Scientific Practice 1
A Tool For Modelling Advective-Reactive-Dispersive Transport In A Column Experiment

Janek Geiger

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Supervised by:

Jonas Allgeier

Dr. Adrian Mellage

1 Problem Description

The tool presented in this documentation solves a one dimensional solute transport problem in a column experiment. Given a constant input concentration, soil, compound and column parameters, as well as the elapsed time, this tool calculates the normed concentration for each point in the column. It is a browser based application and allows the user to make adjustments to the parameters expressing the experimental setup to which the model immediately responds. If a target state of the experiment is reached the concentration distribution data can be exported to a .csv file.

2 Physical Theory

The transport through the column is considered to be one dimensional and is described by the following expression:

$$c(x,t) = \frac{c_{ini}}{2}\mathrm{erfc}\Big(\frac{x - vt}{\sqrt{4Dt}}\Big)\exp(-\lambda t) \tag{1}$$

where:

c = concentration $[\frac{M}{L^3}]$
x = location $[L]$
t = time $[T]$
erfc = complimentary error function
v = seepage velocity $[\frac{L}{T}]$
D = dispersion coefficient $[\frac{L^2}{T}]$
exp = exponential function
λ = reaction coefficient $[T^{-1}]$

Eq. 1 considers advection, dispersion and reaction. The reaction term $\exp(-\lambda t)$ treats the reaction of the compound as first order decay. Advection and dispersion are combined in the argument of the complimentary error function (erfc)[4].

$$\mathrm{erfc}(x) = 1 - \mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty \exp(-\xi^2)d\xi \tag{2}$$

which represents the area under a zero-mean Gaussian bell curve in the intervalls $[x, \infty)$ and $(-\infty, -x]$. The bounds of the integral in Eq. 2 (x and ∞) represent the tail in the positive x-direction. Using the symmetry of the of a zero-mean Gaussian bell curve the tail in negative x-direction can be accounted for by the scaling factor 2. As the function value of the complimentary error functions is in the range [-2, 2], the scaling factor $\frac{1}{2}$ needs to be introduced in order to norm the output of Eq. 1.

As stated above, Eq. 1 considers advection, dispersion and reaction of the compound. It does not implement sorption of any kind and does not distinguish between different reaction kinetics. It assumes a homogeneous soil matrix.

3 Model

The model was developed in Python, but also uses JavaScript, as it is designed for browser application. The python library Bokeh [1] is central to the interactive character of the model. It provides tools for visualization and user-model interaction. The model itself works with sliders (see Figure 1) to receive user input and callbacks to change the model output based on the user input. The initial state of the model is calculated in Python, while for all subsequent states a callback is used to calculate the new state.

