LABORATORY NOTEBOOK

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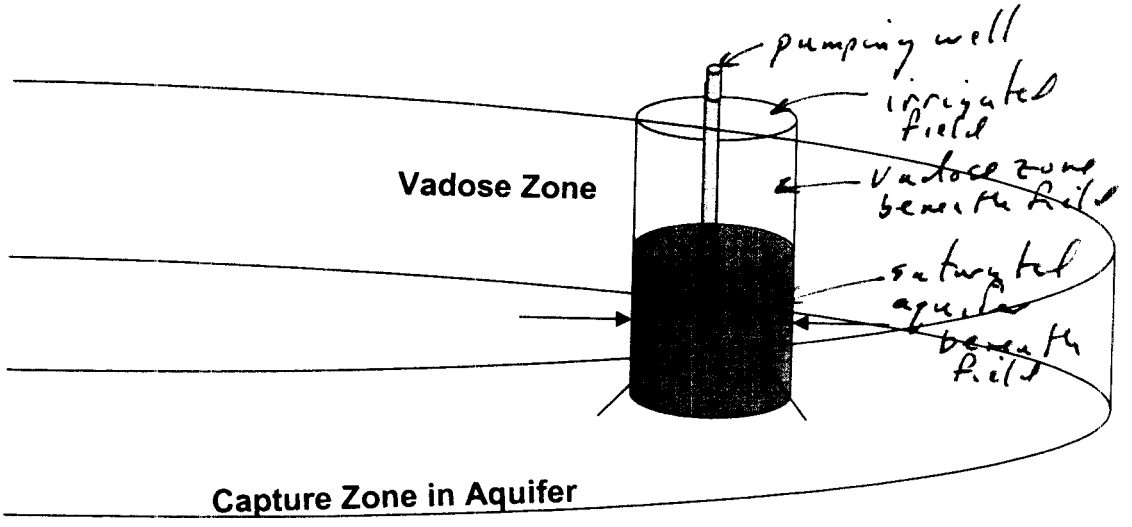
BOOK NO. 20.14002.01.101 PROJECT

Gary R. Walter Gary R. Walter

This notebook opened on 10/22/07 to record development of conceptual and mathematical models related to recycling of dissolved radionuclides beneath irrigated fields. The first conceptual model is shown below



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The conceptual model consists of a single irrigation well pumping at an annual average rate of Q_w. Water pumped from the well is applied to irrigate a circular field at the same rate. A fraction, f, of the water returns to the aquifer as irrigation return flow, the rest is evapotranspired or incorporated into the crop and is removed from the flow system. The pumping well establishes a steady capture zone that fully encompasses a plume of contaminated groundwater.

Irrigation return flow and any dissolved contaminants that were applied to the field move vertically downward and mix with the zone of contaminated water in the aquifer beneath the field.

The following additional assumptions are made:

1. The irrigation return flow has reached steady state as has the concentration in the return flow.

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2. The background concentration of the contaminant in the plume is constant beneath the irrigated field.

3. The cylindrical volume in the aquifer beneath the irrigated field is well-mixed.

Based on this conceptual model and these assumptions, the change in concentration in the cylinder in the aquifer beneath the field is described by the ~~flow~~ CW 10/22/07 following differential equation

This model is revised starting p.15 CW 10/24/07

$$V_T \frac{dC_T}{dt} = Q_p C_p + Q_i C_R - \lambda C_T \quad (1)$$

V_T – volume of saturated cylinder $[L^3]$

C_T – concentration in the saturated cylinder $[M/L^3]$

t – time $[t]$

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Q_p – rate that water flows into the cylinder from the aquifer $[L^3/t]$

C_p – background concentration in the plume $[M/L^3]$

Q_i – rate of irrigation return flow $[L^3/t]$

C_R – concentration in the return flow when it reaches the aquifer $[M/L^3$

λ – first-order decay constant for the contaminant $[1/t]$

The first term on the right hand side (RHS) of (1) represents the mass flow into the cylinder from the aquifer. The second term on the RHS of (1) is the mass flow into the cylinder from irrigation return flow. The last term on the RHS of (1) is decay within the cylinder

