Bioavailability of polycyclic aromatic hydrocarbons in sediments : experiments and modelling

Haftka, J.J.H.

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Abbreviations and symbols

Abbreviations

ABACUS	evaluation of Availability to BiotA for organic Compounds Ubiquitous in Soils and sediments
Amber	Assisted Model Building and Energy Refinement (force field)
Ant	Anthracene
AOC	Amorphous Organic Carbon
BaA	Benzo[*a*]anthracene
BaP	Benzo[*a*]pyrene
BC	Black Carbon
BeP	Benzo[*e*]pyrene
Bz	Benzene
CAS	Chemical Abstract Service
DOC	Dissolved Organic Carbon
DOM	Dissolved Organic Matter
dw	Dry weight
EQS	Environmental Quality Standard
ERL	Environmental Risk Limit
FA	Fulvic Acid
Fla	Fluoranthene
Flu	Fluorene
GC	Gas Chromatography
GCVAP	Gas chromatographic method for determination of vapour pressures
GO	Geometrical Optimization
H/C	Hydrogen to Carbon atomic ratio
HA	Humic Acid
HC_5	Hazardous concentration at which 5% of the species are affected
HOC	Hydrophobic Organic Contaminant
HOY	Lake Höytiäinen, Finland
HPLC	High Performance Liquid Chromatography
IEFPCM	Integral-Equation-Formalism Polarizable Continuum Model (solvation model)
ISO	International Organisation for Standardisation
KET	Lake Ketelmeer, The Netherlands
KON	Lake Kontiolampi, Finland
KUO	Lake Kuorinka, Finland
MC	Monte Carlo

MD	Molecular Dynamics
MEK	Lake Mekrijärvi, Finland
MP2/6-31G(d)	Calculation of electron correlation with second-order Møller-Plesset perturbation theory and description of electron density with Gaussian functions (quantum mechanical computational method)
msPAF	Multisubstance Potentially Affected Fraction
n.d.	Not determined
N-PAH	Nitrogen containing Polycyclic Aromatic Hydrocarbon
NAPL	Non-Aqueous Phase Liquid
NIST	National Institute of Standards and Technology
NOEC	No Observed Effect Concentration
O/H	Oxygen to Hydrogen atomic ratio
OC	Organic Carbon
OECD	Organisation for Economic Cooperation and Development
p,*p*'-DDT	*p*,*p*'-DichloroDiphenylTrichloroethane
PAH	Polycyclic Aromatic Hydrocarbon
PCB	PolyChlorinated Biphenyl
PCDD	PolyChlorinated Dibenzo-p-Dioxin
PCDF	PolyChlorinated DibenzoFuran
PDMS	PolyDiMethylSiloxane
Phe	Phenanthrene
PM3	Parameterized Model number 3 (semi-empirical computational method)
Pyr	Pyrene
QM	Quantum Mechanical calculation
rpm	Rounds per minute
(R)ESP	(Restrained) Electrostatic Potential Fit
SD	Standard Deviation
SE	Standard Error
SER	Standard Error of Regression
S-PAH	Sulphur containing Polycyclic Aromatic Hydrocarbon
SPM	Suspended Particulate Matter
SPME	Solid Phase MicroExtraction
SRM-1650	Standard Reference Material of diesel soot
SSA	Specific Surface Area (m^2/g)
SSD	Species Sensitivity Distribution
SUVA	Specific UltraViolet Absorbance (L/g)
TIP3P	Water model with three interaction sites (atoms) used in force fields
TOC	Total Organic Carbon (mg C/L)
UBL	Unstirred Boundary Layer
UV	UltraViolet radiation

VAR	Lake Varparanta, Finland
VM552	Strain of polycyclic aromatic hydrocarbon-degrading bacterium
WFD	Water Framework Directive

Symbols

a	Edge of periodic periodic box (Å)
a_s, a_l	Empirical regression parameters
A_{270}	Absorbance at 270 nm
A	Aqueous phase
A	Empirical regression parameter
A	Van der Waals repulsive parameter (Å^{12} J/mol)
b_s, b_l	Empirical regression parameters
b	Sorption affinity (m^3/g)
B	Empirical regression parameter
B	Sorbent phase
B	Van der Waals attractive parameter (Å^6 J/mol)
c	Concentration (µg/L)
c	Cooling time used in force field method (ps)
c_{free}	Freely dissolved concentration (µg/L)
c_{PDMS}	Concentration in polydimethylsiloxane fiber (mg/L)
c_S	Aqueous solubility for solid compounds (mg/L)
c_{total}	Total concentration (µg/L)
c_w, c_{water}	Aqueous concentration (µg/L)
C	Empirical regression parameter
C	Sorbate phase
$C_{P,G}$	Constant pressure heat capacity of gas phase (J/mol.K)
$C_{P,L}$	Constant pressure heat capacity of liquid phase (J/mol.K)
$C_{P,S}$	Constant pressure heat capacity of solid phase (J/mol.K)
ΔC	Difference between gas and liquid heat capacities (J/mol.K)
$\Delta C_{P,vap}$	Constant pressure heat capacity difference between gas and liquid phase (J/K.mol)
d	Density (g/cm^3)
D	Dielectric constant (C^2/J.m)
ε, ε_{vdW}	Van der Waals well depth for two similar atoms (kJ/mol)
e	Energy contribution to thermodynamic potential
E	Empirical regression parameter
E, E_{pot}	Potential energy in force field equation (J/mol)
E_{ABC}	Intra- and intermolecular energy of a molecular system of water molecules (A), sorbent (B) and solute (C) (kJ/mol)

