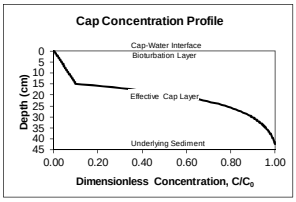
STEADY-STATE CAP DESIGN MODEL
from Lampert and Reible (2009)*
Version 1.19
6/8/2012

Instructions: This spreadsheet determines concentrations and fluxes in a sediment cap at steady-state, assuming advection, diffusion, dispersion, bioturbation, deposition/erosion, sorption onto colloidal organic matter, and boundary layer mass transfer. The deposition velocity is negative in the case of erosion, and is assumed to be constant and to have minimal effect on the thickness of the cap. The cells in GREEN are input cells; these can be changed for the design of interest. Cells in YELLOW are commonly used parameter estimates. These can be changed but note that physically unrealistic parameter values may result. A second worksheet calculates the transient profiles for a semi-infinite case. DO NOT CHANGE THE CELLS IN RED (or the spreadsheet will not function properly). These are calculated values for model outputs. The third worksheet title "array" allows the user to create an array of outputs for a given input (e.g., to study different compounds for a given site).



Contaminant Properties

Contaminant	PHE	
Octanol-water partition coefficient, log K_{ow}	4.57	
Water Diffusivity, D_w	6.0E-06	cm^2/s
Cap Decay Rate, λ_1	0.00	yr^{-1}
Bioturbation Layer Decay Rate, λ_2	0.00	yr^{-1}

Sediment Properties

Contaminant Pore Water Concentration, C_0	1	ug/L
Biological Active Zone fraction organic carbon, $(f_{oc})_{bio}$	0.05	
Colloidal Organic Carbon Concentration, ρ_{DOC}	0	mg/L
Darcy Velocity, V (positive is upwelling)	10	cm/yr
Depositional Velocity, V_{dep} *(positive is deposition of sediments)*	0	cm/yr
Bioturbation Layer Thickness, h_{bio}	15	cm
Pore Water Biodiffusion Coefficient, D_{bio}^{pw}	100	cm^2/yr
Particle Biodiffusion Coefficient, D_{bio}^{p}	1	cm^2/yr

Cap Properties

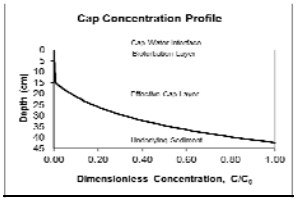
Conventional Cap placed depth	45	cm
Cap Materials -Granular (G) or Consolidated Silty/Clay (C)	G	
Cap consolidation depth	0	cm
Underlying sediment consolidation due to cap placement	15	cm
Porosity, ε	0.4	
Particle Density, ρ_P	2.6	g/cm^3
fraction organic carbon, $(f_{oc})_{eff}$	0.0002	
Depth of Interest, z	15	cm
Fraction organic carbon at depth of interest, $f_{oc}(z)$	0.05	

Commonly Used Parameter Estimates

Organic Carbon Partition Coefficient, log K_{oc}	4.22	log L/kg	
Colloidal Organic Carbon Partition Coefficient, log K_{DOC}	3.85	log L/kg	
Boundary Layer Mass Transfer Coefficient, k_{bl}	0.75	cm/hr	
Dispersivity, α	2.12	cm	(not allowed to be less than 1 cm)
Effective Cap Layer Diffusion/Dispersion Coeff., D_1	77	cm^2/yr	
Bioturbation Layer Diffusion/Dispersion Coeff., D_2	1474	cm^2/yr	

Output

Pore Water Concentration at Depth, $C(z)$	0.101	ug/L
Loading at Depth, $W(z)$	83.8	ug/kg
Average Bioturbation Layer Loading, $(W_{bio})_{avg}$	43	ug/kg
Flux to Overlying Water Column, J	103	$ug/m^2/yr$
Cap-Bioturbation Interface Concentration, C_{bio}/C_0, C_{bio}	10.08%	
Cap-Water Interface Concentration, C_{bl}/C_0, C_{bl}	0.16%	
Average Bioturbation Concentration, $(C_{bio})_{avg}/C_0$, $(C_{bio})_{avg}$	5.20%	
Characteristic Time to~1% of steady state, $t_{advdiff}$	2.8	yr



