Preferential flow in Daisy 2D
Concept and model for tile drained soil

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This note describes briefly the concept, math, and code behind the support in Daisy for estimating drain flow dynamics, as well as the transport of particles and pesticides to tile drains in agricultural fields. See Hansen et al. (1990); Abrahamsen and Hansen (2000); Hansen (2002); Hansen and Abrahamsen (2009) for more general descriptions of Daisy.

1 Conceptual model

The conceptual model is illustrated on figure 1. In this section we will discuss the elements of the model in some more detail.

1.1 Soil

We start with a description of the soil. The soil is divided into a number of zones which are considered homogeneous and static with regard to certain physical attributes, most significantly the soil texture. The main division is the horizons, typically with an Ap horizon (the plowing layer) at top, and a number of other horizons below. The top of the Ap horizon is given special regard, the hydraulic properties will be very dynamic depending on tillage and weather effects. The hydraulic properties for the rest of the Ap horizon will also wary with tillage, but that is not considered. The top of the second horizon is also given special regard, as it will often form a dense plow pan with low hydraulic conductivity. Finally, we have a non-horizontal zone, namely the drain trench, which was formed when the drain tiles were installed.

1.2 Water flow pathways

Starting with the smallest water flow pathways, we have the pathways within the soil aggregates. These have very limited flow capacity, but play an important role during spring and summer, as the main pathways for moving water towards the roots and the soil surface for transpiration and surface evaporation. Next step up in size is the pathways between soil aggregates, in particular soil cracks of various origins, as they provide a continuous path through the soil. We only consider cracks small enough for the capillary forces to have an effect. The cracks can potentially have a much higher flow capacity, but are only activated at near saturated conditions. Cracks are characterized by aperture, density, orientation, and location in soil. The largest pathways considered are earth worm burrows.

