OpusCZ Modeling Methodology

What Does OpusCZ do?

A simultaneous numerical solution of equations representing

- Surface water flow,
- Soil water flow,
- Soil erosion,
- Chemical transport in porous media,
- Chemical transport in surface water flow,
- Pesticide degradation,
- Nutrient cycling, and
- Crop growth and transpiration,

with boundary conditions that approximate natural topography, using appropriate input and time steps.

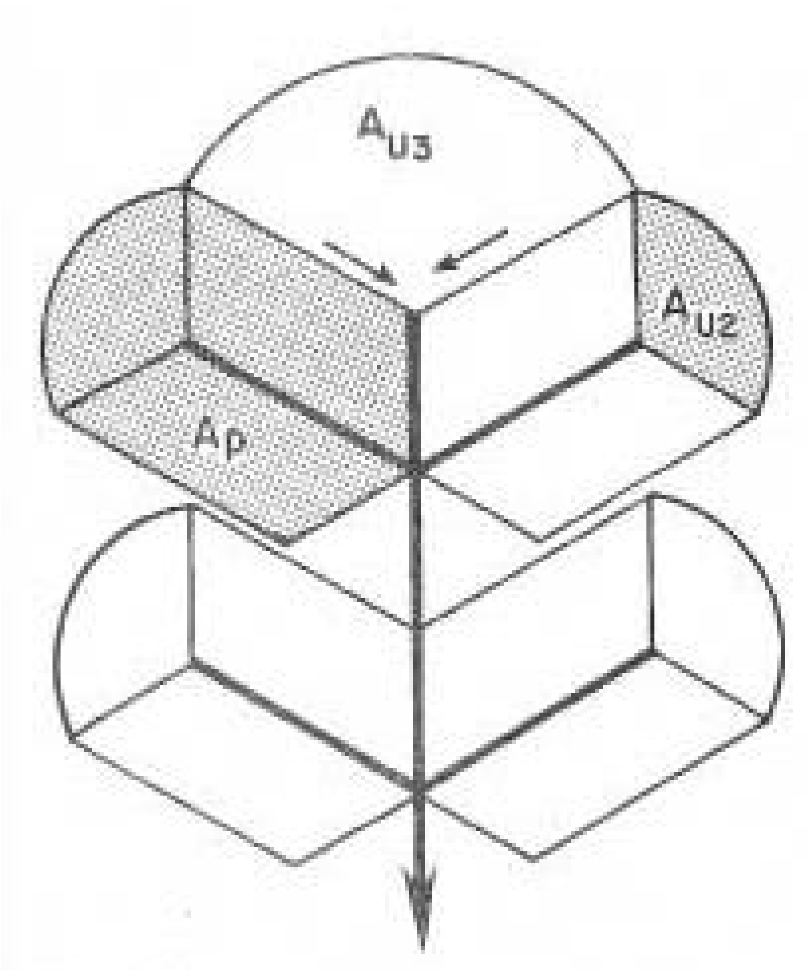
Opus and her Descendants

- Opus: 1992. USDA Ag. Research Service model building on and modernizing methodology from CREAMS
- Opus2: 2003. Developed in New Zealand with improvements to Opus, including better with pesticide simulation.

Müller, K, R.E. Smith, T.K. James, P.T. Holland, and A. Rahman, 2003. Prediction of field atrazine persistence in an allophonic soil with Opus2. Pest Management Science, **60**, pp. 447-458.

