

Fate and Transport—Rapid Overview



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Chemical
Descriptors

- T_b , T_m , MW
- Solvation parameters

Partition and
Rate
Coefficients

- K_a/w , K_{ow} , K_{oc}
- Half lives

Environmental
Fate Model

- Environmental descriptors
- Discharge scenario

Abraham Solvation Parameter Example

E = excess molar refraction

S = polarizability/dipolarity

A = solute hydrogen bond acidity

B = solute hydrogen bond basicity

L = logarithmic gas-hexadecane partition coefficient

V = McGowan's molar volume

Name	CAS-RN	<i>E</i>	<i>S</i>	<i>A</i>	<i>B</i>	<i>V</i>	<i>L</i>
BDE 47 ¹	5436-43-1	-	1.45	0.00	0.34	2.083	10.660
triphenyl phosphate ²	115-86-6	1.83	1.66	0.00	1.10	2.371	11.259
tris(2-chloroethyl)phosphate ³	115-96-8	-	2.09	0.03	0.98	1.761	7.180

UFZ-Helmholtz LSER Database: [https://www.ufz.de/index.php?en=31698&contentonly=1&lserd_data\[mvc\]=Public/start](https://www.ufz.de/index.php?en=31698&contentonly=1&lserd_data[mvc]=Public/start)

¹Stenzel, A., Goss, K.-U., Endo, S. (2013) Environ. Sci. Technol., 47, 1399-1406.

²Abraham, M. H., Acree, W. E. (2013) Sep. Sci. Technol. 48, 884-897.

³Stenzel, A., Goss, K.-U., Endo, S. (2013) Environ. Sci. Technol., 47, 1399-1406.

Key Fate Parameters Estimated

Name	Log Kw/a	Log Koc	Log K b/w	Log Kow	Half life estimate
BDE 47	3.87	3.14	6.73	6.73	weeks-recalcitrant
triphenyl phosphate	7.56	4.15	4.48	4.76	days-months
tris(2-chloroethyl)phosphate	7.57	1.34	1.47	1.34	days-months

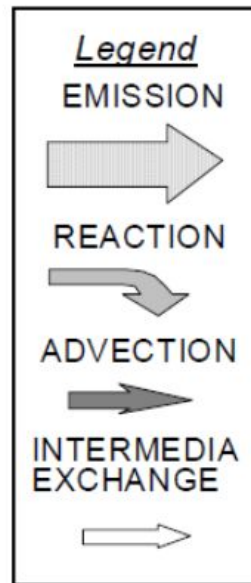
Partition coefficients calculated using Abraham parameters
Half life estimates based on BIOWIN 3 and 4

