Dynamic soil-plant uptake simulation model for monovalent organic chemicals, such as pesticides and pharmaceuticals

Documentation and User Guide

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Content

Two files are provided, named

i) New plant uptake model for ionics 2x2 matrix.xls
is a steady-state solution of the plant uptake from soil, only roots and leaves. It serves for control purposes of the complex numerical model.

ii) Plant uptake one season numerical.xlsx
A fully dynamic coupled water-and-solute transport model for soil and plants, parameterised for one growth season (1st March to 31st July), with numerical matrix solution.

Both files were coded in excel.

Disclaimer

The plant uptake models for ionisable compounds, such as pesticides and pharmaceuticals, contain many parameters that are rarely known in detail and variable in time. The models therefore usually do not predict exact concentrations.

Their main purpose is
- understanding the processes underlying transport in soil and plant uptake
- analysing the most relevant parameters (for a given set of data)
- understanding the complex interplay between water movement, water uptake (into plants) and chemical transport
- education.

The software is distributed under gnu3-license which allows free use. The code is open to allow students to see and change the code.

The author under no circumstances take any liability for the outcome of the model calculations.
A) Steady-state solution “New plant uptake model for ionics 2x2 matrix.xls”

This small steady-state model is far easier than the complex dynamic model. It’s main purpose is control and comparison to the dynamic model, but it can also excellently serve to give a first overview of the general behaviour of a monovalent ionisable compound in the soil-root-leaves system.

A.1 Model description

This short small model combines the cell model (for prediction of partition coefficients, see next chapter A2) with a steady-state soil-root-leaf model (similar to Trapp 2015). Transport of chemical is via xylem from soil to roots to leaves, and via phloem from leaves to roots. In the analytical steady-state solution, the concentration C1 is soil is constant; C2 is roots; C3 is leaves.

The underlying differential equation is
\[ \frac{dC_2}{dt} = k_{12} C_1 - k_2 C_2 + k_{32} C_3 \]
\[ \frac{dC_3}{dt} = k_{23} C_2 - k_3 C_3 + I \]

with the steady-state solution:
\[ C_2 = \frac{(k_{12} + k_{32}) C_1 + I k_{32}}{k_2 + k_{32}} \]
\[ C_3 = \frac{k_{23} C_2 + I}{k_3} \]

where k12 is transfer rate from 1 (soil) to 2 (roots); k2 is loss rate from 2 (roots) and k32 is gain with phloem from leaves. Similar, k3 is gain with xylem from roots to leaves, and k3 is total loss from leaves. Input I (from air) is currently set to zero. The way the rates are derived can be seen directly in the excel file and follows (except for phloem) the descriptions in Trapp (2015) and Hurtado et al. (2016).

The model is implemented in excel. The screen shot is Figure 1. Input is always into the yellow fields. There are cells for chemical input, plant input, and soil input. The unit and a description of the parameter is given in the excel sheet. The chemical input is in the same format as for the dynamic model and is described there (section B).

Figure 1. Screen shot of the analytical steady-state model.
A.2 Partition coefficients and cell model

The description herein refers to the file Plant uptake one season numerical2.xlsx

**Brief:** The cell model is implemented as sub-unit in both the steady-state and the dynamic model (sheet “one season”). It is used to calculate partition coefficients of ionisable compounds (monovalent). It uses its own set of default parameters. Plant-specific data are water, protein and lipid content (cells B46 to E48, highlighted in yellow). Another relevant input parameter is pH (cells B-E44).

The result after \( t = (\text{cell } A25) \) is used to calculate the partition coefficients root to water, xylem to water, phloem to xylem etc. (cells G24 to H43, sheet one season), used in both plant models.

A.2.1 Theory Cell Model

**Neutral compounds.** The partition coefficient is the endpoint of diffusion between two different phases. Neutral organic compounds distribute mainly into the water \( W \) and the lipid phase \( L \) (the latter described by \( K_{ow} \)). The root concentration factor RCF (Briggs et al. 1982) is such a partition coefficient. It can be rewritten to a \( K_{RW} \) (\( L/\text{kg} \)), which describes the equilibrium partitioning between root concentration \( C_R \) (mg/kg fresh weight) and water \( C_W \) (mg/L).

\[
K_{RW} = W_R + L_R a K_{OW}^b = 0.82 + 0.03 \times 1.22 \times K_{ow}^{0.77}
\]

where \( a = 1/\text{density of octanol (unit conversion)} \) and \( b \) is from the RCF Briggs.