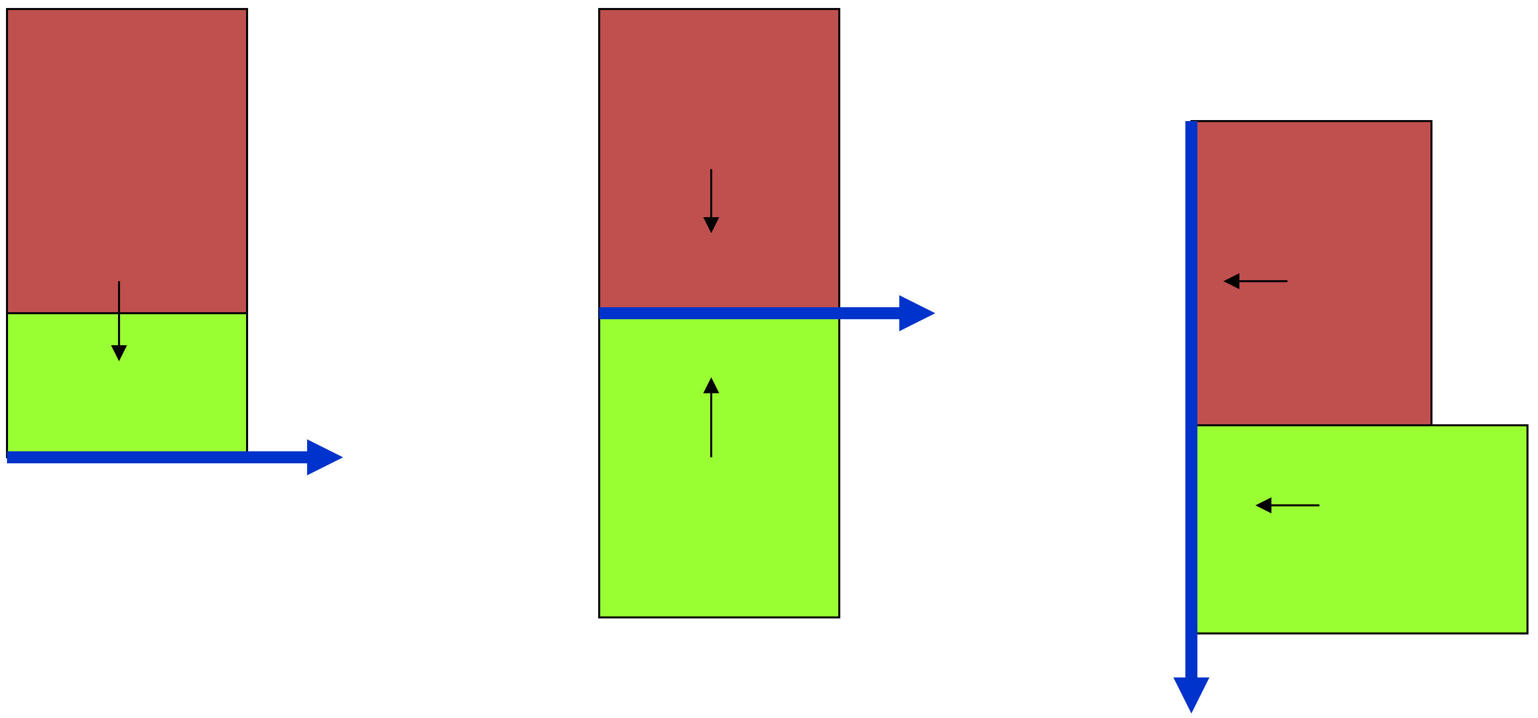
- OpusZ: 2-dimensional version of Opus2 with simplified topology, using joint solution of Richards' equation and surface flow equations.
- OpusCZ: OpusZ with improved chemical transport features, and without subsurface lateral flow simulation.
- K2O2: A combination of OpusZ with KINEROS2, providing large watershed scale simulation ability.