Level III

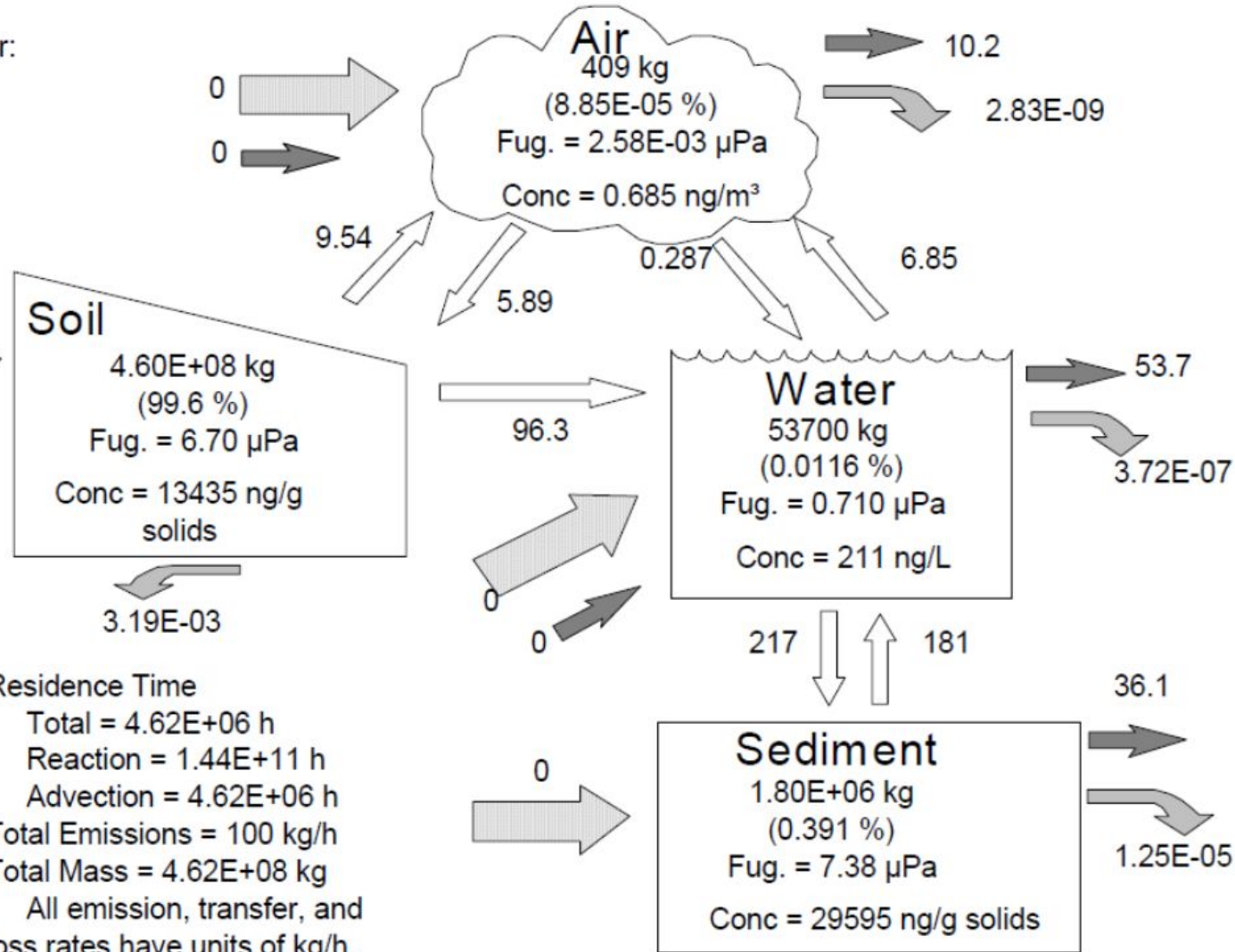
Version 2.80.1

Simulation Identifier:
BDE-47

BDE-47 in Default 1



Residence Time
Total = 4.62E+06 h
Reaction = 1.44E+11 h
Advection = 4.62E+06 h
Total Emissions = 100 kg/h
Total Mass = 4.62E+08 kg
All emission, transfer, and loss rates have units of kg/h.



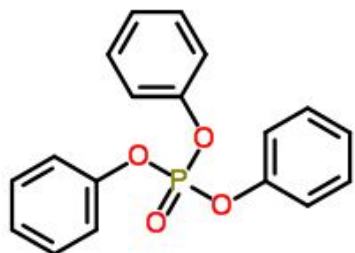
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Level III

