Topic: MIBIREM - WP4: Continue Discussion on chemical modelling of Ghent Site
Date: 2024-03-01
Participants:

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<u>Topics and Meeting progress</u>

- Purpose of meeting: Discussion on the conceptual design of the "*Ghent*" site (data provided by TAUW) for geochemical modeling in PHREEQC and identify the required information for linking geochemical model to simple 1D advective transport equation. We also discussed the possibility to consider "*Ploufragan*" site as another candidate for the geochemical modeling

- **1ˢᵗ: Developing batch dissolution-adsorption model at source location:**
  - Available data in the report "*Composition free product and characteristics*" which are:

    1. The amount of soil contamination and its composition at LUM77 location from 22/11/2002 including the weight percentage of the contaminant composition. (page 10 of the report)
    2. The equilibrium concentration (on base of shaken batches) in water is 31,400 µg/l total hydrocarbons (first paragraph in page 11 of the report)
    3. The composition of emission to groundwater from soil at LUM77 (figure 3.2 in the report)
    4. The information and data on groundwater characterization which were carried out on 27/09/2004 by ESA BVBA (table in page 13 of the report)
    5. The cumulative emissions on base of leaching test (per kg soil) is 0,0014 mg/kg Naphthalene and 0,0002-0,0003 mg/kg Acenapthene (figure 3.4 in the report)

  - Available data in the excel sheet and according to the explanation that Tobias mentioned in his email:

    6. The tab 'Waterbodem' (soil bed / sediment, before removal) and look specifically at the soil contents in WB 2, 4 and 5, can be a quite representative of the initial soil contaminants concentration
    7. the tab 'Peilbuizen' (monitoring wells), specifically Oip5 (= well 50) at the dates 3-2-2020, 30-3-2020 and 4-6-2020. These concentrations might be considered as in equilibrium with the soil contents mentioned in 'Waterbodem' WB2, 4 and 5, because at that time the flow was quite low (after removal of sediment flow increased and maybe non-equilibrium).

- → MM: It is possible to develop a batch model at source location to simulate pure dissolution of Tar composition in water including adsorption (reverse mechanism of adsorption).
- → **Source concentration:** data from page 10 in the report
- →**equilibrium groundwater concentration before canal cleaning (to compare the simulation results with)**: data from the tab 'Peilbuizen' (monitoring wells), Oip5 (= well 50) at the dates 3-2-2020, 30-3-2020 and 4-6-2020
- →SA: There is alternative way to compute distribution coefficient for each contaminant (k_d^i) according to what Suzanne used in her PhD (page 161 in het thesis)
- → AZ: We can develop the model first by computing the k_d values from leaching test as mentioned in the report and then use Suzzane approach to compute k_d values and then compare them together. Although, for the second approach we have to consider new value for organic carbon mass fraction (f_{oc}) based on the information from Ghent site which is 2% also we need to think about the distribution values for BTEX component inside soil, maybe we can start by considering equal distribution.
- → AZ: if the results of this simulation doesn't match the observation concentration at oip 5 then we should look for more accurate groundwater concentration, probably those mentioned in the report in 2004.

- **2ⁿᵈ : Developing 1D box model to link simple advective transport equation to the geochemical model**
  - Conceptual model:
    - →AZ: Let's consider constant supply of source at 40 meter distance from the receptor (well Oip 5) and 1D flow from the source to the receptor.
  - Hydrogeological parameters:
    - →AZ: value for groundwater velocity, porosity and dispersion, from the conservative transport model
  - Adsorption effect:
    - →AZ: considering linear adsorption → retardation factor will be calculated
  - Concentration at source location:
    - →AZ: calculated values from the batch dissolution model
  - Concentration at the receptor Oip 5 after cleaning: (to compare the simulation results with)
    - →AZ: data from the tab 'Peilbuizen' (monitoring wells), Oip5 (= well 50) at the dates 03-06-2021
  - Chemical and/or biochemical reactions to be considered:
    - →MM: For now we cannot consider biodegradation reactions until we have more data for that.

- →AZ: It is good to set up the PHREEQC model to simulate these reactions as well just for the purpose of modeling and even we don't have enough data for Ghent site, but having this model in hand, can be adapted to other site which have more data.

- **Considering Ploufragan site as another candidate for geochemical modeling**
  - →MM: There is possibility of DND collaboration at Ploufragan site, so it can be a good opportunity for modeling. As there is a chance to implement a prototype and pylot there by DND, and they will take some samples and do some experiment which can be combined with the purpose of calibrating the model or gathering more data to test the model.
  - →MM: Now they also have more hydrogeological data from different well locations.
  - →MM: The situation for collaboration with this site is in the proposal stage.
  - →AZ: We can have a look again at this site and after running the Geochemical model on the Ghent site we can then adapt it for Ploufragan site as well, based on the additional data which may be available and the test that are going to be done.

ToDos:

- [MM]: start setting up the draft of batch model in PHREEQC for dissolution-adsorption model at source zone without looking at the data.
- [MM]: prepare the coupling of PHREEQC with Python.
- [SA]: Share the PowerPoint slide on our shared MIBIREM OneDrive as a source for updating each other about the activity that we are doing or adding relevant information to that.
- [AZ]: Add one slide to the PowerPoint with the sketch of the flow model including the velocity and other required parameters.
- [SA]: Clean the Excel file data and gather all the required data for the purpose of the batch dissolution and 1D advective- transport model, and add this data as well to our PowerPoint document. Also, Contact Tobias and ask about the Naftalin which is mentioned 2 times in the Excel sheet?
- [SA]: From the report, cutting the relevant figures and information and putting them on one PowerPoint slide.
- [SA] & [AZ]: Install PHREEQC and after receiving the draft model, try to adjust the model to the data by playing with the parameters.
- [MM]: As next step, start implementing a 1D model
- [MM]: check with Cosimo regarding the timing for the proposal for Ploufragan site and let us know if we need to arrange a meeting together to discuss the possibility of adding activities for the purpose of the modeling in the proposal.

Next Meeting:

- After Easter holiday, we can check our availabilities to meet and update each other.

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