Documentation of nitrate-related input preparation for mHM-Nitrate

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1. Model configuration files

1.1. mhm.nml

- The nitrate simulation is only activated when *processCase(11) = 1*

Fig.1 toggle option for activating nitrate simulation in mhm.nml (a screenshot)

```
!added by X. Yang FOR WQM
!> water quality
!> 0 - deactivited
!> 1 - Nitrogen sub-model(mHM-Nitrate)
processCase(11) = 1
```

- Specify the observation file names for water quality evaluation gauges *(&wqm_evaluation*_gauges) and point-source gauges *(&wqm_addinflow_gauges)*

- Notes
  - (1) the nitrate module make use of the "inflow gauges" structure for considering the point-source input data;
  - (2) all the gauges *id*s should be corresponding to the gauge locations in *./input/morph/idgauges.asc.*

1.2. mhm_paramter.nml

- Nitrate model parameters are added in the end of the parameter list: &nutrientparamter
- Nitrate model parameters are mostly land-use dependent, but here they are grouped into "agricultural" (named with "_agri") and "non-agricultural" types for simplification.
- The instream denitrification rate (*denitrification_aquatic*) and the instream autotrophic N uptake rate (*autotrophicuptk_rate*) are global parameters (i.e., not landuse dependent).
- Notes when using the regionalization approach of instream N uptake by Yang et al., WR:
  - *autotrophicuptk_rate* is activated only by present the global radiation input data, details shown below).
  - In this case, parameter "primaryprod_rate" and "primaryprod_rate_agri" is used as the proportion of the gross autotrophic uptake that is mineralized and returned back to the stream water volume.

1.3. wqm_outputs.nml

Nitrate related state variables and fluxes specified here can be written out as NetCDF format in *./output/WQM_Fluxes_States.nc*. Details has been documented within each toggle.

2. Time series of observations

Gauging stations for both evaluation data and point-source input data
(./input/water_quality/wqm_gauge/)

- Naming of the files for each gauging station: wq_##.txt ("##" should be exactly the corresponding station IDs)
- The header format of each file should be strictly maintained!

e.g., Fig. 2 A screenshot of the observation data file

```
    1:Selke (Abfluss)   DAILY
    nodata  -9999
    n   1   measurements    per day "[1,"    1440]
    start   1993    1    1    0    0    (YYYY    MM   DD   HH   MM)
    end 2016    1    1    0    0    (YYYY    MM   DD   HH   MM)
YYYY    MM   DD   HH   NN   IN
```

- Specific Notes
  - For evaluation data, Nitrate-N (i.e., IN) observations are only allowed as input data
  - For point-source input data, both Total Nitrogen (TN) and IN are allowed. The model will automatically detect the corresponding column names. If only "TN" is presented, then 80% of TN will be assigned to IN by default. This proportion is hard coded and can be adjusted in the source code. See more in *./src/WQM/mo_wqm_read.f90:177-190*
  - Time series of point-source inputs should be continuous, which means the input data should be pre-interpolated.

3. Information of Agricultural Management (*./input/water_quality/*)

3.1. cropdata.txt

This file contains all necessary agricultural farming and management information that should be provided for the nutrient simulation.

- Ln 1 specify the total number of crops/vegetation types, e.g., "*number_of_crops 8*"
- Ln2 the title of information for each crop/vegetation, explained column-by-column:

Column name	Description	Unit
Crop_name	The name of the crops	--
Crop_id	The assigned ID of the crop. This id is being used for the model to identify each crop and extract corresponding information.	--
frtn1	The amount of mineral N for the FIRST application	Kg N ha^{-1} yr^{-1}
frtday1	The date of the FIRST mineral application	Julian date
frtdown1	The proportion of applied N that is assigned to the second soil layer	0-1
frtn2	The amount of mineral N for the SECOND application	Kg N ha^{-1} yr^{-1}
frtday2	The date of the SECOND mineral application	Julian date
frtdown2	The proportion of applied N that is assigned to the second soil layer	0-1

