

Simple proxy model of Lung-Deposited Surface Area (LDSA)

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Lung deposited surface area (LDSA) has been considered to be a better metric to explain nanoparticle toxicity instead of the commonly used particulate mass concentration. LDSA concentrations can be obtained by direct measurements and by estimation from the empirical lung deposition model and measurements of particle size distribution. However, these measurements are neither compulsory nor regulated by the government; as a result, the data of LDSA has been scarce spatially and temporally. In light of this, we develop a novel proxy model, input-adaptive mixed-effects (IAME) model, to estimate LDSA by other already existing air pollutant variables and meteorological conditions.

During the measurement period of two full years 2017–2018, we retrieved LDSA measurements measured by Pegasor AQ Urban and other variables in a street canyon (SC, average LDSA = $19.68 \pm 11.29 \mu\text{g m}^{-3}$) site and an urban background (UB, average LDSA = $11.17 \pm 7.1 \mu\text{g m}^{-3}$) site in Helsinki, Finland. For the continuous estimation of LDSA, IAME is automatised to select the best combination of a maximum of 3 fixed effects, together with 3 temporal categories as random effects, as inputs. Altogether, 696 sub-models are generated and ranked by the coefficient of determination (R^2), mean absolute error (MAE) and centred root-mean-square differences (cRMSD) in order. At the SC site, LDSA concentrations can be mostly estimated by mass concentration of particle of diameters smaller than $2.5 \mu\text{m}$ ($\text{PM}_{2.5}$), total particle number concentration (PNC) and black carbon (BC), all of which are closely connected with the vehicular emissions, while they are found correlating with $\text{PM}_{2.5}$, BC and carbon monoxide (CO) the best at the UB site. The accuracy of the overall model is higher at the SC site ($R^2 = 0.80$, $\text{MAE} = 3.74 \mu\text{m}^2 \text{cm}^{-3}$) than at the UB site ($R^2 = 0.77$, $\text{MAE} = 2.30 \mu\text{m}^2 \text{cm}^{-3}$) because the source of LDSA is more homogeneous at a street canyon. The results also demonstrate that the additional adjustment by taking random effects into account manages to improve the sensitivity of the fixed effect model to the existing diurnal, weekly and seasonal pattern. Due to its adaptive input selection and inclusion of random effects, IAME could serve as virtual sensors of LDSA in support with the reference measurements (Fung, et al., 2021). This continuous and reliable estimation could even provide a foundation for the inclusion of LDSA as one of the indicators in air quality index.