Dimensionless Parameters

Effective Cap Layer Peclet No., Pe_1	3.55
Effective Cap Layer Damkohler No., Da_1	0.00
β = SQRT($Pe_1^2/4+Da_1$)	1.78
Bioturbation Layer Peclet No., Pe_2	0.10
Bioturbation Layer Damkohler No., Da_2	0.00
γ = SQRT($Pe_2^2/4+Da_2$)	0.051
Sherwood Number at Interface, Sh	66.6

Other Parameters

Cap final thickness, h_{cap}	42.31	cm	
Cap Effective thickness w/ot bioturbation layer, h_{eff}	27	cm	
Containment Layer Retardation Factor, R_1	6		
Bioturbation Layer Retardation Factor, R_2	1297		
Effective Advective Velocity, U	10.00	cm/yr	(not allowed to be more negative than that which will offset diffusion)
Characteristic Advection Time-cap layer, t_{adv}	15.3	yr	
Characteristic Diffusion Time-cap layer, t_{diff}	3.4	yr	
Characteristic Reaction Time-cap layer, t_{decay}	infinity	yr	

z/hcap		
0	0.01	1
0.00	0.42	42.31
0.00	0.00	1.00
0.00	0.00	1.00

*Lampert, D.J. and Reible, D.D. 2009. "An Analytical Modeling Approach for Evaluation of Capping of Contaminated Sediments," Soil & Sediment Contamination, 2009, 18(4):470-488.

TRANSIENT MODEL

from Van Genchten 1981*

Instructions: The values in the "Parameter" Cells are linked to those on the "Steady State Conditions" page. DO NOT CHANGE THE CELLS IN RED; feel free to change the cells with GREEN color to create an array of concentration profiles.

Model Equations:

$$\xi = \frac{h_{cap} - z}{h_{cap}} \qquad \tau = \frac{D_1 t}{h_{cap}^2 R_1} \qquad Pe = \frac{U h_{cap}}{D_1} \qquad u = \sqrt{\frac{Pe}{4}}$$

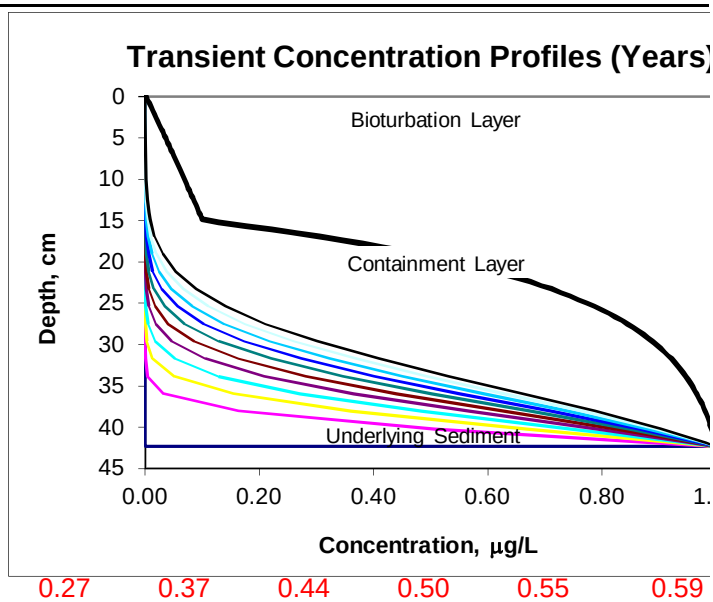
$$C / C_0 = 0.5 \begin{cases} \exp\left[\left(\frac{Pe}{2} - u\right)\xi\right] \mathrm{erfc}\left[\frac{1}{2\tau^{0.5}}(\xi - 2u\right. \\ \exp\left[\left(\frac{Pe}{2} + u\right)\xi\right] \mathrm{erfc}\left[\frac{1}{2\tau^{0.5}}(\xi + 2u\right. \end{cases}$$