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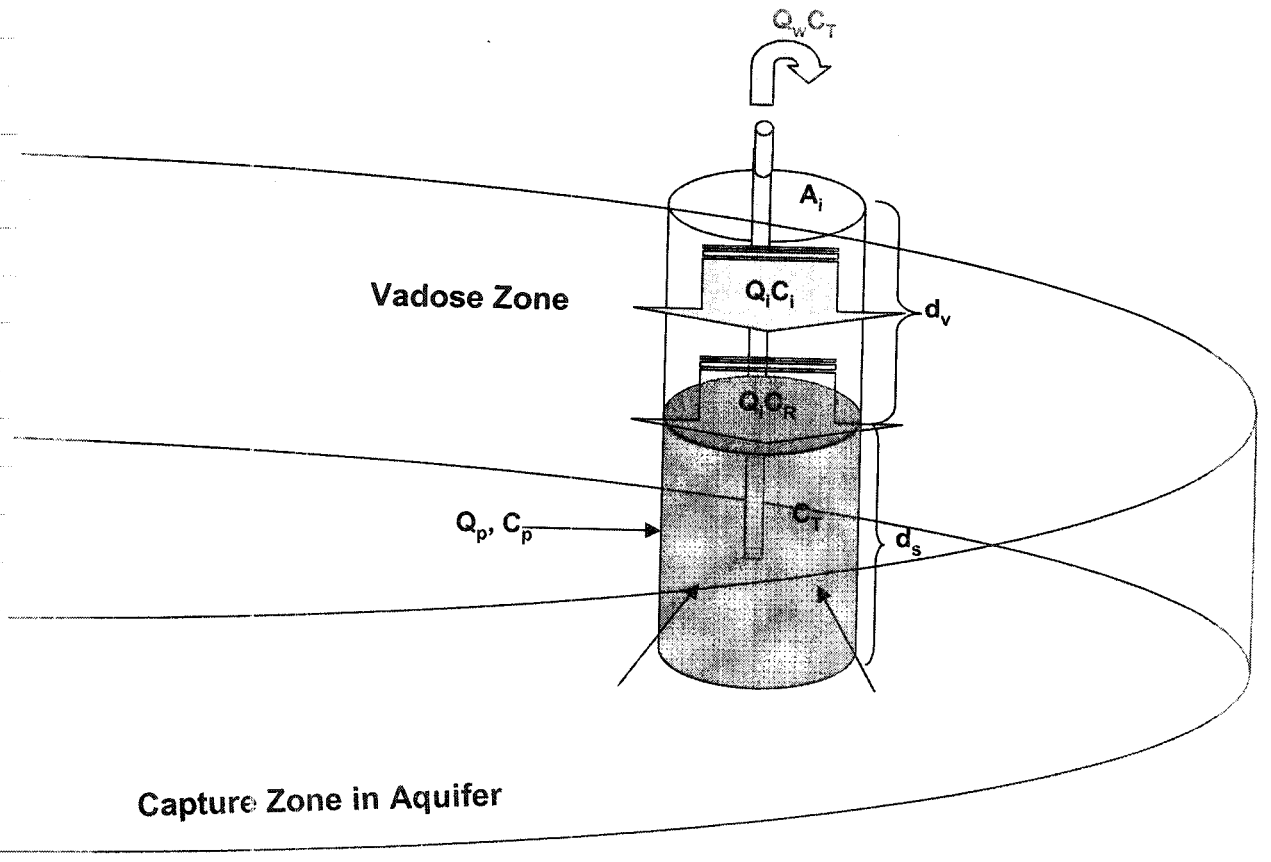
This mathematical model that is illustrated below. 10/22/07



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The concentration in the irrigation return flow reaching the aquifer, C_R, for a decaying contaminant is given by

$$C_R = C_i \exp[-\lambda R_i t_{R_i}] \qquad (2)$$

C_i – concentration at the top of the vadose zone $[M/L^3]$

R_i – retardation factor in the vadose zone $[L^3/M]$

t_{R_i} – unretarded travel time through the vadose zone $[t]$

The concentration entering the vadose zone, C_i, is given by

$$C_i = C_p Q_w / Q_i \qquad (3)$$

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Equation (3) represents evaporative concentration of the mass pumped from the aquifer.