Possible symmetrical topologies

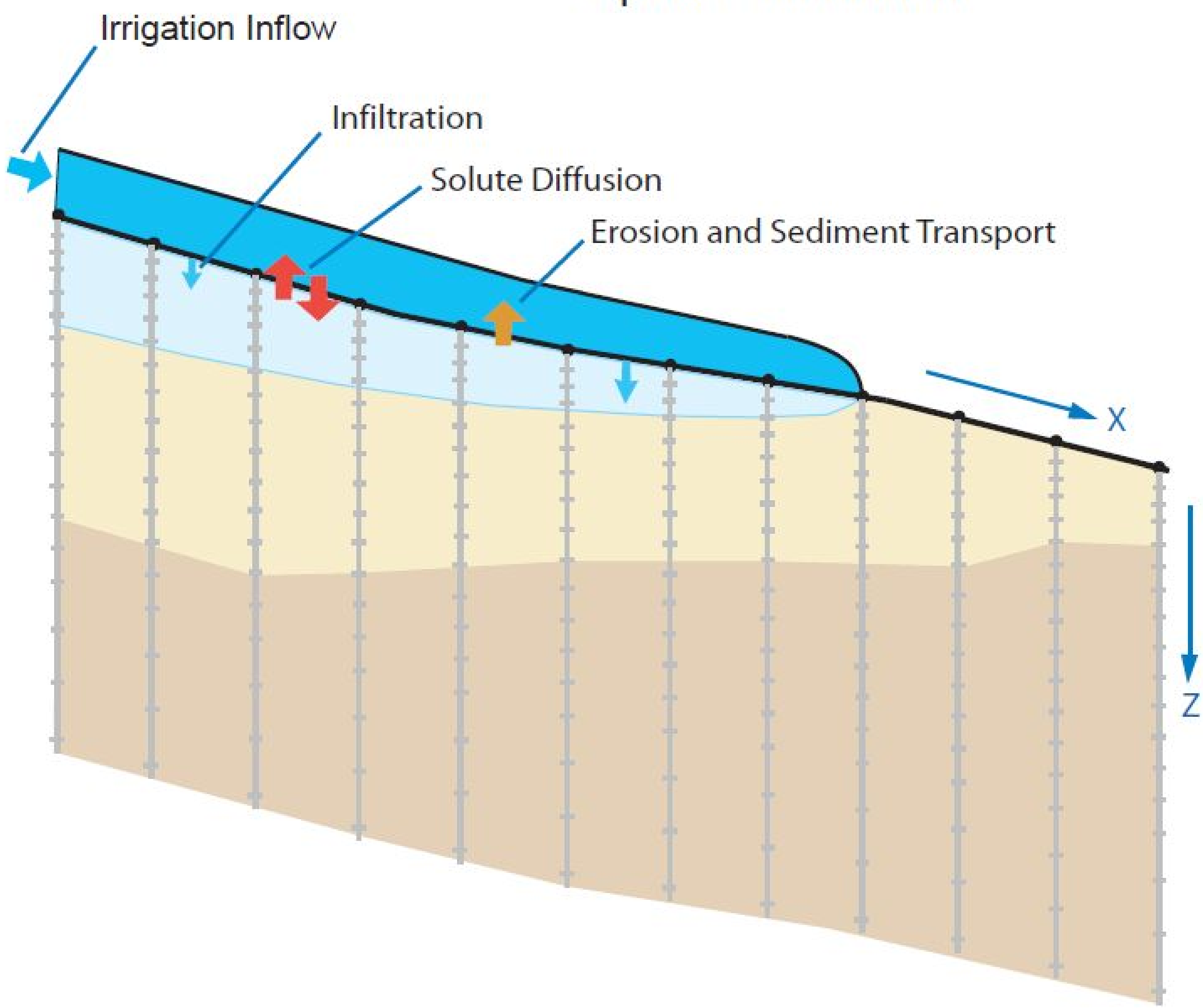


N = 4
M = 2

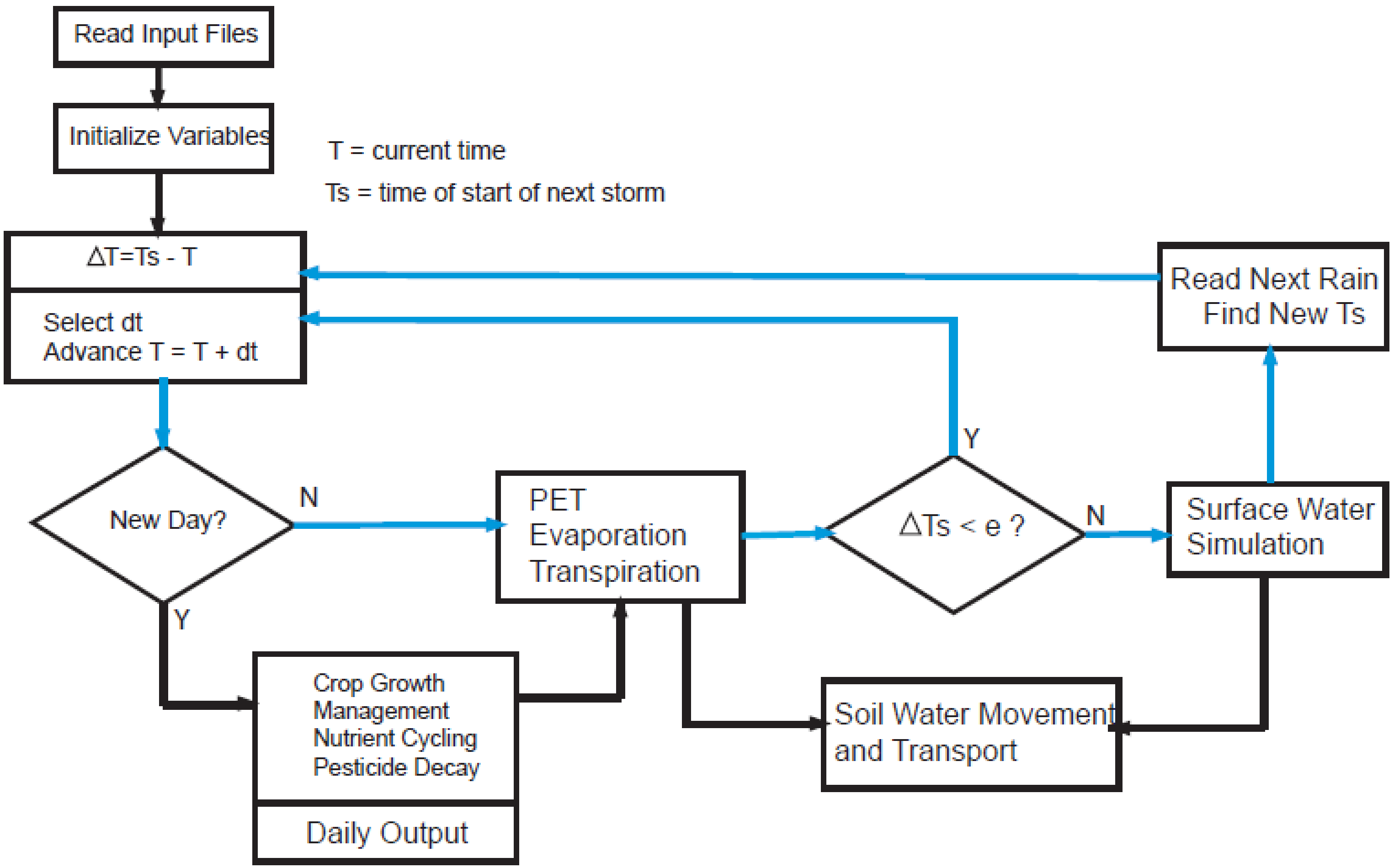
Opus2 Geometries



OpusCZ Simulation



OpusCZ Flow Diagram



Procedural Modifications in OpusCZ

	Opus	**OpusCZ**
Time Management		
	Day cycle with subdivisions	Continuous with variable Δt
Input		
Data Format	Fixed positions	Free Format on each line
Comments	Fixed	Open – * comment lines can be added

