# Adapting the bundle of capillary tubes model (BCTM) for vertical soil solute transport modelling

## A case study

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# Abstract

This study explores an approach for adapting the bundle of capillary tubes soil model for vertical soil solute transport modelling. The soil is split into thin layers allowing vertical water flow between capillaries of differing width with concomitant advective flow of solutes. Diffusion is included to improve realism. Modelling software is developed to apply the proposed adaption. Case studies are performed to test the software. The transport modelling reacts in a way which makes qualitative sense to physical soil factors as well as chemical properties of modelled compounds.

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# Introduction

There are many contaminated soils in Sweden and there is a large on-going project to prioritize among known contaminated areas for possible remediation (Naturvårdsverket, 2012). To remediate all sites is not a realistic alternative, partly for economic reasons but also because remediation comes with an environmental cost which in some cases can be greater than that of the contamination (Naturvårdsverket, 2012).

In order to prioritize rationally decision makes must have reliable and easily interpretable data. Two important factors for determining the environmental risk of contaminated soils are ground water contamination as well as spread into sensitive and or protected areas through the ground water. Vertical transport of contaminants through top soil into ground water must be modelled to provide decision makers with a basis on which they can evaluate the risks posed to the chemical status of ground water and to further model the transport into neighbouring areas (Yadav and Junaid, 2015).

Per- / polyflourinated alkylic substances (PFASs) such as perflourooctanesulfonic acid (PFOS) and perflourooctanoic acid (PFOA) have in recent years been found in alarming concentrations in Swedish drinking water as well as fresh water fish (Livsmedelsverket, 2013). Their transport through ground water can be modelled using well established methods such as described by Edvinsson (2015). A major source of PFOS and PFOA contamination in Sweden is due to fire fighting exercises at airports and military sites (Hansson et al, 2016). There is a large uncertainty surrounding the transport of these substances from the soil surface to the ground water (Brusseau, 2018).

Vertical flow through the vadose zone is often modelled using a classical class of soil models, “a bundle of capillary tubes”(Hunt et al, 2013). This type of model envisions the soil as a collection of vertical tubes with differing radii and corresponding capillary suction and flow rates. It is a simple and useful soil model, however, it does not consider the transport or fluid movement from one pore size to another (Fatt, 1956). This is a major weakness when modelling solute transport since solutes would be modelled as flowing through only one pore size resulting in some particles being transported very quickly through large tubes with high flow rates whilst others are stuck for an extremely long time in narrow tubes with almost no flow.

Hunt et al (2013) argues that the legitimacy of soil physics depends on it being a branch of physics, metaphorically lending legitimacy from its parent discipline. This is unsatisfactory, the field of soil physics must have a claim on legitimacy on its own merits or it should be abandoned. Furthermore Hunt et al argue that the traditional bundle of capillary tubes model, which has been predominant in soil physics, lacks a connection to the physical reality of soils and thus hinders reasoning and prediction. I propose an adjustment of the bundle of capillary tubes model which should allay the criticism from Hunt and retain the useful properties of BCTM without adding too much complexity.

The main problem with direct application of BCTM for vertical soil solute transport modelling is the absence of solute movement between tubes of different widths. In order to rectify this solutes have to be able to move between tubes of differing width. The simplest solution would be to introduce a diffusion coefficient between the tubes which would allow the particles stuck in the narrow tubes to diffuse into larger tubes with higher flow rates through which they would then be transported. However, whilst such a solution would fix one end of the problem it would exacerbate the issue of high speed transport through wide tube pathways.

In order to solve this issue the water flow was remodelled based on a few simple principles. The soil was split into centimetre thick layers, each modelled as a bundle of capillary tubes, water flowing from layer to layer would be distributed between tubes in accordance to their suction i.e. in inverse order of magnitude (smallest first). Using this approach the preferential pathways for water flow would depend on water content and tube size distribution which is modelled as a function of grain size distribution.

The purpose of this paper is to examine a possible adaptation of BCTM for modelling vertical soil solute transport to include these important processes and still retain some of the simplicity which makes it suitable for applied purposes. The general idea for the adaptation is as follows: The soil is split into thin layers, from the surface to the groundwater level. Each layer is defined by its capillary tube size distribution and a sorption isotherm. Solute transport is modelled as the result of diffusion and advection. Diffusion is modelled both within and between layers. Water retention is modelled as a result of capillary suction as in BCTM. Water flow is modelled through the tubes using soil physics and between them by the assumption that due to their higher suction thinner tubes fill up before thicker tubes.

# Method

Modelling software was built based on the adaptation of BCTM for vertical soil solute transport modelling software in order to test the viability of the approach. The code was written in C++ using the open source wxWidgets library for the graphics user interface and the CodeBlocks interactive development environment. The software was then tested by running simulations of an extreme set of soil horizons to see whether the results make qualitative sense. It was further tested by running simulations of real contaminated soils based on data provided by Niras.

## The Vertical Soil Solute Transport Modeller

The implementation of the general solution which was built into the vertical soil solute transport modeller (VSSTM) and is presented here consists of a set of constituent models which combine into a meta model. The meta model produces the vertical transport rate which is plugged into a simple numerical model to plot the solute concentration as a function of depth and time. The constituent models are mathematical functions that map from a well-defined domain to another and can be used interchangeably with alternative models as long as their domains correspond. E.g. the diffusion model described here can be replaced by any other diffusion model which depends on the same input as long as its output can be modified to come out in the same form and range. This approach was chosen to enable future refinement as well as adaptation for different soils and climates.

