Gas-particle partitioning of semivolatile polycyclic aromatic hydrocarbons in polluted and unpolluted air in central Europe and the Aegean: observation vs. model prediction

POURYA SHAHPOURY[1], GERHARD LAMMEL[1,2], AYSUN SOFUOĞLU[3], YETKIN DUMANOĞLU[4], LINDA LANDLOVÁ[2], MARIE D. MULDER[2], PETRA PŘIBYLOVÁ[2], ROMAN PROKEŠ[2], ADELA HOLUBOVÁ ŠMEJKALOVÁ[5,6], C. SAIT SOFUOĞLU[3], MILAN VÁŇA[5,6]

Email: p.shahpoury@mpic.de

[1]Max Planck Institute for Chemistry, Multiphase Chemistry Department, 55128 Mainz, Germany

[2]Masaryk University, Research Centre for Toxic Compounds in the Environment, 62500 Brno, Czech Republic

[3]Izmir Institute of Technology, Chemical Engineering Department, 35430 Urla, Turkey

[4]Dokuz Eylul University, Environmental Engineering Department, 35160 Buca, Turkey

[5]Czech Hydrometeorological Institute, 39422 Košetice, Czech Republic

[6]Global Change Research Centre, Academy of Sciences of the Czech Republic, 60300 Brno, Czech Republic

Gas-particle partitioning is an important mechanism, which affects the transport and fate of semivolatile organic compounds (SOCs). This preferential partitioning depends on parameters such as the compound's molecular structure as well as particulate matter (PM) physical and chemical properties, and can be explained by various empirical and theoretical models. These include Junge-Pankow (JP), Harner-Bidleman (HB), Dachs-Eisenreich (DE)/Lohmann-Lammel (LL), and poly-parameter linear free energy relationship (ppLFER) models. To explain the SOC partitioning, each model considers compound physico-chemical properties or PM characteristics. Despite the past efforts in determining the most appropriate model, discrepancies remain, as each model neglects certain intermolecular interactions. The aim of the present research was to determine what model better predicts the gas-particle partitioning of polycyclic aromatic hydrocarbons (PAHs). To this end, air samples (gas and particulate phase) were collected from four sites in central Europe, namely Brno, Košetice, Kyjov, and Gt. Hungarian Plain, as well as two coastal sites, Finokalia and Urla. ∑15 PAH mean concentrations and particulate mass fractions (Θ) were 52.3 (Θ = 0.23; n = 4), 17.85 (Θ = 0.25; n = 162), 46.6 (Θ = 0.31; n = 4), and 2.13 ng m^{-3} (Θ = 0.13; n = 22) for the central European sites, and 0.94 (Θ = 0.46; n = 11) and 3.7 ng m^{-3} (Θ = 0.27; n = 22) for the costal sites, respectively. Initial results showed that JP and ppLFER models are overall better in predicting PAH gas-particle partitioning.

Keywords: Semivolatile organic compounds, aerosol chemical composition, linear free energy relationship