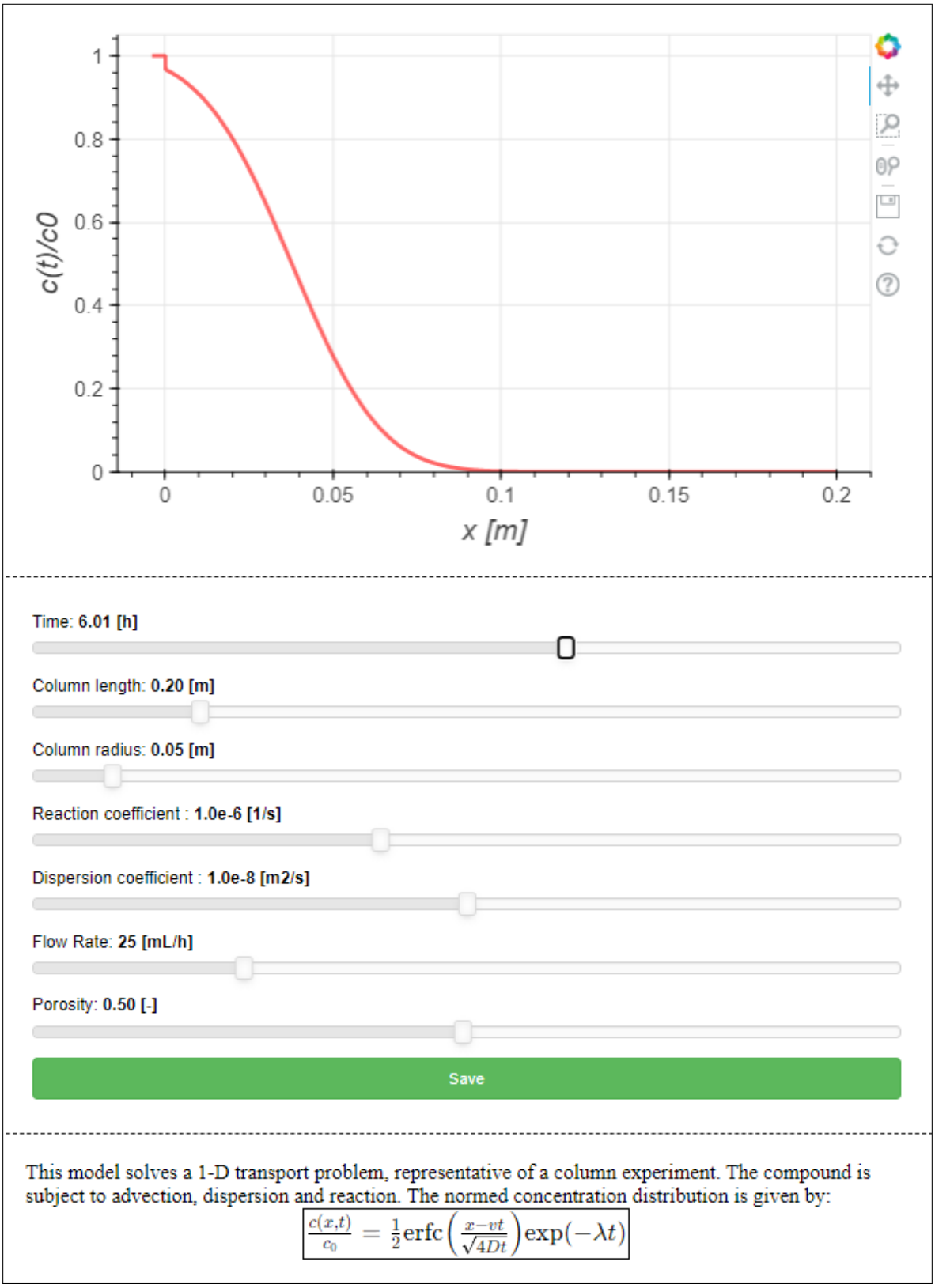

Figure 1: Initial state of the model

The callback is written in JavaScript so that it can be run on a browser. As JavaScript does not have a built in complimentary error function, the model accompanying html template calls the math library mathjs [2] in order to compute user based changes to the model (see Section 4). In order to respond to changes made by the user the callback re-evaluates Eq. 1 and updates the setup specific model data. These changes are plotted immediately and do not require a re-run of the model. After the experiment specific parameters are entered or a desired model outcome is reached, the model data can be exported to a .csv file containing the spatial coordinate x and the relative concentration y. This is realised via a save button (see Figure 1) which is a tool of the bokeh library as well. The specific application of this tool is credited to a forum post[3].

4 User Interface

The initial state of the user interface (UI) is depicted in Figure 1. Parameters that can be adjusted are the elapsed time in the experiment, column specific parameters as the column length, its radius, the flow rate and the porosity of the soil matrix and compound specific parameters with the reaction coefficient and the dispersion coefficient. Changes to these parameters can be performed with sliders, as depicted in Figure 1. Note that the scales of the reaction coefficient, the dispersion coefficient and the time slider are logarithmic. In the case of the two coefficients this choice was made, as the values for both of these coefficients stretch over several orders of magnitude for different compounds. In the case of elapsed experiment time, the choice of a logarithmic time scale was made, as the early time behaviour of a column experiment is often of greater interest than the late time behaviour until a breakthrough of the compound is reached.

Example In this paragraph two examples of experimental setups are presented. The experiment specific parameters are identical with the exception of the reaction coefficient and are taken from a range of values that are representative of a column experiment in a laboratory.

Table 1: Example parameters for conservative and reactive compound

	Time [h]	Length [cm]	Radius [cm]	Flow Rate [$\frac{\mathrm{mL}}{\mathrm{h}}$]
1	13.8443	0.2	0.05	25
2	13.8443	0.2	0.05	25

	Porosity [-]	Dispersion [$\frac{\mathrm{m}^2}{\mathrm{s}}$]	Reaction Coefficient [$\frac{1}{\mathrm{s}}$]
1	0.5	1e-8	1e-8
2	0.5	1e-8	1e-5

Case 1 in Table 1 represents the conservative compound with a first-order decay reaction coefficient of 1e-8 and case 2 represents the reactive compound with a respective value of 1e-5. While an ideal conservative compound is not subject to reactive degradation, the lowest value in the allowed rage was selected to represent conservative behaviour.