## Mechanistic Model

### *Conceptual Meta Model*

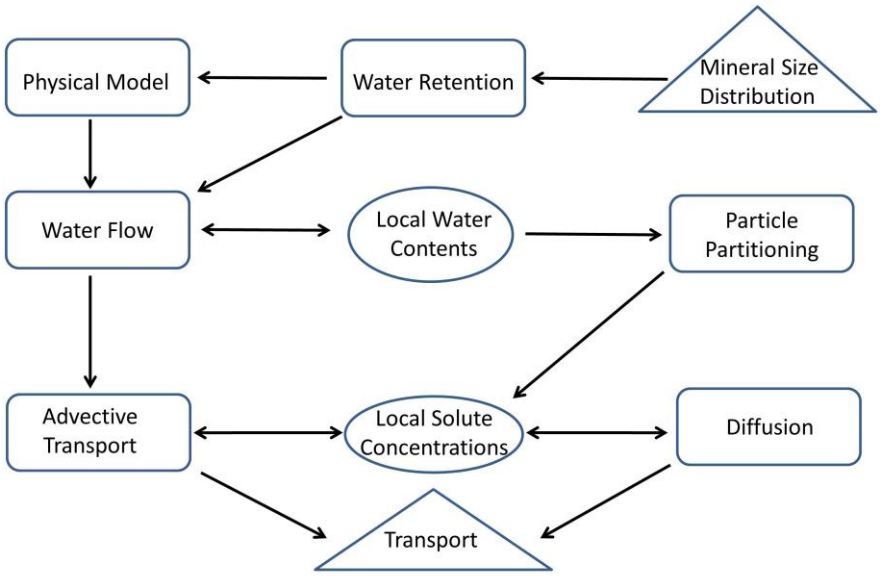

**Figure 1 shows the conceptual meta model. Rounded boxes are constituent models, ovals are key variables, and triangles are input or output.**

A model for water retention as a function of mineral size distribution is used to define the characteristic curve (water retention as a function of pressure). A physical model as described in the general solution is then generated to match the characteristic curve. Water flow is modelled based on the water retention and physical model. The flow modelling defines the local water content for each tube size in each layer at every point in time. Based on the local water content and the chemical properties of the modelled compound the compound is locally partitioned between sorbed and solved state. The diffusion model acts to even out the solute concentration within each layer and between adjacent layers. Advective transport is a simple multiplicative function of the water flow and local solute concentrations. The transport is simply the sum of advective and diffusive transport.

### *Water retention and the physical model*

The VSSTM allows for the definition of up to five soil horizons which are defined by their grain size distribution, organic content, void ratio, and density. Water retention is calculated from this data using van Genuchten and Mualem's model (VGM) as described by Mohammadi and Meskini-Vishkaee (2013). A tube size distribution is generated using the Monte Carlo method so that the capillary rise matches the water retention curve obtained through VGM and the volume allotted to each tube size is equal. The tube geometry is left undefined except for the bottleneck minimal radius which defines the water retention and flow rate. The tube size distribution is defined by bottleneck radii assigned to the twenty modelled tube size categories in such a way that each size category is assigned an equal portion of the total pore volume.

The amount of tubes within each size category is calculated from the arbitrary assumption that the volume of each tube is the cylindrical volume defined by the bottleneck radius multiplied by 1.5 and the layer's width. The total surface area is calculated from the conservative assumption that all mineral grains are round, excluding the clay which is handled separately. The surface area is assigned to the tube size categories as a linear function of their radii based on a cylindrical model of the tube geometry. The minimum water content in each tube is modelled to be the Langmuir film which is calculated as the surface area multiplied with the Langmuir thickness (Langmuir, 1938).

The basic modelling unit is the tube size category within each layer, they will henceforth be referred to as "pores". The sets of tubes of the same size are handled as singular pores for computational reasons. Conceptually a pore in this context can be thought of as a kind of average.

### *Sorption isotherm*

The modelled compound can be either solved in water or sorbed to clay, organic matter, or mineral surfaces. A simple linear sorption model was utilized because it can be implemented in a computationally sparse manner and is a good approximation of freundlich isotherms at most environmental concentrations (Xie et al, 2011). Equation 1-3 were used, under the assumption that equilibrium is reached in each pore between each time step (1 day).

$$K_D = \frac{K_{mineral} * A_{mineral} + K_{Clay} * Clay + K_{OC} * OC}{Water\ volume} \qquad \text{(Eq. 1)}$$

$$Compound_{sorbed} = \frac{K_D * Compound_{total}}{K_D + 1} \qquad \text{(Eq. 2)}$$

$$Compound_{Solute} = \frac{Compound_{total}}{K_D + 1} \qquad \text{(Eq. 3)}$$

Each pore has its own partitioning coefficient ($K_D$) calculated from partitioning coefficients between water and organic matter ($K_{OC}$), water and clay by weight ($K_{Clay}$) and between water and mineral surfaces by area according to equation 1. Clay is technically a subset of the mineral category but is handled separately because it has a very large and variable surface to weight ratio as well as sorption potential which makes it critical for estimating the total partitioning coefficient ´(Brusseau, 2018). Because it is handled separately it can easily be modified based on data about what type of clay there is in the modelled soil.

*Diffusion model*

The diffusion is modelled in two steps, first out, then in. Since the physical model lacks topography the diffusion process is simplified. Diffusion out is modelled layer by layer through comparing the solute concentration in each pore to the average concentration in the same layer as well as adjacent layers. The pores which have a higher concentration than these averages contribute to the diffusion into them, as shown in figure 2. The diffusion in is then handled layer by layer through splitting the diffusion in between the pores with less than average concentrations as seen in figure 2. This diffusion model is used instead of modelling diffusion between each individual pore to reduce the amount of calculations involved in each time step.

