Sensitivity analysis of a model characterizing nanoparticle agglomeration, dispersion and deposition processes in the atmosphere

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Introduction

An increasing amount of nanoscale materials such as engineered nanoparticles (ENPs) are produced for various industrial applications and everyday products. Recent studies have shown that some ENPs may cause adverse effects on human health (Card *et al*, 2008) and the environment (Hegde *et al*, 2016). Present risk assessment models generally assume chemically inert compounds, therefore they neglect many nanoparticle specific processes, such as coagulation, wet and dry deposition and gas-to-particle conversions that affect ENPs after their release into the atmosphere, see Fig. 1. In addition, current models lack proper testing and calibration, thus can yield in uncertain risk estimates (Hristozov *et al*, 2016).

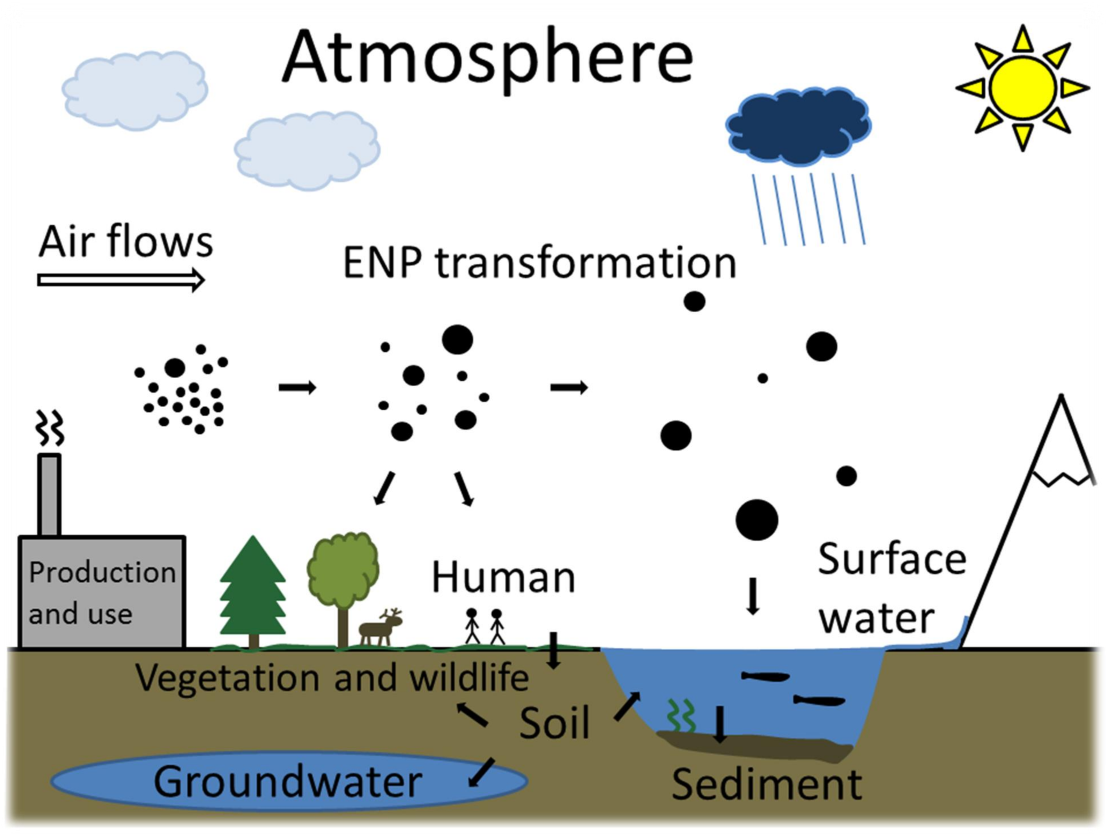

Figure 1. A schematic of ENP dispersion and transformation in the atmosphere with possible transport and exposure routes.

Modeling tool

In this study, the nanoparticle Agglomeration, Dispersion and Deposition model (ADD, Anttila and Dal Maso, 2015) is further developed to be used in risk assessment of an atmospheric release of ENPs. It is based on the Gaussian dispersion equation (Stockie, 2011)

$$N_{tot}(x,y,z,t) = \frac{N_0}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z}\exp\left(\frac{-(x-Ut)^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2}\right)\left(2\cdot\exp\left(\frac{-z^2}{2\sigma_z^2}\right)\right),$$

which introduces a non-recurring point source N_0 at *(x,y,z,0)*. The model has been refined to compute the predicted environmental concentration (PEC) in soil and the nanoparticle dose in the human respiratory system due to an emission of airborne ENPs, see Fig. 2.

