
Appendix 1

1.1 LIST OF SYMBOLS AND ABBREVIATIONS

A_i	area of phase i, m ²
ALPM	automated log-P measurement
AS	absorption spectrophotometry
BCF	bioconcentration factor
bp	boiling point, °C
C	molar concentration, mol/L or mmol/m ³
C ^S	saturated aqueous concentration, mol/L or mmol/m ³
C _L	liquid or supercooled liquid concentration, mol/L or mmol/m ³
C _S	solid molar concentration, mol/L or mmol/m ³
C _A	concentration in air phase, mol/L or mmol/m ³
C _W	concentration in water phase, mol/L or mmol/m ³
¹⁴ C	radioactive labelled carbon-14 compound
CC	countercurrent chromatography
COD	chemical oxygen demand
CPC	centrifugal partition chromatography
D	D values, mol/Pa·h
D _A	D values for advection, mol/Pa·h
D _{Ai}	D values for advective loss in phase i, mol/Pa·h
D _R	D value for reaction, mol/Pa·h
D _{Ri}	D value for reaction loss in phase i, mol/Pa·h
D _{ij}	intermedia D values, mol/Pa·h
D _{VW}	intermedia D value for air-water diffusion (absorption), mol/Pa·h
D _{RW}	intermedia D value for air-water dissolution, mol/Pa·h
D _{QW}	D value for total particle transport (dry and wet), mol/Pa·h
D _{RS}	D value for rain dissolution (air-soil), mol/Pa·h
D _{QS}	D value for wet and dry deposition (air-soil), mol/Pa·h
D _{VS}	D value for total soil-air transport, mol/Pa·h
D _S	D value for air-soil boundary layer diffusion, mol/Pa·h
D _{SW}	D value for water transport in soil, mol/Pa·h
D _{SA}	D value for air transport in soil, mol/Pa·h
D _{Ti}	total transport D value in bulk phase i, mol/Pa·h
DOC	dissolved organic carbon
DOM	dissolved organic matter
DSC	differential scanning calorimetry
DTA	differential thermal analyzer
E	emission rate, mol/h or kg/h
EPICS	equilibrium partitioning in closed system
F	fugacity ratio
f	fugacity, Pa
f _i	fugacity in pure phase i, Pa
f-const.	fragmental constants

fluor.	fluorescence method
G	advective inflow, m ³ /h
G _B	advective inflow to bottom sediment m ³ /h
ΔG _v	Gibbs's free energy of vaporization kJ/mol or kcal/mol
GC	gas chromatography
GC/FID	GC analysis with flame ionization detector
GC/ECD	GC analysis with electron capture detector
GC-RT	GC retention time
gen. col.	generator-column
H, HLC	Henry's law constant, Pa·m ³ /mol, or atm m ³ /mol
ΔH _{fus}	enthalpy of fusion, kJ/mol
ΔH _{subl}	enthalpy of sublimation, kJ/mol
ΔH _v	enthalpy of vaporization, kJ/mol or kcal/mol
HPLC	high pressure liquid chromatography
HPLC/MS	HPLC analysis with mass spectrometer detector
HPLC/UV	HPLC analysis with UV detector
HPLC/fluor.	HPLC analysis with fluorescence detector
HPLC-k'	HPLC-capacity factor correlation
HPLC-RI	HPLC-retention index correlation
HPLC-RT	HPLC-retention time correlation
HPLC-RV	HPLC-retention volume correlation
IP	ionization potential
IR	infrared absorption
J	intermediate quantities for fugacity calculation
K	Kjeldahl method
k	reaction rate constant
k _i	first-order rate constant in phase i, h ⁻¹
k _A	air/water mass transfer coefficient, air-side, m/h
k _W	air/water mass transfer coefficient, water-side, m/h
K _{AR/W}	aerosol/water partition coefficient
K _{AW}	dimensionless air/water partition coefficient
k _H	Henry's law constant with units of vapor pressure
K _B	bioconcentration factor
K _h	association coefficient
K _{OC}	organic-carbon sorption partition coefficient
K _{OM}	organic-matter sorption partition coefficient
K _{OA}	octanol/air partition coefficient
K _{OW}	octanol/water partition coefficient
K _{SD/W}	sediment-water partition coefficient
K _{SSD/W}	suspended sediment/water partition coefficient
K _{SW}	soil/water partition coefficient
K _p or K _d	sorption coefficient
k ₁	uptake/accumulation rate constant, d ⁻¹ (day ⁻¹)
k ₂	elimination/clearance/depuration rate constant, d ⁻¹
k _b	biodegradation rate constant, d ⁻¹
k _h	hydrolysis rate constant, d ⁻¹
k _p	photolysis rate constant, d ⁻¹
k _{OH}	photooxidation rate constant for hydroxyl radical
k _{NO3}	photooxidation rate constant for NO ₃ radical
k _{O3}	photooxidation rate constant for ozone
L	lipid content of fish
LSC	liquid scintillation counting
LSS	liquid scintillation spectrometry
m _i	amount of chemical in phase i, mol or kg
M	total amount of chemical, mol or kg