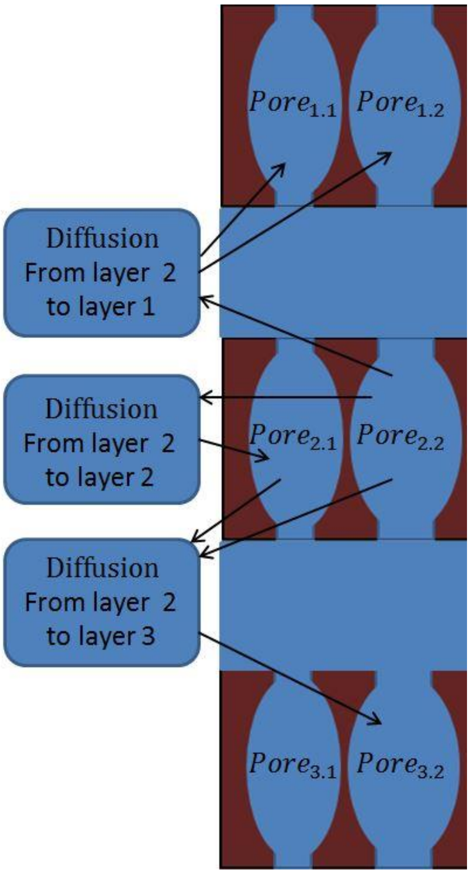

**Figure 2 illustrates the diffusion model.**

Quantitatively the diffusion out is modelled using Fick’s law with a diffusion coefficient calculated using Millington and Quirk’s formula for diffusion in soil as a function of porosity and saturation (Millington and Quirk, 1961). The concentration gradient used in the diffusion formula is the difference between the pore concentration and the pertinent layers average concentration. The distance is calculated using the difference between the pores layer width for diffusion between layers and the pore diameters for inter layer diffusion. The diffusion in is split between the pores with less than average concentrations as a linear function of the difference between their concentrations and the average.

*Water flow and advection*

The boundary conditions are rather straightforward; at the surface there is a water input defined by the user and the ground water table is assumed to be constant and able to receive whatever flow is coming from the lowest modelled layer. Allowing for a varying ground water table would have either necessitated making the model three dimensional, including inclines and ground water drains such as wells and rivers among other things, or introduced an unnecessary arbitrary variable. For the case study a 30 day cycle of randomly generated precipitation values with an average of 2 mm per day was used. Evapotranspiration is modelled to be constant over time as well as depth at 1 mm per square meter and day. Within each layer the evapotranspiration is split between the tubes as a linear function of their water content by volume. The evapotranspiration model is kept simple to focus on the other aspects of the modelling, 1 mm per day is close to the average for Sweden estimated by SMHI (1998).

Since the outflow from a layer must equal the inflow into the layer below the maximum allowable output from each layer must be calculated before the flow is modelled. This is done through calculating the maximum input each layer can handle starting from the bottom. Because the ground water is modelled to be able to absorb any amount of input water the bottommost layer has no limit on how much water it is allowed to output. Its maximum input is thus defined by the sum of the air volume and the maximum flow rate, i.e. the saturated hydraulic conductivity. Layers above have their maximum input defined as the lowest of either the maximum input into the layer below plus air volume or the saturated flow rate plus air volume.

Once the maximum flow is determined the next step is determining whether the flow is saturated or unsaturated. If the input of water into a layer exceeds its air volume flow is modelled to be saturated, otherwise it is considered unsaturated.

Saturated flow is modelled in two or three phases depending on whether the flow is limited by input water from above or the hydraulic conductivity of the layer. If the hydraulic conductivity is the limiting factor the flow is modelled in two simple phases. First the input water fills any volumes previously occupied by air. Then the water flows through each pore according to its hydraulic conductivity as described below. If the water input from above is limiting the flow a third phase of flow is introduced in which pores which do not retain water are drained.

The water flow rate at saturation is calculated according to Darcy’s law. The saturated hydraulic conductivity of the soil, K, is calculated using a formula by

Chapuis (2004). The relative flow rate through pores of different width is calculated using Poiseuille’s law according to which the flow rate through a tube is proportional to the fourth power of its radius (Zhe et al, 2019).

Unsaturated flow is modelled in a two-step process. The outflow is handled for each tube followed by the inflow. Pores for which the capillary rise exceeds their elevation in relation to the ground water level retain their water and have zero flow in unsaturated conditions as illustrated in figure 3 layer 1 and 2. At saturation water flows through even the smallest pores since it is assumed that there is contiguous water mass pushed through the pore due to a pressure differential, contrast layer 2 and 3 in figure 3. The unsaturated flow is calculated on a pore by pore basis as their saturated flow multiplied by their level of saturatio. If the flow exceeds the free water volume, the water volume minus the Langmuir film, it is reduced to the free water volume.

