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Stochastic Assessment for Non-Point Source Contamination of Heterogeneous Aquifer: Instructions for Inputs and Outputs

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This document provides useful instructions to generate the input files of the different software used to model transport from a nonpoint source into a heterogeneous aquifer within a stochastic framework.

We refer to the manuscripts attached to this document if further information about the mathematical and conceptual background of the study is needed.

1. T-PROGS

The same T-PROGS model is used for all studies made in the project. In our study, we do not use any data to condition the geostatistical model, but T-PROGS is proposing this option. Two set of parameters have to be generated in order to run the program: MCMOD inputs and TSIM inputs. MCMOD and TSIM inputs were generated using the GUI available for the TPROGS software. T-PROGS manual provides the scientific background and the detailed instructions on how to generate the needed inputs. A set of example parameter files and the *tsim* executable in provided in the folder 1_TPROGS. The software *tsim* will generate a single file with the facies spatial distribution for all realizations (output file with extension "*.asc*").

The only post-process required here to proceed with our stochastic analysis is to split this output file into a file per realization and convert the facies index to a corresponding value of hydraulic conductivity. A Matlab script does this:

tsim_to_Kmat.mat: Generates hydraulic conductivity fields to be later used to generate the input of the Modflow model

2. MODFLOW

Some inputs are common to all realizations. It should be created once only, depending on the model main characteristics, and be used for any simulation. These files will be copied in the sub-folder used to run Modflow-2000 (MF2K) during the Monte Carlo simulation. These files, common to all realizations are: *BAS, DIS, GMG, MNWI, OC.* We refer to the Modflow online

manual for details about these packages. An example of each file is provided in the folder 2_MF2K.

Some other input files depend on the hydraulic conductivity field, such as the recharge rate, the well package and the K-weighted fluxes leaving the domain and are, therefore, realization dependent. Some parameters used as input to compute the flow field is also dependent on the land use.

These provided Matlab scripts help generate the series (for all realization) of input files:

get_landuse_cons.m: Generates a series of *RCH* files, which are MF2K input files with spatial variability of the recharge rate; and generates the spatial distribution of the particle density used for the transport modeling.

In our study, the local recharge rate depends on the soil and the crop types. The soil type is defined as the first (top) layer of the hydraulic conductivity field previously generated.

This Matlab script also generates a random spatial distribution of a series of crop over the domain, used to generates the spatial distribution of the particle density used for the transport modeling.

KweightedFHB.m: Generates a series of *FHB* packages, which specify the spatial distribution of prescribed fluxes to be applied at the bottom of the domain in order to simulate non-represented extraction. The local flux is proportional to the local hydraulic conductivity.

mnw2_pack.m: Generates the *MNW2* packages for each realization with different pumping rate, screen length, and top depth. 3 extraction wells are implemented in each simulation. The well location is selected in order to always have 10ft of gravel/sand for each 100 gpm of pumping rate. If this is not doable at the given well location, the algorithm changes this location until the criteria is fulfilled.

get_nam.m: Generates the name file (specifies input and output files names) for each realization.

3. RW3D

get_nameRW3D.m:

get_paramRW3D.m:

get_landuse_cons.m:

4. OUTPUTS

5. Translation to pesticide contamination

Hydrus 1D
Add degradation (in RW3D)
Add sorption (in RW3D)