

NanoFASE

NanoFASE WSO Environmental Exposure Model

Overview

The *NanoFASE water-soil-organism (WSO)* model predicts the fate and bio-uptake, across space and in time, of NMs entering the soil and aquatic environments. It works by coupling submodels for environmental compartments: soils, rivers, bed sediments, lakes, estuaries and the sea, and simulating the transport of NMs between these compartments. The model takes account of the fact that within each compartment, NMs can transform between different forms and states, and be taken up by the biota present (Svendsen et al. 2020, Cheimarios et al. 2020).

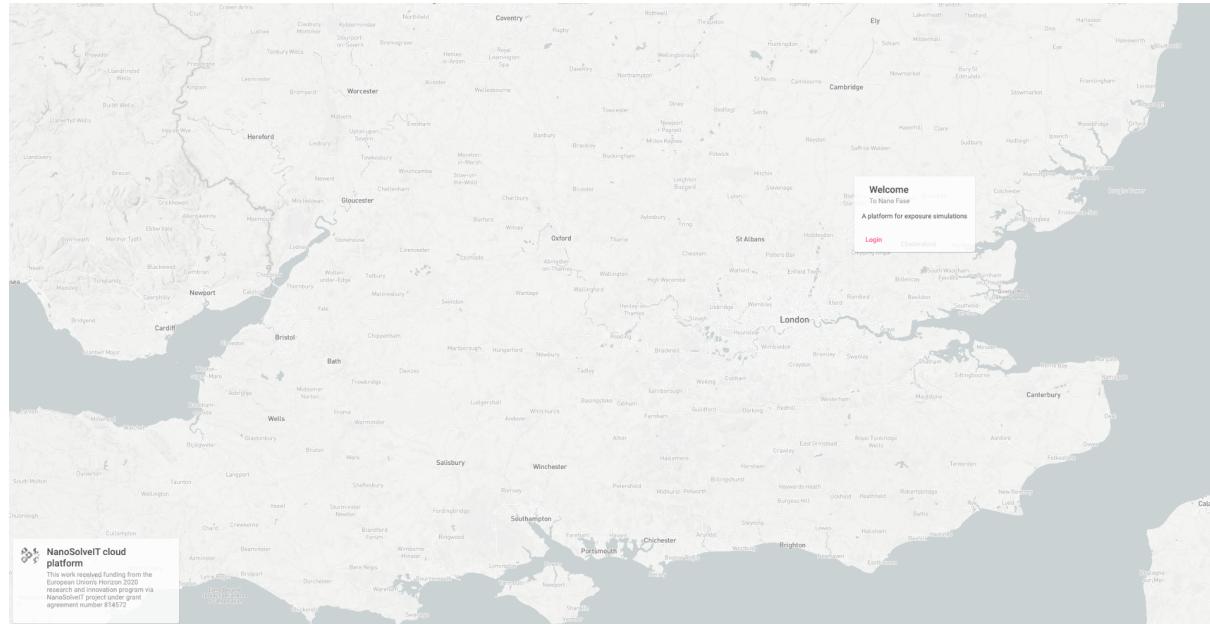


Figure # The NanoFase landing Page

Underlying models

The computational workflow employs several models. First is the Nanofase Environmental Exposure model and several bio uptake models. The NanoFase model represents the state-of-the-art in ENM environmental exposure modelling, providing spatial and temporal predictions across multiple environmental compartments. The key output variables are the predicted environmental concentrations (PECs). These are combined with PBPK models for better understanding of the bio-uptake by and biological effects of NMs on organisms and ecosystems. Both form a key part of environmental NM risk assessment.

All the inputs and outputs of the models are represented through real time rendering maps from a graphical user interface for better interpretations of the results. Also, everything is available through API's, allowing further integration with other services.

Tool description

The workflow for the user over the GUI is as follows:

1. User logs in to the system to access personal modelling space
2. Adds emissions (if necessary)
3. Constructs a scenario that includes all the desired emissions
4. Runs the simulations
5. Inspects results on screen / render the outputs

Add emissions

In order to define an emission, the user first selects between point or areal emission. In the first case, a point emission is added on the map by clicking on the desired location, while the areal emission is defined by forming the desired polygon that specifies the emission on the map.

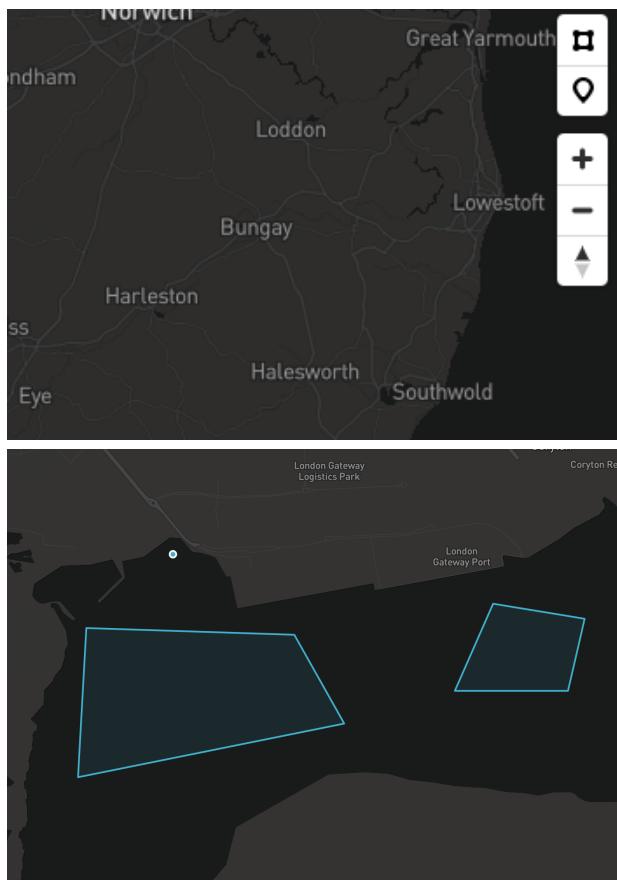


Figure # Choosing the desired action (point / areal emission) and adding on the map

Upon completion, the user is prompted through a pop up dialog to add the characteristics of each emission source. A title, a description , the nanomaterial involved and the actual emission value are filled in and generate the GeoJSON encoding needed. When complete, the json is stored through an API for later usage.