Methodological Changes in OpusCZ

	Opus	OpusCZ
Topological		
Elements	Multiple but symmetrical	1 or 2 segments in tandem
Variability	None – all identical in soil and plants	Different soils, depths, and mangement
Furrowing	Separate topology for furrowed case	No special furrow topology
Soil Hydrology		
Input	Daily or continuous rain options	Continuous rain data only
Soil water flow	Explicit solution between storms	Implicit solution every time step
Spatial variation	Single solution for each element	Solution at each node along surface
Infiltration	Analytic infiltration model	Richards' solution
Time management	External to soil model	Internal in soil model
Chemical Modeling		
Movement	Explicit Model	Implicit model
Soil-surface interaction	Approximate, parametric	Diffusion solution
Adsorption Isotherm	Linear only	Linear or Non-linear
Volatilization	Not treated	Henry's Law
Degradation	Bulk value	2-part, sigmoidal, and phase separate options
Degradation metabolites	Not treated	2 or more allowed

Chemical Movement in Soil

$$\frac{\partial\left(C_L q\right)}{\partial z} + \frac{\partial\left(C_L + \rho_B C_A\right)}{\partial t} = \delta_C$$

where:

- C_L is concentration dissolved in water, kg/L,
- C_A is concentration adsorbed to soil particles, kg/kg,
- z is depth measured downward, mm,
- q is water flux through soil, mm/T,
- ρ_B is soil bulk density, kg/L,
- δ_C is local gain (or loss) of chemical,. T^{-1}

and t is time.

Soil Solute and Surface Water interaction

$$\frac{\partial(AC_R)}{\partial t} + \frac{\partial(QC_R)}{\partial x} = w\left[\omega(C_L - C_R) - f(C_R) + RC_W\right]$$