Sensitivity analysis

A sensitivity analysis, using the one-at-a-time (OAT) method (Saltelli et al, 2008), is performed on the ADD model. The main goal of the analysis is to map changes in model output, i.e., PEC and the lung-deposited number of particles (LDN), as a function of input parameters. The analysis reveals, e.g., how accurate the model input data should be in order to achieve reliable results.

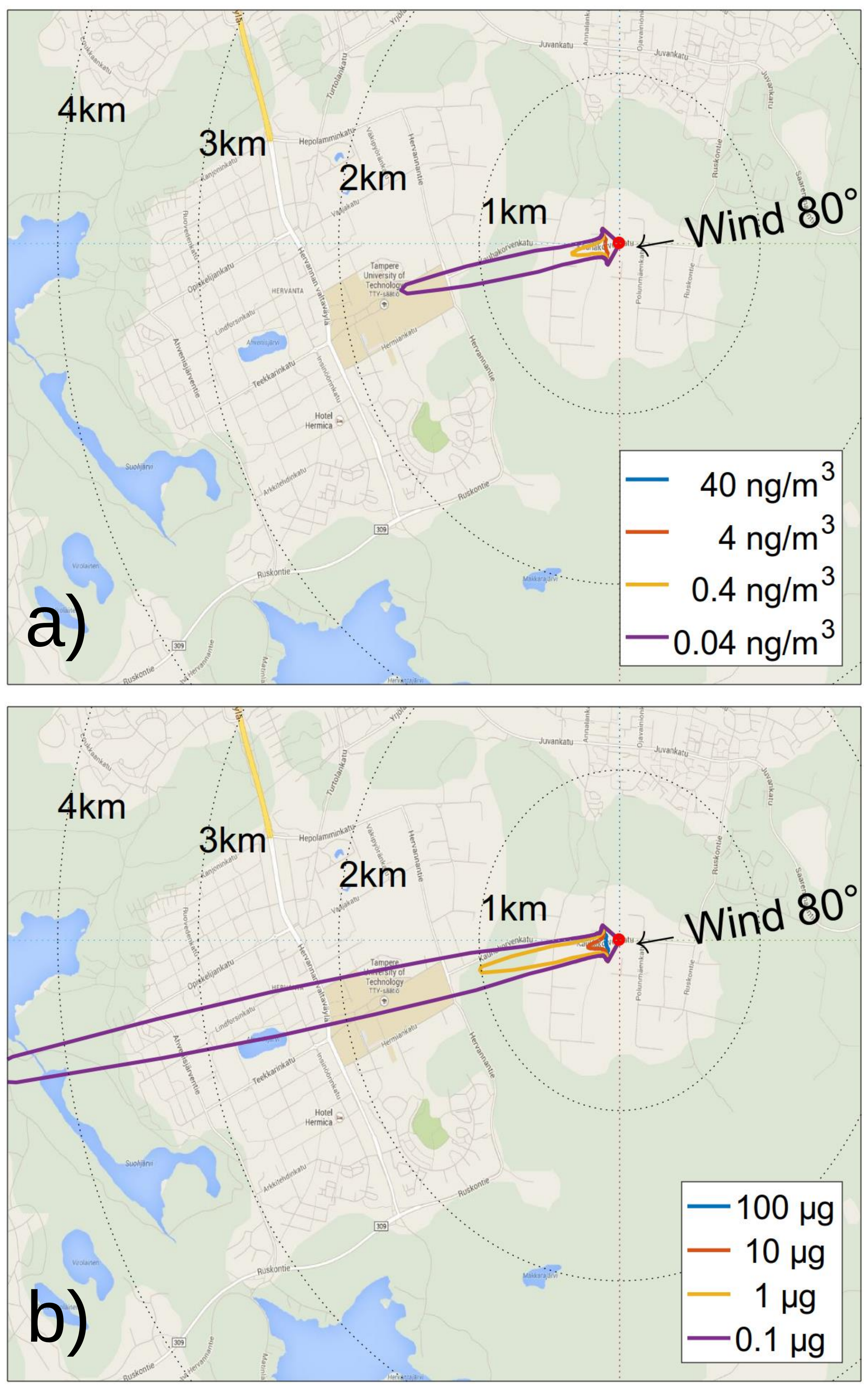

Figure 2. (a) PECs in soil and (b) lung deposited mass on a map of Hervanta, Finland. Background map from: maps.google.fi.