Similar, for leaves: \( K_{lw} = W_L + L_L a K_{OW}^b \) with \( b = 0.95 \) (Briggs et al. 1982).

The value \( b \) is entered in sheet “Input” cell B20 or B21 (default: 0.85).

**Ionisable compounds.** For ionisable compounds, this simple regression does no longer hold. There are (at least) two molecule species to consider, and one of them is charged. And while diffusion of a neutral molecule across membranes can be described with Fick’s 1st law of diffusion, it requires the Nernst-Planck law for the ions (Trapp 2004). The following equations relate to monovalent ions. For bivalent ions see Trapp, Rosania et al. (2008).

**Dissociation.** The activity ratio between ionic (index d) and neutral molecule (index n) is calculated by the Henderson-Hasselbalch equation

\[
\log \frac{a_d}{a_n} = i(pH - pK_a)
\]

where \( a \) is the activity, \( d \) is the index for dissociated (synonym ionic), \( n \) for neutral, \( i \) is +1 for acids and -1 for bases; \( pK_a \) is the negative logarithm (\( \log_{10} \)) of the dissociation constant.

It follows for the fraction of neutral molecules \( F_n \) that

\[
F_n = \frac{1}{1 + 10^{i(pH-pK_a)}} \quad \text{and} \quad F_d = 10^{i(pH-pK_a)}
\]

**Activity.** In non-dilute solutions, the activity \( a \) is lower than the concentration \( C \). \( a = \gamma \times C \), where \( \gamma \) is the activity coefficient (\( \cdot \)). The activity coefficient of the ion, \( \gamma_d \), can be calculated with the modified Debye-Hückel equation / Davies approximation:

\[
\log \gamma_d = -A \times z^2 \left( \frac{\sqrt{I}}{1 + \sqrt{I}} - 0.3 \times I \right) \quad \text{for } I \leq 0.5 \text{ M, and } A \text{ is 0.5 for } 20^\circ \text{ and 1 atm.}
\]

The activity coefficient of the neutral compound, \( \gamma_n \), is found by the Setchenov equation: \( \gamma_n = 10^{kd} \)
Using $a = \gamma \times C_{\text{free}}$, we receive for the relation between the activity $a_n$ of the neutral molecules and the total concentration the "activity capacity" $f$:

$$f_n = \frac{a_n}{C_i} = \frac{1}{W / \gamma_n + K_n / \gamma_n + 10^{(pH-PK_a)} \times (W + K_d) / \gamma_d}$$

and

$$f_d = \frac{a_d}{C_i} = f_n \times 10^{(pH-PK_a)}$$

where $K$ is the adsorption (to lipids and to proteins, L/L).

### A.3 Diffusive exchange of electrolytes across membranes and “Partition Coefficients”

The diffusive flux of **neutral molecules** (index $n$) across membranes, $J_n$, is described by *Fick’s 1st Law of Diffusion*: $J_n = P_n (a_{n,o} - a_{n,i})$ where $J$ is the unit net flux of the neutral molecules $n$ from outside ($o$) to inside ($i$) of the membrane (kg m$^{-2}$ s$^{-1}$), $P_n$ is the permeability of the membrane (m s$^{-1}$) for neutral molecules, and $a$ is the activity of the compound (kg m$^{-3}$).

The unit net flux of the **ions** (index $d$, for dissociated) across electrically charged membranes, $J_d$, is described by the *Nernst-Planck equation*. An analytical solution for constant electrical fields is (Goldman 1943, Hodgkin and Katz 1949, Briggs et al. 1961)

$$J_d = P_d \frac{N}{e^N - 1} (a_{d,o} - a_{d,i} e^N)$$

where $P_d$ is the permeability of the membrane (m s$^{-1}$) for dissociated molecules, $N = z E F / (R T)$ (origins from *Nernst*); $z$ is the electric charge (synonym valency, for acids -, for bases +), $F$ is the Faraday constant (96 484.4 C mol$^{-1}$), $E$ is the membrane potential (V), $R$ is the universal gas constant (8.314 J mol$^{-1}$ K$^{-1}$) and $T$ is the absolute temperature (K). It can be seen that the electrical charge affects the velocity of transfer (multiplied with $P$) but also the gradient (multiplied with $a_d$). Exchange stops when $e^N$ the *Nernst ratio* is reached.

