**Air–water exchange and gas-particle partitioning of polycyclic aromatic hydrocarbons (PAHs) in coral reef areas of the South China Sea Ziyue Feng1,2,3, Chenglong Wang1,2,3, Wanzhi Wang1,2,3, Chuchu Zhang1,2,3, Jiajia Wang3, Xinqing Zou1,2,3,4,\*, Guanghe Fu1,2,3,\***

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Text 2.4 Calculation details of *Kwater* and *Kair*

*Kwater* and *Kair* can be calculated as follows [*Mackay et al., 1983; Wu et al., 2019*]:

when U10 ≤ 4.2 m/s, where U10 is the wind speed at 10 m

(1)

when U10 > 4.2 m/s

, (2)

where *Kwater.CO2* is the mass transfer coefficient of CO2 in water, whose value depends on U10:

6.5×10-4 (U10 < 4.2 m/s)

(0.79U10-2.6)×10-3 (4.2 ≤ U10 ≤ 13 m/s)

(1.6U10-13.6)×10-3 (U10 > 13 m/s).

*Dwater.CO2* and *Dwater.pollut* are the molecular diffusivities of CO2 and pollutant in water, respectively, and can be calculated using [*Schwarzenbach et al., 2003*]:

, (3)

where *Mi* (g/mol) is the molar mass of different pollutants. *Kair* can be calculated using

, (4)

where *Kair.water* (cm/s) is the mass transfer coefficient of water, *Dair.pollut* (cm2/s) and *Dair.water* (cm2/s) are the diffusion coefficients of pollutant and water in the air, respectively, given by [*Fuller et al., 1966*]

(5)

(6)

, (7)

where *Mair*, *Mpollut*, and *Mwater* are the molar masses of air, pollutant, and water, respectively; and *Vair*, *Vpollut*, and *Vwater* are the molar volumes of air, pollutant, and water, respectively. Physicochemical properties of PAH congeners were shown in Table S8.

Reference

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