CONTAINMINANT TRANSPORT

MECHANICAL ASPECTS

ADVECTION

$$\bar{v} = \frac{Kdh}{\phi_e dl} = \text{average linear velocity}$$

DISPERSION/DIFFUSION

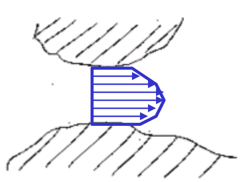
due to variable advection that occurs in the transition zone between two domains of the fluid with different compositions (diffusion is caused by chemical gradients)

Later we will look at some fundamental Some NONMECHANICAL ASPECTS : Decay & Sorption

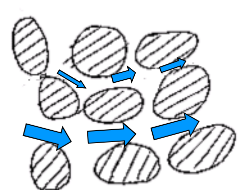
In the direction of flow we consider

LONGITUDINAL DISPERSION:

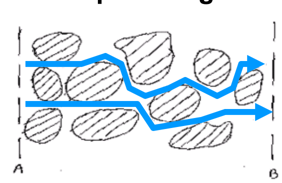
Velocity variation within pores:



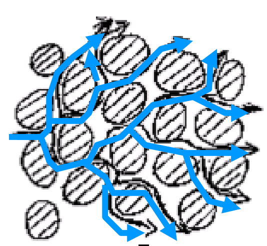
Velocity variation between pores:



Variation of flow path lengths



TRANSVERSE DISPERSION (normal to the flow path):



Splitting of flow paths

These physical mixing processes are combined and referred to as "Mechanical Dispersion"

Mechanical dispersion is related to average pore velocity by dispersivity (α)

$$Mechanical\ Dispersion = D = \alpha\bar{v}$$

dispersivity (α)

units of length

increases with increased heterogeneity and thus with travel distance

Diffusion:

Movement of dissolved species from areas of high concentration to low concentration

Fick's Law:

$$\mathbf{Flux = F = -D\frac{\partial C}{\partial l}}$$

D in open water for common groundwater ions
~1×10^{-9} to 2×10^{-9} m^2/sec

D* represents D in porous media, and is reduced due to tortuosity and effective porosity

D* ~ 2×10^{-11} to 5×10^{-10} m^2/sec

$$\text{some suggest } D^* = D\frac{\phi_e}{\tau}$$

$$\tau = \frac{\text{actual path}}{\text{direct path}}$$

Transport Equations

The combined mechanical and chemical diffusion process is treated with a Fick's Law approach

$$F = -D_l \frac{\partial C}{\partial l}$$

But here D is Hydrodynamic Dispersion expressed as

$$D_l = \alpha_l \overline{v_l} + D^*$$

Studies indicate scale dependence of dispersivity, α

Dispersivities at various scales & measured by various methods as compiled by Stan Davis et al. Table B1 in the book, "Ground Water Tracers"

Single-Well Injection Withdrawal Test

Type of Aquifer	Location	αL (meters)	Reference
Alluvial	Lyons, France	0.1-0.5	Fried, 1975

Multiple-Well Tracer Test (including two-well tracer tests)

Type of Aquifer	Location	Distance Between Injection and Observation Wells (meters)	αL (meters)	Reference
Chalk	Dorset, England	8	3.1	Ivanovich and Smith, 1978
Alluvial	Lyons, France	6 & 12	4.3	Fried, 1975
Alluvial	Eastern France	6 & 12	11.0	Fried, 1975
Fractured dolomite	Carlsbad, NM	55	38.0	Grove and Beetem, 1971
Fractured carbonate	So. Nevada	121	15.0	Classen and Cordes, 1975
Fractured crystalline	Savannah River Plant, S.C.	538	134.0	Webster et al., 1970