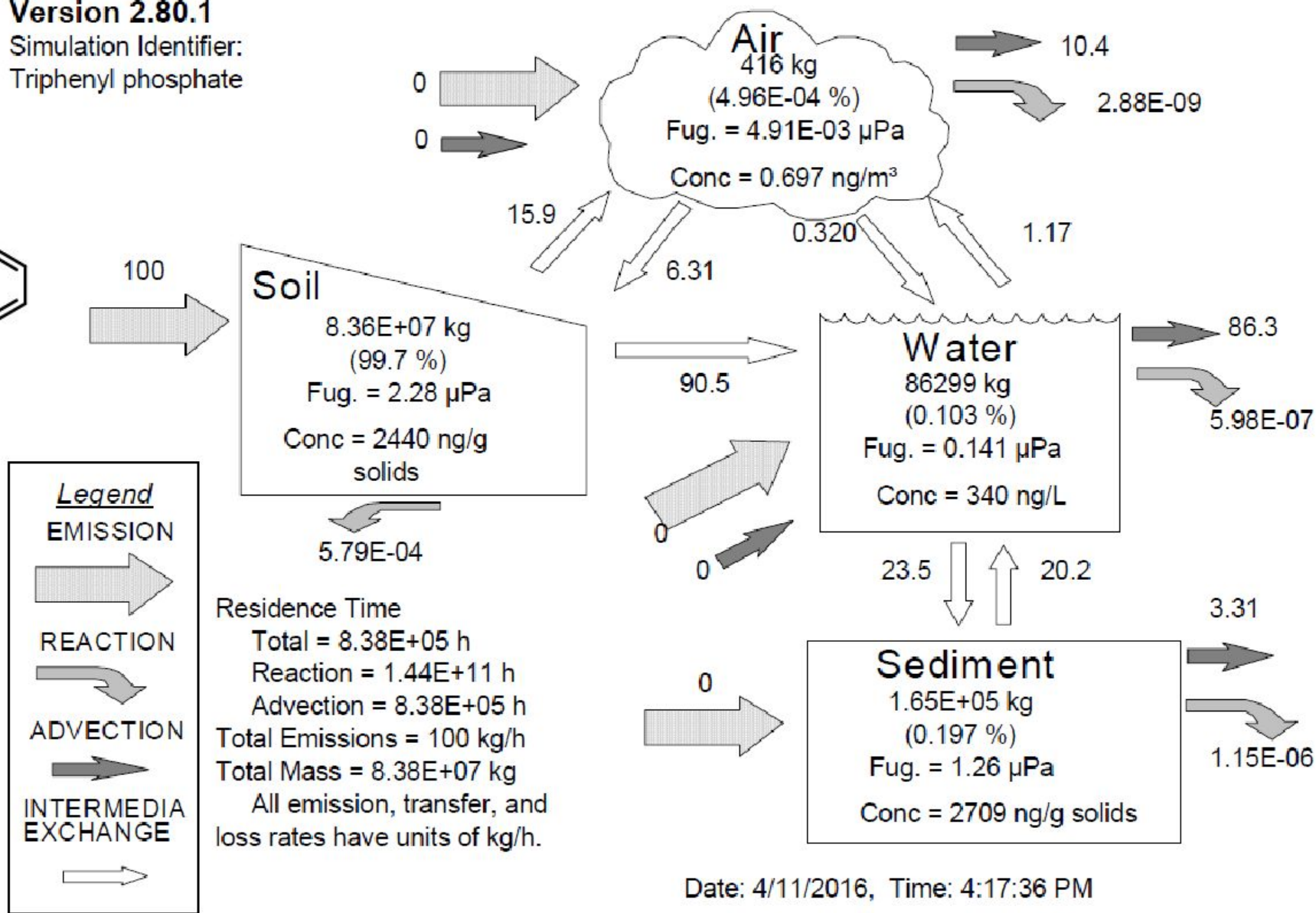
Version 2.80.1

Simulation Identifier:

Triphenyl phosphate



Triphenyl phosphate in Default 1

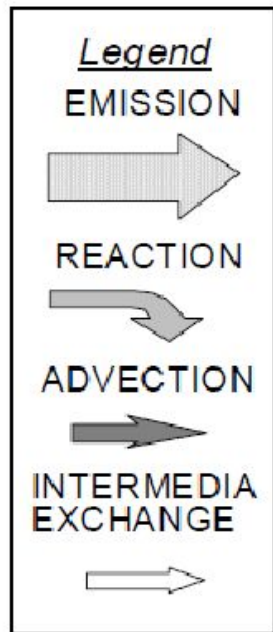
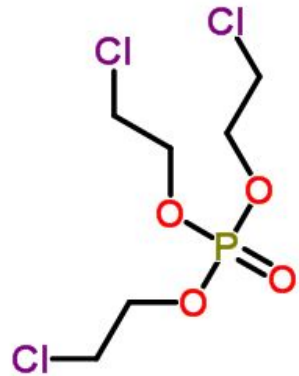