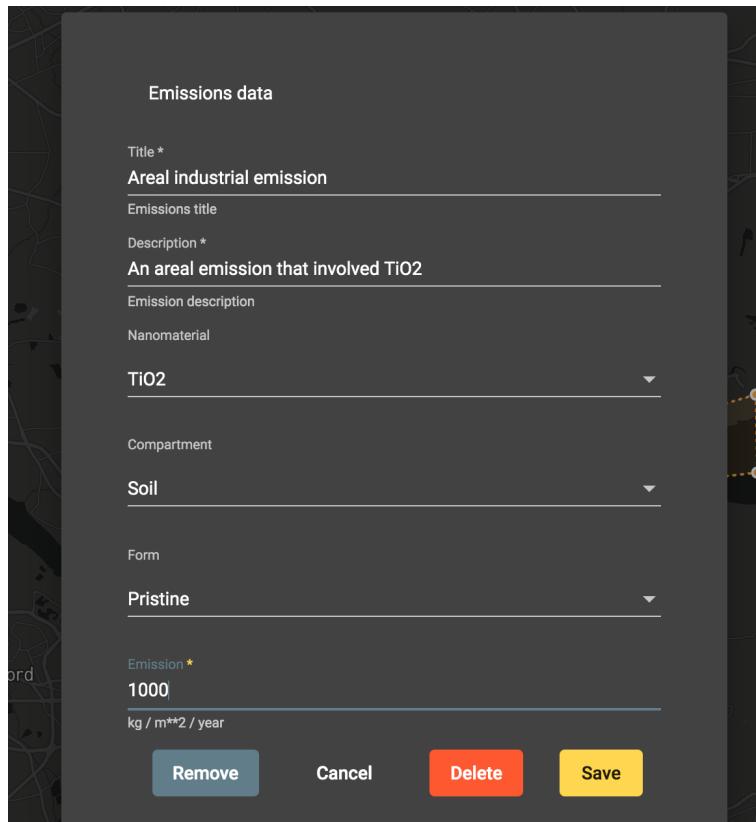


Figure # The Metadata of a point emission. (An example dialog)

```
{
  "_id" : "2ad325b0410f4049cca64d5",
  "properties" : {
    "title" : "point 1",
    "description" : "p1",
    "nanomaterial" : "TiO2",
    "compartment" : "Surface water",
    "form" : "Pristine",
    "temporalProfile" : "P2",
    "emission" : "100",
    "date" : NumberLong("1594206068943"),
    "saved" : true
  },
  "geometry" : {
    "coordinates" : [
      0.459833933046554,
      51.5056585580292
    ],
    "type" : "Point"
  },
  "type" : "Feature",
  "userId" : "a-user-id"
}
```

Figure # The GeoJSON of a point emission.

Construct the scenario

A simulation will probably consist of many emissions sources, since real world scenarios involve multiple sources of nanomaterial emission. When all desired emissions have been added to the map, they are stored as a scenario which is used as input to a simulation. Both the emissions and the scenarios are stored and can be enriched with more emissions or update the existing ones.

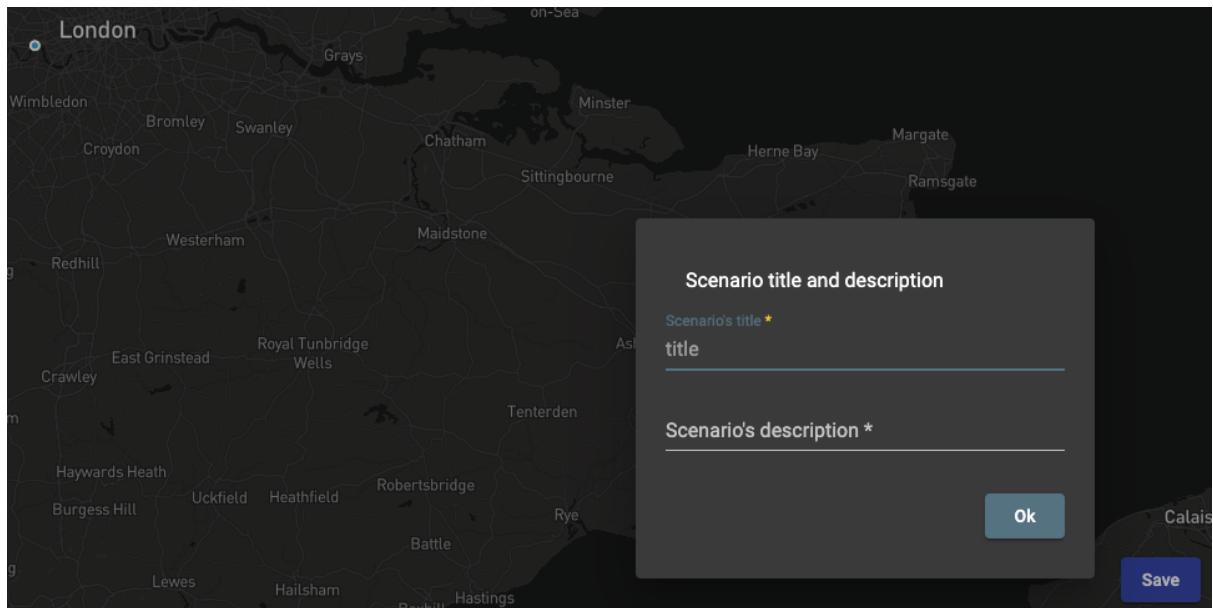


Figure # Creating a scenario.

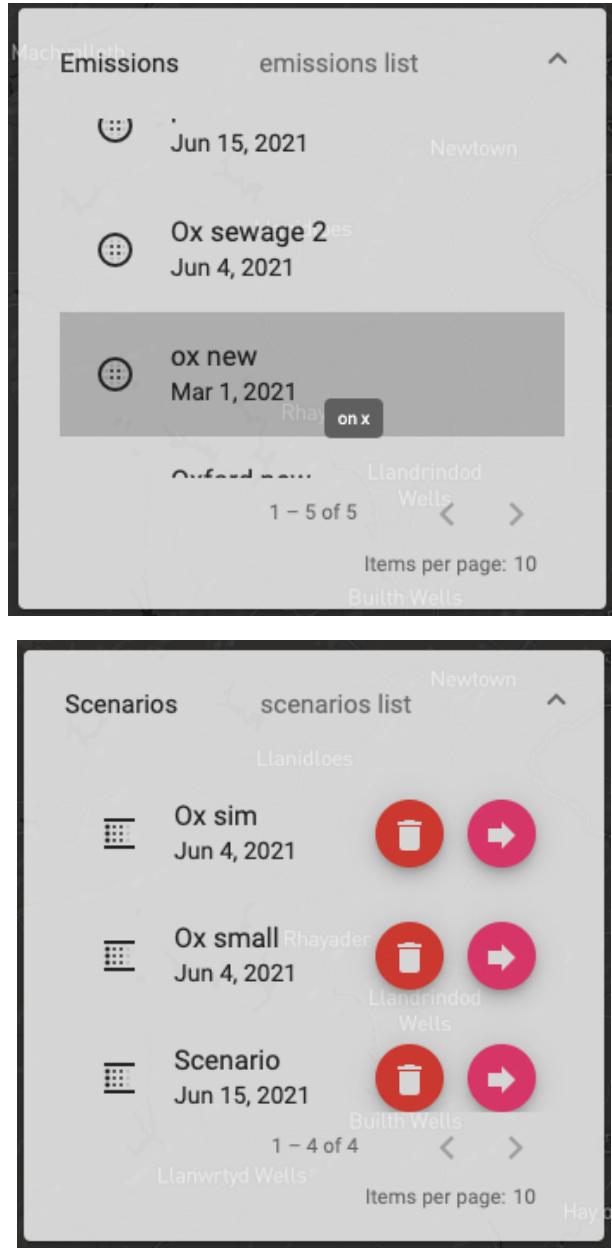


Figure # Emision and scenario lists..