Advection is simply modelled by keeping track of where the water is coming from and how much solute it contains based on its concentration. Any water that flows into a pore carries with it a certain amount of solute just as any water flowing out of it does. For flow between the layers the average solute concentration out is applied to the inflow into the layer below.

$$J_A = Q \times C \qquad \text{(Eq. 4)}$$

$J_A =$ Advective flow $(g/s)$
$Q =$ Water flow $(m^3/s)$
$C =$ Concentration $(g/m^3)$

$$\sum_i Qut_{1.i} = Q_B = \sum_i Qin_{1,i}$$

$Q_B =$ The flow B $(m^3/s)$ between layer 1 and 2

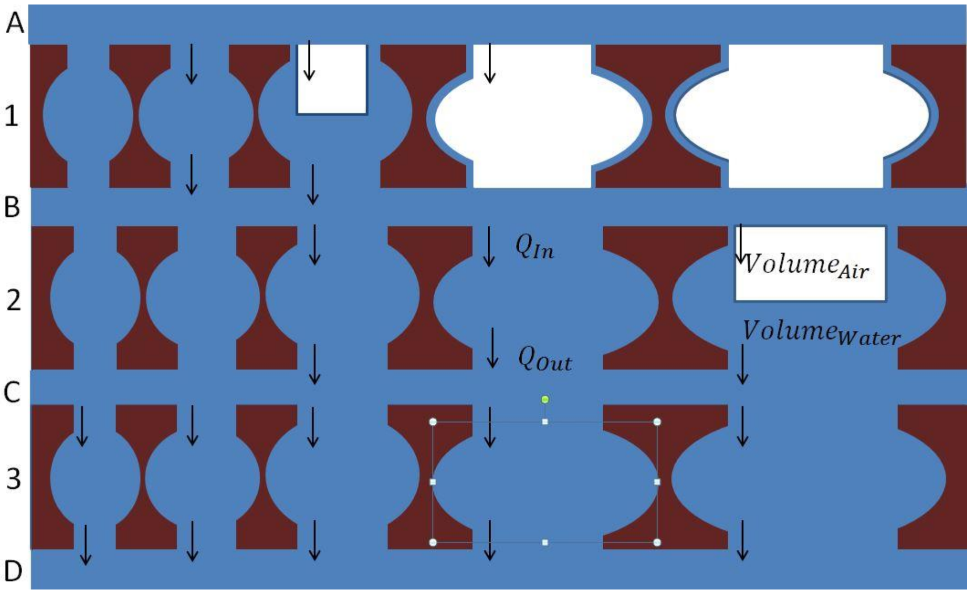

**Figure 3 illustrates the flow model through three layers (1-3). Water fills smaller pores first, flows through pores large enough not to retain water, layer 1 and 2, unless the layer is saturated in which case it flows through all pores, layer 3.**

$$C_B = \frac{\sum_i (Qut_{1.i} C_{1.i})}{Q_B} \qquad \text{(Eq. 5)}$$

$C_B =$ The solute concentration $(g/m^3)$ in the flow $Q_B$

*Programming implementation of the model*

After generating the initial state of the model (the physical model, initial water content and initial concentrations of the modelled compound) the model runs for a pre-set amount of time steps (days). Each step starts by partitioning the modelled compound, achieving local equilibrium between sorbed and solved states. This is followed by modelling the diffusion, and the water flow with concomitant advection. Finally the evapotranspiration is modelled before the next iteration begins. The implementation of these principles into a modelling program resulted in a very computation heavy solution which makes long term modelling impractical. For that reason a second layer of the model was implemented to numerically compute the transport as a function of the rates determined in the mechanistic model.

### Numerical Model

The numerical model utilizes the transport rate from the mechanistic model to extrapolate the solute movement into the future in a much less computation heavy manner. The average rate of vertical transport through each layer towards the end of the mechanistic modelling ($T_i$) is used to define the downwards flux ($J_{i,t}$) of the modelled compound as described in equation 6-7.

$$J_{i,t} = M_{i,t} \times T_i \quad \text{(Eq. 6)}$$
$$M_{i,t+1} = M_{i,t} + J_{i-1,t} - J_{i,t} \quad \text{(Eq. 7)}$$

## The case studies

VSSTM was tested through modelling the environmental fate of two chemicals through a synthetic soil as well as through two real soil profiles. This was done through entering soil and contaminant parameters into the VSSTM and plotting the result using Microsoft Excel. The synthetic soil consists of three very different horizons, to test the transport rates of different compounds through radically different soil substrates. The real soil profiles are based on soil and contaminant spread data provided by Niras. The transport modelling through them represent the intended use of the VSSTM with real data.

Varying the model parameters, see whether VSSTM reflects the soil and compound parameters in a way that makes sense.

**Table 1 shows the soil and contaminant spread parameters used in the case study modelling in tabulated form**

| Soil and Horizon | Width $m$ | PFOA $\mu g/kg$ | PFOS $\mu g/kg$ | OC % | Clay % | Silt % | Sand % | Gravel % |
|---|---|---|---|---|---|---|---|---|
| Silt | 1 | 100 | 100 | 1 | 0 | 99 | 0 | 0 |
| Sand | 1 | 100 | 100 | 0 | 0 | 0 | 100 | 0 |
| Sand OC | 1 | 100 | 100 | 25 | 0 | 0 | 75 | 0 |
| S1 H1 | 1.00 | 0.10 | 350 | 0.40 | 3 | 10 | 57 | 30 |
| S1 H2 | 1.07 | 1.6 | 690 | 0.68 | 3 | 13 | 84 | 0 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| S2 H1a | 0.40 | 1.7 | 220 | 0.86 | 2 | 15 | 40 | 44 |
| S2 H1b | 0.40 | 0.40 | 100 | 0.86 | 2 | 15 | 40 | 44 |
| S2 H2 | 0.20 | 4.0 | 2500 | 0.91 | 3 | 19 | 74 | 3 |
| S2 H3 | 0.90 | Eq. 8 | Eq. 9 | 0.26 | 1 | 7 | 89 | 3 |

