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# NanoBio: a Biokinetic model for ENM distribution in freshwater ecosystems

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*A brief tutorial*

NanoSolveIT H2020 Nanoinformatics Project

[info@nanosolveit.com](mailto:info@nanosolveit.com)

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## Overview

This web application was developed in the context of the NanoSolveIT project for simulating the biodistribution of Engineered Nanomaterials (ENMs) in freshwater ecosystems. The biokinetic model used (nanoBio) has been developed by [Garner et al. \(2018\)](#) for describing the biodistribution of either TiO<sub>2</sub>, ZnO or CuO ENMs in freshwater ecosystems. The system includes seven species: two phytoplankton species (*S. capricornutum* and *F. crotonensis*), a zooplankton (*D. magna*), a benthic invertebrate (*H. azteca*), a bivalve (*V. constricta*), a planktivorous fish (*P. promelas*) and an upper trophic level fish (*O. mykiss*). The ecosystem also includes water, particulate matter and sediment and the ENMs can produce the corresponding dissolved metal ion via dissolution. Each species is exposed to either the ENM or the dissolved ion via the water, suspended particulates or dietary ingestion. Each organism is modeled as a two-compartmental model, one for describing the uptake, elimination and accumulation of ENMs and one for describing the uptake, elimination and accumulation of dissolved metal ion. Dissolution inside the organism is also considered by linking of the two subcompartments. For a more details please read the corresponding publication, available at <https://doi.org/10.1021/acssuschemeng.8b01691>

The tool can be easily accessed through the link:

<https://nanobio.cloud.nanosolveit.eu/>

## Instructions


The User Interface (UI) of the web service is presented in Figure 1. The application consists of two modules, the exposure scenario and the simulation information module. The user is requested to provide some input to both modules in order to simulate a complete biodistribution scenario stemming out of an environmental exposure event.

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Logout

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NanoSolveIT  
Cloud Platform

This work received funding from the European Union's Horizon 2020 research and innovation program via [NanoSolveIT project](#) under grant agreement number 614572.

### Upload an Exposure Scenario

Please upload a csv file containing the exposure scenario



### Set the Simulation Parameters

Please provide the necessary simulation information

Simulation start (days)  
0

Time increment (days)  
1

Simulation end (days)  
.....

ENM Selection  
.....

**Figure 1:** The UI of the NanoBio web service.

### Step 1: Defining an environmental exposure scenario

The environmental exposure module offers the user the ability to upload an exposure scenario in the form of a csv file. The user can first download a template containing the necessary columns to be filled (Figure 2). Specifically, the user is asked to provide 5 time series, including time, ENM water concentration, dissolved ion concentration, suspended sediment concentration and finally sediment concentration. Figure 3 presents a demonstration case in which the user is interested only in providing the water concentration of an ENM. After constructing the desired csv containing the exposure scenario, it can be uploaded on the web service by pressing the upward red arrow and selecting the desired csv file from the local user machine (Figure 4).

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For a more details  
<https://doi.org/10.1021/acssuschem>