E_{gas}	Energy of gas phase (kJ/mol)
E_{inter}	Energy of intermolecular interactions (kJ/mol)
E_{intra}	Energy of intramolecular interactions (kJ/mol)
E_{liq}	Energy of liquid phase (kJ/mol)
E_{w}	Energy of aqueous phase (kJ/mol)
ΔE_{cav}	Energy of cavity formation (kJ/mol)
ΔE_{hyd}	Energy of hydration (kJ/mol)
ΔE_{sol}	Energy of solution (kJ/mol)
ΔE_{vap}	Energy of vaporization (kJ/mol)
F	Empirical regression parameter
F	Helmholtz free energy (kJ/mol)
ΔF	Free energy difference (kJ/mol)
γ^{∞}	Activity coefficient at infinite dilution
g	Gravitational constant (9.80665 m/s^2)
G^{E}_{w}	Excess Gibbs free energy of dissolution into water (kJ/mol)
ΔG	Gibbs free energy of phase transfer (kJ/mol)
ΔG_{sorp}	Gibbs free energy of sorption (kJ/mol)
h	Heating time used in force field method (ps)
H^{E}_{DOM}	Excess enthalpy of dissolution into dissolved organic matter (kJ/mol)
H^{E}_{PDMS}	Excess enthalpy of dissolution into polydimethylsiloxane fiber (kJ/mol)
H^{E}_{w}	Excess enthalpy of dissolution into water (kJ/mol)
ΔH	Enthalpy of phase transfer (kJ/mol)
ΔH, ΔH_{vap}	Enthalpy of vaporization (kJ/mol)
ΔH_{fus}	Enthalpy of fusion (kJ/mol)
ΔH_{hyd}	Enthalpy of hydration (kJ/mol)
ΔH_{sol}	Enthalpy of solid phase dissolution (kJ/mol)
ΔH_{sorp}	Enthalpy of sorption (kJ/mol)
ΔH_{sub}	Enthalpy of sublimation (kJ/mol)
i	Test compound
I	Kováts retention index
φ	Proper or improper dihedral angle (rad)
k_1	Absorption rate coefficient (1/h)
k_2	Desorption rate coefficient (1/h)
k_b	Boltzmann constant (1.3806504×10^{-23} J/K)
k_θ	Angle bending force constant ($kJ/mol.rad^2$)
k_r	Bond stretching force constant (kJ/mol.Å)
K_{BC}, $K_{BC,water}$	Black carbon to water sorption coefficient (L/kg)
K_{DOC}	Dissolved organic carbon to water partition coefficient (L/kg)
K_{H}	Henry's law constant ($Pa.m^3/mol$)
$K_{HA,water}$	Humic acid to water partition coefficient (L/kg)

$K_{HA,air}$	Humic acid to air partition coefficient (L/kg)
K_{ow}	Octanol to water partition coefficient (L/L)
K_{PDMS}	Polydimethylsiloxane to water partition coefficient (L/L)
K_{TOC}	Total organic carbon to water partition coefficient (L/kg)
K^x	Mole fraction based partition coefficient (mol/mol)
λ	Coupling parameter
μ^∞	Thermodynamic potential at infinite dilution (kJ/mol)
m	Atomic mass (g)
MW	Molecular weight (g/mol)
n, N	Number of measurements
n	Number of moles (mol)
n, N_C	Number of carbon atoms
N	Cartesian coordinates
N, N_{at}	Number of atoms
P, P_L	Liquid vapour pressure (Pa)
P_{GC}	Vapour pressure determined with gas chromatography (Pa)
P_S	Solid vapour pressure (Pa)
P_t	Mean carrier gas pressure (Pa)
θ	Bending angle (rad)
q	Partial atomic charge ($e = 1.6021773\times10^{-19}$ C)
Q_{max}	Maximum adsorption capacity (mol/g)
r	Bond length (Å)
r	Number of Monte Carlo simulation steps
r	Run time used in force field method (ps)
r^2	Squared correlation coefficient
R	Correlation coefficient
R	Ideal gas constant (8.31441 J/K.mol)
R	Non-bonded atomic distance (Å)
R^*	Minimum energy separation between two similar atoms (Å)
s	Electrostatic scaling factor
sg	Subgroup
S^E_w	Excess entropy of dissolution into water (J/mol.K)
ΔS	Entropy of phase transfer (J/mol.K)
ΔS_{fus}	Entropy of fusion (J/mol.K)
ΔS_{sol}	Entropy of solid phase dissolution (kJ/mol)
ΔS_{sorp}	Entropy of sorption (J/mol.K)
τ	Coupling constant to a simulated heat bath (ps)
t	Time (h)
t'_R	Retention time adjusted with hold-up time of unretarded component (min.)
T	Absolute temperature (K)

T_{mp}	Melting point temperature (K)
T_m	Mean temperature of measurement (K)
v	Atomic velocity (Å/ps)
v	Molar volume (cm^3/mol)
v/v	Volume to volume ratio (L/L)
V	Volume ($Å^3$)
V_n	*n*-Fold torsional potential barriers (J)
V_{PDMS}	Volume of polydimethylsiloxane fiber (µl)
V_{water}	Volume of water (L)
w/v	Weight to volume ratio (kg/L)
x	Mole fraction in stationary phase
x_{eq}	Equilibrium mole fraction (mol/mol)
y	Mole fraction in carrier gas
z	Number of carbon atoms in *n*-alkanes
Z	Number of water molecules

Note: The superscript '0' in free energy (G), enthalpy (H) and entropy (S) denotes standard temperature (T = 298.15 K) and pressure (P = 1 bar) conditions.

"I have a very, very strange feeling (in the stomach and elsewhere...)
when reading line 304."
Anonymous reviewer