Note that $Q_p = (1-f) Q_w$ and $V_T = A_i d_s \phi$ where ϕ is the aquifer porosity

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Using (2) and (3), (1) can be written as.

$$\frac{dC_T}{dt} = \frac{Q_p C_p}{V_T} + \frac{Q_w \exp[-\lambda R_i t_{R_i}]}{V_T} C_T - \lambda C_T \quad (4)$$

$$= \frac{Q_p C_p}{V_T} + \left[\frac{Q_w \exp[-\lambda R_i t_{R_i}]}{V_T} - \lambda\right] C_T \quad (5)$$

Letting

$$a = \frac{Q_p C_p}{V_T} \; ; \; b = \left[\frac{Q_w \exp[-\lambda R_i t_{R_i}}{V_T} - \lambda\right]$$

(5) can be written as

$$\frac{dC_T}{dt} = a + bC_T$$

$$\frac{1}{a + bC_T} dC_T = dt \quad (6)$$

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The concentration at time t_1 after the return flow mass pulse first reaches the aquifer, t_0, can be found by integration (6)

$$\int_{C_p}^{C_T} \frac{1}{a+bC_T}\, dC_T = \cancel{\int_{t_0}^{t_1} dt} \quad \int_{t_0}^{t_1} dt \qquad (7)$$

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$$\frac{1}{b} \ln[a+bc]\Big|_{C_p}^{C_T} = (t_1 - t_0)$$

(Abramowitz and Stegun, Handbook of Mathematic Functions, 1972)

$$\ln\left\{\frac{a+bC_T}{a+bC_p}\right\} = b(t_1 - t_0)$$

$$a + bC_T = (a+bC_p)\exp[b[t_1 - t_0]]$$

$$C_T = \frac{(a+bC_p)}{b}\exp[b(t_1-t_0)] - \frac{a}{b} \qquad (8)$$

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The retardation factor in the vadose zone is defined as

$$R_i = 1 + \frac{\rho_b K_D}{\theta}$$

ρ_b – dry bulk density [M/L^3]

K_D – distribution coefficient [L^3/M]

θ – water content [unitless]

The unretarded travel time through the vadose zone is computed as

$$t_{R_i} = A_i \theta / Q_w$$

A_i – irrigated area

The model solution (eq'n (8)) was implemented in an Excel spreadsheet called

"GRW recirculation model.xls"

An example of the spreadsheet calculations for an unretarded, non-decaying contaminant is shown on p. 10

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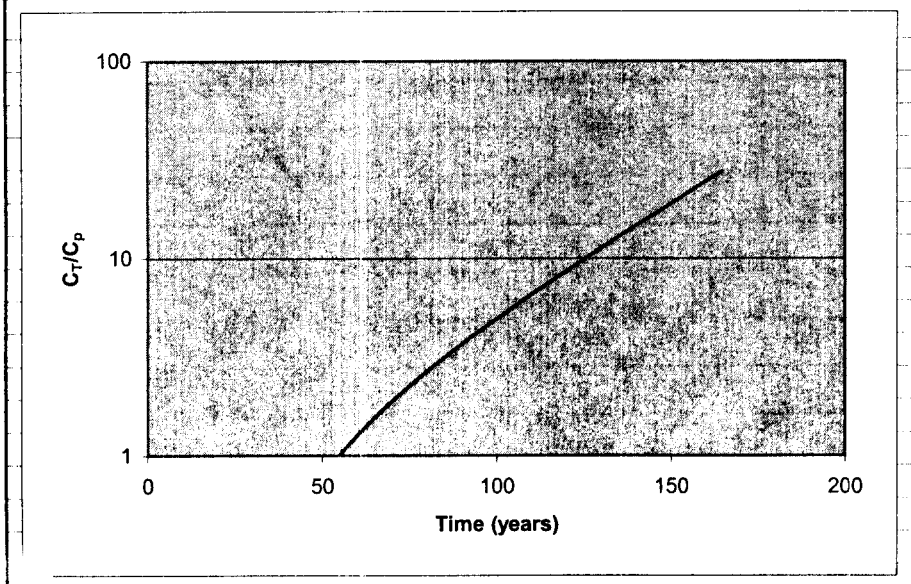
Parameter	Value	Units
Concentration in plume outside of irrigation area (C_p)	1	mass unit/Ac-ft
Irrigation rate (Q_w)	3000	Ac-ft/yr
Fraction irrigation return flow (f)	0.05	none
Net pumping from plume $Q_p = (1-f)Q_w$	2850	Ac-ft/yr
Decay rate (λ)	0.00E+00	1/yr
Distribution coefficient of contaminant in vadose zone (K_d)	0	V/M
Thickness of vadose zone (d)	328	ft
Bulk water content of vadose zone (Θ)	0.05	none
Bulk density of vadose zone(ρ_b)	1.6	M/V
Retardation factor in vadose zone ($R_i = 1+ K_d \rho/\Theta$)	1	none
Area irrigated (A_i)	500	Ac
Unretarded travel time in vadose zone ($t_{Ri}=(A_i*\Theta)/Q_w$)	54.66667	yr
First arrival time ($t_0=t_{Ri}R_i$)	54.66667	yr
Thickness of saturated zone contributing to well (d_a)	984	ft
Porosity of aquifer (Θ_a)	0.25	
Volume of saturated zone below irrigated field ($V_T = A_i\, d_a\, \Theta_a$)	123000	Ac-ft
"a" factor (Q_pC_p/V_T)	0.023171	
"b" factor ($Q_w \exp[-\lambda R_i t_{Ri}]-\lambda)/V_T$	0.02439	
Time expansion factor	1.1	
Delta t	5	yr