The contaminant spread data for soil 2 horizon 3 is missing and is thus modelled using linear interpolation between the closest existing concentration values, equation 8 and 9.

$$C = 4.0 + (depth - 1.0)/(1.9 - 1.0) \times (0.01 - 4.0) \qquad \text{(Eq. 8)}$$
$$C = 2500 + (depth - 1.0)/(1.9 - 1.0) \times (110 - 2500) \qquad \text{(Eq. 9)}$$

**Table 2 shows the mineral size distribution from table 1 in the more detailed form which was used in the modelling.**

| Soil and Horizon | Fine Silt % | Medium Silt % | Coarse Silt % | Fine Sand % | Medium Sand % | Coarse Sand % | Fine Gravel % | Medium Gravel % |
|---|---|---|---|---|---|---|---|---|
| Silt | 33 | 33 | 33 | 0 | 0 | 0 | 0 | 0 |
| Sand | 0 | 0 | 0 | 33 | 33 | 33 | 0 | 0 |
| Sand OC | 0 | 0 | 0 | 25 | 25 | 25 | 0 | 0 |
| S1 H1 | 2 | 3 | 5 | 6 | 21 | 30 | 15 | 15 |
| S1 H2 | 2 | 2 | 9 | 28 | 50 | 06 | 0 | 0 |
| S2 H1 | 2 | 4 | 9 | 8 | 17 | 15 | 18 | 26 |
| S2 H2 | 4 | 7 | 8 | 25 | 37 | 12 | 2 | 1 |
| S2 H3 | 1 | 1 | 5 | 17 | 64 | 8 | 1 | 1 |

Hellsing et al (2016) experimented with sorption of PFOA and PFOS to alumina and silica. They fitted their results using Langmuir sorption isotherms. However, since the VSSTM requires a linear sorption coefficient the isotherms where linearized by assuming the concentrations are low enough for there to be no competition for sorption sites. The $K_{Mineral}$ coefficients used for modelling the transport of PFOA and PFOS, table 3, are the averages of the linearized coefficients for silica and alumina. The $K_{Clay}$ values, table 3, were derived from the experimental values of Zhao et al (2014) analogously to the $K_{Mineral}$ values. The sorption isotherms were linearized by assuming infinitesimal concentrations and the average taken from three kinds of clay, montmorillonite, kaolinite, and hematite. The $K_{OC}$ values used in the modelling, table 3, were taken straight from Milinovic et al (2015). The diffusion coefficients, table 3, are from a study by Pereira et al (2014).

**Table 3 shows the partitioning and diffusion coefficients used in the modelling**

| PFAS | $K_{Mineral}$ $(mL/m^2)$ | $K_{Clay}$ $(mL/g)$ | $K_{OC}$ $(mL/g)$ | D $(m^2/s)$ |
|---|---|---|---|---|
| PFOS | 0.005 | 807100 | 710 | $0.31 \times 10^{-9}$ |
| PFOA | 0.002 | 588533 | 91 | $0.32 \times 10^{-9}$ |

# Results

Figure 4 shows how PFOA transport is modelled through a synthetic soil consisting of three horizons with a 1 metre width each.

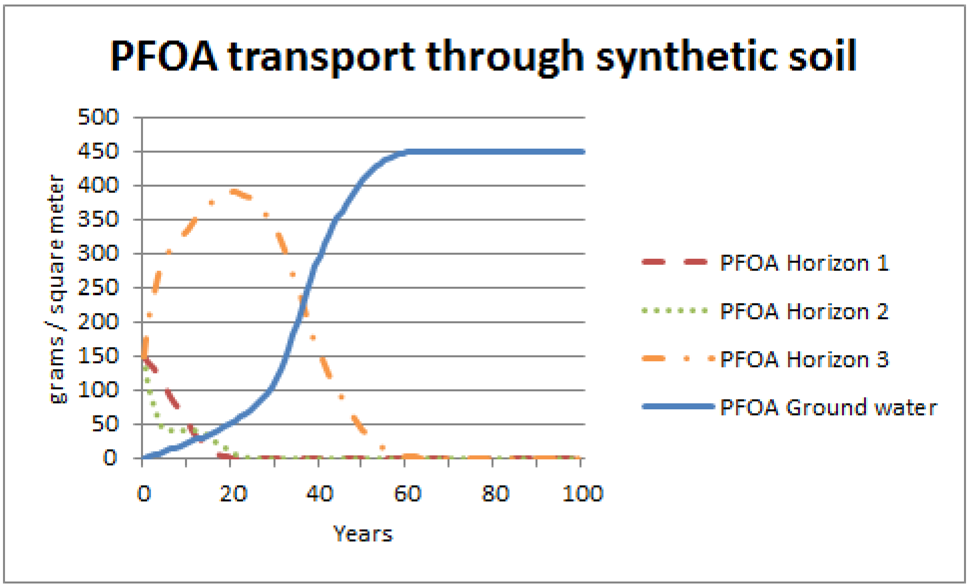

**Figure 4 shows the modelled movement of PFOA through a synthetic soil over time.**

PFOA flows relatively swiftly through the first horizon in spite of the high silt content because sorption and the concomitant retardation depend mostly on the clay and organic content resulting in low equilibrium sorption in horizon 1 (table 4). The initial reduction of PFOA in horizon 2 is swifter due to its incredibly low equilibrium sorption (table 4) caused by the pure sand which has a very small surface area compared to the silt in horizon 1. After a few years it reaches a plateau which can be attributed to the low concentration resulting in a PFOA leakage that equals the constant leakage from horizon 1. The third horizon has a high sorption coefficient which results in it buffering the PFOA transport, storing the leachate from the horizons above, slowly releasing it into the ground water over 40 years' time after the horizons above have been completely leached.