Running a simulation

When a scenario is present on the map the application is ready to run a simulation. The user is prompted through a dialog to submit the metadata of the simulation, like the title, description and start date of the simulation. The user can optionally add bio uptake simulation results in the output, along with the duration window of the bio uptake simulations. The default output of the NanoFase model is 365 days. For the bio uptake predictions the simulation can produce predictions for more than 365 days.

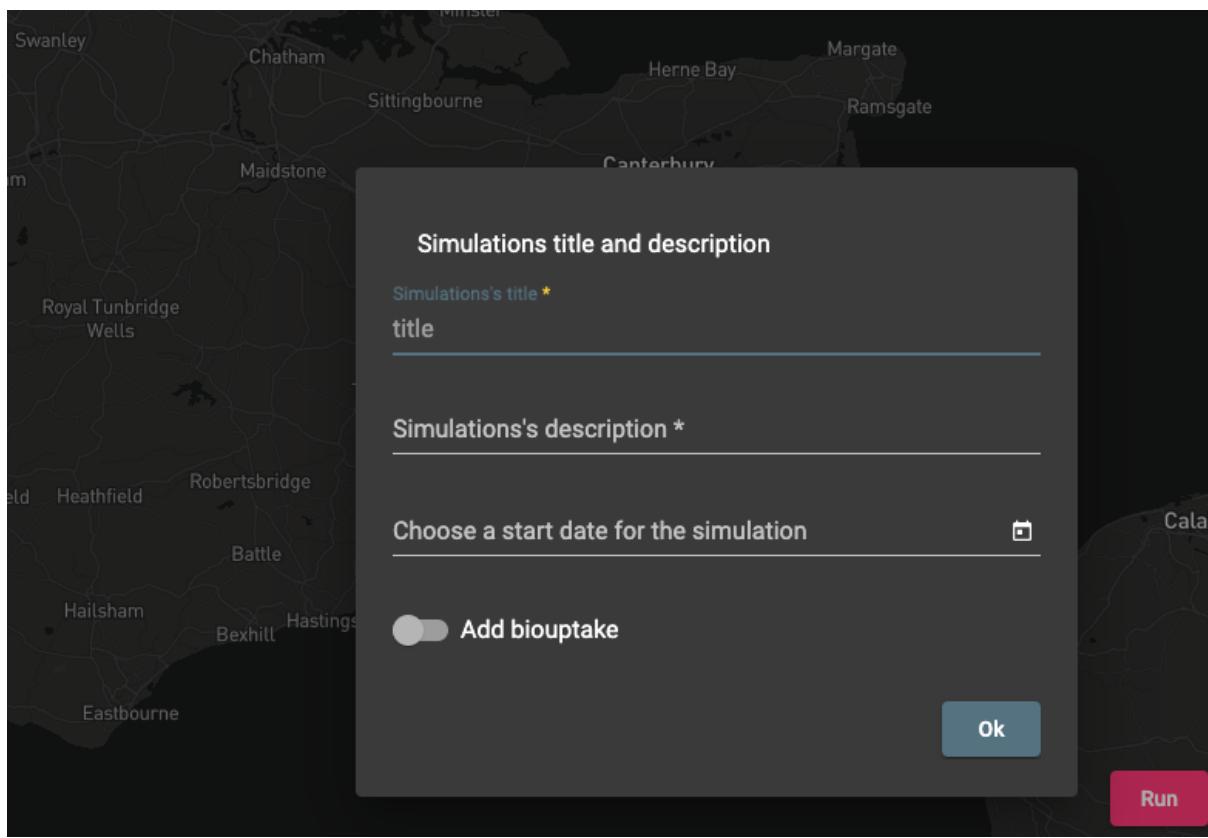


Figure # Simulations metadata and bio uptake outputs..

Accessing the results through visualisations

Once the simulation is finished, the results can be inspected through the user interface. The simulation takes some time to be complete since the data that is produced reaches hundreds of megabytes and both production and manipulation is time consuming. The simulation completion percentage is available at any time through the user interface. When the first results become available, the inspection and rendering process can be realised.

Every simulation is stored and is available through a list containing the user's simulations, allowing revisiting each simulation. Each simulation gets an id, which allows the formation of a unique URL. In that way, sharing is enabled and other users can visit the outputs of a simulation. This functionality gives access to users of multiple levels. For example, a regulator may not have access to a series of emissions to submit them and run a simulation but it is critical to have access to the results to define a risk about a new plant etc.

The URL's have the form <https://nanofase.cloud.nanosolveit.eu/simulation/<simulationId>> and are accessible from everyone.