Time	C_T/C_p
54.66667	1
60.16667	1.279942307
65.66667	1.600073177
71.16667	1.966162084
76.66667	2.384806773
82.16667	2.863552159
87.66667	3.411026308
93.16667	4.037095932
98.66667	4.75304421
104.1667	5.571774136
109.6667	6.50804106
115.1667	7.57871861
120.6667	8.803102799
126.1667	10.20325977
131.6667	11.80442351
137.1667	13.63545056
142.6667	15.72934014

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The example on p. 12 shows the ~~case~~ case for a retarded, decaying
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contaminant. In this case, the saturated zone concentration stabilizes with time. Note, however, that the residence time in the vadose zone is very long.

Whether or not the concentration increases or stabilizes depends on the value of b in eq'n (8).

For $b > 0$, the concentration keeps increasing. For $b \leq 0$ the value stabilizes. For a given set of pumping and return flow rates, and soil/aquifer conditions, b depends on the decay rate and the distribution coefficient for a specific contaminant.

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The graph on p. ~~12~~ shows the value of b as a function of K_D and λ based on the other constant parameters in the table on p. 10. The graph on p. 12 was prepared using the "function" feature in Surfer 8. The Surfer file is "sensitivity to Kd.srf"

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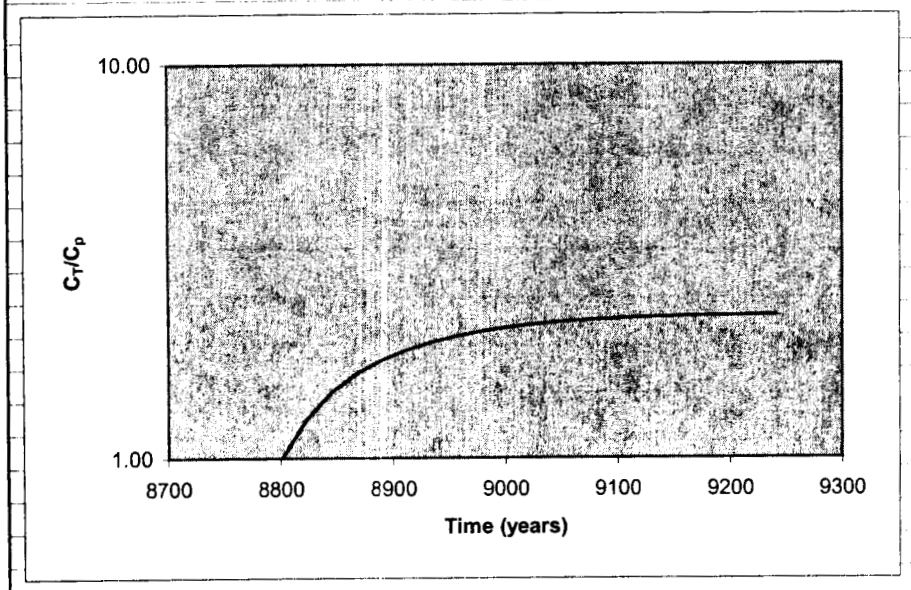
Parameter	Value	Units
Concentration in plume outside of irrigation area (C_p)	1	mass unit/Ac-ft
Irrigation rate (Q_w)	3000	Ac-ft/yr
Fraction irrigation return flow (f)	0.05	none
Net pumping from plume $Q_p = (1-f)Q_w$	2850	Ac-ft/yr
Decay rate (λ)	1.00E-02	1/yr
Distribution coefficient of contaminant in vadose zone (K_d)	5	V/M
Thickness of vadose zone (d)	328	ft
Bulk water content of vadose zone (Θ)	0.05	none
Bulk density of vadose zone(ρ_b)	1.6	M/V
Retardation factor in vadose zone ($R_i = 1 + K_d \rho/\Theta$)	161	none
Area irrigated (A_i)	500	Ac
Unretarded travel time in vadose zone ($t_{Ri}=(A_i*\Theta)/Q_w$)	54.66667	yr
First arrival time ($t_0=t_{Ri}R_i$)	8801.333	yr
Thickness of saturated zone contributing to well (d_a)	984	ft
Porosity of aquifer (Θ_a)	0.25	
Volume of saturated zone below irrigated field ($V_T = A_i\, d_a\, \Theta_a$)	123000	Ac-ft
"a" factor (Q_pC_p/V_T)	0.023171	
"b" factor ($Q_w \exp[-\lambda R_i t_{Ri}]/V_T-\lambda$)	-0.01	
Time expansion factor	1.1	
Delta t	20	yr