**Table 4 shows the resultant equilibrium partitioning at full water saturation in each modelled horizon.**

| Soil and horizon | $K_D$ PFOA | $K_D$ PFOS |
|---|---|---|
| Synthetic Silt | 26 | 37 |
| Synthetic Sand | 0.04 | 0.09 |
| Synthetic Organic | 103 | 761 |
| Soil 1 Horizon 1 | 88 | 132 |
| Soil 1 Horizon 2 | 73 | 116 |
| Soil 2 Horizon 1 | 61 | 108 |
| Soil 2 Horizon 2 | 69 | 114 |
| Soil 2 Horizon 3 | 26 | 44 |

In figure 5 we see the results of modelling transport of PFOS through the same synthetic soil. The results are similar but the retention in horizon three is severely prolonged due to the high organic content and much higher $K_{OC}$ value of PFOS compared to PFOA, table 3.

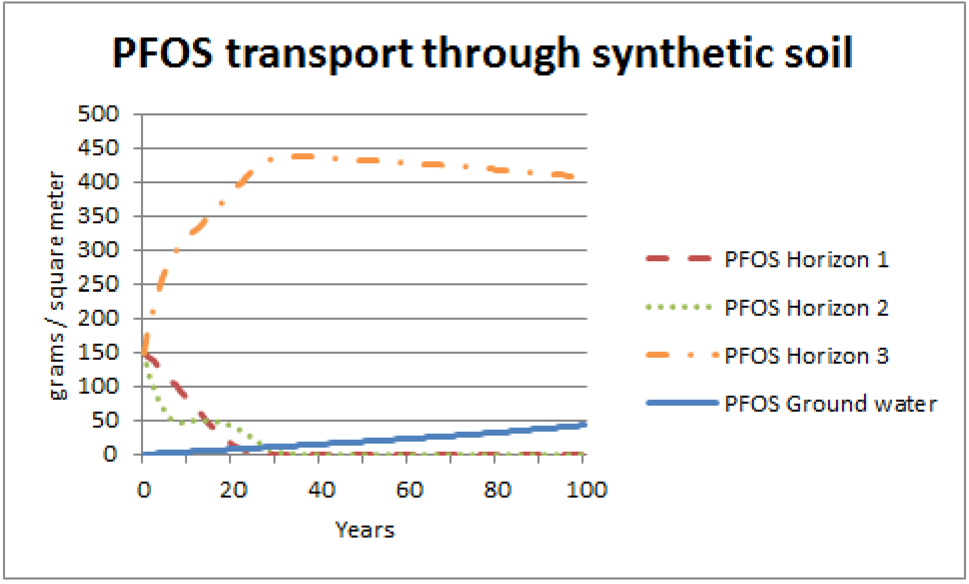

**Figure 5 shows the modelled movement of PFOS through a synthetic soil over time.**

In figure 6 we can see the modelled ground water leachate of a real soil. The initial concentration in horizon 1 is too small for its leachate to significantly affect the PFOA concentrations in horizon 2 or the ground water leachate. In this simple scenario the leachate approximates exponential decay.

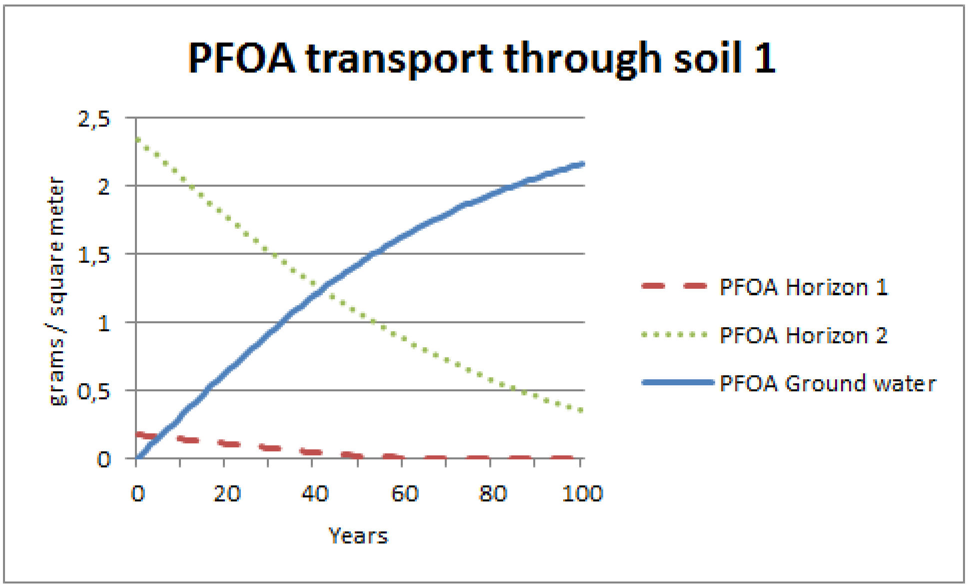

**Figure 5 shows the modelled transport of PFOA through soil 1 over time.**

Comparing figure 7 and table 4 we can clearly see that the modelled retardation of PFOS is not a simple function of $K_D$ values. The PFOS content in horizon 2 stays at a plateau for about 60 years in spite of the lower sorption and higher content compared to horizon 1 which by itself would mean higher transport out than in and consequently lowered PFOS content. The leachate out of horizon 1 almost matches that of horizon 2, probably because of the higher water flow closer to the surface caused by evapotranspiration. The nearly constant PFOS content in horizon 2 causes a nearly linear ground water leaching.