mann1	The amount of manure (organic fertilizer) for the FIRST application	Kg N ha^{-1} yr^{-1}
manday1	The date of the FIRST manure application	Julian date
mandown1	The proportion of applied N that is assigned to the second soil layer	0-1
mann2	The amount of manure (organic fertilizer) for the SECOND application	Kg N ha^{-1} yr^{-1}
manday2	The date of the SECOND manure application	Julian date
mandown2	The proportion of applied N that is assigned to the second soil layer	0-1
manfIN	The proportion of inorganic content in the applied manure	0-1
frtperiod	The period that the applied fertilizer (both mineral and organic) is evenly added to the corresponding soil N pools after the applied date	Days (e.g., 60 days)
resn	The N amount of crop/plant residues in organic forms	Kg N ha^{-1} yr^{-1}
resday	The date of the residues entering into soil N pools	Julian date
resdown	The proportion of residual N that is assigned to the second soil layer	0-1
resfast	The proportion of residual N that is assigned to the liable (active) Soil organic N pool	0-1
resperiod	The period that the received residues (organic) are evenly added to the corresponding soil N pools after the applied date	days
up1,up2,up3	The three parameters for the logistical potential plant/crop growth function (potential N uptake function, see codes in *./src/WQM/mo_water_quality.f90: subroutine agri_management()*, or check the HYPE model descriptions: http://www.smhi.net/hype/wiki/doku.php? id=start: hype_model_description:hype_np_soil#potential_vegetation_uptake_of_nitrogen)	--
uppsoil	The proportion of potential N uptake that is assigned to the first soil layer	0-1
plantd	The plant date of the crop	Julian date
emergd	The emerge date, especially for winter crops (can be "0" for spring crops)	Julian date
havestd	The harvest date of the crop	Julian date
catch_crop	The catch crop ID (NOT IMPLEMENTED YET!!)	
ccplantd	The plant date of catch crop (NOT IMPLEMENTED YET!!)	Julian date
cchavestd	The havrest date of catch crop (NOT IMPLEMENTED YET!!)	Julian date

- Ln3 and onwards: the specific information for each crop/vegetation type.

3.2. rotation_info.txt and rotation_class.asc

As description in the associated publication (Yang et al., 2018 WRR), an explicit structure for crop rotation is implemented in the mHM-Nitrate model. Therefore, the two inputs should be provided:

- rotation_info.txt gives the information of rotation types and the crop sequence for each rotation type
    - ln1: the total number of rotation types
    - ln2: the title of information for each rotation type, explained column-by-column:

Column name	Description
rotation_id	The ID of each rotation type, should be in consistent with those in the rotation map, i.e., "rotation_class.asc"

ncrops	The total number of crops in each rotation type
crop1, crop2, …	The crop ID sequence of each rotation type. The crop IDs should be correspondent to the IDs in “cropdata.txt”

- rotation_class.asc gives the spatial distribution of each rotation types (as the same ASCII format as other morphological inputs in *./input/morph/*). Note that (1) the spatial resolution should be kept as the same as other geographic inputs, from an easier coding perspective; (2) the ids should be correspondent to these in rotation_info.txt.

3.3. initial_values.txt

Some more initial storage conditions of soil N pools have to be provided to the model. These initial conditions are assigned as land-use dependent. The columns are described as:

Column name	Description	Unit
mhm-LAI	The IDs of land use types, which should be in consistent to those defined in *./input/morph/LAI_classdefinition.txt*	
init_concIN	The initial IN (i.e., Nitrate-N) concentration of the third soil layer	mg l^{-1}
init_concON	The initial dissolved ON (i.e., organic N) concentration of the third soil layer	mg l^{-1}
init_fastN	The initial solid liable ON storage for each soil layer	mg N m^{-2}
init_humusN	The initial solid humus ON storage for the top soil layer	mg N m^{-2}
hnhalf	The parameter of assigning initial humus ON storages for lower soil layers (see *./src/WQM/mo_water_quality.f90: subroutine wqm_initialise*)	

3.4. geoformation.txt

The hydrological platform mHM model (https://www.ufz.de/mhm), as a catchment hydrological model, has largely simplified the deep groundwater dynamics. Alternatively, information of the geological units is required for considering the baseflow generation.

Nitrate accumulation/storage along the soil profile is depending not only on the landuse, but also on the geological formation. For instance, if a shallow bedrock (i.e., relatively impermeable) is presented, the nitrate-enriched soil waters, e.g., due to agricultural activities, cannot be percolated into deep groundwater. This results in relatively low Nitrate concentrations in baseflow component, although in agricultural dominant areas. In contrast, in loess agricultural areas, Nitrate concentrations in baseflow can be largely elevated.

Therefore, the initial IN storage in deeper groundwater (i.e., the third layer) should also consider the geological formation. The *geoformation.txt* provides the rough permeability of each geological unit type (1 – relatively permeable and 2- impermeable bedrock). The “GeoParam” and “ClassUnit” should be exactly the same as in *./input/morph/geology_calissdefinition.txt*

3.5. global_radiation.txt (an optional inputs for instream N uptake)

*This is an optional input if the regionalization approach by Yang et al., 2019 Water Research is being used.

**If this file is presented in the input files (*./input/water_quality/*), the model will automatically calculate in-stream autotrophic N uptake (i.e., primary production) based on the new approach. Otherwise, the original approach based on the HYPE description is used.

- The header format should be strictly maintained!

```
    1:Selke (Global radiation)   DAILY
    nodata  -9999
    start   2010    1   1   0   0   (YYYY   MM  DD  HH  MM)
    end 2016    1   1   0   0   (YYYY   MM  DD  HH  MM)
Date    G-R
```