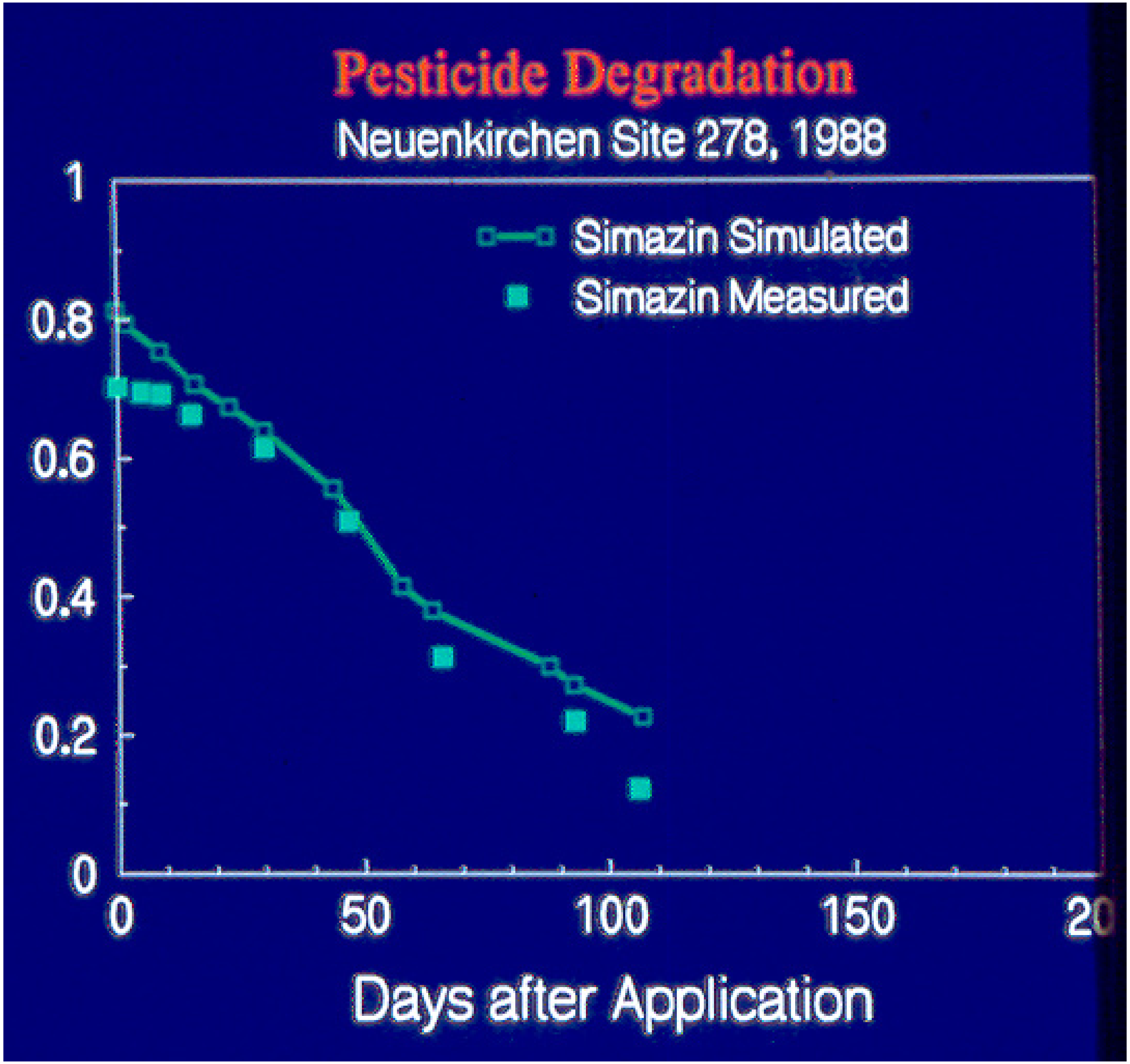
where

A	is cross sectional area of flow,
t	is time,
x	is distance along flow path,
w	is width of flow,
f	is infiltration rate,
Q	is discharge [L^3/T]
R	is rainfall rate
C_R	is concentration in surface runoff water
C_L	is dissolved concentration in surface soil
Cw	is concentration in rainfall input, if any, and
ω	is film diffusion coefficient.[L/T]

Surface interaction of soil adsorbed chemicals

$$\frac{\partial\left(AC_S C_{aR}\right)}{\partial t} + \frac{\partial\left(QC_S C_{aR}\right)}{\partial x} = w\left(\beta d C_{A1} - e_D C_{aR}\right) + q_S C_e$$

C_S	is concentration of particle size class in surface water,
C_{aR}	is concentration of adsorbed chemical on suspended sediment,
C_{A1}	is concentration of adsorbed chemical in surface soil,
β	is relative particle class weighting based on particle specific surface,
d	is gross splash and erosion detachment rate of particle class,
e_D	is gross deposition rate for particle size class (negative for erosion), and
$q_S C_e$	is an external supply (if any) of adsorbed material.



Pesticide Degradation
Neuenkirchen Site 278, 1988
1
0.8
0.6
0.4
0.2
0
Simazin Simulated
Simazin Measured
0
50
100
150
Days after Application

