Respiratory deposition estimates of airborne per- and poly-fluoroalkyl acids (PFAS) powered by Enalos Cloud Platform

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1. Introduction

Exposure to per- and poly-fluoroalkyl acids (PFAS), present in particulate matter such as soils and dust, or in the gaseous phase as vapor, has been observed to yield potential detrimental effects on both the environment and human health.[1] Several studies have addressed waste streams as critical sources of PFAS in the environment.[2, 3] Lin et al.[4] conducted a study wherein they sampled air and size segregated particulate matter from the largest landfill and three Waste Water Treatment Plants (WWTPs) in Hong Kong. These samples were then compared to those obtained from coastal and natural reserve sites to assess any differences.

The objective of the present study is to use the particulate size data of PFAS collected by Lin et al.[4] from various WMIs, as well as coastal and natural reserve sites, to assess the deposition rates of PFAS in different regions of the human respiratory tract when individuals inhale PFAS in these outdoor environments.

2. Methodology

To assess the deposition efficiency and flux of inhaled PFAS within the human respiratory tract, the simplified equations derived from the International Commission on Radiological Protection (ICRP) model are utilized.[5] This model provides calculations for the deposition flux and efficiency of inhaled particles across three distinct regions of the respiratory tract: the head airways (HA), the tracheobronchial region (TB), and the alveolar region (AR). The deposition efficiency of particles across these three distinct regions is calculated as follows:

$$DE_{HA} = IF \times \left[\frac{1}{1+\exp\left(6.84+1.183\ln D_P\right)} + \frac{1}{1+\exp\left(0.924-1.885\ln D_P\right)} \right] \quad (1)$$

$$DE_{TB} = \left(\frac{0.00352}{D_P} \right) \left[\exp\left(-0.234\left(\ln D_P + 3.40\right)^2\right) + 63.9\exp\left(-0.819\left(\ln D_P - 1.61\right)^2\right) \right] \quad (2)$$

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$$DE_{AL} = \left(\frac{0.0155}{D_P}\right)\left[\exp\left(-0.415\left(\ln D_P + 2.84\right)^2\right) + 19.11\exp\left(-0.482\left(\ln D_P - 1.362\right)^2\right)\right] \quad (3)$$

$$IF = 1 - 0.5\left[1 - \frac{1}{1 + 0.00076 \times D_P^{2.8}}\right] \quad (4)$$

Where D_P (μm) is the diameter of the particle and *IF* is the inhalable fraction of all particles. The D_P in the above equations is the mass median aerodynamic diameter (MMAD) of each PFAS compound. The deposition flux (*DF*, pg h^{-1}) of particle-bound PFAS in the respiratory tract is estimated by:

$$DF_i = \sum\left(DE_i \times C_i\right) \times V \quad (5)$$

Where DF_i is the particle deposition efficiency in each region for DP_i (the average diameter of each particle size fraction), C_i is the concentration of PFAS in each size fraction, and *V* is the human breathing rate under normal conditions (0.45 m^3 h^{-1}).[6]

The equations discussed above, which are used to predict lung deposition in the HA, TB, and AL regions/compartments using the ICRP model, have been incorporated into the Enalos Cloud Platform.[7, 8] This integration has been achieved through the development of a web application: https://enaloscloud.novamechanics.com/proplanet/lungdeposition/, which was created as part of the PROPLANET project (Funded by the European Union under the GA no 101091842).