Results

The results show that PEC in soil (Fig. 3) is most sensitive for variations in the total particle material mass released to the air *M*, size of the released particle plume d_{lim}, particle size d_0, wind speed *U* and Pasquill stability class *Sta* (Gifford, 1961). In contrary, varying the atmospheric boundary layer height B_{lh}, particle fractal dimension D_f, particle density ρ, shape factor χ, dispersion parametrization *Di* or air temperature *T* does not cause significant changes in the PECs.

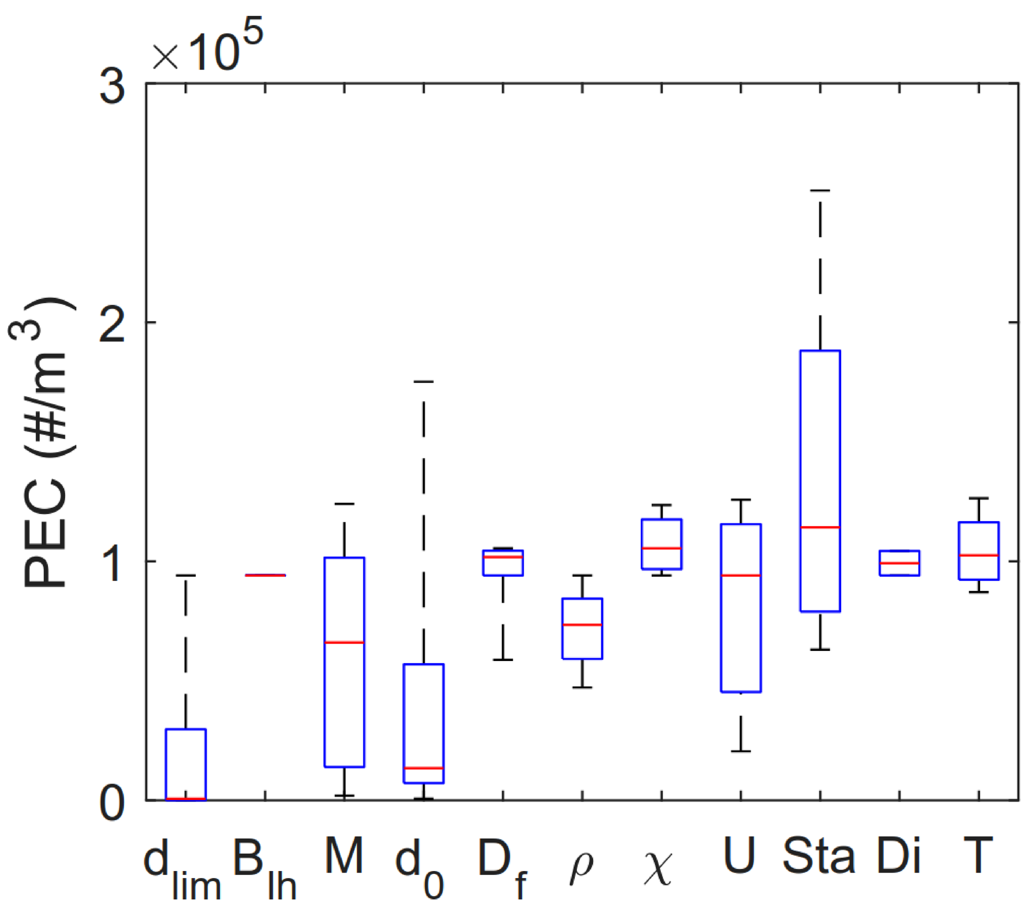

Figure 3. PEC in soil, 200 meters from the particle source, for different input parameter values. Red lines represent median values, the edges of blue boxes are 25 and 75 percentiles and the tails point out min and max values.

Similar outcome is also observed for LDN with an exception that varying the particle density ρ causes notable change in the lung deposition, see Fig. 4b.