Time	C_T/C_p
8801	1.00
8823	1.26
8845	1.47
8867	1.64
8889	1.77
8911	1.88
8933	1.97
8955	2.03
8977	2.09
8999	2.14
9021	2.17
9043	2.20
9065	2.22
9087	2.24
9109	2.26
9131	2.27
9153	2.28

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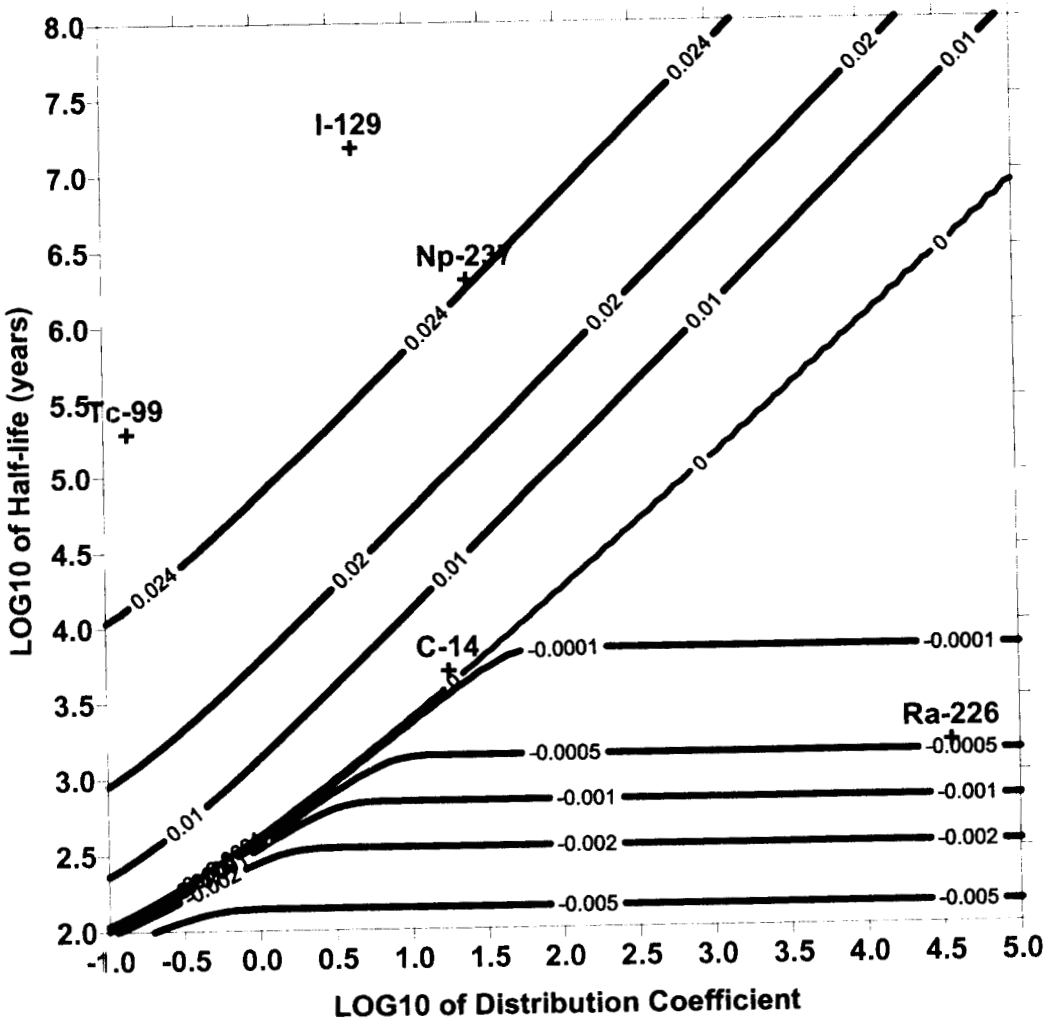

