Readme

Variable boundary condition with root water uptake

# Four HYDRUS (2D/3D) simulation files are needed:

All files should have the same exact FE mesh, root distribution, upper and lower boundary conditions. The boundary condition at the suction cup is defined for each simulation. In the present code, irrigation is applied from an upper boundary condition ‘Variable Flux 2’. Length units ‘cm’. Uncheck “Press enter at the end”.

1. *washRun –* a relatively long simulation that brings the system to a place where the soil solution sampling will begin. Boundary condition at the suction cup: no flow. Time units can be chosen.
2. *fnameI –* the initial simulation at day 1, time 00:01, it will run until vacuum application. Boundary condition at the suction cup: no flow. Time units ‘min’. Uncheck T-level information. Interval output of 10 min.
3. *contRun –* this is the simulation that runs between the sampling periods. Boundary condition at the suction cup: no flow. Time units ‘min’. Uncheck T-level information. Interval output of 10 min.
4. *simulation –* one minute simulation for each time step of the suction cup sampling event. The name of this simulation should be ‘\H3D2\_something\_1’, where there should be a number of files ‘\H3D2\_something\_1’ to ‘\H3D2\_something\_*n’*, where *n* is the maximum time in minutes that the sampling should continue. Boundary condition at the suction cup: constant head. Time units ‘min’. Uncheck T-level information. Interval output of 1 min.

# Building the time variable boundary conditions function ‘buildAtmosphAll\_ET’:

This matrix includes the irrigation, ET and vacuum application time.

Inputs:

1. Days – number of days that sampling is performed
2. hourI – time of the day, in hours, at which the irrigation starts
3. irrDur – duration of the irrigation event in hours
4. hourS – time of the day, in hours, at which the vacuum is applied.
5. dayET – day ET in cm/day
6. ETdur – duration of ET in hours (suggested 12 hours)
7. LF – leaching fraction as in Irrigation=ET\*LF
8. ETarea – surface area associated with transpiration, as defined at the Time Variable Boundary Conditions in the simulations in cm2 .
9. irrArea – actual area of irrigation at the variable flux 2 in cm2.
10. ETi – time in hours that the 12 hour ET begins (suggested 6am)

# Other inputs at the scriptAll\_ET script:

1. P1 – initial pressure applied at the VBC in cm
2. V1 – the total volume of the suction cup system in cm3
3. CO2i – atmospheric CO2 concentration in mol/mol
4. time – maximum time in minutes allowed for the suction cup sampling

# Functions to be called:

*runInitial* – runs initial simulation

*nodesN* – gets the total number of nodes

*nodesVBC* – gets the number of nodes at the VBC (constant head)

*buildAtmosphAll\_ET* - build the matrix with the time variable boundary conditions for all the entire period

*mainCodeF\_ET* - function that runs the sampling event

*resultsInitial* – saves one time the results from the initial simulation

*domain\_initial* - this function reads the previous run final water content and concentration (if standard solute transport is considered) in the profile and re-writes them as initial conditions in the next run

*atmosphF\_ET* – writes variable boundary conditions in first simulation

*domainChemInitial* – imports the chemical initial conditions from a previous simulation (UNSATCHEM)

*saveVar* – saving outputs water flow

*saveSolute* – saving each solute outflow

*cupSolution* – separate each type of outflow and puts together all solutes

*obsNod* – saves data from observation nodes

*getH* - Gets pressure Head for the boundary condition in next run

PHREEQC – runs chemical equilibrium inside the cup with PHREEQC

*domain\_w* – like domain initial but in the loop

*domainChem* – like domainChemInitial but in the loop

*continueRun\_ET* - continue simulation after suction period

*domainChemContinue* – initial solute distribution for simulation in between sampling events

*domain\_cont* – initial pressure heads for simulation in between sampling events

*soluteDataLongR* – save results from simulations in between sampling events

*mainCodeF\_ET* – runs one sampling event, from initial vacuum application until either no more water goes into the cup or the defined maximum sampling time arrives

# Extra files:

1. HYDRUS (2D/3D) + UNSATCHEM batch file
2. ~~PHREEQC batch file~~ Phreeqc should be installed in the computer and the path updated in the ‘PHREEQC’ Matlab function.
3. ‘phreeqcFile.File’ input file for PHREEQC
4. ‘level\_01.dir’ file for running HYDRUS in batch
5. Pos\_data – vector with 720 values between 0 and 1 with a sinusoidal distribution (half a period)