Single-Well Tracer Test with Surface Geophysics

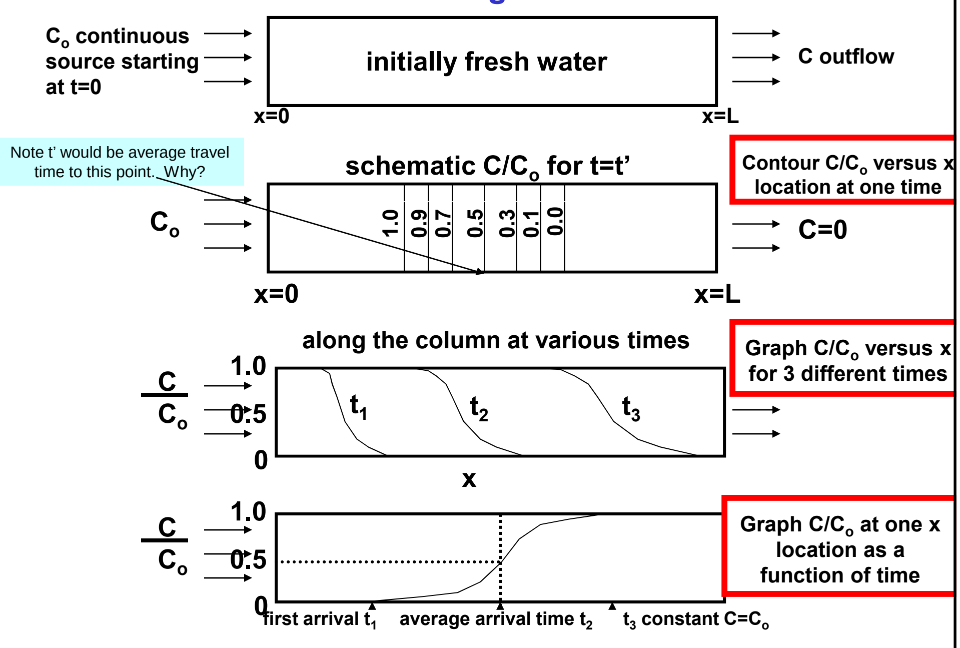
Type of Aquifer	Location	Distance Traveled by Tracer (meters)	αL (meters)	αT (meters)	Reference
Alluvial	Lyons, France	~ 80 m	5-12	0.009-14.5	Fried, 1975

Table B1 CONTINUED Dispersivities at various scales & measured by various methods from "Ground Water Tracers"

Dispersivities Measured on a Regional Scale by Model Calibration

Type of Aquifer	Location	Approximate Distance Traveled by Solute (meters)	αL (meters)	αT meters	Reference
Alluvial	Lyons, France	1,000	12	4	Fried, 1975
Limestone	Brunswick, GA	1,500	61	18	Bredehoeft & Pinder, 1973
Alluvial	Rocky Mtn. Arsenal, CO	4,000	30	30	Konikow, 1977
Alluvial	Arkansas River Valley, CO	5,000	30	9	Konikow & Bredehoeft, 1974
Glacial deposit	Long Island, NY	1,000	21.3	4.3	Pinder, 1973
Basalt	Snake River	4,000	91	137	Robertson, 1974

Break through Curves



Mechanical Transport Equations can be derived by considering an elemental volume as we did for the flow equations

We leave the derivation to a later course & consider the practical analytical forms

$$\frac{\partial C}{\partial t} = D_l \frac{\partial^2 C}{\partial l_l^{\,2}} + D_t \frac{\partial^2 C}{\partial l_t^{\,2}} + D_v \frac{\partial^2 C}{\partial l_v^{\,2}} - \overline{v}_l \frac{\partial C}{\partial l}$$

C	**concentration in fluid**
t	**time**
l	**spatial coordinate**
D	**dispersion tensor**
$\overline{\mathbf{v}}$	**interstitial velocity**
l_l	**reflects the flow direction**
l_t	**reflects the direction transverse laterally to flow**
l_v	**reflects the direction transverse vertically to flow**

Note differing form of flow equations

$$\frac{\partial h}{\partial t} = \frac{T}{S}\left[\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2}\right]$$

Equation for mechanical transport in 1-D

$$\frac{\partial \mathbf{C}}{\partial \mathbf{t}} = \mathbf{D}_{\mathbf{x}} \frac{\partial^2 \mathbf{C}}{\partial \mathbf{x}^2} - \overline{\mathbf{v}}_{\mathbf{x}} \frac{\partial \mathbf{C}}{\partial \mathbf{x}}$$

C	**concentration in fluid**
t	**time**
x	**spatial coordinate**
D	**dispersion tensor**
$\overline{\mathbf{v}}$	**interstitial velocity**

Analytical Solution for transport in 1-D flow field
continuous source
1D spreading
without chemical reaction

This is an appropriate model for transport along a sand column
It will over estimate C at x if applied to a case with spreading in the transverse lateral or vertical directions