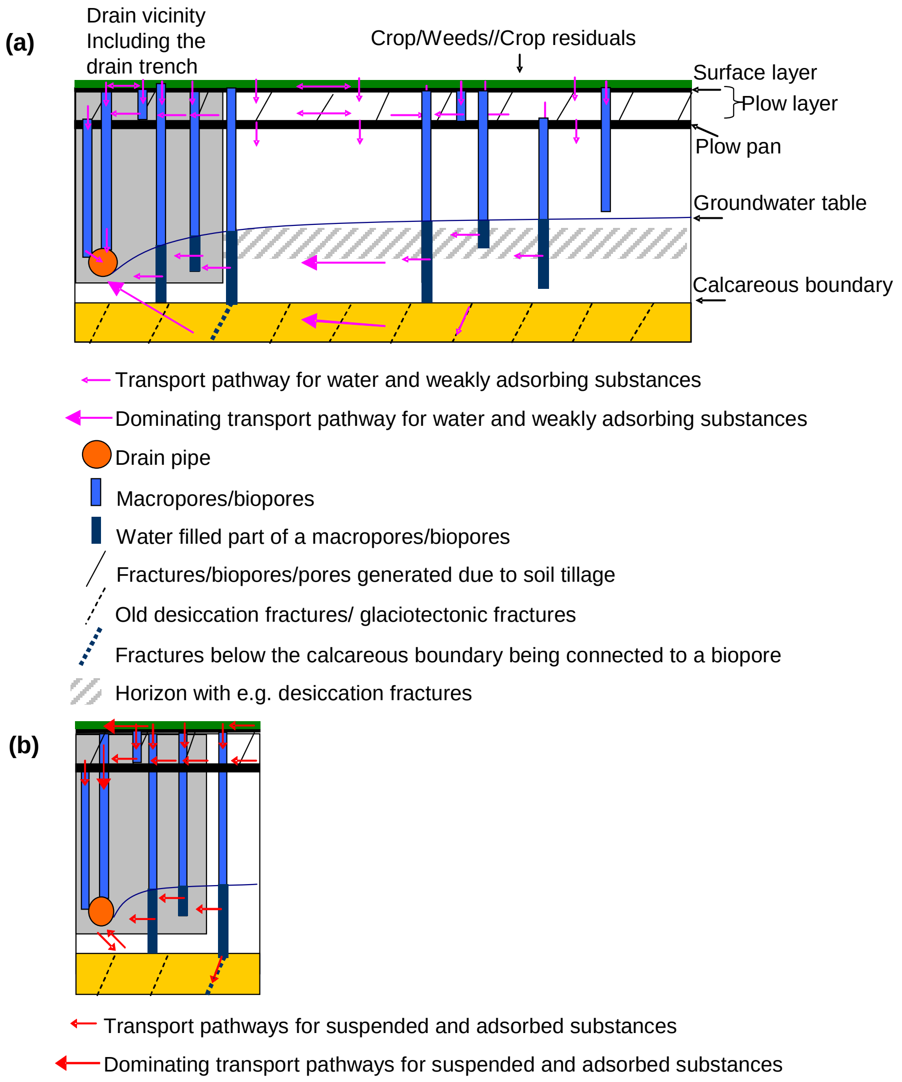

Figure 1: Conceptual model of important structure elements in a situation with saturation at drain depth. The model include indications of transport pathways (a): for water and weakly adsorbing substances and (b): for suspended and strongly adsorbing substances.

These are large enough that capillary forces no longer play a role, and have a very high flow capacity, but must be initiated by locally saturated conditions, and are mostly limited to vertical flow. Finally we consider old root channels. These will largely overlap with the cracks (for the smaller root channels) and earth worm burrows (for the larger root channels). Together, large root channels and earth worm burrows are referred to as biopores.

The main limitation for flow through biopores is the speed at which the water can enter or leave. The biopores may start from the soil surface, or end in the drain tiles, or in a system of root channels and cracks that is well connected to the drains. In the first case, the flow capacity of water into the biopores from the surface is very high, in the second case the flow capacity of water out of the biopores to the drain tiles is very high. For this reason, biopores that start at the surface and are well connected to the drain tiles are of particular importance. Biopores are characterized by size, density, location in soil, and whether or not they are connected to drain pipes.

The biopores will typically be activated when saturated soil is located above unsaturated soil. This will (again, typically) happen at the border between two horizons. In that respect, the surface and plow pan are of particular interest. If a rain event has a low intensity, the water will enter the soil through the pathways within and between soil aggregates. If the rain intensity is higher than the flow capacity of these pathways, the water will accumulate in the surface, and once a certain roughness threshold is reached, move horizontally towards the nearest biopore connected to the surface. We ignore the situation where a rain drop falls directly upon a biopore. If the rain intensity is higher than the flow capacity of water out of the biopore, water will begin to build up within the biopore, which will increase the rate of water leaving the biopore. Once the biopore is full, water will start accumulating on the surface again, and once another roughness threshold is reached, move further away towards biopores that have a better flow capacity of water out of the biopores. Something similar may happen on top of the plow pan. Once the soil at the bottom of the plowing layer is saturated, biopores that penetrate the plow pan will be activated, and water will move through the soil toward these biopores. And again, when the local biopores are filled, water may start moving towards the drain connected biopores. The same can happen elsewhere in the soil, but the surface and plow pan are considered the two most important barriers. Once a biopores has become activated, it may continue to extract water from the surrounding soil through connected film flow inside the biopores, until the soil becomes too dry, as demonstrated in Tofteng. et al. (2002); Gjettermann et al. (2004).

As described above, drain flow can occur whenever the biopores are activated, that is when we have localized saturated conditions above the drain pipes. The drain season is when we have saturated conditions at drain depth. Between drains we may have saturated conditions above drain depth. This pressure potential will cause a horizontal flow towards the drain pipes, mostly through the flow pathways that goes between soil aggregates, in particular cracks.

1.3 Colloids and pesticide transport

Chemicals (such as pesticides) dissolved into the water mostly follows the flow of the water, with the addition of diffusion between water with different concentrations, which is a relatively slow process compared to advection. In Daisy, we ignore diffusion in cracks and in biopores. However, of particular interest here is diffusion between water in cracks and water inside soil aggregates. Depending on the timing, this might cause water with a high solute concentration to bypass soil volumes with relatively clean water, or allow solutes to be protected within the soil aggregates while relatively clean water pass by in the cracks and biopores.