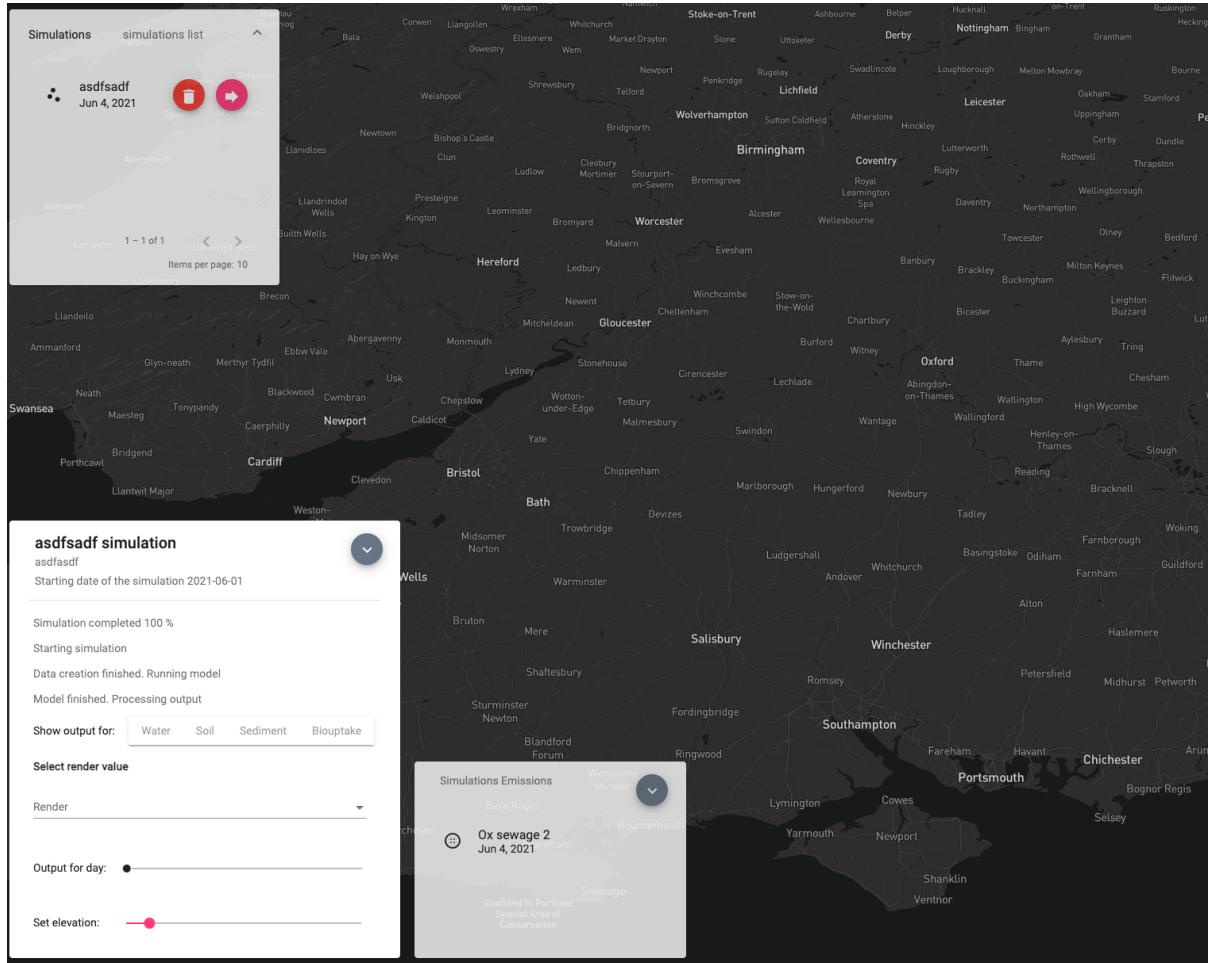


Figure # Simulation windows on the user interface.

For better rendering and inspection of the outputs of the simulation only one variable is rendered each time. The outputs are separated in four or three groups respectively to the input. The water outputs, the soil, the sediment and the bio uptake outputs if available. On each output type the variable to be rendered is chosen. Each output has different outputs. For example the bio uptake outputs have variables for the concentration of nanomaterials for each organization whereas the water has variables like dissolved nanomaterial etc and others. Two sliders are available that facilitate the rendering of the variables. One for the days and one for the elevation of the rendered outputs.

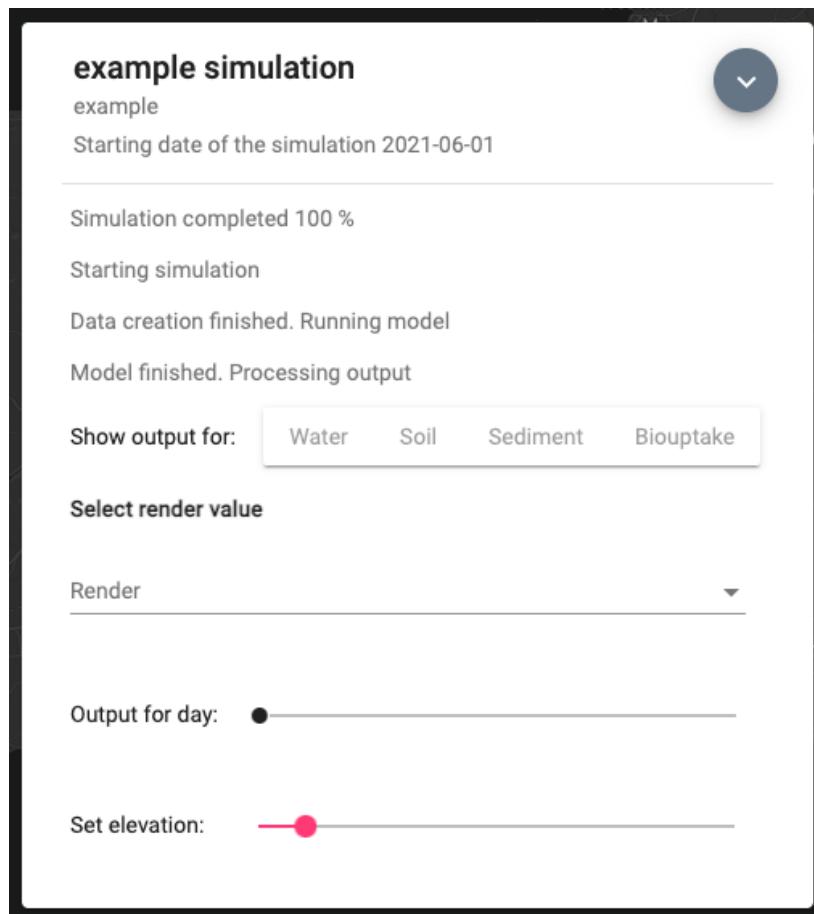


Figure # Simulation windows on the user interface.

Rendered outputs

Once the above options are selected the results are rendered on the map of the Graphical User Interface.

Below we present an example for the concentration of TiO₂ in the Thames catchment that occurred from a point emission in the river near Oxford. The more red and high the polygons are, the higher is the concentration of the material in the specified catchment. By clicking a point the actual data are presented and time / concentration charts are created. The outputs of the specific point throughout the whole simulation are presented in an easy interpreted form. All the variables can be rendered and viewed this way.