It will predict the break through curves we looked at earlier

$$C = \frac{C_o}{2}\left(\operatorname{erfc}\left(\frac{x - \overline{v_x} t}{2\sqrt{D_x t}} \right) + \exp\left(\frac{\overline{v_x} x}{D_x} \right) \operatorname{erfc}\left(\frac{x + \overline{v_x} t}{2\sqrt{D_x t}} \right) \right)$$

erfc is the complimentary error function

Error Function

Tables are listed in the back of ground water hydrology books

Complementary Error Function (erfc)

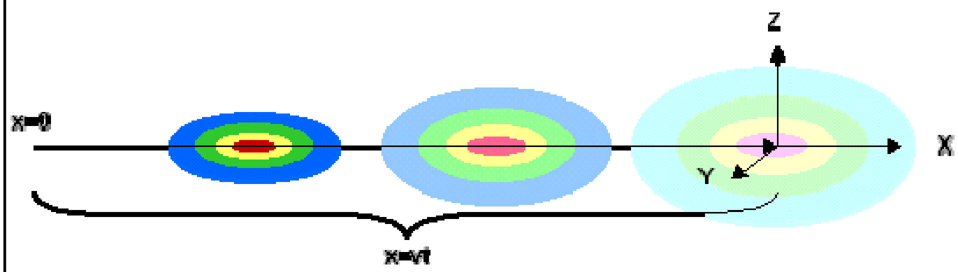
$$\operatorname{erf}(\beta) = \frac{2}{\pi} \int_0^{\beta} e^{-\epsilon^2}\, d\epsilon$$

$$\operatorname{erf}(-\beta) = -\operatorname{erf} \beta$$

$$\operatorname{erfc}(\beta) = 1 - \operatorname{erf}(\beta)$$

β	erf (β)	erfc (β)
0	0	1.0
0.05	0.056372	0.943628
0.1	0.112463	0.887537
0.15	0.167996	0.832004
0.2	0.222703	0.777297
0.25	0.276326	0.723674
0.3	0.328627	0.671373
0.35	0.379382	0.620618
0.4	0.428392	0.571608
0.45	0.475482	0.524518
0.5	0.520500	0.479500
0.55	0.563323	0.436677
0.6	0.603856	0.396144
0.65	0.642029	0.357971
0.7	0.677801	0.322199
0.75	0.711156	0.288844
0.8	0.742101	0.257899
0.85	0.770668	0.229332
0.9	0.796908	0.203092
0.95	0.820891	0.179109
1.0	0.842701	0.157299
1.1	0.880205	0.119795
1.2	0.910314	0.089686
1.3	0.934008	0.065992
1.4	0.952285	0.047715
1.5	0.966105	0.033895
1.6	0.976348	0.023652
1.7	0.983790	0.016210
1.8	0.989091	0.010909
1.9	0.992790	0.007210
2.0	0.995322	0.004678
2.1	0.997021	0.002979
2.2	0.998137	0.001863
2.3	0.998857	0.001143
2.4	0.999311	0.000689
2.5	0.999593	0.000407
2.6	0.999764	0.000236
2.7	0.999866	0.000134
2.8	0.999925	0.000075
2.9	0.999959	0.000041
3.0	0.999978	0.000022

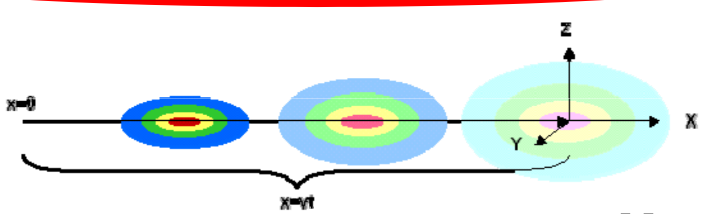
Analytical Solution for transport in 1-D flow field
slug source
3D spreading
without chemical reaction



Analytical Solution for transport in 1-D flow field
slug source
3D spreading
without chemical reaction

$$C\left(x = vt + X, y = Y, z = Z\right) = \frac{M}{8(\pi t)^{\frac{3}{2}}\sqrt{D_x D_y D_z}} \exp\left(-\frac{X^2}{4D_x t} - \frac{Y^2}{4D_y t} - \frac{Z^2}{4D_z t}\right)$$