In the current model version, $P_d$ is estimated from the Kow and is 3162 times lower than the $P_n$. Recent studies show that this does not hold, and the polar surface area of the molecule is probably a better predictor. However, no regression is available yet.

The **total flux** $J$ of the compound across the membrane is of course the sum of the fluxes of the neutral molecule and the ion, $J_n$ and $J_d$:

$$J = P_n (a_{n,o} - a_{n,i}) + P_d \frac{N}{e^N - 1} (a_{d,o} - a_{d,i} e^N)$$

This total flux is calculated for every membrane, i.e. the outer cell membrane (plasmalemma), the vacuole membrane (tonoplast) and phloem and xylem.

The cell model delivers the concentration ratio between cell organelle and outside water as result (cell B24 to E25), from which the partition coefficients of ionising chemicals in cells G24 to H43 are composed.
B) Dynamic model “Plant uptake one season numerical.xlsx”

This dynamic model calculates water and substance fluxes for one growth season (March to July). It requires a large volume of data which depend and relate to each other. The default dataset is consistent and based on field data. For the change of chemical, only a few data need to be entered.

The model is implemented in three excel sheets named “Input”, “Output” and “one season” which are described in the following chapters.

Sheet “Input”: Input of all time-invariant data, such as chemical properties, properties of soil layers, and plant properties that do not vary with time.

Sheet “Output”: Tables and Graphs of the results, like concentrations in soil and plant with time, water budget.

Sheet “one season”: Entering of time-variable input data (e.g., precipitation), mirror of the input data from sheet “Input”, and all calculations of transport in soil and plant.

B.1 Sheet “Input”

All data except those changing with time are entered in sheet “Input”, that is (see Figure 2) chemical data, soil data and plant data. It is wise to change data only in a consistent manner, e.g., when changing chemical data, to change them all, same for plant and soil parameter.

Figure 2. Segments of the sheet “input”, ignore cells in grey, but enter data in the yellow cells.
## Chemical data input Cell A7 to B20
- cell B8 is log Kow is the partition coefficient octanol water of the neutral molecule species in the unit L/L;
- cell B9 is log Kow of the ion. Typically 3.5 log units lower than log Kow neutral. A good source for both values is the log D estimation of ACD.
- cell B11 Kaw air-water is the partition coefficient between air and water (L/L), also known as dimensionless Henry’s Law constant. Enter here the value for the neutral molecule only. Because, that is what estimation routines give (e.g., ACD), and the ion is not volatile, never. The Kaw is later multiplied with fn fraction neutral for loss from leaves to air.
- cell B12 K HSA adsorption to proteins (L/mol). For weak acids, adsorption to proteins is typically far more relevant than adsorption to lipids. For the given substance with log Kow = -2.6 and the default K HSA of 2000 L/mol, adsorption to proteins is 35 times more relevant than that to lipids. Do not set K HSA to zero, or numerical troubles results.
- cell B14 Molar mass M in g/mol. The molar mass is used to calculate diffusivity. For M > 390 g/mol, plant uptake is inhibited. This has to be considered by the user.
- cell B15 pKa (acid dissociation constant) in pure water (the value is later corrected for pKa in membranes). Also for bases, enter here pKb and not pKb.
- cell B17 valency z, also known as charge number. Enter -1 for a monovalent acid, and +1 for a monovalent base.
- cell B20 slope b (on the log Kow for the calculation of partitioning into plant lipids). Default value of 0.85 is a compromise between the value 0.77 for roots and 0.96 for leaves (Briggs et al. 1982).

## Soil pH and Koc
The value in B27 is calculated by the method in Franco and Trapp (2008), using soil pH in B25. The user can enter its own value in B28, which is the one that the model will use.