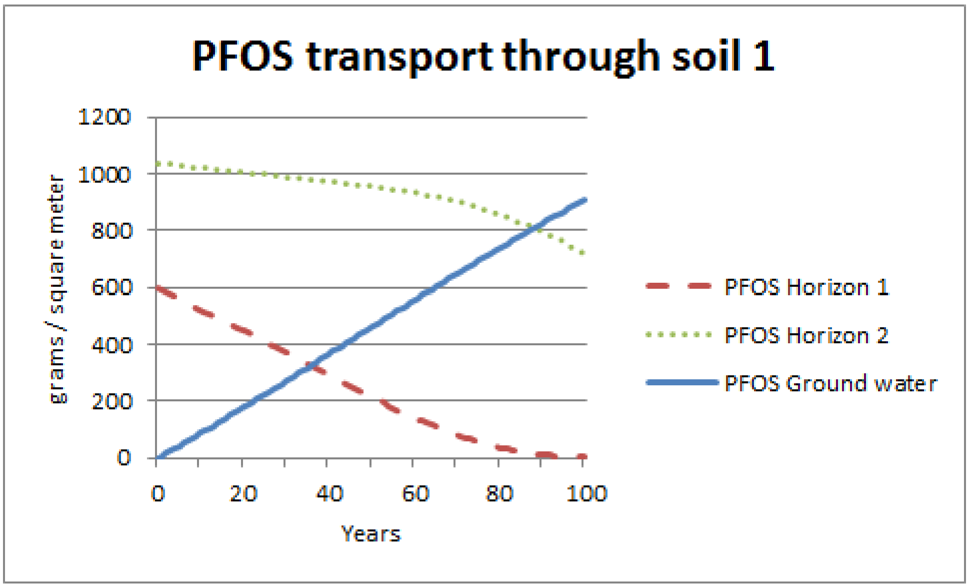

**Figure 6 shows the modelled transport of PFOS through soil 1 over time.**

Similarly to the dynamic in figure 7 the PFOA content in horizon 2, figure 8, increases due to significantly higher leachate from horizon 1 in spite of the $K_D$ values being similar, table 4.

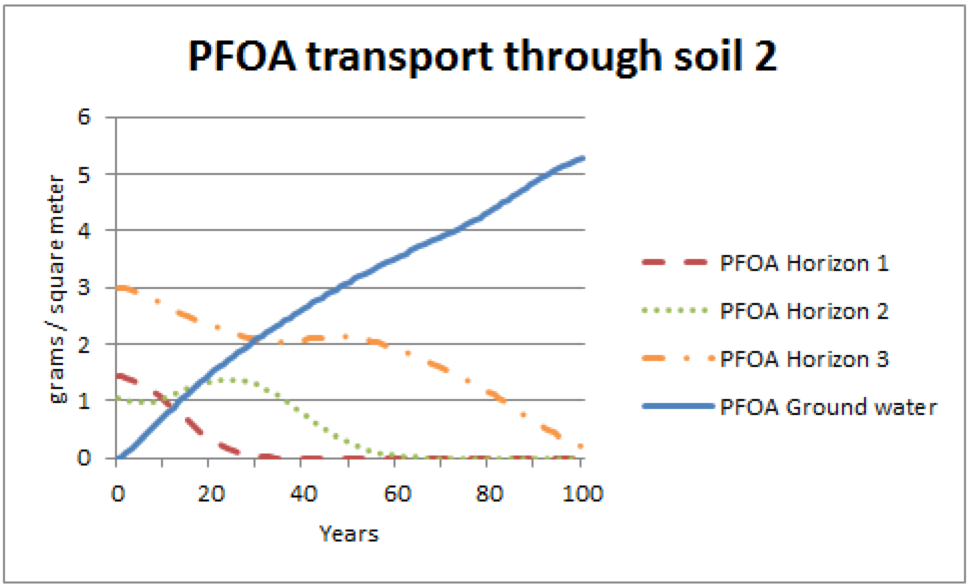

**Figure 8 shows the modelled transport of PFOA through soil 2 over time.**

Comparing figure 8 and 9 with the $K_D$ values in table 4 it seems counterintuitive that PFOS leaches into the ground water quicker than PFOA. However, this is due to the majority of PFOS being in the third horizon at the start of the modelling.