IMPORTANT! X Y Z = distance from center of mass



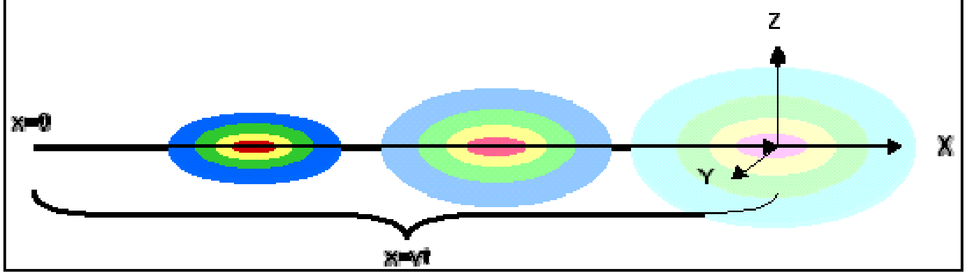
Maximum concentration will occur at the center of mass
Where X=Y=Z=0

$$C_{max} = \frac{M}{8(\pi t)^{\frac{3}{2}}\sqrt{D_x D_y D_z}}$$

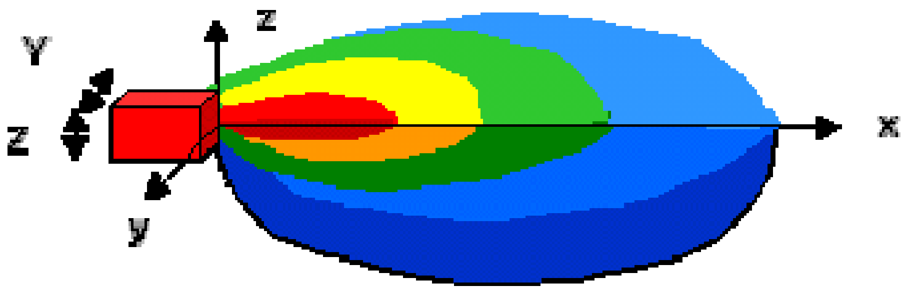
So we just considered an Analytical Solution for transport in
1-D flow field
slug source
3D spreading
without chemical reaction

$$C\left(x = vt + X, y = Y, z = Z\right) = \frac{M}{8(\pi t)^{\frac{3}{2}}\sqrt{D_x D_y D_z}} \exp\left(-\frac{X^2}{4D_x t} - \frac{Y^2}{4D_y t} - \frac{Z^2}{4D_z t}\right)$$

X Y Z = distance from center of mass in each direction



NEXT Analytical Solution for transport in
1D flow field
continuous source
3D spreading
without chemical reaction



Analytical Solution for transport in

uniform 1D flow
continuous source

3D spreading

without chemical reaction

see previous graphic

Upper case Y and Z Are the source width and height

$$C(x,y,z,t) = \frac{C_o}{8}\left(\operatorname{erfc}\left(\frac{x-\overline{v}_x t}{2\sqrt{D_x t}}\right)\right)$$

$$\left(\operatorname{erf}\left(\frac{y+\frac{Y}{2}}{2\sqrt{D_y \frac{x}{\overline{v}}}}\right)-\operatorname{erf}\left(\frac{y-\frac{Y}{2}}{2\sqrt{D_y \frac{x}{\overline{v}}}}\right)\right)$$

$$\left(\operatorname{erf}\left(\frac{z+\frac{Z}{2}}{2\sqrt{D_z \frac{x}{\overline{v}}}}\right)-\operatorname{erf}\left(\frac{z-\frac{Z}{2}}{2\sqrt{D_z \frac{x}{\overline{v}}}}\right)\right)$$

Analytical Solution for transport in
uniform 1D flow
continuous source
3D spreading
without chemical reaction

If source is on the water table such that spreading is only downward

Omit (/2) on Z terms

$$C(x,y,z,t) = \frac{C_o}{8}\left(\operatorname{erfc}\left(\frac{x-\overline{v}_x t}{2\sqrt{D_x t}}\right)\right)$$

$$\left(\operatorname{erf}\left(\frac{y+\frac{Y}{2}}{2\sqrt{D_y \frac{x}{\overline{v}}}}\right)-\operatorname{erf}\left(\frac{y-\frac{Y}{2}}{2\sqrt{D_y \frac{x}{\overline{v}}}}\right)\right)$$

$$\left(\operatorname{erf}\left(\frac{z+Z}{2\sqrt{D_z \frac{x}{\overline{v}}}}\right)-\operatorname{erf}\left(\frac{z-Z}{2\sqrt{D_z \frac{x}{\overline{v}}}}\right)\right)$$