Chemicals that are sorbed to soil particles move together with the soil particles, which is to say, mostly not at all. However, soil particles may be released by various means, of which only one is considered in the model: Clay particles released as a result of the impact of rain drops on the soil surface. As the particles are large, they will tend to be filtered quickly if they enter soil aggregates, less quickly when moving between soil aggregates, and not at all when moving within biopores. Chemicals are thus generally found in three forms in the soil. Dissolved, sorbed to immobile soil, and sorbed to mobile soil particles.

2 Mathematical model

In Daisy, the flow pathways within soil aggregates are referred to as the primary domain. The flow pathways between soil aggregates, including cracks, are referred to as the secondary domain. Together these two domains where the capillary forces are active is called the matrix domain. The large biopores where the capillary forces no longer are significant constitute the tertiary domain.

The mathematical model for 2D water flow and solute transport is described in Mollerup et al. (2011); SAFIR (2009); Mollerup (2010) with increasing level of details. The model behind colloid generation and filtration can mostly be found in Jarvis et al. (1999).

3 Software model

The Daisy tutorial (Abrahamsen, 2011b) describes how to set up Daisy for a one dimensional column. In this section we will give an overview of how the new features discussed in this paper are specified. A complete reference can be found in Abrahamsen (2011a).

3.1 Soil

Assume we already have defined three horizons, “Ap”, “B”, and “C”. We can then use these to define the surface and plow pan by adjusting the hydraulic conductivity and bulk density.

```
(defhorizon "Surface" "Ap"
  (hydraulic original (K_sat 0.17 [cm/h])))

(defhorizon "Plow pan" "B"
  (dry_bulk_density 1.70 [g/cm^3])
  (hydraulic original (K_sat 0.04 [cm/h])))
```

If no better information exists, leave the surface unchanged and set the saturated hydraulic conductivity of the plow pan to 10% of the value for the B horizon.

If we want a dynamic surface horizon, it become more complicated. The `M_vG_compact` hydraulic model allows the Mualem – van Genuchten parameters to be a function of the porosity (Θ_{sat} or `Theta_sat`). For example, the van Genuchten n parameter is calculated as $n = n_{\mathrm{ref}} \times n_{\mathrm{mod}}(\Theta_{\mathrm{sat}})$. n_{mod} is specified as a piecewise linear function defined by number of points of the form (Θ_{sat} *value*).

```
(defhorizon Surface Ap
  (hydraulic M_vG_compact
             (Theta_res 0 [%])
             (Theta_sat 0.39 [])
             (ref_alpha 0.01 [cm^-1])
             (ref_n 1.1 [])
             (ref_K_sat 2.25 [cm/h])
             (mod_alpha (0 1) (1 1))
             (mod_n  (0 1) (1 1))
             (mod_K_sat  (0.3 0.001) (0.35 0.01) (0.39 1))))
```

In this example, `K_sat` is decreased to 1% when `Theta_sat` is decreased to 35%, and decreased to 0.1% when `Theta_sat` is decreased to 30%. You can set the porosity with a pseudo-manager operation.

```
(wait (at 2000 06 01))
(set_porosity (depth -1 [cm]) (porosity 0.35))
```

In general, you should decrease the porosity after the first rain event, and reset it to the normal level after tillage. The new pseudo-horizons are specified like the normal horizons.

The drain trench is defined the same way as you specify a normal horizon. However, since it partly overlap with the horizons is enabled differently, based on both horizontal and vertical limits.

```
(Soil (MaxRootingDepth 150 [cm])
      (horizons (-3.00 "Surface")
                (-25.00 "Ap")
                (-33.00 "Plow pan")
                (-120 "B")
                (-200 "C"))
      (zones ((box (top finite -33 [cm]) (bottom finite -120 [cm])
                   (left finite  0 [cm]) (right finite    25 [cm]))
              "Drain trench")))
```

3.2 Cracks and pathways between soil aggregates

Daisy can handle three different situation with regard to cracks and pathways between soil aggregates (collectively referred as the secondary domain). The first is the simplest, there are no cracks. We then use pressure head to specify the border between the primary domain (pathways within soil aggregates) and the secondary domain (h_{lim}). We also specify an exchange rate for solutes between the primary and secondary domain (α).

```
(defsecondary no_cracks pressure
```

```
    (alpha 0.001 [h^-1]))
    (h_lim 2 [pF]))

  (defhorizon Ap ;; More ...
    (secondary no_cracks))
```