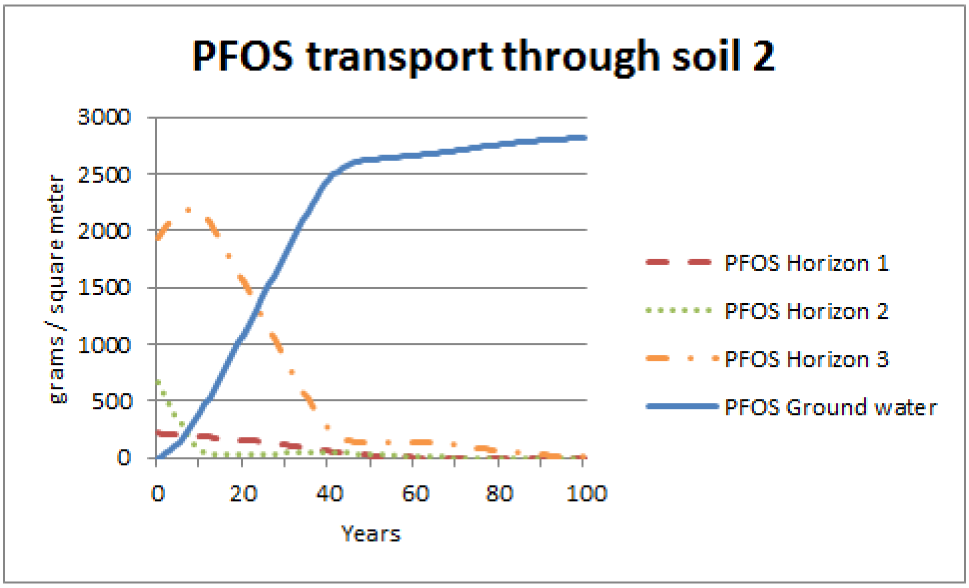

**Figure 9 shows the modelled transport of PFOS through soil 2 over time.**

Ocular comparison between the PFAS contents in horizon 1 over time clearly shows that PFOS is transported more slowly than PFOA. Horizon 3 empties more quickly of PFOS than PFOA because PFOA is transported into it from above in much larger quantities, relative to the total amount.

# Discussion

The case studies show that the VSSTM can provide simple output which is easily interpreted and has a strong connection to the physical soil parameters as well as the modelled compounds sorption coefficients. The graphical representation of environmental fate over time provides a useful basis for decision making concerning contaminated soils. The ground water leachate as a function of time can be used as input for ground water transport modelling. VSSTM can be considered to have proven the usefulness of the proposed adaption of BCTM provided the predictions are accurate.

The results show that VSSTM responds to input parameters in a way that makes qualitative sense. Due to budget and time constraints the results have not been compared to empirical data which means that the transport rates may be over- or underestimated. However, the arbitrary parameters can be adjusted to fix the diffusion and transport rates. To maximize the accuracy of predictions these parameters can be used as fitting parameters for any specific soil based on simple laboratory soil core transport experiments. VSSTM would then function as an extrapolation tool to go from laboratory transport rates to field scale environmental fate modelling.

Due to a combination of time, budget, and data constraints VSSTM couldn’t be properly tested, there are several aspects that would need rigorous testing before VSSTM could be held up as conclusive evidence that the general solution is a valid. Foremost is the need to test the predictions quantitatively which could be achieved through core leachate tests in a set up with a ground water table. Secondly the effect of calibration also needs to be examined. VSSTM also needs to be trimmed down for a quicker run time to prove that the approach doesn’t necessitate quite so long time to run. Finally there is a need for rigorous sensitivity analysis which is non-trivial since the model is non-linear, which precludes “one at a time” sensitivity analysis (Saltelli et al, 2006).

The general solution is conceptually simple, as is evidenced by it being explained in a short paragraph. Its implementation in VSSTM is more complicated but since it consists of simple constituent models it can be broken apart, understood piecemeal and then be put back together. The VSSTM is a compromise between simplicity and realism. It is decidedly more complicated than the BCTM but in return it may produce results which more accurately describe soil solute transport whilst remaining conceptually simpler than percolation theory. VSSTM has one major drawback; it is so computation heavy that it takes a normal computer up to an hour to run a single simulation. This precludes repetition heavy methods for testing out scenarios or sensitivity analysis. However, this problem is largely caused by the author's inexperience at programming and could be largely mitigated by cleaning up the code and making a few simplifications.

The VSSTM could be refined through modifying the constituent models based on empirical data. As it is an implementation of the general solution proposed to the adaptation problem it may illustrate problems with the general solution but it doesn't define its merit. This approach to modelling vertical transport is useful for applied purposes such as deciding how to handle a contaminated soil because it relies on easily measured input, provides output that is easy to interpret and relies on principles that are easy to understand. The modular nature of VSSTM means that it is simple to improve upon and to calibrate for any particular type of soil or include factors such as degradation for contaminants with short environmental half-lives.

To what extent the mechanics of flow and transport in the model reflects real soil transport is important to examine. This information is necessary to determine which modelled results are modelling artefacts and which grant insight and or good transport rate results. One of the flow mechanics which follow directly from the modelling assumptions is that the smallest pores which are too large to retain water at any given depth are responsible for a large portion of the water flow due to "filling up" before the larger pores. This mechanic has an impact on the transport rate since the smaller pores have proportionally larger surface areas and thus higher local $K_D$ values, larger retardation rates and lower transport rates. This ought to funnel the transport into larger pores with higher transport rates closer to the ground water table where the water retention is greater. Whether this reflects actual soil transport dynamics or is merely a modelling artefact has implications for the modelled transport rate as a function of depth and consequently the expected ground water leakage.

Hunt et al (2013) argues that the approach in soil physics of applying different models to every process modelled makes it difficult to tackle problems involving multiple processes due to the implied "lack of conceptual unity in our understanding". I beg to differ, as long as the interaction between processes is properly characterized in our meta models there is no lack of unity in our understanding. On the contrary the conceptual understanding of the processes interaction is laid bare in the mathematical expressions of the models interaction which allows us to focus on it. This approach is embraced in VSSTM with its highly modular approach.

# Conclusions

The modelling tool (VSSTM) built based on the adaptation of BCTM for vertical soil solute transport modelling produces results which reflect the input parameters in a way that makes qualitative sense. The results need to be quantitatively verified but if the predictions made by the VSSTM can be shown to have decent precision this approach based on the bundle of capillary tubes model and soil physics will be shown to be useful for practical applications in modelling environmental fate.

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