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 Lammel, 2004].

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

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

where: $\varphi^{ad}$ is the fraction of particulate phase of the compound; $S$ is the aerosol surface phase of the compound; $p^0_p$ 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, $\mu$g/m$^3$, 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 $\gamma_{oct}/\gamma_{OM}$ 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]

\[ \varphi_{ab+bc}^{ab+bc} = K_p^{ab+bc} \cdot \frac{TSP}{(1 + K_p^{ab+bc}TSP)} \]

where \( TSP \) is the concentration of suspended particulate matter, \( \mu g/m^3 \), 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:

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

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

\[ \log K_{SA} = -0.85 \log \rho^0_L + \log(998/a_{soot}) + 8.94, \]

where \( a_{soot} \) is assumed to be 18.21 m²/g [Efstathiou et al., 2016].

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