### Upload an Exposure Scenario

Please upload a csv file containing the exposure scenario



### Set the Simulation Parameters

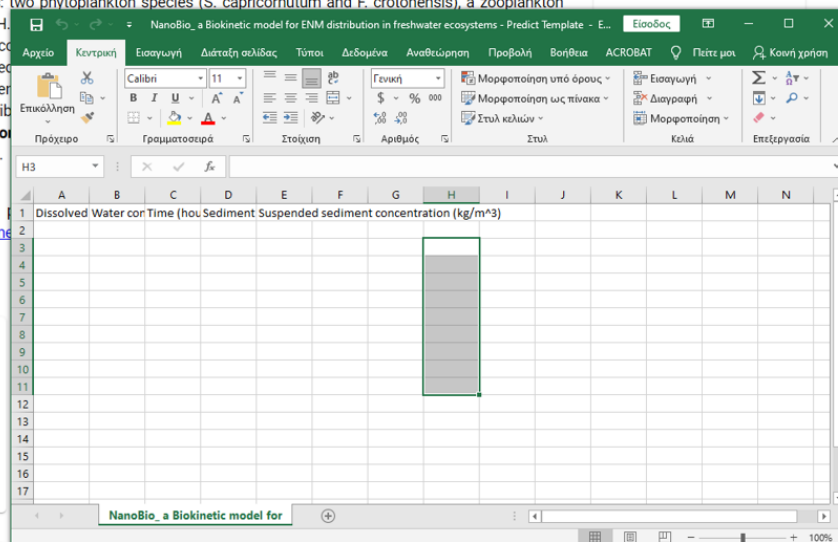
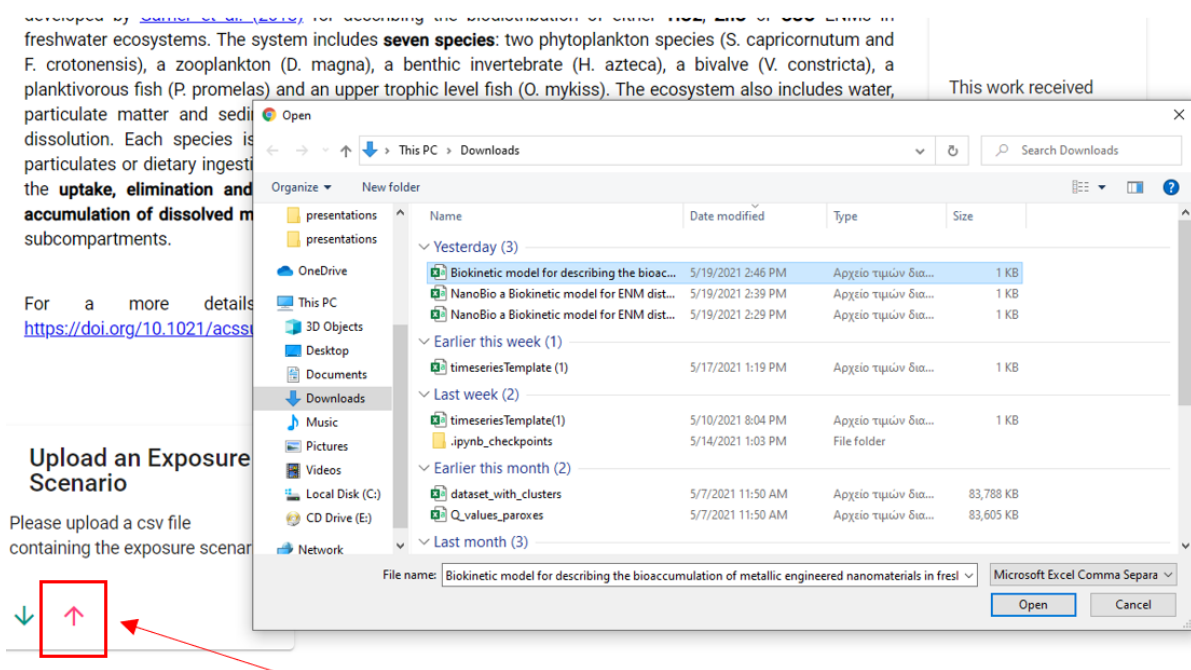


Figure 2: Downloading the csv template.

|    | A            | B  | C  | D   | E   |
|----|--------------|--|--|---|---|
| 1  | Time (hours) | Water concentration (kg/m <sup>3</sup> ) | Dissolved ion concentration (kg/m <sup>3</sup> ) | Sediment concentration (kg/m <sup>3</sup> ) | Suspended sediment concentration (kg/m <sup>3</sup> ) |
| 2  | 0            | 10                                       | 0  | 0   | 0   |
| 3  | 5            | 10                                       | 0  | 0   | 0   |
| 4  | 10           | 10                                       | 0  | 0   | 0   |
| 5  | 15           | 15                                       | 0  | 0   | 0   |
| 6  | 20           | 15                                       | 0  | 0   | 0   |
| 7  | 25           | 14                                       | 0  | 0   | 0   |
| 8  | 30           | 20                                       | 0  | 0   | 0   |
| 9  | 35           | 25                                       | 0  | 0   | 0   |
| 10 | 40           | 27                                       | 0  | 0   | 0   |
| 11 | 45           | 12                                       | 0  | 0   | 0   |
| 12 | 50           | 5  | 0  | 0   | 0   |
| 13 | 55           | 10                                       | 0  | 0   | 0   |
| 14 | 60           | 15                                       | 0  | 0   | 0   |
| 15 |              |  |  |   |   |
| 16 |              |  |  |   |   |
| 17 |              |  |  |   |   |
| 18 |              |  |  |   |   |

Figure 3: Example on how to complete the csv file.