The spatial concentration distribution after t = 13.8 hours is depicted in Figure 2. In order to compare the solution of the tool with the analytical solution of Eq. 1, a .csv file was generated with the experimental setup, shown in Table 1 and exported to the software Matlab [5]. The column in the model is subdivided into 1000 distinct points. The normed concentration is evaluated for each of the points, given a change in experiment parameters. For values in between the 1000 points the plotted line is interpolated. In Matlab, the command fplot allows the plotting of a function in a given interval. With this command the analytical data in Figure 2 is generated.

This can be seen in the subplots of Figure 2 that show a zoomed section of the original plot in the interval x = [0.1 0.1002] m. With the aforementioned spatial discretization of a

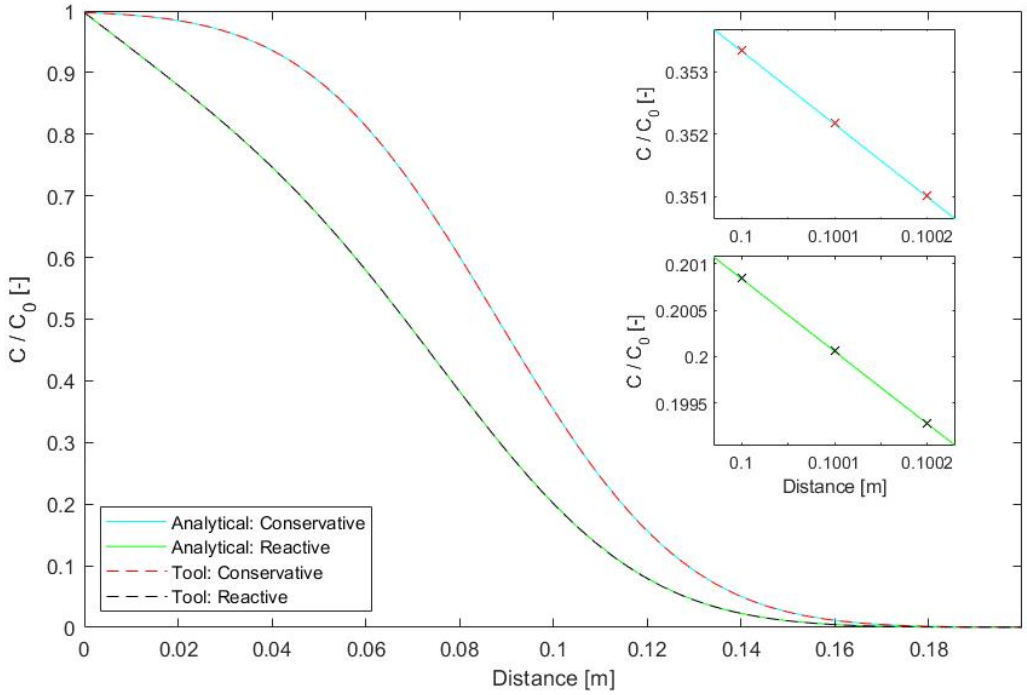

Figure 2: Spatial concentration distribution of a conservative and a reactive compound after 13.8 hours

thousand points in the column this yields three points in the interval that are marked with an x. From Figure 2 with its subplots a nearly perfect agreement between both data sets for both the conservative and the reactive compound can be observed. Furthermore the effect of first-order decay can be observed as well, as the spatial concentration distribution shows a lower normed concentration for the reactive compound 2 compared to the conservative compound 1.

5 Future Improvements

Eq. 1 expresses a simplified 1-D transport problem. It does not consider sorption of any kind. In subsequent versions of the model, the implementation of sorption is possible. As there are several approaches to the modeling of sorption it is advised to give the user the option of choosing between different types of sorption, e.g. Langmuir sorption of Freundlich sorption, or to neglect sorption in total.

Another improvement is the generation of breakthrough curves. This can be implemented via a second graph, where the breakthrough curve of a user specified time point is shown. This should come with the option of selecting several time points in order to compare breakthrough curves at different times.

If the user is working with insufficient information, the tool can be extended to estimate certain parameters. For example, if the dispersion coefficient of a compound is not known, it can be estimated with the following realtion:

$$D = \alpha v + D_e \tag{3}$$

with the dispersivity α, the velocity v and the molecular diffusion coefficient D_e.

Lastly, the option of choosing between several common laboratory experiments can be implemented as well.

The tool can be accessed via `https://github.com/JanGei/ColumnTestModel`

References

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