**Mass Transport**

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*Task 1: 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**

**Clean water**

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

Moving to the **Intervals** pane

**The first interval runs from 0 to 2 years. The second interval runs from 2 to 10 years.**

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

**Click to expand**

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

**Water contains**

**20 mg kg–1 Pb2+**

**Clean rinse water**

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

***n* = 30% porosity**

***αL* = 1 m**

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

**Domain is divided into 400 nodal blocks, 1 km long**

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

***qx* = 30 m3 m–2 yr–1**

**(*vx* = *qx*/*n* = 100 m yr–1)**

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

**Double-click axis label, select variable type “Components in fluid”, choose variable “Pb++”. Set “mmol/kg” units and a linear axis.**

**Double-click label, select Display “X position”.**

**Set units to “m”. Go to “Time Level” pane, select Display “One value at several times”, then choose a time level—or several—and click “Apply”.**

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 **Format → Animate…**

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

*Task 2: Effects of dispersion*

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.

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