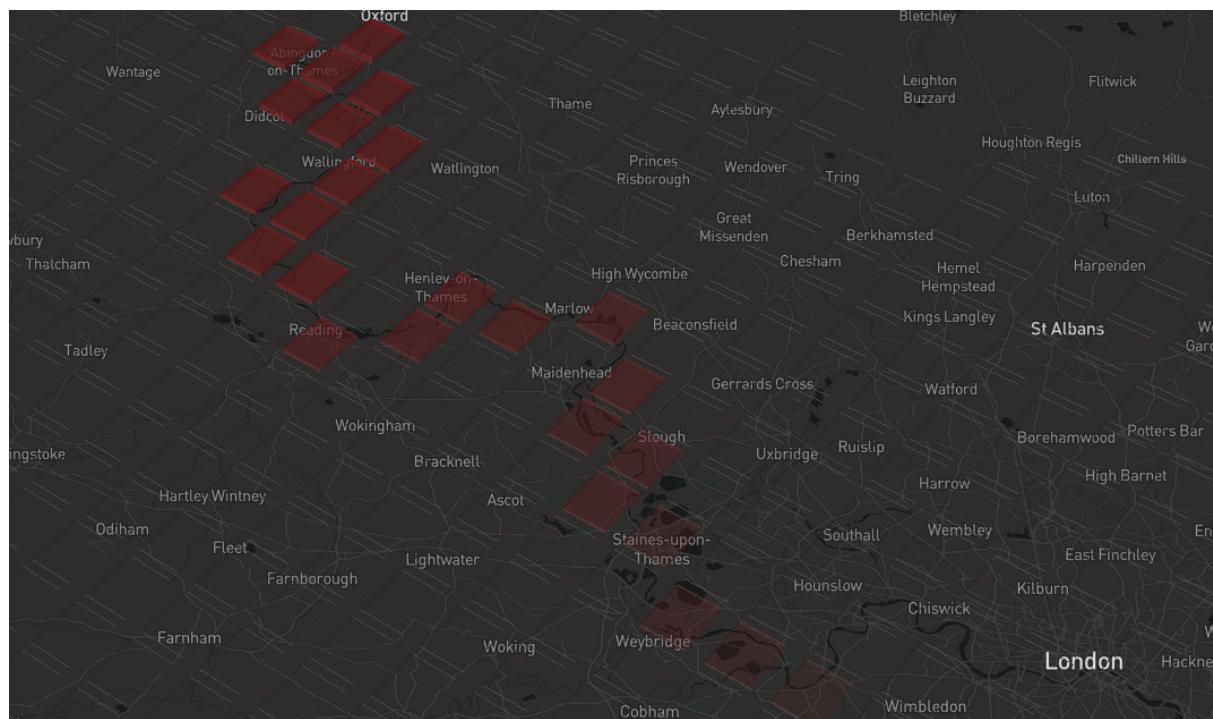


Figure # Rendered outputs on the Thames catchment.



Figure # Time / Concentration charts for a specific polygon on the map .

More interesting are the outputs for the Bio Uptake models. Bio-uptake by and biological effects of NMs on organisms and ecosystems are rendered. In order to conduct the risk on the specific parts the pod (point of departure) value for each organization is entered and the renderings take

a color code corresponding to the submitted value. Red are the polygons on the map that have over-passed the pod value and yellow to green the polygons that the concentration is less than the pod value.

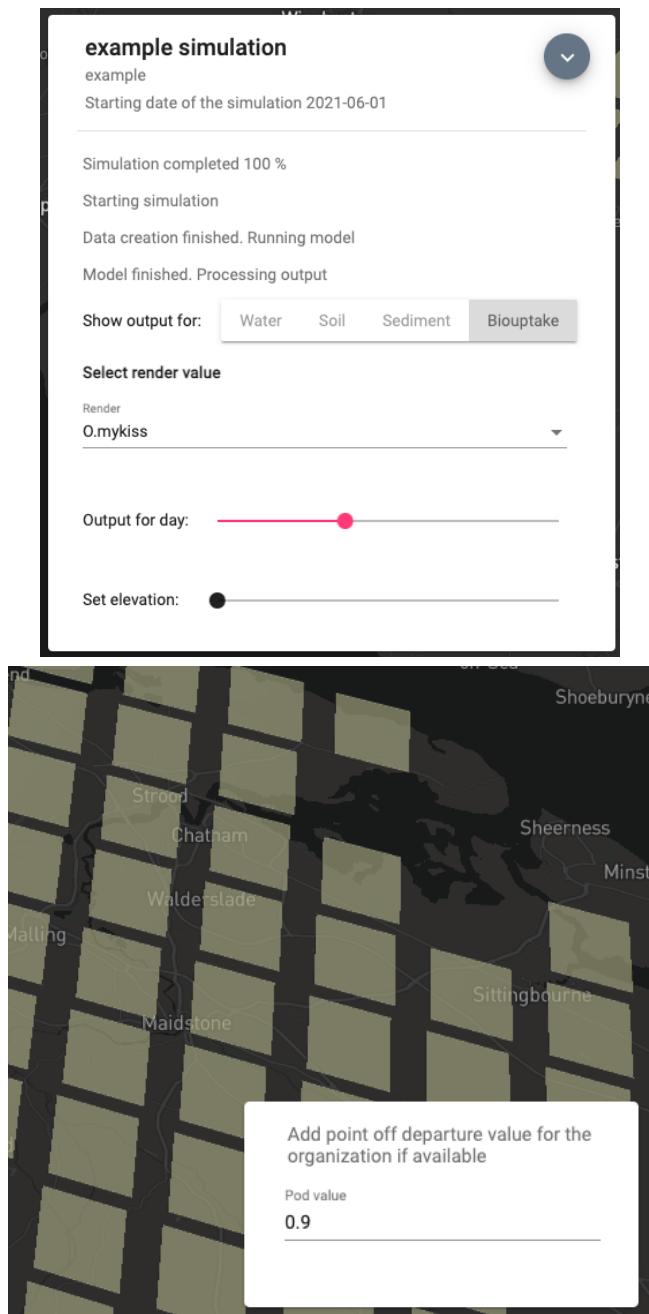


Figure # Enabling Bio-Uptake rendering for O.mykiss and submitting a POD value for the organization .