Analytical Solution for transport in uniform 1D flow continuous source 3D spreading without chemical reaction

$$C(x,y,z,t) = \frac{C_o}{4}\left(\operatorname{erfc}\left(\frac{x - \bar{v}_x t}{2\sqrt{D_x t}}\right)\right)$$

$$\left(\operatorname{erf}\left(\frac{y + \frac{Y}{2}}{2\sqrt{D_y \frac{x}{\bar{v}}}}\right) - \operatorname{erf}\left(\frac{y - \frac{Y}{2}}{2\sqrt{D_y \frac{x}{\bar{v}}}}\right)\right)$$

If source is of full vertical extent in a confined aquifer

OR

if you are far from a limited extent source in a confined aquifer

Change Co/8 to Co/4

Omit z terms

Decay

$$\frac{dN}{dt} = -\lambda N$$

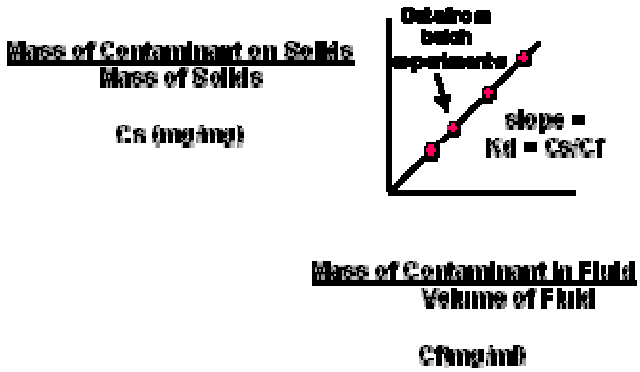
$$\text{or} \quad N = N_o e^{(-\lambda t)}$$

$$\text{where} \quad \lambda = \frac{0.693}{T_{\frac{1}{2}}}$$

decay constant

0.693 is the natural log of 0.5

Retardation - Adsorption



Units K_d

$\frac{\text{ml}}{\text{mg}}$

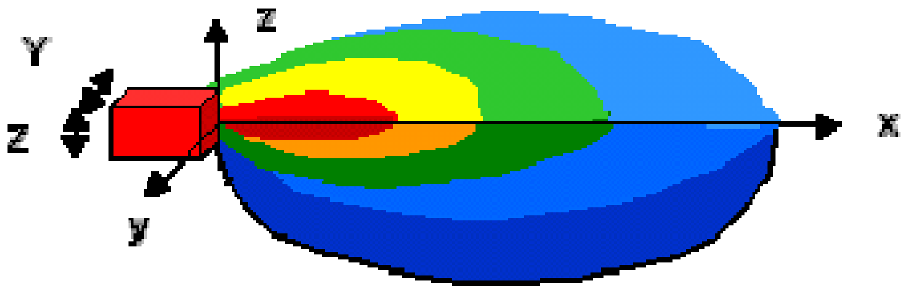
$$R = \frac{V_{water}}{V_{contaminant}} = \left(1 + \frac{\rho_b}{\phi_e} K_d\right)$$

Equation for transport in 1-D with
Decay, Retardation, Reaction, Source
Divide D's and V's by R

$$\frac{\partial C}{\partial t} = \frac{D_x}{R}\frac{\partial^2 C}{\partial x^2} - \frac{\bar{v}_x}{R}\frac{\partial C}{\partial x} + \frac{W(C - C')}{R\phi b} + \frac{CHEM}{\phi} - \lambda C$$

C	concentration in fluid
t	time
b	aquifer thickness
x	spatial coordinate
D	dispersion tensor
R	retardation coefficient
$\bar{v}$	interstitial velocity
W	source fluid flux
ϕ	porosity
C'	concentration of source fluid
CHEM	chemical reaction source/sink per unit volume of aquifer
lambda	decay constant

Analytical Solution for transport in uniform 1D flow continuous source 3D spreading With Decay



Analytical Solution for transport in uniform 1D flow continuous source 3D spreading with Decay

$$C(x,y,z,t) = \frac{C_o}{8} \exp\left(\frac{x}{2\alpha_x}\left(1-\sqrt{1+\frac{4\lambda\alpha_x}{\bar{v}}}\right)\right)$$

$$\left(erfc\left(\frac{x-\bar{v}t\left(1+\sqrt{\frac{4\lambda\alpha_x}{\bar{v}}}\right)}{2\sqrt{\alpha_x \bar{v} t}}\right)\right)$$

$$\left(erf\left(\frac{y+\frac{Y}{2}}{2\sqrt{\alpha_y x}}\right) - erf\left(\frac{y-\frac{Y}{2}}{2\sqrt{\alpha_y x}}\right)\right)$$

$$\left(erf\left(\frac{z+\frac{Z}{2}}{2\sqrt{\alpha_z x}}\right) - erf\left(\frac{z-\frac{Z}{2}}{2\sqrt{\alpha_z x}}\right)\right)$$