Parameters

$t_{avd/diff}$	2.8 yr	2.77142 ss time
Pe	5.5	
Da	0.0	
u	3	

Dimensionless Calculations

zeta \ tau	0	0.002	0.004	0.006	0.009	0.011	0.013	0.015	0.017
1	0.00	0.00	0.00						
0.95	0.00	0.00	0.00						
0.9	0.00	0.00	0.00						
0.85	0.00	0.00	0.00						
0.8	0.00	0.00	0.00						
0.75	0.00	0.00	0.00						
0.7	0.00	0.00	0.00						
0.65	0.00	0.00	0.00						
0.6	0.00	0.00	0.00						
0.55	0.00	0.00	0.00						
0.5	0.00	0.00	0.00						
0.45	0.00	0.00	0.00						
0.4	0.00	0.00	0.00						
0.35	0.00	0.00	0.00						
0.3	0.00	0.00	0.00						
0.25	0.00	0.00	0.01						
0.2	0.00	0.00	0.05						
0.15	0.00	0.03	0.15	0.27	0.37	0.44	0.50	0.55	0.59
0.1	0.00	0.16	0.36	0.48	0.57	0.63	0.68	0.71	0.74
0.05	0.00	0.51	0.67	0.74	0.79	0.82	0.85	0.87	0.88
0.01	0.00	0.90	0.94	0.95	0.96	0.97	0.97	0.98	0.98
0.001	0.00	0.99	0.99	1.00	1.00	1.00	1.00	1.00	1.00
0	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00



Concentration Profiles

depth \ time	0.0	0.3	0.6	0.8	1.1	1.4	1.7	1.9	2.2
0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2.11574498	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4.23148995	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6.34723493	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8.4629799	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10.5787249	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12.6944699	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

14.8102148	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16.9259598	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
19.0417048	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01
21.1574498	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.02
23.2731947	0.00	0.00	0.00	0.00	0.00	0.01	0.02	0.03	0.05
25.3889397	0.00	0.00	0.00	0.00	0.01	0.02	0.03	0.06	0.08
27.5046847	0.00	0.00	0.00	0.00	0.02	0.04	0.07	0.10	0.14
29.6204297	0.00	0.00	0.00	0.02	0.05	0.09	0.13	0.17	0.22
31.7361746	0.00	0.00	0.01	0.05	0.11	0.16	0.22	0.27	0.32
33.8519196	0.00	0.00	0.05	0.13	0.21	0.28	0.35	0.40	0.45
35.9676646	0.00	0.03	0.15	0.27	0.37	0.44	0.50	0.55	0.59
38.0834096	0.00	0.16	0.36	0.48	0.57	0.63	0.68	0.71	0.74
40.1991545	0.00	0.51	0.67	0.74	0.79	0.82	0.85	0.87	0.88
41.8917505	0.00	0.90	0.94	0.95	0.96	0.97	0.97	0.98	0.98
42.2725846	0.00	0.99	0.99	1.00	1.00	1.00	1.00	1.00	1.00
42.3148995	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

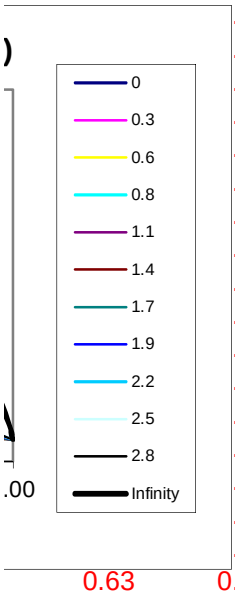
*Van Genuchten, M.T. 1981. “Analytical solutions for chemical transport with simultaneous adsorption, zero order production and first order decay.” Journal of Hydrology, 49(3):213-233.

$$\frac{{}^{2}}{-} + \frac{\varepsilon\lambda h_{cap}^{2}}{D_1}$$

$$u\tau)\Big] + \Big\}$$

$$u\tau)\Big] \quad \Big\}$$

0.019	0.021
	.00
	.00
	.00
	.00
	.00
	.00
	.00
	.01
	.02
	.03
	.05
	.09
	.14
	.21
	.30
	.41
	.53
0.63	0.66
0.77	0.79
0.89	0.90
0.98	0.98
1.00	1.00
1.00	1.00



2.5	2.8
0.00	0.00
0.00	0.00
0.00	0.00
0.00	0.00
0.00	0.00
0.00	0.00
0.00	0.00

0.00	0.01
0.01	0.02
0.02	0.03
0.04	0.05
0.07	0.09
0.11	0.14
0.17	0.21
0.26	0.30
0.37	0.41
0.49	0.53
0.63	0.66
0.77	0.79
0.89	0.90
0.98	0.98
1.00	1.00
1.00	1.00

STEADY-STATE CAP DESIGN MODEL -- Array/Multiple Contaminant Worksheet

Instructions: Copy column "C" to create multiple solution rows; then change the parameters/chemical of ir
Column "B" is linked to the front worksheet. This example shows the effect of log Kow.