The second option is that we have cracks with no particular orientation (vertical or horizontal). In that case effective aperture and density of the cracks, along with α as before. The aperture will form the basis of the division between the domains, and together with density is will also be used for calculating the hydraulic conductivity within the secondary domain.

```
  (defsecondary has_cracks cracks
    (aperture 78 [um])
    (density 10 [m^-1])
    (alpha 0.001 [h^-1]))

  (defhorizon B ;; More ...
    (secondary has_cracks))
```

The third option is that we have cracks with a clear horizontal or vertical orientation. In that case, we use the vertical conductivity as basis, and specify the horizontal conductivity through the `anisotropy` horizon parameter. The anisotropy parameter affects both conductivity in the primary and the secondary domain, but significant horizontal water movement is only expected in saturated or near saturated conditions, where the secondary domain will dominate.

```
  (defhorizon C ;; More ...
    (secondary no_cracks)
    (anisotropy 12))
```

If the cracks are vertical, you may want to use a bimodal hydraulic model, such as `M_BaC_Bimodal` or `M_vGp` (Børgesen et al., 2006).

3.3 Biopores

The biopores are divided into classes with common properties. The properties are where they start, where they end, their diameter, and whether they are well connected to drains. For biopores well connected to drains we also need to know the position of the drains. For biopores that are not well connected to the drains, we need to know the hydraulic conductivity of the biopore wall. The conductivity is specified relative to the surrounding soil matrix, and the thickness of the wall is assumed to be 10% of the diameter. We also specify the density, as a function of distance to drain (x).

In the following we define three biopore classes. The first class consist of short, narrow biopores, going from the soil surface to the borrom of the plowing layer. This class is uniformly distributed. The next two classes are long wide biopores that start at the soil surface and go down to 1.25 meter below. The biopores less than approximately 25 cm from the drain are considered well connected to the drains. The rest are not. Finally we define a tertiary domain consisting of these three classes, and name it “MyBiopores”. There is no limit to the number of biopore classes you can have, but simulation time will suffer if you have too many, and there is an increased risk of instability.

```
(defbiopore "short"
  (matrix (height_start 0 [cm])
          (height_end -25 [cm])
          (diameter 2 [mm])
          (density 100 [m^-2])
          (K_wall_relative 1 [%])))

(defbiopore "long"
  (matrix (height_start  0 [cm])
          (height_end -125 [cm])
          (density 10 [m^-2])
          (diameter 4 [mm])
          (density (plf x (range [m^-2])
                          (domain [cm])
                          (points (20 0) (30 15))))
          (K_wall_relative 1 [%])))

(defbiopore "connected"
  (drain (height_start  0 [cm])
         (height_end -125 [cm])
         (diameter 4 [mm])
         (density (plf x (range [m^-2])
                         (domain [cm])
                         (points (20 15) (30 0))))
         (pipe_position -110 [cm])))

(deftertiary MyBiopores biopores
  (classes ("short") ("long") ("connected")))
```

3.4 2D movement

The `Movement` parameter is where is where you specify the geometry and enable the biopores. The `rectangle` movement model provides a 2D grid where you specify the endpoints with `zplus` and `xplus`. You also specify the location of the drain here, depth first. And finally, this is where you enable the tertiary domain.

```
(Movement rectangle
  (Geometry (zplus -1.5 -3 -5.5 -10 -14 -18 -22 -25
                   -27 -30 -33 -40 -50 -60 -75 -90 -100 -120
                   -125 -150 -170 -200 [cm])
            (xplus 25 50 100 150 300 500 650 800 [cm]))
  (drainpoints (-110.0 [cm] 1 [cm]))
  (Tertiary MyBiopores))
```

This is also where you specify the numeric details of the transport algorithms, which can be important for stability.