## Degradation rates
Cell A31 ..B35. The user can enter degradation rates for Temp = 20 °C in soil and plant. The values are corrected for ambient temperature with the constant in cell B36 according to k(Temp) = k (20°C) x constant(Temp - 20)

## Soil Water input data
Cells A38 to F42 please enter data relevant for the water budget in soil, namely
- layer thickness (default 0.2 m)
- PWP (L/L) permanent wilting point is the water content of a soil layer below which plants cannot extract water anymore
- FC (L/L) Field capacity is the water content of a soil layer above which water starts to flow (leach) deeper. FC and PWP are entered for a sandy loam, i.e., a typical agricultural soil.
- Initial water content (L/L). The initial water content is a very sensitive parameter for leaching, and also for plant uptake (the plant can only take up chemical with water, and thus only from layers where there is water above PWP). The entered value is between PWP and FC.
- Density (kg/L). The value is only used for unit conversion.

## Soil chemical input data A46 to E52
Please enter here initial concentration (mg/kg dw) of all five soil layers and temperature of soil layer 2 to 5 (temperature of layer 1 is set equal to air temperature). Grey fields are unit and temperature conversion, please keep as is.

Organic carbon input is currently in the dynamic section “One season” from O40 to FK 44
Fixed data for plant growth and uptake cells E8 to F36
Those plant data that are constant over the whole simulation period are entered also in sheet “input”. It is not useful to change individual parameters e.g., only final mass of roots, but not also of stems and leaves), because the parameters are for the same plant and belong together. Some are explained here in detail:
- EF8: Transpiration coefficient (L/kg fw), determines how much water is transpired per kg fresh weight biomass formed. It is thus one of the most relevant parameters for concentrations in plants (more water at same growth means higher concentration), the default value of 55 L/kg is for wheat.
- EF9: Germination day: no plant growth before that day, default day 2)
- E17 to F22: data for stem
- E24 to F28: data for leaves
- E30 to F35: data for fruits (grain, corn)
- EF36: Root specific surface area. The value is used to calculate permeability of root towards water PW (from Q = P x area), but only for control. A default value for PW is entered elsewhere (sheet one season H45). Default value and calculated value match quite well.

That’s it for sheet “input”. At the bottom of the sheet are two figures, so that the user can see the effect of its changes immediately. However, far more results are shown in the second sheet “Output”. 
B.2 Sheet “Output”

In the sheet “Output” the user finds numerical (cells A3..B42) and graphical output (7 Figures).

**Numerical output**
- cell B3: the output is for the time given in that cell (default 152 d after start)
- cell B4: date of output (start day is 1st of March)
- cell B6 to B10: concentrations in five soil layers, unit mg/L
- cell B12 to B15: concentrations in plant (root, stem, leaves, fruits) in mg/kg fresh weight
- cell B17 and B18: concentrations in leaves and fruits including attached soil particles
- cell B20 to B31: concentrations soil and plant in mg/kg dry weight
- cell B34: concentration in top soil layer at day 16; this is used to calculate BCF values (plant concentration at the end of the period). Day 16 is March 16, and this was - recently - the day after spray application. Can be adapted as needed.
- cell B35 to B38: BCF bioconcentration factor = concentration in plant (end, dw) / concentration in soil (day 16, dw)
- cell B41: leaching of chemical out of first (top soil) layer to underlying layer
- cell B42: leaching of chemical out of lowest (fifth) soil layer

**Figures**

All Figures have headings describing the content. The x-axis is the time scale (days after start) and the y-axis is as labeled, with unit.

![Figure 1](image1.png)

**Figure 1.** Concentration in plants from day 2 to end. Ignore error message "values of zero cannot be shown" or set initial concentration (sheet “one season” cells O10 to O15) to a reasonable value, please.

![Figure 2](image2.png)

**Figure 2.** Concentration (mg/L) in all five soil layers over time. This figure is very helpful - together with the figure on transpiration from layers - to interpret the depression of plant (root) concentrations from day 80 to day 127 in Figure 1.

![Figure 3](image3.png)

**Figure 3.** Leaching of chemical out of layer 1 and of layer 5 can be interpreted best in relation to the three following figures. A leaching from layer 1 occurs after heavy rain-falls. No leaching from layer 5 because the chemical has (not yet) reached the lowest layer after 152 days.
Figures 4, 5, 6 and 7: Water balance (precipitation, actual evaporation from top soil layer, leaching of water from layer 5 to groundwater GW, and transpiration of water by plants, unit L/d); Water content of soil layers (L/L); Transpiration per layer (L per period, here L per one day) and Plant mass.

