Supplementary file

Contaminant transport model

$$D_x \frac{\partial^2 C_1(x,y,z,t)}{\partial x^2} + D_y \frac{\partial^2 C_1(x,y,z,t)}{\partial y^2} + D_z \frac{\partial^2 C_1(x,y,z,t)}{\partial z^2} - v \frac{\partial C_1(x,y,z,t)}{\partial x} - \mu_1 R_1 C_1(x,y,z,t)$$

$$= R_1 \frac{\partial C_1(x,y,z,t)}{\partial t}, 0 \le x \le \infty, 0 \le y \le W, 0 \le z \le H$$

$$D_x \frac{\partial^2 C_i(x,y,z,t)}{\partial x^2} + D_y \frac{\partial^2 C_i(x,y,z,t)}{\partial y^2} + D_z \frac{\partial^2 C_i(x,y,z,t)}{\partial z^2} - v \frac{\partial C_i(x,y,z,t)}{\partial x} - \mu_i R_i C_i(x,y,z,t)$$

$$+ g_{i-1\to i} \mu_{i-1} R_{i-1} C_{i-1}(x,y,z,t) = R_i \frac{\partial C_i(x,y,z,t)}{\partial t}, 0 \le x \le \infty, 0 \le y \le W, 0 \le z \le H$$

$i = 2,\ 3,\ 4,\ 5$

Parameters	Description	Unit
L, W, H	domain length, width and height	m
$C_i(x,y,z,t)$	concentration of the *i*th species in the aqueous phase	mg/L
x, y, z	spatial coordinates	m
t	time	year
D_x, D_y, D_z	dispersion coefficients in the *x*, *y* and *z* directions	m^2/year
v	constant pore-water velocity in the *x* direction	m/year
μ_i	first-order degradation reaction rate constant of the *i*th species	1/year
$g_{i-1\to i}$	yield coefficient which describes the mass produced from parent species *i*-1 to species *i*	-
R_i	retardation factor of the *i*th species	-

Source: Liao et al, Exact analytical solutions with great computational efficiency to three-dimensional multispecies advection-dispersion equations coupled with a sequential first-order reaction network, *Advances in Water Resources*, Volume 155, 2021. https://doi.org/10.1016/j.advwatres.2021.104018

Health risk assessment

Exposure calculation

Ingestion :

$$ADD = C_w \times \frac{IR \times EF \times ED}{BW \times AT}$$

Inhalation :

$$EC = C_a \times \frac{ET \times EF \times ED}{AT}$$

Dermal absorption :

$$ADD = DA \times SA \times \frac{EV \times EF \times ED}{BW \times AT}$$

$$DA = 2 \times FA \times K_p \times C_w \times \sqrt{6 \times \frac{\tau \times t}{\pi}} \times CF, \qquad t \leq 2.4\tau$$

$$DA = FA \times K_p \times C_w \times \left[\frac{t}{1+B} + 2 \times \tau \left(\frac{1 + 3 \times B + 3 \times B^2}{(1+B)^2}\right)\right] \times CF, \qquad t > 2.4\tau$$

Risk calculation

Carcinogenic risk :

$$CR = ADD \times CSF = EC \times IUR$$
$$TCR = \sum CR$$

Non-carcinogenic risk :

$$HQ = ADD/RfD = EC/RfC$$
$$HI = \sum HQ$$

Parameters	Full name	Unit
C_w	concentration in groundwater	mg/L
C_a	concentration in air	μg/m³ or mg/m³
DA	absorbed dose per event	mg/cm^2
ADD	average daily dose	mg/kg-day
EC	exposure concentration	μg/m³ or mg/m³
IR	ingestion rate	L/day
SA	skin surface area	cm^2
FA	absorbed fraction	-
K_p	dermal permeability coefficient	cm/hour
B	ratio of the permeability coefficient of a compound through the stratum corneum relative to its permeability coefficient across the viable epidermis	-
τ	lag time	hour
t	event duration	hour
EV	event frequency	1/day
ET	exposure time	hours/day
EF	exposure frequency	days/year
ED	exposure duration	years
AT	average time	days(hours)
CF	unit convert factor	L/cm³

CSF	cancer slope factor	$(mg/kg\text{-}day)^{-1}$
RfD	reference dose	(mg/kg-day)
IUR	inhalation unit risk	$(\mu g/m^3)^{-1}$
RfC	reference concentration	(mg/m^3)
CR	cancer risk	-
TCR	total cancer risk	-
HQ	hazard quotient	-
HI	hazard index	-

Source:

USEPA, Risk Assessment Guidance for Superfund Volume I Human Health Evaluation Manual (Part A), 1989

USEPA, Risk Assessment Guidance for Superfund Volume I: Human Heatlh Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment), 2004

USEPA, Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part F, Supplemental Guidance for Inhalation Risk Assessment), 2009