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The parameters used to plot the specific isotopes are listed below

isotopes.xls

	A	B	C
1	Log10(Kd)	t1/2	Isotope
2	0.65	7.18	I-129
3	-0.85	5.3	Tc-99
4	1.4	6.3	Np-237
5	1.25	3.7	C-14
6	4.55	3.2	Ra-226

The values for Kd are taken from Soil-Related Input Parameters for the Biosphere Model ANL-NBS-MD-000009 Rev03 September 2006

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The mathematical model started on page 3, eq'n (1) is missing two important terms.

The first is the rate of mass removal from the aquifer which is

$$-Q_w C_T$$

and the second is a term for the permanent removal of mass due to such processes as erosion, incorporation into bio mass which will be represented as

$$-\alpha Q_w C_T$$

α is fracture of mass permanently removed
Incorporating these additional terms into eq'n (5) gives

$$\frac{dC_T}{dt} = \frac{Q_p C_p}{V_T} + \frac{Q_w}{V_T} \exp[-\lambda R_i t_{Ri}] C_T - \frac{Q_w}{V_T} C_T - \alpha \frac{Q_w}{V_T} C_T - \lambda C_T \qquad (9)$$

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Rearranging (9) gives

$$\frac{dC_T}{dt} = \frac{Q_p C_p}{V_T} + \left[\frac{Q_w}{V_T}\left\{\left(e^{-\lambda R_i t_{Ri}} - 1 - \alpha\right)\right\} - \lambda\right] \cdot C_T$$

letting $a = \frac{Q_p C_p}{V_T}$

$$b = \left[\frac{Q_w}{V_T}\left\{e^{-\lambda R_i t_{Ri}} - 1 - \alpha\right\} - \lambda\right]$$

The solution to (9) is of the same form as eq'n (8) on p. 8

Note that if $\lambda = 0$ and $\alpha = 0$,

~~the solution is~~ aw 10/24/07

eqn (9) becomes simply

$$\frac{dC_T}{dt} = \frac{Q_p C_p}{V_T}$$

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$$C_T = \frac{Q_p C_p}{V_T} \cancel{(t_d} \; (t_1 - t_0) \qquad (10)$$

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The spreadsheet model was revised according to the reformulations. The reformulated result for a conservative solute is shown on ~~p. 17~~ p. 18
[illegible] 10/24/07

The result for technicium-99 assuming $\alpha = 0.05$ is shown on p. 19

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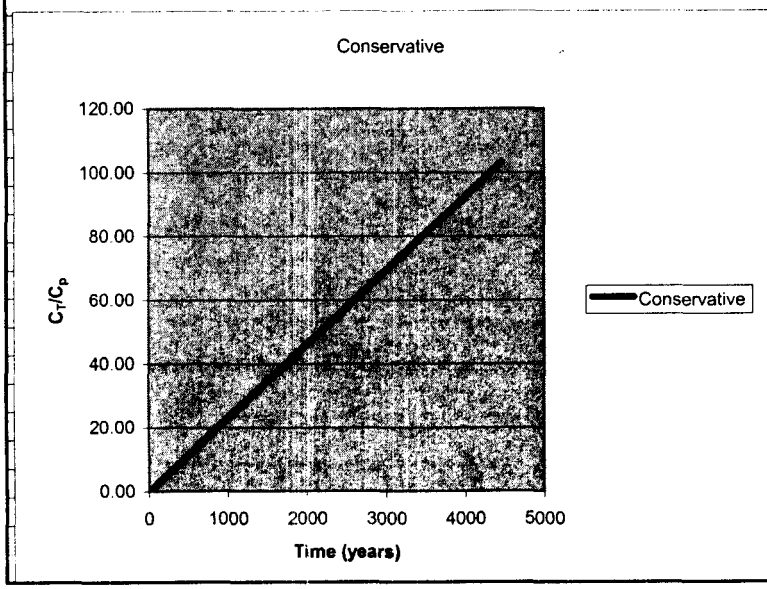
Parameter	Value	Units
Concentration in plume outside of irrigation area (C_p)	1	mass unit/Ac-ft
Irrigation rate (Q_w)	3000	Ac-ft/yr
Fraction irrigation return flow (f)	0.05	none
Net pumping from plume $Q_p = (1-f)Q_w$	2850	Ac-ft/yr
Mass removal fractions (α) (must be > 0, set to small value for no mass loss)	1.00E-08	
Decay rate (λ)	0.00E+00	1/yr
Distribution coefficient of contaminant in vadose zone (K_d)	0	V/M
Thickness of vadose zone (d)	328	ft
Bulk water content of vadose zone (Θ)	0.05	none
Bulk density of vadose zone(ρ_b)	1.6	M/V
Retardation factor in vadose zone ($R_i = 1 + K_d \rho/\Theta$)	1	none
Area irrigated (A_i)	500	Ac
Unretarded travel time in vadose zone ($t_{Ri}=(A_i*\Theta)/Q_w$)	54.67	yr
First arrival time ($t_0=t_{Ri}R_i$)	54.67	yr
Thickness of saturated zone contributing to well (d_a)	984	ft
Porosity of aquifer (Θ_a)	0.25	
Volume of saturated zone below irrigated field ($V_T = A_i\, d_a\, \Theta_a$)	123000	Ac-ft
"a" factor (Q_pC_p/V_T)	0.023171	
"b" factor ($Q_w (\exp[-\lambda R_i t_{Ri}]-1)-\alpha)/V_T-\lambda$)	-2.44E-10	
Time expansion factor	1.1	
Delta t	200	yr