Inputs

Contaminant	PHE	PHE	PHE	PHE
Octanol-water partition coefficient, log K_{ow}	4.57	4.58	4.59	4.6
Water Diffusivity, D_w	0.000006	0.000006	0.000006	0.000006
Cap Decay Rate, λ_1	0	0	0	0
Bioturbation Layer Decay Rate, λ_2	0	0	0	0
Contaminant Pore Water Concentration, C_0	1	1	1	1
Biological Active Zone fraction organic carbon, $(f_{oc})_{bio}$	0.05	0.05	0.05	0.05
Colloidal Organic Carbon Concentration, ρ_{DOC}	0	0	0	0
Darcy Velocity, V (positive is upwelling)	10	10	10	10
Depositional Velocity, V_{dep}	0	0	0	0
Bioturbation Layer Thickness, h_{bio}	15	15	15	15
Pore Water Biodiffusion Coefficient, D_{bio}^{pw}	100	100	100	100
Particle Biodiffusion Coefficient, D_{bio}^{p}	1	1	1	1
Conventional Cap placed depth	45	45	45	45
Cap Materials -Granular (G) or Consolidated (C)	G	G	G	G
Cap consolidation depth	0	0	0	0
Underlying sediment consolidation	15	15	15	15
Porosity, ε	0.4	0.4	0.4	0.4
Particle Density, ρ_P	2.6	2.6	2.6	2.6
fraction organic carbon, $(f_{oc})_{eff}$	0.0002	0.0002	0.0002	0.0002
Depth of Interest, z	15	15	15	15
Fraction organic carbon at depth of interest, $f_{oc}(z)$	0.05	0.05	0.05	0.05

Estimates

Organic Carbon Partition Coefficient, log K_{oc}	4.22	4.23	4.24	4.25
Colloidal Organic Carbon Partition Coefficient, log K_{DOC}	3.85	3.86	3.87	3.88
Boundary Layer Mass Transfer Coefficient, k_{bl}	0.75	0.75	0.75	0.75
Dispersivity, α	1.00	1.00	1.00	1.00
Effective Cap Layer Diffusion/Dispersion Coeff., D_1	66	66	66	66
Bioturbation Layer Diffusion/Dispersion Coeff., D_2	1462	1490	1517	1546

Outputs

Pore Water Concentration at Depth, $C(z)$	0.457	0.460	0.464	0.468
Loading at Depth, $W(z)$	379.7	390.7	402.0	413.6
Average Bioturbation Layer Loading, $(W_{bio})_{avg}$	43	43	43	43
Flux to Overlying Water Column, J	101	101	101	101
Cap-Bioturbation Interface Concentration, C_{bio}/C_0	10.03%	9.86%	9.69%	9.52%
Cap-Water Interface Concentration, C_{bl}/C_0	0.15%	0.15%	0.15%	0.15%
Average Bioturbation Concentration, $(C_{bio})_{avg}/C_0$, $(C_{bio})_{avg}$	5.18%	5.09%	5.00%	4.91%
Characteristic Time to ~1% of pre-cap, $t_{adv/diff}$	3.1	3.2	3.3	3.4

Effective Cap Layer Peclet No., Pe_1	4.15	4.16	4.17	4.18
Effective Cap Layer Damkohler No., Da_1	0.00	0.00	0.00	0.00
β = SQRT(Pe_1^2/4+Da)	2.08	2.08	2.08	2.09
Bioturbation Layer Peclet No., Pe_2	0.10	0.10	0.10	0.10
Bioturbation Layer Damkohler No., Da_2	0.00	0.00	0.00	0.00
γ = SQRT(Pe_1^2/4+Da)	0.051	0.050	0.050	0.049
Sherwood Number at Interface, Sh	67.1	65.9	64.7	63.5
Cap final thickness, h_{cap}	42.31	42.37	42.42	42.47
Cap Effective Depth, h_{eff}	27	27	27	27
Containment Layer Retardation Factor, R_1	6	6	6	6
Bioturbation Layer Retardation Factor, R_2	1297	1324	1352	1380
Effective Advective Velocity, U	10.00	10.00	10.00	10.00
Characteristic Advection Time-cap layer, t_{adv}	15.3	15.6	15.9	16.3
Characteristic Diffusion Time-cap layer, t_{diff}	4.0	4.1	4.1	4.2
Characteristic Reaction Time-cap layer, t_{decay}	infinity	infinity	infinity	infinity

ıterest.

PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE
4.61	4.62	4.63	4.64	4.65	4.66	4.67	4.68	4.69	4.7
0.000006	0.000006	0.000006	0.000006	0.000006	0.000006	0.000006	0.000006	0.000006	0.000006
0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0
1	1	1	1	1	1	1	1	1	1
0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
0	0	0	0	0	0	0	0	0	0
10	10	10	10	10	10	10	10	10	10
0	0	0	0	0	0	0	0	0	0
15	15	15	15	15	15	15	15	15	15
100	100	100	100	100	100	100	100	100	100
1	1	1	1	1	1	1	1	1	1
45	45	45	45	45	45	45	45	45	45
G	G	G	G	G	G	G	G	G	G
0	0	0	0	0	0	0	0	0	0
15	15	15	15	15	15	15	15	15	15
0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4
2.6	2.6	2.6	2.6	2.6	2.6	2.6	2.6	2.6	2.6
0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002
15	15	15	15	15	15	15	15	15	15
0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
4.26	4.27	4.27	4.28	4.29	4.30	4.31	4.32	4.33	4.34
3.89	3.90	3.90	3.91	3.92	3.93	3.94	3.95	3.96	3.97
0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.75
1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
66	66	66	66	66	66	66	66	66	66
1575	1604	1635	1666	1697	1729	1762	1796	1830	1865
0.471	0.474	0.478	0.481	0.484	0.488	0.491	0.494	0.497	0.500
425.4	437.5	449.8	462.5	475.4	488.6	502.1	515.9	530.0	544.5
44	44	44	44	44	44	44	45	45	45
101	101	101	101	101	101	101	101	101	101
9.35%	9.19%	9.03%	8.87%	8.72%	8.56%	8.41%	8.27%	8.12%	7.97%
0.15%	0.15%	0.15%	0.15%	0.15%	0.15%	0.15%	0.15%	0.15%	0.15%
4.83%	4.74%	4.66%	4.58%	4.50%	4.42%	4.34%	4.27%	4.19%	4.12%
3.4	3.5	3.6	3.7	3.8	3.9	3.9	4.0	4.1	4.2

4.18	4.19	4.20	4.21	4.21	4.22	4.23	4.23	4.24	4.24
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2.09	2.10	2.10	2.10	2.11	2.11	2.11	2.12	2.12	2.12
0.10	0.09	0.09	0.09	0.09	0.09	0.09	0.08	0.08	0.08
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.048	0.047	0.046	0.045	0.044	0.043	0.043	0.042	0.041	0.040
62.4	61.2	60.1	59.0	57.9	56.8	55.7	54.7	53.7	52.7
42.51	42.56	42.61	42.66	42.70	42.75	42.79	42.83	42.87	42.92
28	28	28	28	28	28	28	28	28	28
6	6	6	6	7	7	7	7	7	7
1409	1439	1469	1500	1532	1564	1597	1630	1664	1699
10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00
16.6	17.0	17.3	17.7	18.1	18.5	18.9	19.3	19.7	20.1
4.3	4.4	4.5	4.7	4.8	4.9	5.0	5.1	5.2	5.3
infinity	infinity	infinity	infinity	infinity	infinity	infinity	infinity	infinity	infinity

PHE	
4.71	
0.000006	cm^2/s
0	yr^{-1}
0	yr^{-1}
1	ug/L
0.05	
0	mg/L
10	cm/yr
0	cm/yr
15	cm
100	cm^2/yr
1	cm^2/yr
45	cm
G	
0	cm
15	cm
0.4	
2.6	g/cm^3
0.0002	
15	cm
0.05	

4.35	log L/kg
3.98	log L/kg
0.75	cm/hr
1.00	cm
66	cm^2/yr
1900	cm^2/yr

0.503	ug/L
559.2	ug/kg
45	ug/kg
101	$ug/m^2/yr$
7.83%	
0.15%	
4.04%	
4.3	yr

4.25	
0.00	
2.13	
0.08	
0.00	
0.040	
51.7	
42.96	cm
28	cm
7	
1735	
10.00	cm/yr
20.5	yr
5.5	yr
infinity	yr