

Gas-particle partitioning (POPs)

For the description of POP partitioning between the gaseous and particulate phase in the atmosphere the three model parameterizations can be applied: the Junge-Pankow model [Junge, 1977; Pankow, 1987], the K_{OA} absorption model [Pankow, 1994,1997; Harner and Bidleman, 1998], and dual model of absorption to organic matter and adsorption to black carbon in the aerosol particles [Dachs and Eisenreich, 2000; Lohmann and Lammer, 2004].

Junge-Pankow adsorption model [Junge, 1977, Pankow, 1987]

$$\varphi^{ad} = c \frac{S}{(p_L^0 + cS)}$$

where: φ^{ad} is the fraction of particulate phase of the compound;
 S is the aerosol surface density, m²surface/m³air;
 p_L^0 is the subcooled liquid vapor pressure of the compound, Pa;
 c is a parameter assumed to be equal to 0.172 Pa·m.

K_{OA} absorption model [Pankow, 1994; 1997; Harner and Bidleman, 1998]

$$\varphi^{ab} = K_p^{OM} \frac{TSP}{(1 + K_p^{OM} TSP)}$$

where TSP is the concentration of suspended particulate matter, µg/m³,

and K_p^{OM} is given by:

$$K_p^{OM} = 10^{-12} \cdot f_{OM} \cdot M_{oct} \cdot \gamma_{oct} \cdot K_{OA} / (M_{OM} \cdot \gamma_{OM} \cdot \rho_{oct}),$$

where f_{OM} is the fraction of organic matter in aerosol, and $\rho_{oct} = 0.82$ kg/L is the density of octanol.

It can be assumed that γ_{oct}/γ_{OM} equals 1 [Harner and Bidleman, 1998], and M_{oct}/M_{OM} equals 0.26 [Efstathiou et.al., 2016; Harner and Bidleman, 1998] assume this ratio to be equal to 1). With these assumptions the following formula can be used:

$$\log K_p^{OM} = \log K_{OA} + \log f_{OM} + 11.91).$$

Dual model of absorption to OM and absorption to BS [Dachs and Eisenreich, 2000; Lohmann and Lammel, 2004]

$$\varphi^{ab+bc} = K_p^{ab+bc} \frac{TSP}{(1 + K_p^{ab+bc} TSP)},$$

where TSP is the concentration of suspended particulate matter, $\mu\text{g}/\text{m}^3$, and K_p^{ab+bc} is given by:

$$K_p^{ab+bc} = 10^{-12} (K_{oa} \cdot f_{OM} \cdot M_{oct} \cdot \gamma_{oct} / (M_{OM} \cdot \gamma_{OM} \cdot \rho_{oct}) + f_{BC} \cdot a_{atm_BC} \cdot K_{SA} / (a_{soot} \cdot \rho_{BC})),$$

where f_{OM} is, as earlier, the fraction of organic matter, and f_{BC} is the fraction of black (elemental) carbon in aerosol. Assuming, in addition to the above assumptions, the ratio of surface densities a_{atm_BC}/a_{soot} to be 1, we rewrite the latter equation in the form:

$$K_p^{ab+bc} = 10^{-12} (0.32 f_{OM} \cdot K_{oa} + 0.55 f_{BC} \cdot K_{SA}),$$

The soot-air partition coefficient can be calculated by the relation [van Noort, 2003]:

$$\log K_{SA} = -0.85 \log p_L^0 + \log(998/a_{soot}) + 8.94),$$

where a_{soot} is assumed to be $18.21 \text{ m}^2/\text{g}$ [Efstathiou et al., 2016].

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