Time	C_T/C_p
55	1.00
275	6.10
495	11.20
715	16.29
935	21.39
1155	26.49
1375	31.59
1595	36.68
1815	41.78
2035	46.88
2255	51.98
2475	57.07
2695	62.17
2915	67.27
3135	72.37
3355	77.46
3575	82.56
3795	87.66
4015	92.76
4235	97.85
4455	102.95



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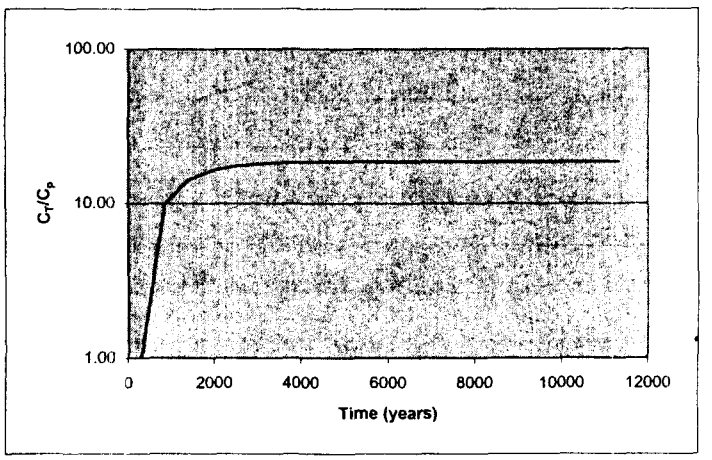
Technicium-99

Parameter	Value	Units
Concentration in plume outside of irrigation area (C_p)	1	mass unit/Ac-ft
Irrigation rate (Q_w)	3000	Ac-ft/yr
Fraction irrigation return flow (f)	0.05	none
Net pumping from plume $Q_p = (1-f)Q_w$	2850	Ac-ft/yr
Mass removal fractions (α) (must be > 0, set to small value for no mass loss)	0.05	
Decay rate (λ)	3.47E-06	1/yr
Distribution coefficient of contaminant in vadose zone (K_d)	0.14	V/M
Thickness of vadose zone (d)	328	ft
Bulk water content of vadose zone (Θ)	0.05	none
Bulk density of vadose zone(ρ_b)	1.6	M/V
Retardation factor in vadose zone ($R_i = 1 + K_d \rho/\Theta$)	5.48	none
Area irrigated (A_i)	500	Ac
Unretarded travel time in vadose zone ($t_{Ri}=(A_i*\Theta)/Q_w$)	54.67	yr
First arrival time ($t_0=t_{Ri}R_i$)	299.57	yr
Thickness of saturated zone contributing to well (d_a)	984	ft
Porosity of aquifer (Θ_a)	0.25	
Volume of saturated zone below irrigated field ($V_T = A_i\, d_a\, \Theta_a$)	123000	Ac-ft
"a" factor (Q_pC_p/V_T)	0.023171	
"b" factor (Q_w (exp[$-\lambda R_i t_{Ri}$]-1)$-\alpha$)/$V_T-\lambda$)	-1.25E-03	
Time expansion factor	1.1	
Delta t	500	yr