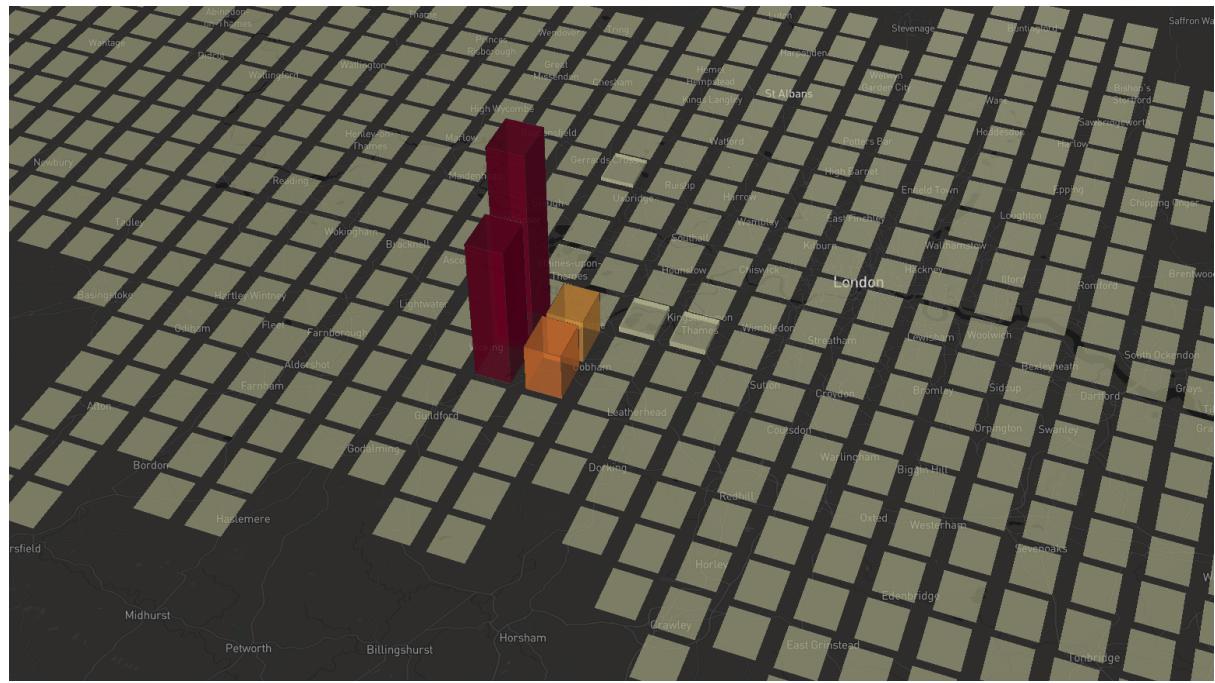


Figure # Rendering the outputs of the Bio-Uptake models in contrast to a POD value.

For better interpretation of the outputs of the model three themes for the application are available. A “dark” theme, a “light” theme and a “green” theme. For better interpretation the end user can choose from those three.

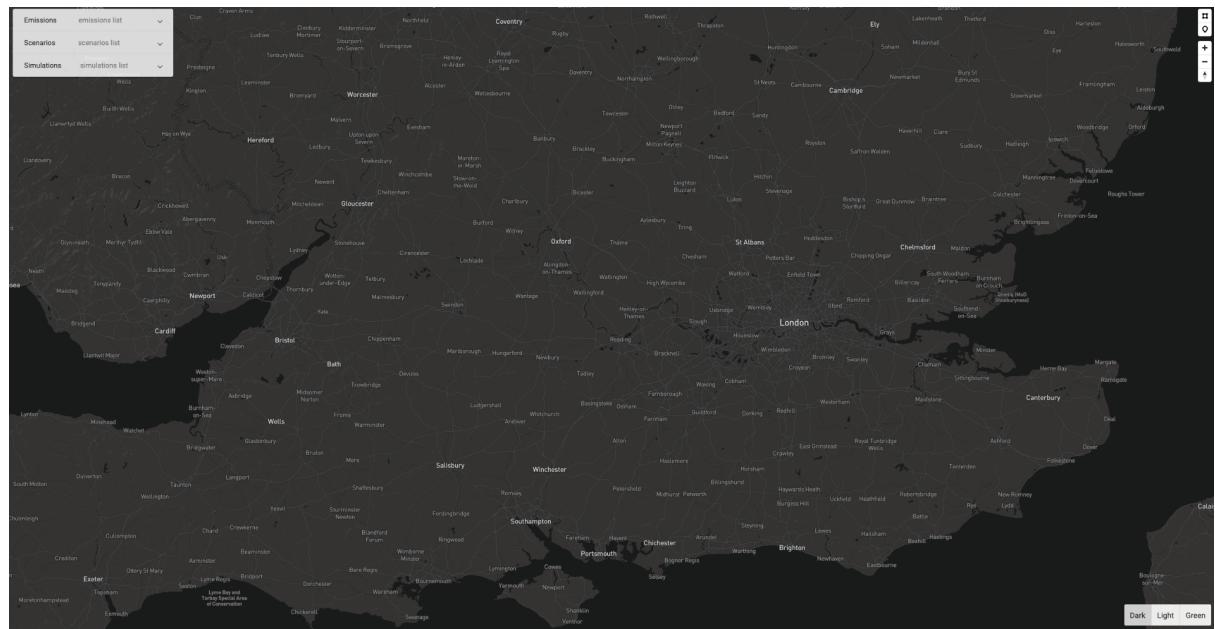


Figure # Dark theme.

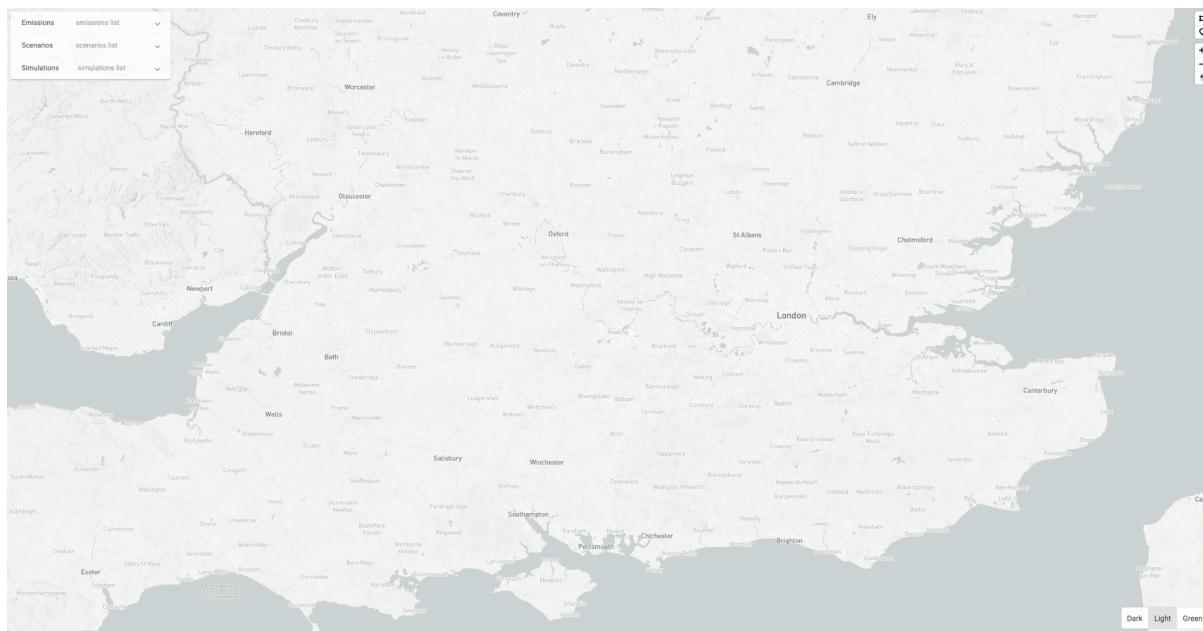


Figure # Light theme.