These figures are best viewed together and give insight into the water movement in the system. In the present parameterisation, the simulation starts with half-full soil layers (Figure 5). Due to continued rain events, at initially very low transpiration (Fig. 4), the top soil layer and next layer 2 fill up. Some leaching of water to GW, some actual evaporation. Then around day 30, plants grow intensively (Figure 7), and growth is related to the use of water and thus transpiration. Until day 65, the plants are satisfied with taking up water from the top soil layer (Figure 6), which then is emptied (Figure 5), and plants draw water from the underlying layer 2. Heavy rainfalls (Figure 4) add water to the top layer around day 70 (May) but the intense transpiration by plants empties layer 1 again and then also layer 2. From day 80 on the plants are forced to take water from layer 3, 4 and 5 - in these layers, the water is yet free of chemical (if the Kd of 44 L/kg is correct), and the concentrations in plant root decrease (compare previous figure). Later on, heavy rainfall in summer bring occasional water above PWP into the top layer, but the bulk of water is taken up from deeper soil.

It is this combination of water budget, chemical fate in soil and plant uptake from varying layers that makes simulations with this coupled model so very interesting - at least for the author of these lines, that is gardener and can confirm such a pattern exists also in field situations. Enjoy the simulations!
B.3 Sheet “One season”

B.3.1 Overview
The third sheet “one season” is the core of the model, where all calculations are performed. It is a quite large sheet. The structure is shown in Figs. 8 and 9 and is like this: left hand is the mirror of chemical data and the cell model. Next to the middle is the plant partition coefficients and the mirror of fixed (time-invariant) plant input data (coming from sheet 1, input). Then, from column O to column FK is the dynamic model. Each column is one model. Therefore, the simulation period can be expanded (or shortened) by marking a complete column and scrolling to the right. Some cells need to be adapted because excel tends to make a 0,0,0 ... to a 0,0,0,1,2,3 (please check if you expand).

Figure 8. Overview sheet “one season”, upper part

Figure 9. Overview sheet “one season”, lower part
B.3.2 Input of data changing with time

For convenience, and in order to be able to track all data better, the input data are mirrored in this sheet. There remain some time-variable input data that can be modified in this sheet, namely:

- cell A25, cell model: output time for the cell model: change not recommended
- cells B44 to E48: properties of plant cells. To some degree, different plant species and variety can be considered here (e.g., low/high protein content, low/high lipid content). The current parameterisation is with low lipid but high protein content. Setting protein content to 0 will result in numerical problems, with the current, polar chemical.
- cell O1: delta t, the time interval. A key parameter that, if changed, requires to adapt all time-variable input!
- cell O10 to O15: initial concentrations in plants. Default zero.
- cell O18 to FK 22: pulse input (mg); here, a pesticide spray input or any other input to top soil or to roots, stem, plants and leaves can be simulated. Typical interception values (retention of spray in sub-surface plants) are 25%, the rest is added to top soil. The base area is 1 m². Default: no input.
- cells O31,32,34 to FK31,32,34: input of the water budget data, namely Precipitation (L/d), potential Evaporation (L/d), and Surface run-off (L/d). Do not fill in line 33, actual Evaporation, because it is calculated, dependant on the water content of the top soil layer.
- cells O35,36 to FK35,36 Temperature (air + soil layer 1) (°C) and Relative humidity (-).
  The current data set is based on the field measurements by INRA in Feucherolles, France (near Paris) and is published in Legind et al. (2011) (year 1999/2000, a relatively wet year). Some data, e.g., soil depth, PWP and FC, have been modified.
- cells O40 to FK45: enter soil organic carbon (g/g) in these cells. Default: top layer 0.02 g/g, all lower layers 0.01 g/g.
- cell O90 phloem surface area to volume ratio (default 10 000 m² per m³)
- cell O97, ratio of phloem to xylem water flow, default 0.05 L/L. The user is advised not to change these values without care. They have high relevance for the resulting concentrations (of weak acids), and also for the numerical stability of the matrix solution.

That's it!