3.5 Colloids and pesticides

In Daisy terminology, a "chemistry" refers to a collection of substances and reactions. A "chemical" is just a name of for a something that can be tracked by Daisy, in the following we define "chemicals" that to track different forms of the same chemical. For colloids, we just define one substance (colloids) and two reactions (generation and filtration).

```
(defchemical colloid common
  "Mobile colloids."
  (diffusion_coefficient 4.6e-6 [cm^2/s])
  (decompose_rate 0 [h^-1]))

(defreaction colloid-generation colgen_Jarvis99
  "Release of colloids in soil surface from heavy rain."
  (kd 15 [g/J])       ;Detachment rate coefficient.
  (kr 0.05 [g/m^2/h]) ;Replenishment rate coefficient.
  (zi 0.05 [cm])      ;Surface layer thickness.
  (colloid colloid))

(defreaction colloid-filter filter_velocity
  "Filtration of colloids in the soil matrix."
  (fc_primary 80 [m^-1])   ;Filter coefficient primary domain.
  (fc_secondary 40 [m^-1]) ;Ditto for secondary domain.
  (mobile colloid))

(defchemistry colloids default
  (trace colloid)
  (reaction colloid-generation colloid-filter))
```

For sorbing pesticides, things get more complicated. The pesticides move differently depending on whether they are dissolved, or sorbed, and if sorbed whether they are sorbed to a colloid, or to the soil matrix. So they have three forms, dissolved, immobile, and colloid bound. We also define a base form from which they are all derived, and define the decompose rate here (assuming the decompose rate is the same for all forms). The pesticide can change between all three forms. The dissolved form can be sorbed or desorbed to either the soil matrix or colloids. A `soil_enrichment_factor` parameter determines how much more likely a colloid is to receive the pesticide compared to an immobile soil particle. A K_{OC} or K_d determines the equilibrium between the sorbed and desorbed forms. A `k_sorption`, and if different `k_desorption`, parameter determine the rate at which equilibrium is reached. Finally, immobile pesticides will be transformed to colloid bound pesticides at the same rate immobile soil particles are transformed into colloids, and colloid bound pesticides will become immobile at the same rate colloids are filtered in the soil matrix.

```
(defchemical Pendimethalin-base herbicide
  "Base parameterization for all Pendimethalin forms."
  (decompose_halftime 90 [d]))          ;27-186 [d]

(defchemical Pendimethalin Pendimethalin-base
```

```
  "Dissolved pendimethalin."
  (adsorption none))

(defchemical Pendimethalin-immobile Pendimethalin-base
  "Pendimethalin sorbed to immobile soil."
  (adsorption full))

(defreaction Pendimethalin-immobile-sorption sorption
  "Sorption equilibrium between dissolved and immobile Pendimethalin."
  (sorbed Pendimethalin-immobile)
  (solute Pendimethalin)
  (K_OC 15744 [ml/g])                   ;6700-29400 [ml/g]
  (k_sorption 0.05 [h^-1]))

(defchemical Pendimethalin-colloid Pendimethalin-base
  "Pendimethalin sorbed to colloids."
  (adsorption none)
  (diffusion_coefficient 4.6e-6 [cm^2/s]))

(defreaction Pendimethalin-colloid-sorption Pendimethalin-immobile-sorption
  "Sorption equilibrium between dissolved and colloid-bound Pendimethalin."
  (colloid colloid)
  (soil_enrichment_factor 10000 [])
  (sorbed Pendimethalin-colloid)
  (k_sorption 0.05 [h^-1]))

(defreaction Pendimethalin-filter colloid-filter
  "Filtration of colloid-bound pendimethalin in the soil matrix."
  (mobile Pendimethalin-colloid)
  (immobile Pendimethalin-immobile))

(defreaction Pendimethalin-colloid-generation bound_release
  "Release immobile Pendimethalin as colloids in mixing layer."
  (colloid colloid)
  (immobile Pendimethalin-immobile)
  (bound Pendimethalin-colloid))

(defchemistry Pendimethalin default
  "Pendimethalin in both immobile, solute and colloid form."
  (trace Pendimethalin Pendimethalin-immobile Pendimethalin-colloid)
  (reaction Pendimethalin-immobile-sorption
            Pendimethalin-filter
            Pendimethalin-colloid-generation
            Pendimethalin-colloid-sorption))
```

The defined chemistries are enabled in the column definition. You must list colloids before any pesticides that can be bound to colloids. You can list as many pesticides as you want, but simulation time will increase linearly with the number of pesticides.

```
(Chemistry multi (combine colloids Pendimethalin))
```

References

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