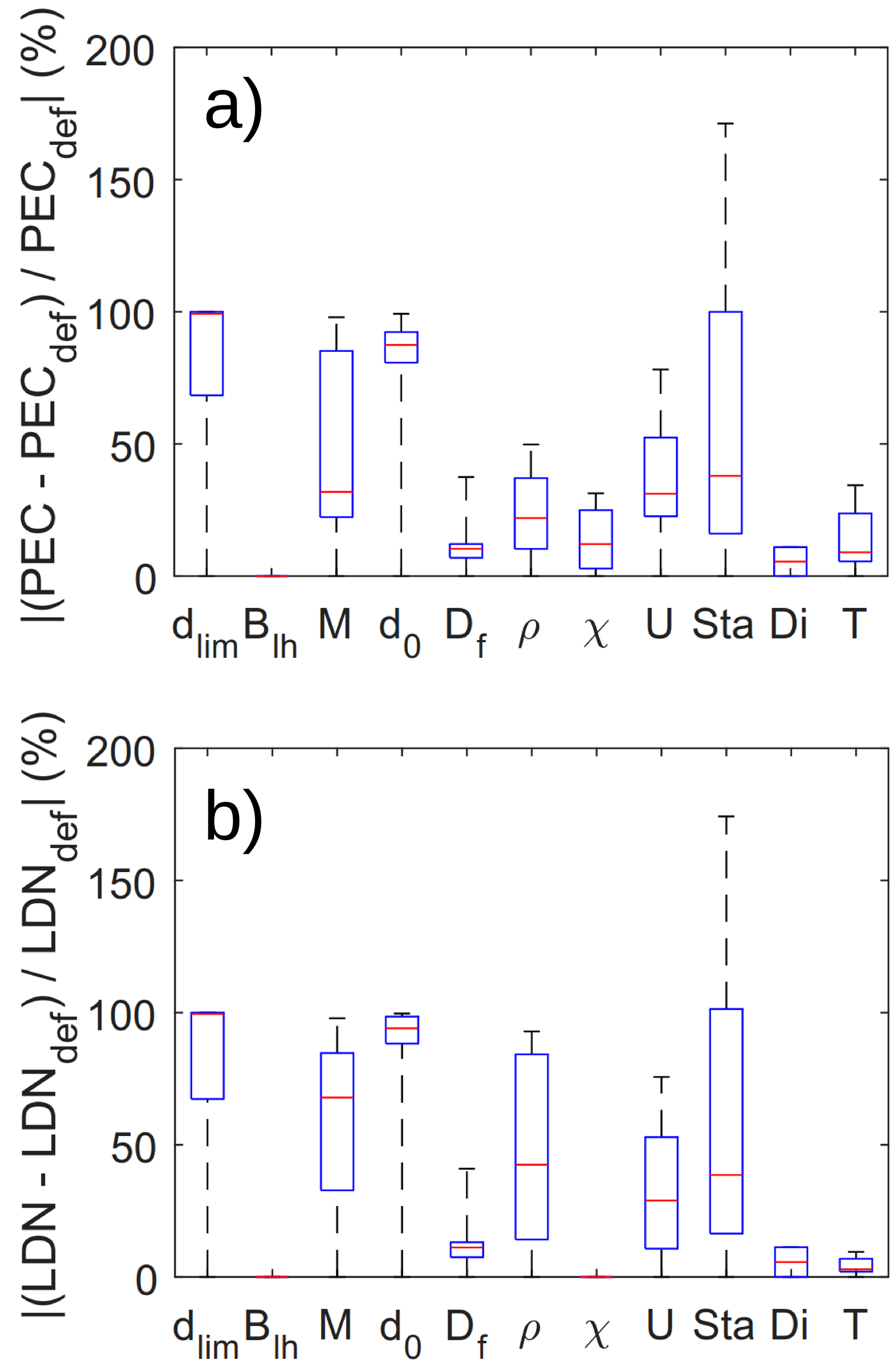

Figure 4. Model output sensitivity of (a) the PEC in soil and (b) lung deposited number of particles (LDN) for different input parameters. The sensitivity is defined as a percentage difference between model output (PEC, LDN) and that with default input values (PEC_{def}, LDN_{def}). The color representation is same as in Fig. 3.

Conclusions

Sensitivity analysis provides information that can be used as a guide to generating new exposure and hazard data. As a result, it increases accuracy and reliability of risk assessment models. The methodology presented here can be applied to all currently available nano-specific environmental and human risk assessment models.

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