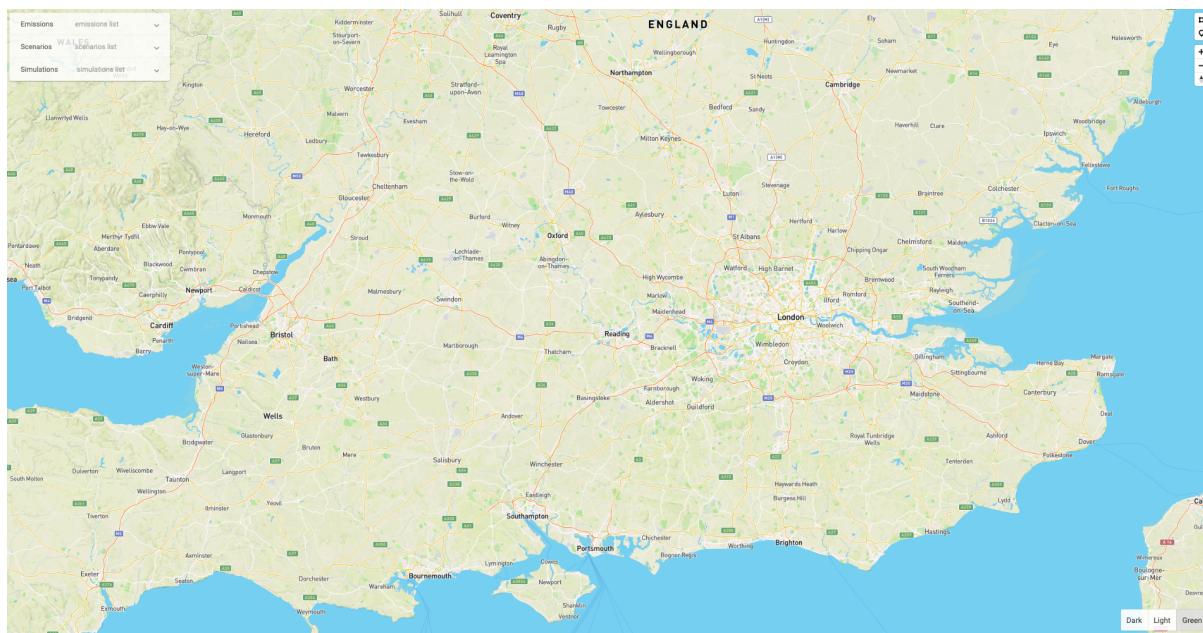


Figure # Green theme.

Input

- As input to the map the user defines the emissions desired either as points or polygons (point / areal emission) and saves them as a scenario.
- When a scenario is present on the map the user can run a simulation upon the specified scenario and add Bio Uptake predictions if wanted.

Output

- By choosing the type of the predictions that need to be rendered and the variable then by selecting the day through a slider the output starts to be rendered at the map.
- By clicking a polygon all the values on the specific part of the map are shown through a pop up dialog. Also time / concentration charts can be generated for the specific part of the map.

Example

Create the emissions on the map by choosing the corresponding actions

- A. Choose whether the emission will be a point or a polygon (areal). Click on the map to submit the emission.
- B. Submit the metadata of the emission (Title, description, Nanomaterial, Form, Emission etc)

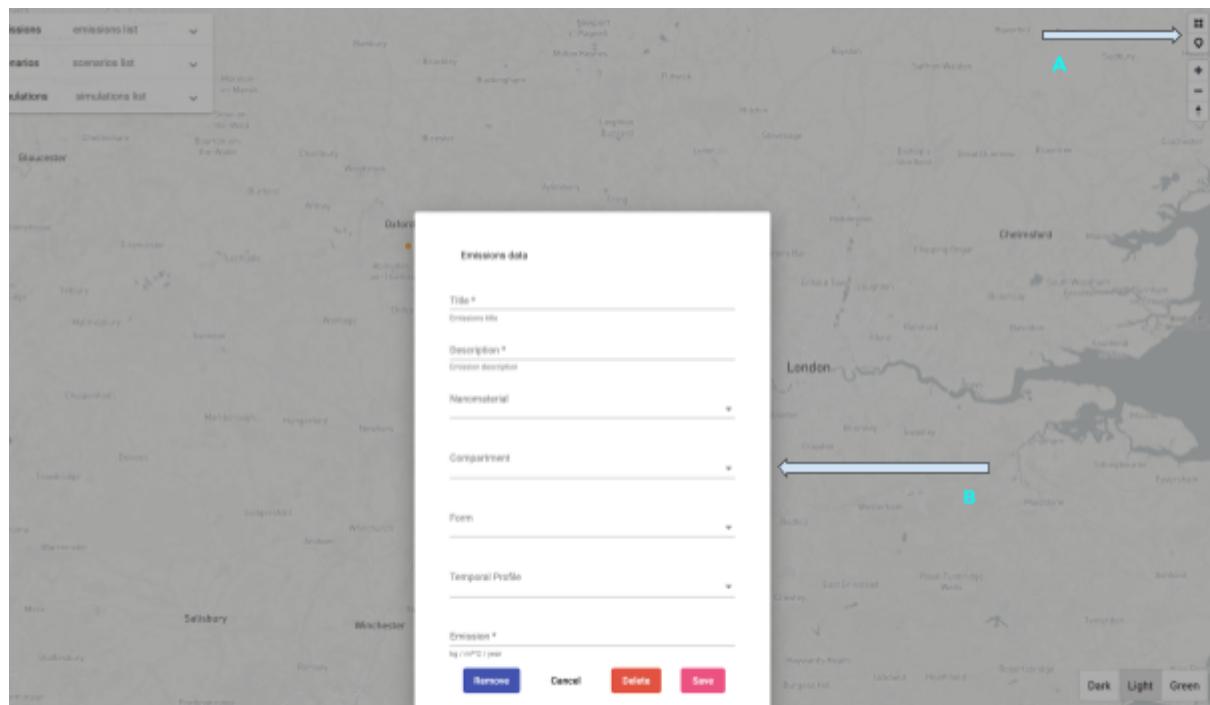


Figure # Submitting an emission.

Save the emissions as a scenario and give a title and a description of the scenario.