MCI	molecular connectivity indices
MO	molecular orbital calculation
mp.	melting point, °C
MR	molar refraction
MS	mass spectrometry
MW	molecular weight, g/mol
n_C	number of carbon atoms
n_{Cl}	number of chlorine atoms
P	vapor pressure, Pa (Pascal)
P_L	liquid or supercooled liquid vapor pressure, Pa
P_S	solid vapor pressure, Pa
Q	scavenging ratio
QSAR	quantitative structure-activity relationship
QSPR	quantitative structure-property relationship
RC	Radiochemical method
RP-HPLC	reversed phase high pressure liquid chromatography
RP-TLC	reversed phase thin layer chromatography
S	water solubility, mg/L or g/m ³
ΔS_{fus}	entropy of fusion, J/mol·K or cal/mol·K (e.u.)
$S_{octanol}$	solubility in octanol
SD	standard deviation
SPARC	a computational expert system that predicts chemical reactivity
$t/^{\circ}C$	temperature in degree centigrade
t	residence time, h (hour)
t_o	overall residence time, h
t_A	advection persistence time, h
t_B	sediment burial residence time, h
t_R	reaction persistence time, h
$t_{1/2}$	half-life, s, h, min, d, month or yr
T_{ij}	intermedia transport rate, mol/h or kg/h
T	system temperature, K
T_B	boiling point, K
T_M	melting point, K
TLC	thin-layer chromatography
TMV	total molecular volume per molecule, Å ³ (Angstrom ³)
TN	titration method
TSA	total surface area per molecule, Å ²
U_1	air side, air-water MTC (same as k_A), m/h
U_2	water side, air-water MTC (same as k_W), m/h
U_3	rain rate (same as U_R), m/h
U_4	aerosol deposition rate, m/h
U_5	soil-air phase diffusion MTC, m/h
U_6	soil-water phase diffusion MTC, m/h
U_7	soil-air boundary layer MTC, m/h
U_8	sediment-water MTC, m/h
U_9	sediment deposition rate, m/h
U_{10}	sediment resuspension rate, m/h
U_{11}	soil-water run-off rate, m/h
U_{12}	soil-solids run-off rate, m/h
U_R	rain rate, m/h
U_Q	dry deposition velocity, m/h
U_B	sediment burial rate, m/h
UV	UV spectrometry
UNIFAC	UNIQUAC functional group activity coefficients
V_i	volume of pure phase i, m ³

V_S	volume of bottom sediment, m^3
V_{Bi}	volume of bulk phase i, m^3
V_I	intrinsic molar volume, cm^3/mol
V_M	molar volume, cm^3/mol
v_i	volume fraction of phase i
v_Q	volume fraction of aerosol
VOC	volatile organic chemicals
W	molecular mass, g/mol
Z_i	fugacity capacity of phase i, $mol/m^3 Pa$
Z_{Bi}	fugacity capacity of bulk phase i, $mol/m^3 Pa$

1.2 GREEK CHARACTERS

π -const.	substituent constants for K_{OW} estimation
γ	solute activity coefficient
γ_o	solute activity coefficient in octanol phase
γ_w	solute activity coefficient in water phase
ρ_i	density of pure phase i, kg/m^3
ρ_{Bi}	density of bulk phase i, kg/m^3
χ	molecular connectivity indices
ϕ_{OC} or f_{OC}	organic carbon fraction
ϕ_i	organic carbon fraction in phase i