If R>1 Divide $\bar{v}$ by R

Note this includes a simplification of D=α$\bar{v}$

$D_y \frac{x}{\bar{v}}$ if D^* is ignored then equivalent to $\alpha_y \bar{v} \frac{x}{\bar{v}}$ which $= \alpha_y x$

Upper case Y and Z Are the source width and height

Same modifications apply for downward & no vertical spreading

$$C(x,y,z,t) = \frac{C_o}{2}\exp\left(\frac{x}{2\alpha_x}\left(1-\sqrt{1+\frac{4\lambda\alpha_x}{\bar{v}}}\right)\right)\left(erfc\left(\frac{x-\bar{v}t\left(1+\sqrt{\frac{4\lambda\alpha_x}{\bar{v}}}\right)}{2\sqrt{\alpha_x \bar{v} t}}\right)\right)\left(erf\left(\frac{Y}{2\sqrt{\alpha_y x}}\right)\right)\left(erf\left(\frac{Z}{2\sqrt{\alpha_z x}}\right)\right)$$

Analytical Solution for transport in uniform 1D flow continuous source 3D spreading with Decay

Upper case Y and Z Are the source width and height

ON THE CENTER LINE

i.e. y = z = 0

If R>1 Divide $\bar{v}$ by R

$$C(x,y,z,steadystate) = \frac{C_o}{4}\exp\left(\frac{x}{2\alpha_x}\left(1-\sqrt{1+\frac{4\lambda\alpha_x}{\bar{v}}}\right)\right)\left(erf\left(\frac{y+\frac{Y}{2}}{2\sqrt{\alpha_y x}}\right)-erf\left(\frac{y-\frac{Y}{2}}{2\sqrt{\alpha_y x}}\right)\right)\left(erf\left(\frac{z+\frac{Z}{2}}{2\sqrt{\alpha_z x}}\right)-erf\left(\frac{z-\frac{Z}{2}}{2\sqrt{\alpha_z x}}\right)\right)$$

Analytical Solution for transport in uniform 1D flow continuous source 3D spreading with Decay

Upper case Y and Z Are the source width and height

AT STEADY STATE

i.e. Mass is decaying as fast as it is being supplied at the source

If R>1 Divide $\bar{v}$ by R

Analytical Solution for transport in

uniform 1D flow

$$C(x,y,z,t)=\frac{C_o}{8}\exp\left(\frac{x}{2\alpha_x}\left(1-\sqrt{1+\frac{4\lambda\alpha_x}{\bar{v}}}\right)\right)\left(erfc\left(\frac{x-\bar{v}t\sqrt{1+\frac{4\lambda\alpha_x}{\bar{v}}}}{2\sqrt{\alpha_x\bar{v}t}}\right)\right)\left(erf\left(\frac{y+\frac{Y}{2}}{2\sqrt{\alpha_y x}}\right)-erf\left(\frac{y-\frac{Y}{2}}{2\sqrt{\alpha_y x}}\right)\right)\left(erf\left(\frac{z+\frac{Z}{2}}{2\sqrt{\alpha_z x}}\right)-erf\left(\frac{z-\frac{Z}{2}}{2\sqrt{\alpha_z x}}\right)\right)$$

$$C(x,y,z,steadystate)=C_o\exp\left(\frac{x}{2\alpha_x}\left(1-\sqrt{1+\frac{4\lambda\alpha_x}{\bar{v}}}\right)\right)\left(erf\left(\frac{Y}{4\sqrt{\alpha_y x}}\right)\right)\left(erf\left(\frac{Z}{4\sqrt{\alpha_z x}}\right)\right)$$

STEADY STATE ON THE CENTER LINE

i.e. Mass is decaying as fast as it is being supplied at the source

i.e. y = z = 0

If R>1 Divide $\bar{v}$ by R

THINK IN TERMS OF ORGANIZING THE ANALYTICAL SOLUTIONS IN TERMS OF

THE TYPE OF SOURCE:

SLUG OR CONTINUOUS

TYPE OF SPREADING:

1D, 2D, 3D

TYPE OF CONTAMINANT BEHAVIOR:

DECAYING, ADSORPING

(and if so steady-state? center-line?)