Time	C_T/C_p
300	1.00
850	9.72
1400	14.11
1950	16.32
2500	17.44
3050	17.99
3600	18.28
4150	18.42
4700	18.49
5250	18.53
5800	18.54
6350	18.55
6900	18.56
7450	18.56
8000	18.56
8550	18.56
9100	18.56
9650	18.56
10200	18.56

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The revised solution indicates that concentrations will reach a single value for non-zero values of α and λ. The ultimate value can be determined by setting dC_T/dt to zero in eq'n (9') and solving for C_T/C_P

$$0 = a + b\,C_T$$

$$\frac{-a}{b} = C_T$$

$$\frac{-Q_P C_P}{V_T}\,\frac{1}{\left[\frac{Q_W}{V_T}\left\{e^{-\lambda R_i t_{R_i}} - 1 - \alpha\right\} - \lambda\right]} = C_T$$

$$(11) \quad \frac{-Q_P}{V_T}\left[\frac{Q_W}{V_T}\left\{e^{-\lambda R_i t_{R_i}} - 1 - \alpha\right\} - \lambda\right]^{-1} = \frac{C_T}{C_P}$$

Eqn (11) is plotted as a function of KD and $t_{1/2}$ on p. 21 using the surfer8 function tool. File is

"sensitivity to Kd.srf"

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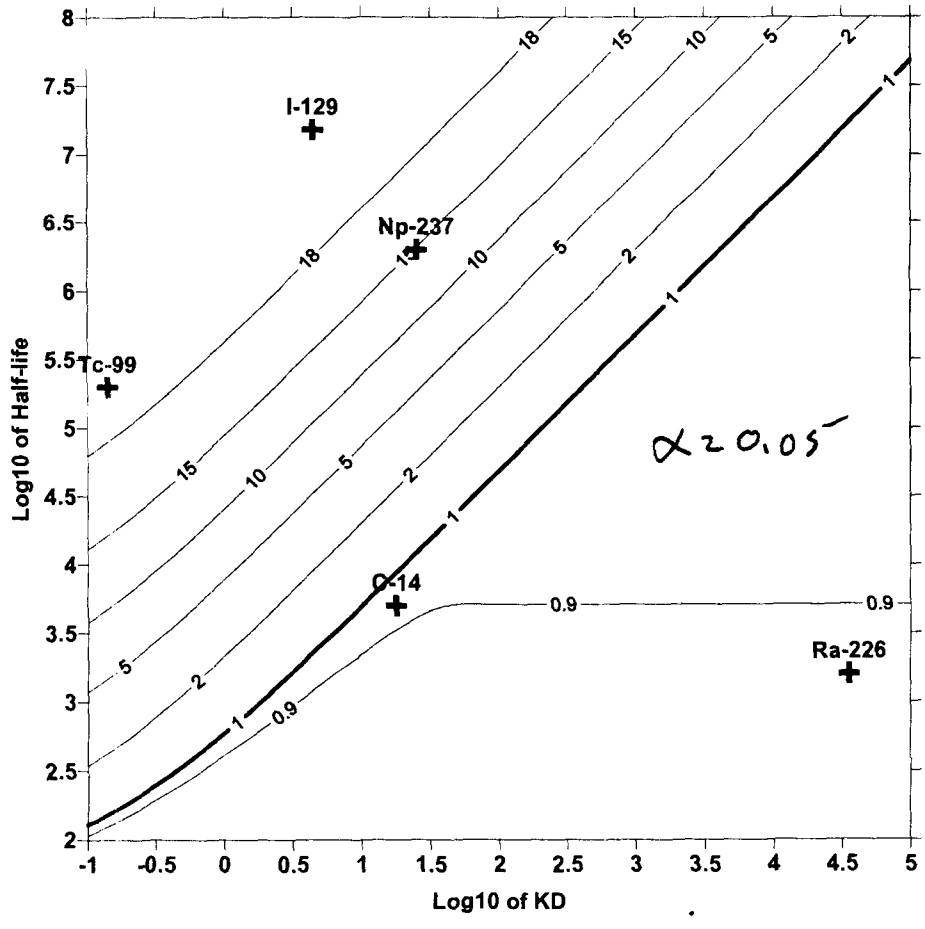

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