**Figure 4:** Uploading a csv file.

Following successful upload of the exposure csv, a visualisation module allowing plotting of the exposure concentration-time profiles appears to the right side of the application (Figure 5). The user can set the x- and y-axis by selecting the desired variables to be visualised from a dropdown menu. In addition, all time series, i.e. the ENM water concentration, dissolved ion concentration, suspended sediment concentration and sediment concentration, can be visualised simultaneously by selecting the “All TimeSeries” box. After setting the desired variables, an interactive plot appears to the right, in which the user can hover over each point to obtain the exact value and zoom in or out of the plot (Figure 6).

### Upload an Exposure Scenario

Please upload a csv file containing the exposure scenario

↓ ↑

### Visualise the exposure scenario

Set the X and Y axis of the plot

X Axis

Y Axis

☐ All TimeSeries

### Set the Simulation Parameters

Please provide the necessary simulation information

Simulation start (days)

0

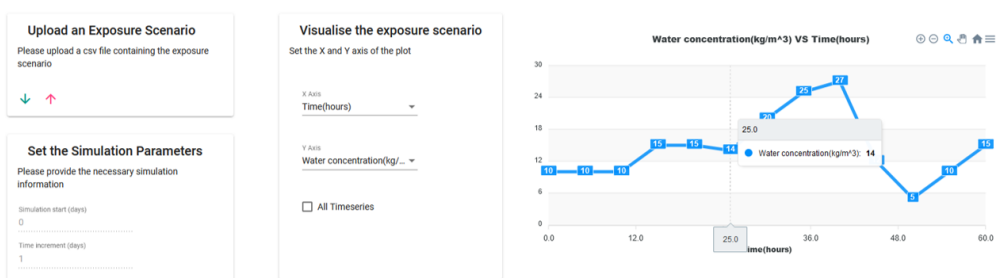
**Figure 5:** Exposure visualisation module.

This web application was developed in the context of the NanoSolveIT project for **simulating the biodistribution of Engineered Nanomaterials (ENMs) in freshwater ecosystems**. The biokinetic model used (nanoBio) has been developed by [Gamer et al. \(2018\)](#) for describing the biodistribution of either **TiO<sub>2</sub>**, **ZnO** or **CuO** ENMs in freshwater ecosystems. The system includes **seven species**: two phytoplankton species (*S. capricornutum* and *F. crotonensis*), a zooplankton (*D. magna*), a benthic invertebrate (*H. azteca*), a bivalve (*V. constricta*), a planktivorous fish (*P. promelas*) and an upper trophic level fish (*O. mykiss*). The ecosystem also includes water, particulate matter and sediment and the ENMs can produce the corresponding dissolved metal ion via dissolution. Each species is **exposed** to either the **ENM** or the **dissolved ion** via the water, suspended particulates or dietary ingestion. Each organism is **modeled as a two-compartment model**, one for describing the **uptake, elimination and accumulation of ENMs** and one for describing the **uptake, elimination and accumulation of dissolved metal ion**. Dissolution inside the organism is also considered by linking of the two subcompartments.

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**Figure 6:** Interactive visualisation of the exposure time series.

## Step 2: Providing the simulation details

The additional information needed for the simulation to run is the ENM of interest, among TiO<sub>2</sub>, ZnO and CuO, and the last time point of the simulation time vector. By default, the starting point is set to zero and the time increment is set to 1 day. Figure 7 illustrates the provided information for a scenario concerning TiO<sub>2</sub> and witnesses the progression of the biodistribution among the relevant aquatic species over a time period of 60 days. At last, the user can hit the “Run the Simulation” button to obtain the simulation results.