Level III

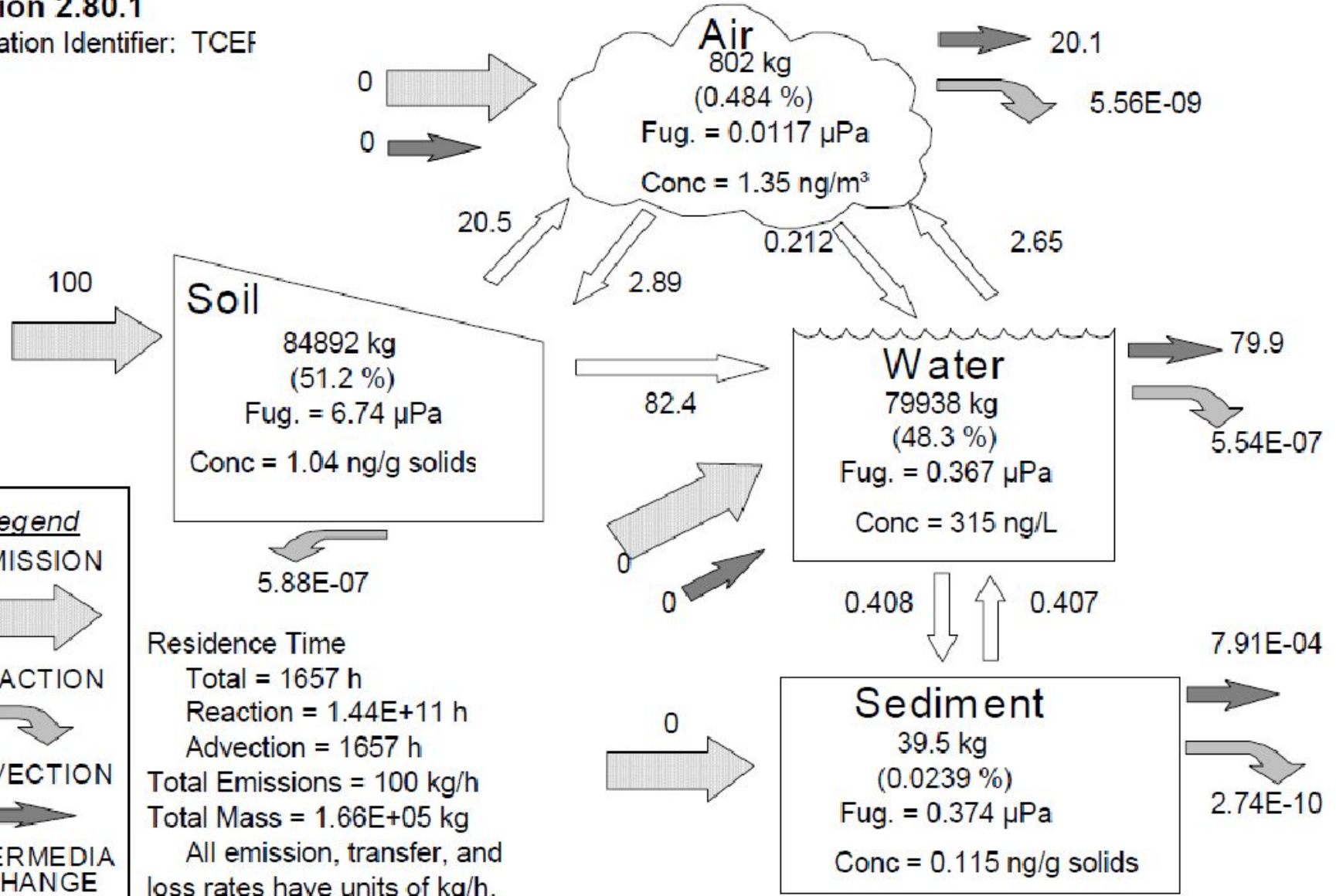
Version 2.80.1

Simulation Identifier: TCEF

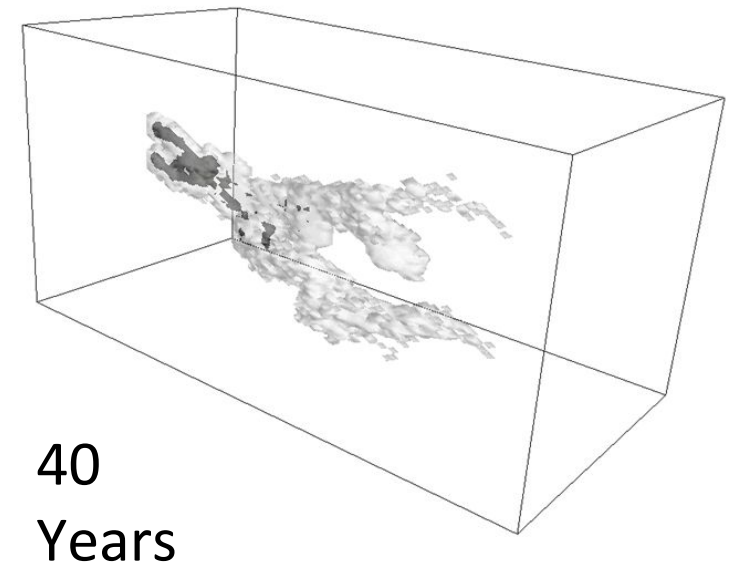
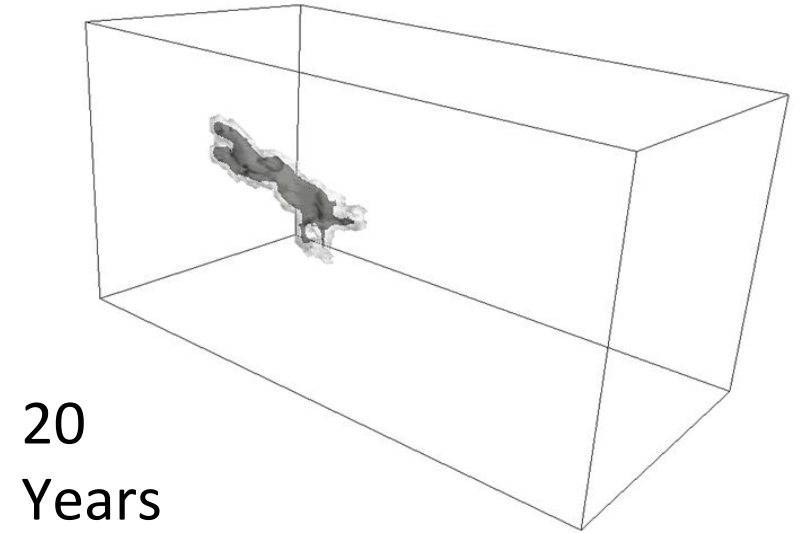
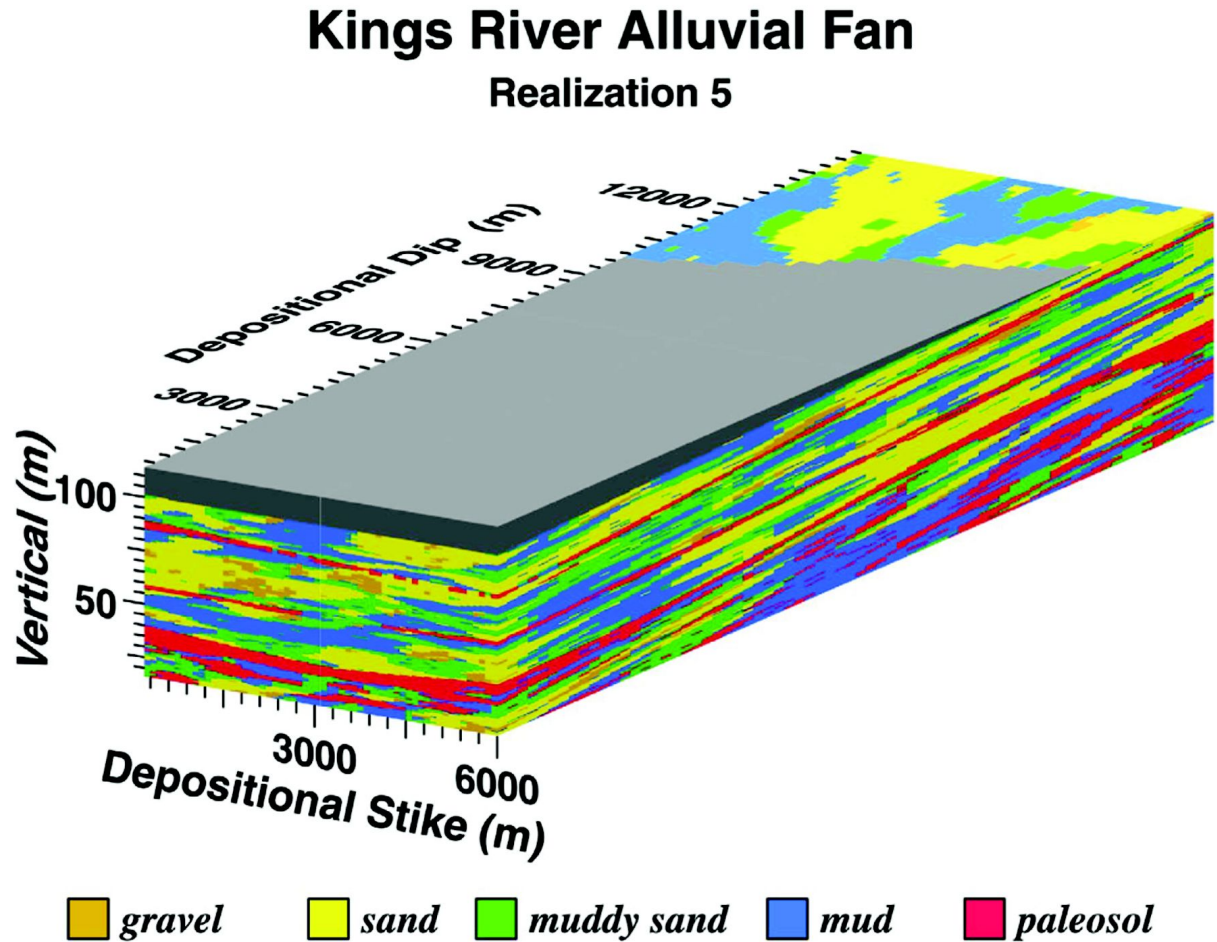
tris(2-chloroethyl)phosphate in Default 1



Residence Time
Total = 1657 h
Reaction = 1.44E+11 h
Advection = 1657 h
Total Emissions = 100 kg/h
Total Mass = 1.66E+05 kg
All emission, transfer, and loss rates have units of kg/h.



Reality is Heterogeneous



Courtesy: Prof. Graham Fogg

Additional Complications

- Nonideal Sorption
 - nonlinear isotherms
 - rate limitations
 - hysteresis
- Mixture Effects
 - cosolvency
- Biodegradation:
 - pathway prediction
 - cometabolism