C Model theory

C.1 Reading

The models are all explained in published papers. In order to save space and efforts, this documentation therefore refers to these published papers for detailed description of the underlying theory.

i) Cell Model

The basics of the cell model for pesticide plant uptake have been described in the review paper Trapp (2004). The best description, and the one that the code follows very closely, is however found in a medical paper, Trapp and Horobin (2005).

ii) Tipping buckets

The tipping buckets soil model for transport of water and solutes was described in the book Trapp & Matthies (chapter 7.5). It is also described in the open-access publication Legind et al. (2011). The latter also details the coupling of soil and plant model. Also the parameterisation of the model is taken from that study, and the meteorological values are listed in the SI. Thus, no further description is required here.
iii) Plant uptake model
The cascade model idea was described in Rein et al. (2011). There, also the way to calculate plant growth and transpiration is explained. The matrix of the plant model remains almost as described in that paper (Table 1), except for the phloem flow. There is, however, a small but very significant difference: the introduction of phloem flow leads to non-diagonal matrix elements. The resulting matrix cannot be solved with the analytical solutions derived in Rein et al. (2011). Therefore, a numerical solution had been introduced instead. Currently, Arno Rein and Wolfgang Larisch work on an analytical solution for a closed 3 x 3 (4 x 4) matrix. If ready, we will implement that solution which will provide more stability and accuracy.

An application of the plant uptake model is found in Trapp and Eggen (2013). There, the meteorological input data are also listed in the SI.

A study on the influence of the plant input data is Trapp (2015). Surprisingly, the combination of soil and plant parameters was as important, or more important, than the chemical properties for the uptake into radish plants at a field site in Bohemia.

iv) Videos, exercises and teaching material
Every 3 to 4 years, course 12906 “Plant uptake of Chemicals” is taught as summer course at DTU. The lectures have been videoed, and all course material is online available, here

year 2013  homepage.env.dtu.dk/stt/PhD%20course%202013website/index.htm
year 2015  homepage.env.dtu.dk/stt/2015/index.htm

C.2 Limitations

C.2.1 Accuracy of data and results
Plant uptake models have first been developed for neutral, and typically non-polar compounds (Trapp and Matthies 1995). These compounds were relatively persistent and had as main process lipophilic sorption. The models were successful in predicting the fate of such substances if the input parameters were sufficiently accurate, e.g., Trapp and Matthies (1995), Kulhanek et al. (2005), Trapp (2015). In many cases, uptake from air dominated levels of chemicals in plants.

In planta degradation can significantly lower uptake (Hurtado et al. 2016, Jacobsen et al. 2015) but is rarely known. The accuracy of the plant uptake models declines dramatically if the relevant environmental and plant parameters are not adapted to the experimental situation in lab or field, as shown in Trapp (2015). However, such data is in most cases not available (plant growth data are surprisingly difficult to get).

C.2.2 Numerical instability
The matrix has been solved numerically. Excel is not in particular well suited for this, and therefore, the number of time steps per day is limited to 30. This means, any rates larger than 0.03 d⁻¹ may lead to trouble with the numerical solution. Such rates occur when adsorption is very low (Kow < -3 or K HSA close to 0).

C.2.2 Problems with ionisable compounds.
This model is the first official release of Stefan Trapp of a plant uptake model for ionisable and ionic substances. Earlier model prototypes have been used in Prosser et al. (2014) and Polesel et al. (2015) but lacked phloem flow. The results for weak acids are therefore different, otherwise there is little change. All results for mostly ionised substances have to be handled with care: the log Kow (or log D) is an insufficient and not reliable parameter to predict adsorption and membrane permeability of ions (see, e.g., Droge and Goss 2013). As better parameter, the (topological) polar surface area TPSA has been suggested (Palm et al. 1997, Ertl 2007). As a rule of thumb, drugs or pesticides with a TPSA < 60 Å² show good membrane permeation (in humans), those with TPSA > 150 Å² show very little (Ertl 2007). It is likely that this parameter, TPSA, is also superior for predictions of plant uptake, but no study has established a relation between TPSA and permeation or adsorption. We have therefore, to live with the imprecision of the log Kow or log D. Results can be close to reality, but they may also fail due to this, please see disclaimer.
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Acknowledgements: Thanks to Bayer Crop Science and Simon Heine for support and suggestions
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