3. Results and Discussion

The deposition flux of inhaled PFAS (pg h^{-1}) and its relative abundance (%) is calculated using the ICRP model, as implemented in the Enalos Cloud Platform[7, 8] (https://enaloscloud.novamechanics.com/proplanet/lungdeposition/). This can be seen in the figure provided below. The deposition flux at the landfill is found to be higher, as expected, owing to the elevated concentration levels of total PFAS. This is followed by the two wastewater treatment plant (WWTP) locations and the natural sites, encompassing the coast and rivers regions. In general, the deposition flux of inhaled PFAS associated with coarse particles was found to be higher in the HA (76% - 92%) and TB regions (46% - 67%), while fine particles were the primary contributors in the AL region (34% - 64%). The relative abundance of inhaled particulate PFAS in the ultrafine fraction increased in the alveolar region, aligning with prior investigations on halogenated and organophosphate flame retardants.[9, 10]

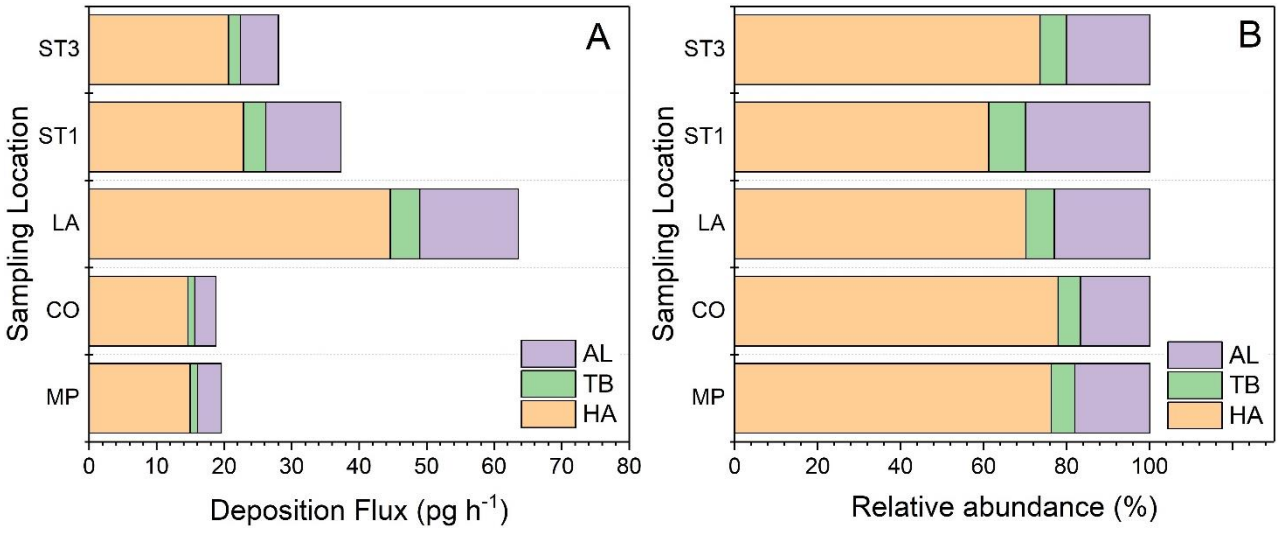

Figure 1: (A) Deposition flux of inhaled PFAS (pg h^{-1}). (B) Relative abundance (%) of inhaled PFAS at different sampling locations.

4. Conclusions

To summarize, in this study the ICRP model is utilized through the Enalos Cloud Platform[7, 8] to assess the deposition of inhaled PFAS particles in the human respiratory tracts. The findings revealed that larger particles are predominantly deposited in the HA region, whereas ultrafine PFAS particles are significantly present in the AL region. It is noteworthy that coarse particles (>0.5 μm) are more prevalent in natural environments such as rivers and coasts, while finer particles (<0.5 μm) are more abundant in landfill and wastewater treatment plant (WWTP) sites (LA, ST1, ST3). These deposition patterns raise concerns regarding inhalation exposure risks and potential implications for human health. The higher concentrations of PFAS in landfill and WWTP areas contributed to an increased deposition flux of PFAS in the human lungs.

In future endeavors, there are plans to carry out epidemiological investigations aimed at establishing a direct link between PFAS exposure through inhalation and specific health effects. These studies will contribute to a better understanding of the risks associated with particles of different sizes that are contaminated with PFAS. Additionally, it is intended to utilize alternative models, such as the National Committee on Radiation Protection (NCRP) model[11] and the Multiple-Path Particle Dosimetry (MPPD) model.[12]

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