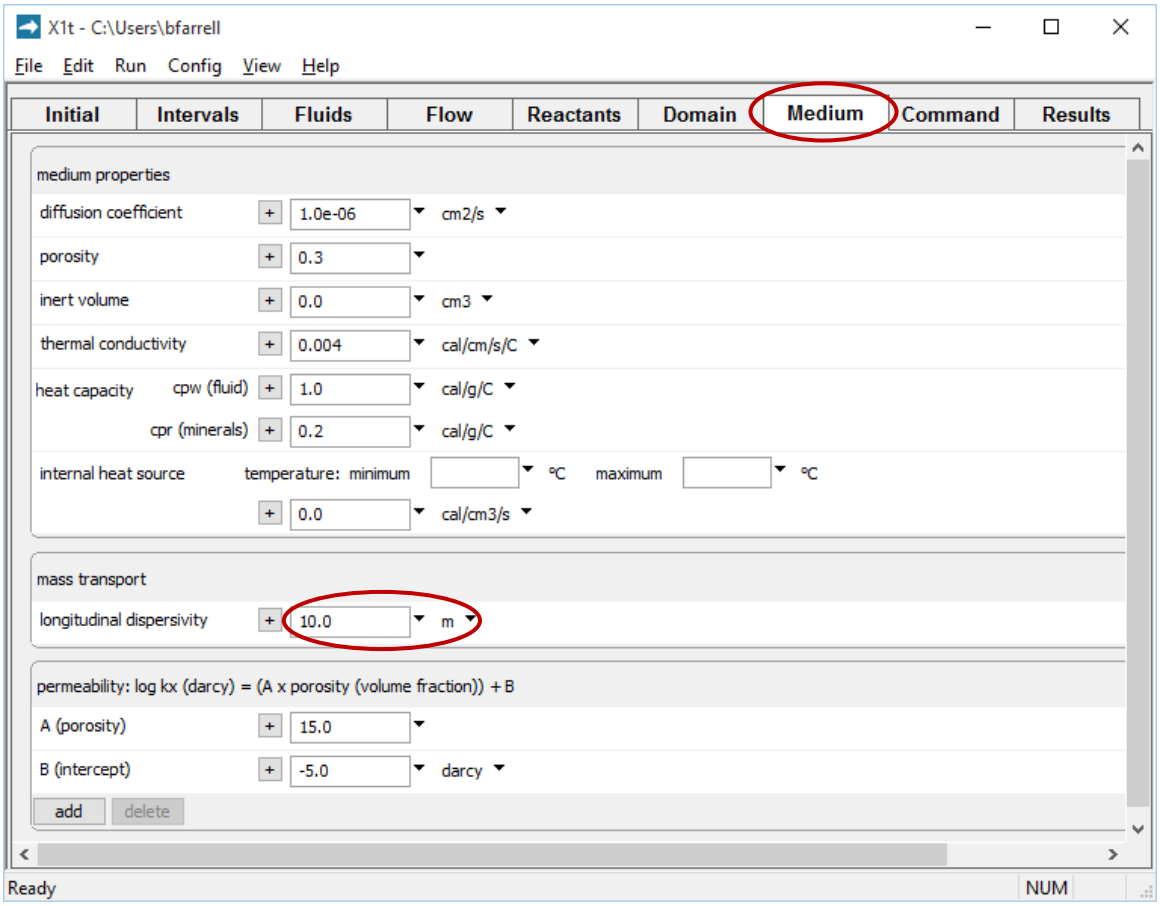


and click on the **Run** button. How does the shape of the pulse change as it traverses the aquifer from left to right?

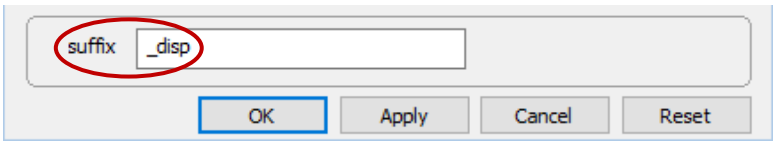
Mass transport — Effects of dispersion (continued from previous exercise)

How does dispersion affect contaminant migration? Let's find out.

Go to the **Medium** pane and change the entry for dispersivity from "1 m" to "10 m"



On **Config → Output…** set a new suffix "_disp"



Click **OK**, then on the main window select **Run → Go**. When **X1t** finishes, launch **Xtplot** to render the results. Compared to the first model, how have the results changed?

You can compare side-by-side instances of **Xtplot**. Double-click on "X1t_plot_pulse.xtp" to render your earlier results. If you feel ambitious, you can build up a composite diagram in MS PowerPoint to show both results in one diagram.