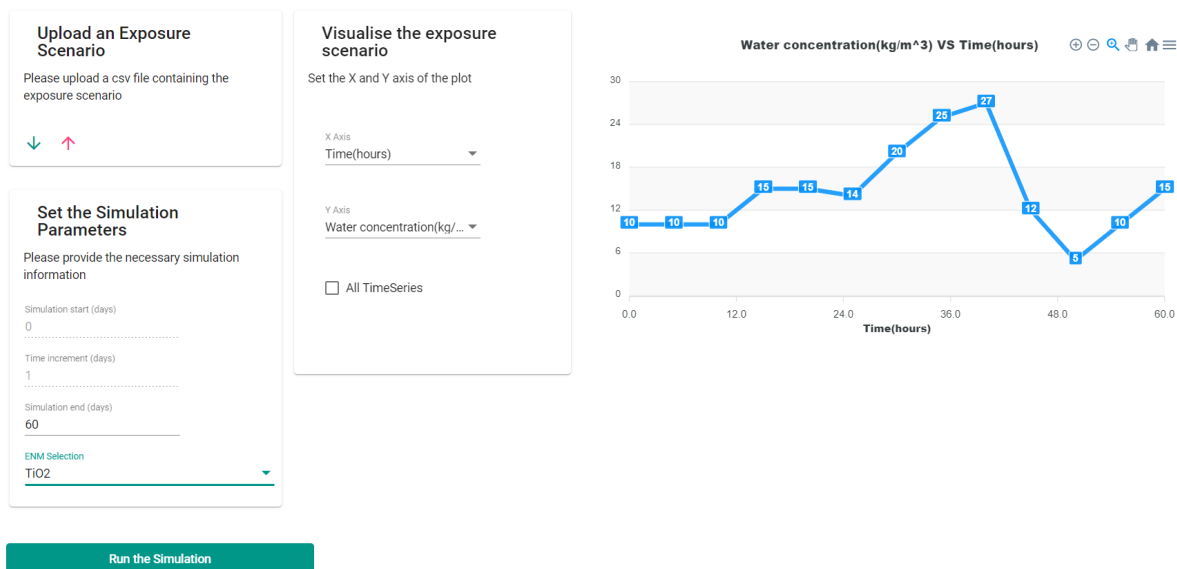


Figure 7: Setting the simulation information.

After the simulation results become available, as in the case of the exposure scenario, the user can select which species' biodistribution to plot in the corresponding visualisation box. The user can again hover over the time series to obtain exact values, zoom in and out and download the csv containing the simulation results (Figure 9). Finally, in order to change any simulation parameters or upload a new exposure scenario, the page must be be refreshed.

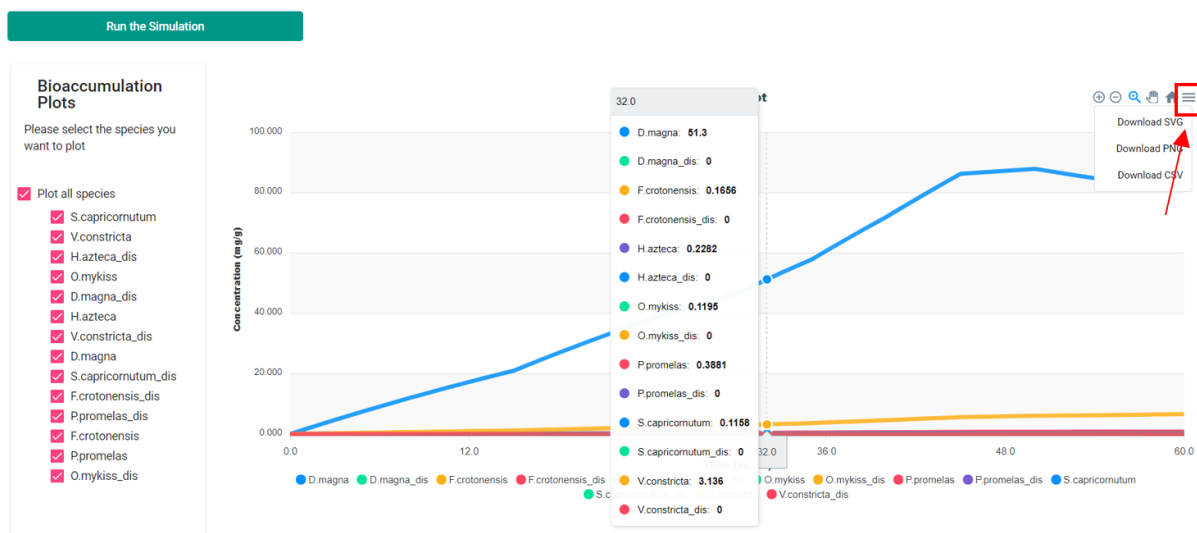


Figure 8: Bioaccumulation plots module and download capabilities.

Support

