

NANOPARTICLE EXPOSURE MODELS: ENVIRONMENTAL MODEL

A. Gallo, M. Domat, M. Gutiérrez, F. Aceti

User manual

November 2018



EXPOSURE MODELS

OCCUPATIONAL EXPOSURE MODELS

Predicting the concentration of nanoparticles in a work environment while a task is carried out

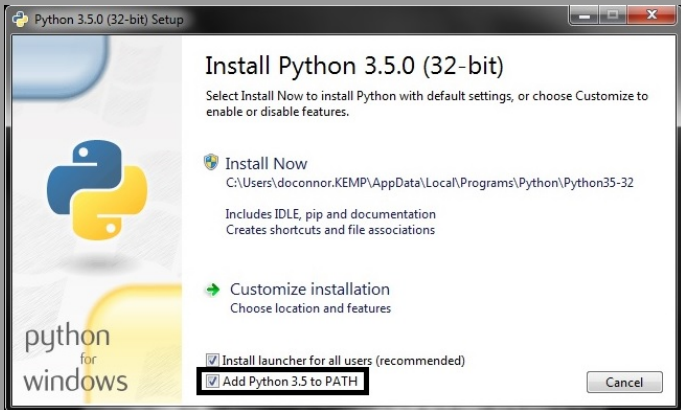
ENVIRONMENTAL EXPOSURE MODELS

Prediction of the amount of nanoparticles that are released into the environment: water, air, soil

[HTTPS://WWW.PYTHON.ORG/DOWNLOADS/](https://www.python.org/downloads/)

Please download last Python version and install it

Make sure to select “Add Python X.X to path”





[HTTP://SUDEENANODESK.EUROPEANPROJECTS.
NET/PLATFORM/EXPOSURE_MODELS](http://sudenanodesk.europeanprojects.net/platform/exposure_models)

INSTALL THE MODEL

- 1 Once downloaded, uncompress the file .zip: a folder will be created named:

environmental_model

- 2 Double click in the file `setup.bat`:
All dependencies will install and the Graphical User Interface (GUI) will open

It can take 2/3 minutes to finish!
Only the first time the model is run

GRAPHICAL USER INTERFACE (GUI)

Environmental model



Process definition

Diameter

Temperature

 ⓘ

Precipitation rate

Mass

Melting point

Project name

Timescale



- Hour +

Time units

 ⓘ

Vapour pressure

 ⓘ

Density

PROCESS DEFINITION

Environmental model

Process definition

Diameter [nm]

Temperature [K]

NM precipitation speed [m/s]

Mass [kg]

Melting point [K]

Project name

the process lasts for hours, days... (default month)

Time units [month]

Vapour pressure [Pa]

Density [kg/m³]

NM vapour pressure [Pa]

temperature in K

NM mass in g

name of the project (po

hours, days... that the process lasts

NM density [kg m⁻³]

RUN

EXECUTE THE MODEL

RUN

Click RUN to execute the model

- It will operate with the input data
- A .pdf file with input and output data will be generated
- Everything will be saved in the same folder where the code has been run

REPORT IN .PDF



Environmental model results

project

Input

Diameter: 20.0 nm

Density: 4.23 kg cm⁻³

Time interval: 6 Weeks

Melting point: 274 K

Mass: 50 kg

Precipitation rate: 2.22e-08 m s

Temperature: 300 K

Vapour pressure: 232 Pa

Output

Mass of material used in the synthesis process

$$M_{raw} = 56.243 \text{ kg}$$

Predictive environmental concentrations

$$PEC_{air} = 6.940e-15 \text{ kg/m}^3$$

$$PEC_{water} = 9.986e-11 \text{ kg/m}^3 ; PEC_{water} = 1.057e-12 \text{ kg/m}^3$$

$$PEC_{soil} = 4.758e-10 \text{ kg/m}^3 ; PEC_{soil} = 6.798e-11 \text{ kg/m}^3$$

Mass in the different environments

$$M_{air}(0) = 10.343 \text{ kg/m}^3 ; M_{air}(6 \text{ Week}) = 0.016 \text{ kg/m}^3$$

$$M_{soil}(0) = 2.381 \text{ kg/m}^3 ; M_{soil}(6 \text{ Week}) = 12.024 \text{ kg/m}^3$$

$$M_{water}(0) = 7.011 \text{ kg/m}^3 ; M_{water}(6 \text{ Week}) = 7.668 \text{ kg/m}^3$$

$$M_{sed}(0) = 0.000 \text{ kg/m}^3 ; M_{sed}(6 \text{ Week}) = 0.002 \text{ kg/m}^3$$

$$M_{tot}(0) = 19.735 \text{ kg/m}^3 ; M_{tot}(6 \text{ Week}) = 19.710 \text{ kg/m}^3$$

$$M_{loss} = 0.126 \%$$

REPORT IN .PDF

Deposition constant

$$K_{\text{soil}} = 1.694\text{e-}06$$

$$K_{\text{soil,hum}} = 2.153\text{e-}11 \text{ kg/m}^3 ; K_{\text{soil,dry}} = 1.694\text{e-}06 \text{ kg/m}^3$$

$$K_{\text{water}} = 8.874\text{e-}08$$

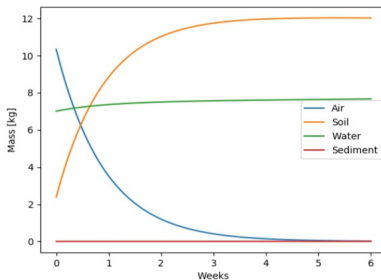
$$K_{\text{water,hum}} = 6.660\text{e-}13 \text{ kg/m}^3 ; K_{\text{water,dry}} = 8.874\text{e-}08 \text{ kg/m}^3$$

Emission during the life cycle

$$E_{\text{m,air}} = 10.343 \text{ kg}$$

$$K_{\text{m,soil}} = 2.381 \text{ kg}$$

$$K_{\text{m,water}} = 7.011 \text{ kg}$$



Evolution of the NM (mass) during the selected time