Chemical Degradation Types

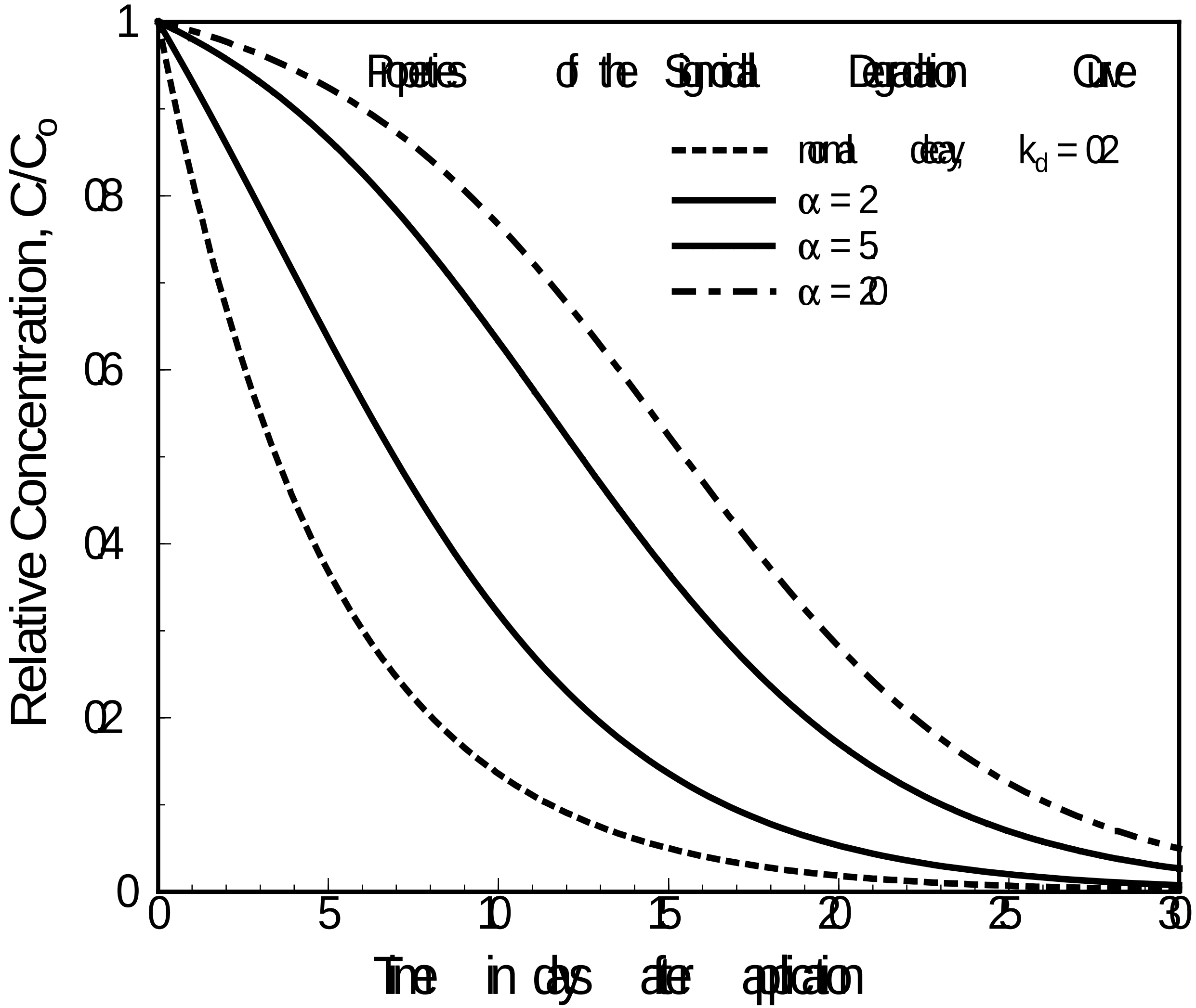
Compound First-order Model:

$$C(t) = C_o \left[(1-\alpha) e^{k_1 t} + \alpha e^{k_2 t} \right]$$

Sigmoidal Degradation Model:

$$\frac{C(t)}{C_o} = \frac{1+\alpha}{\alpha + e^{k_1 t}} \qquad \alpha = \frac{e^{k\delta t} - 1}{1-y} \qquad y = C/C_o$$

Sigmoidal Degradation



Adsorption Isotherms

Linear and Freundlich: $$C_a = K_F {C_S}^{\eta}$$

Langmuir: $$C_a = \frac{K_L C_S}{(\beta + C_S)}$$

Volatization (simplified)

$$\frac{E_C}{E_W} = \frac{H_C}{2.7 \times 10^{-5}}$$

In Summary

- Hydraulic and chemical methodology is more realistic than in Opus
- Crop and nutrient /residue model retained from Opus
- A large number of simulation options are available, but
- A large number of parameters and input data need to be measured or well known for models of this type to give realistic results.
- Models of this type are sophisticated scientific tools, but not “black boxes”