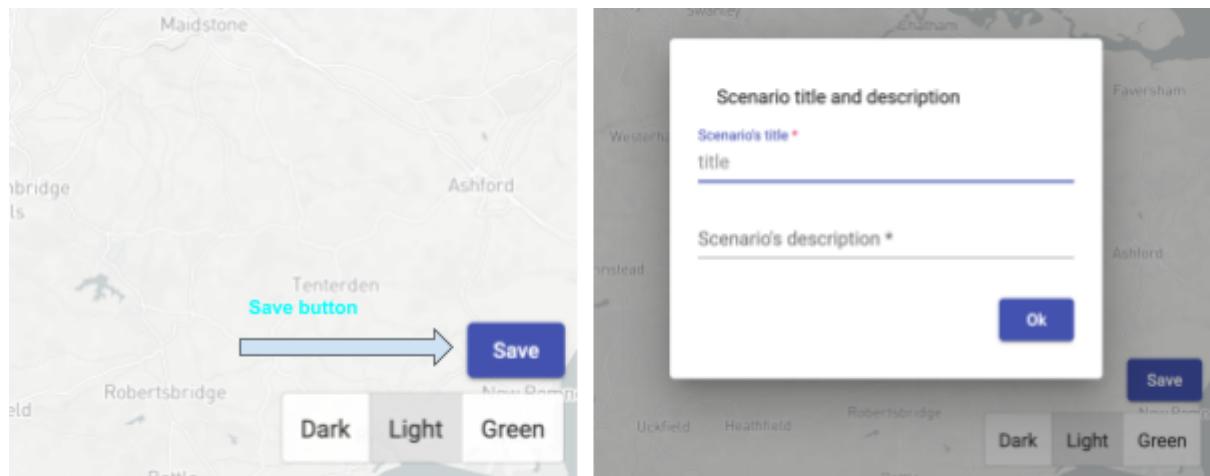


Figure # Save the emissions as a scenario.

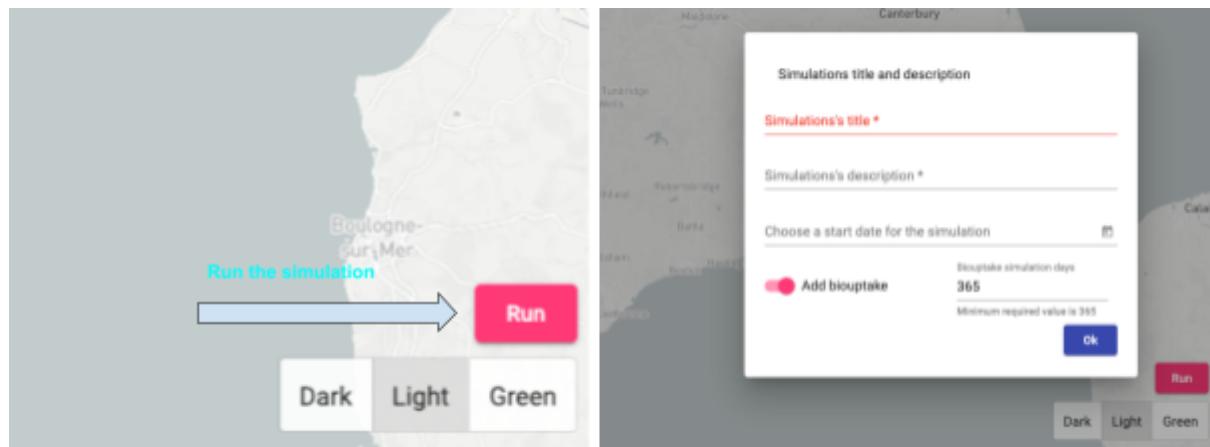


Figure #Run the simulation when a scenario present on mep. Submit the metadata and add bio uptake predictions.

Rendering the outputs of the simulation

- Choose the simulation from the users simulation list
- Choose the outputs to be rendered (Water / Soil / Sediment / Bio Uptake)
- Choose the variable to be rendered.

- D. Choose the day for the output.
 E. Submitting a POD value if available for the specified organisation.

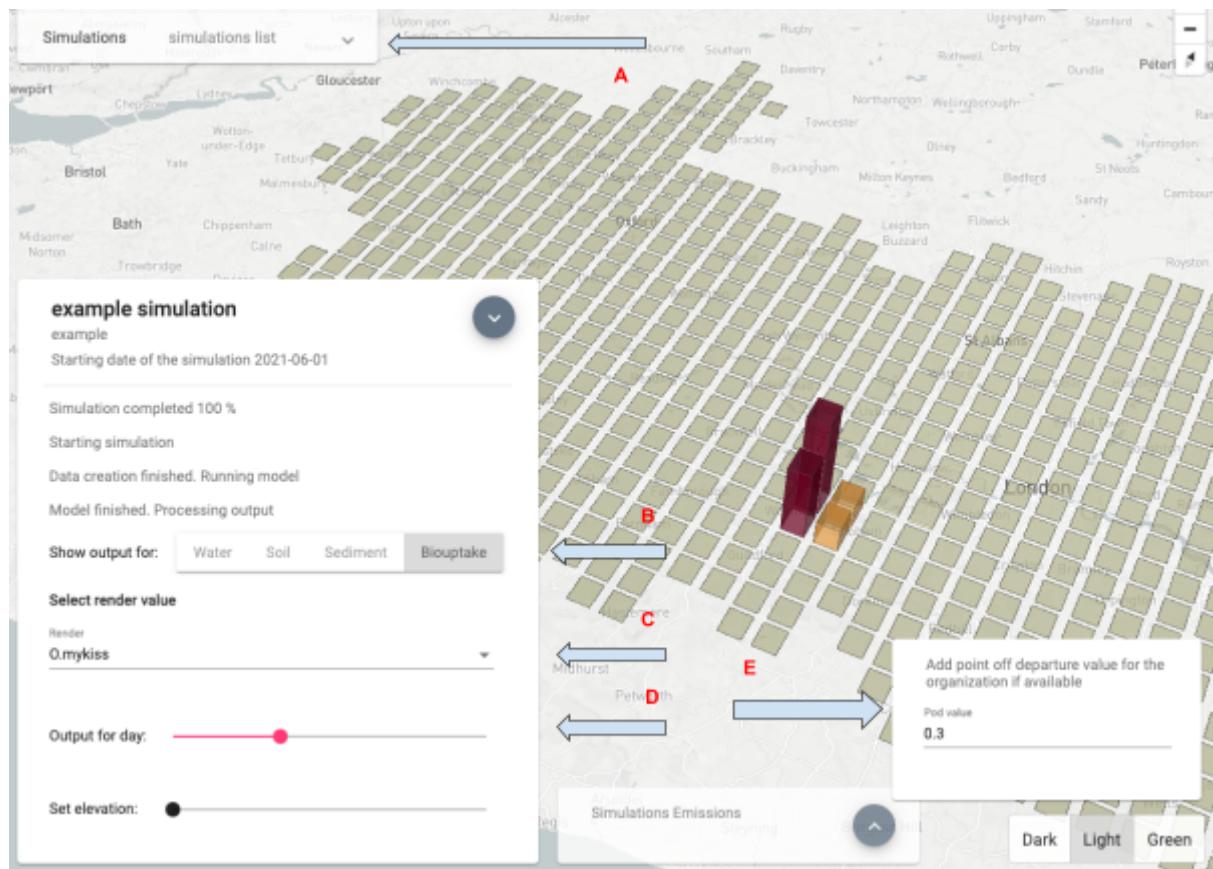


Figure #Rendering the outputs of a simulation.