A Mass Balance Approach Updating the SWAT Pesticide Module for Applications to EMCONs

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Objective

- Updating pesticide model in SWAT
- Rederive the Lavoisier mass balance in the pesticide component of SWAT
- Run numerical simulations comparing the current pesticide model in SWAT and the newly developed Lavoisier mass balance model

Significance of SWAT

- Predict long-term impact of management practices on basin
- Chemical fate in surface and ground waters
- Increasing importance with increase in herbicides, pesticides & EMCON's
    - Examples used
        - Herbicide: Monsanto's Round Up (glyphosate)
        - EMCON (Growth Hormone): trenbolone
        - Pesticides: malathion, methoxychlor, DiBrClpropane

HRU

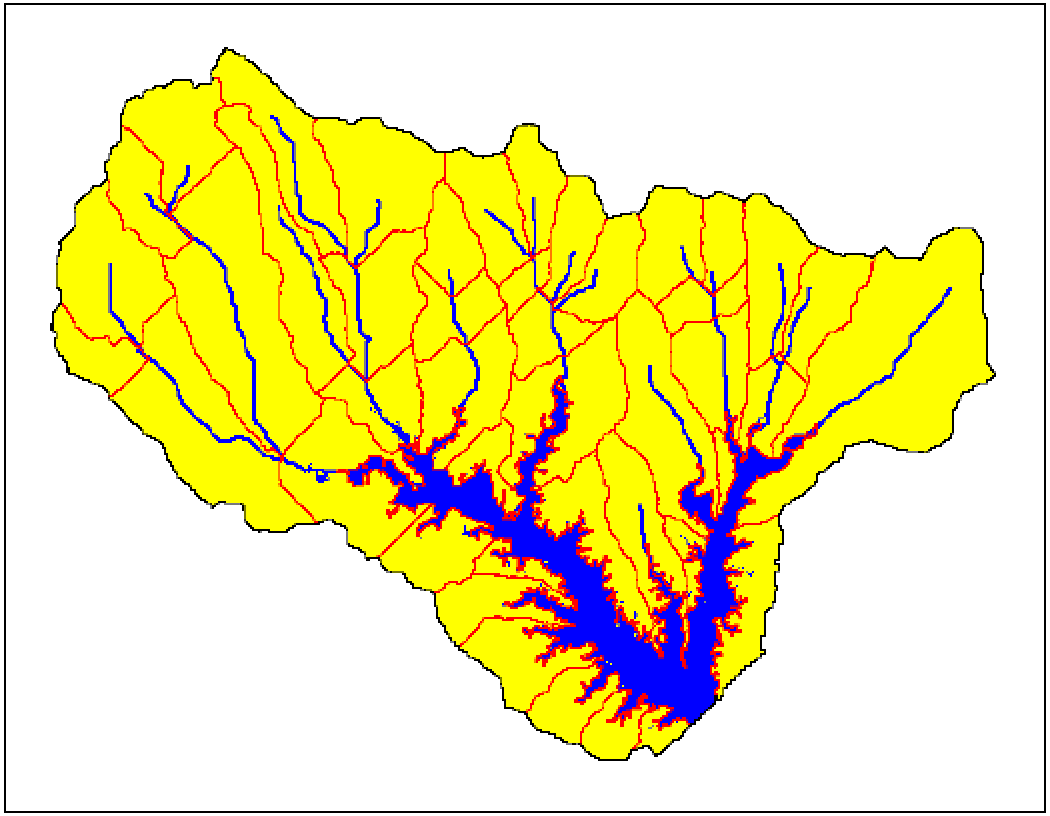


Figure 0.2: Subbasin delineation of the Lake Fork Watershed.

[Swat Theoretical Documentation, 2005]

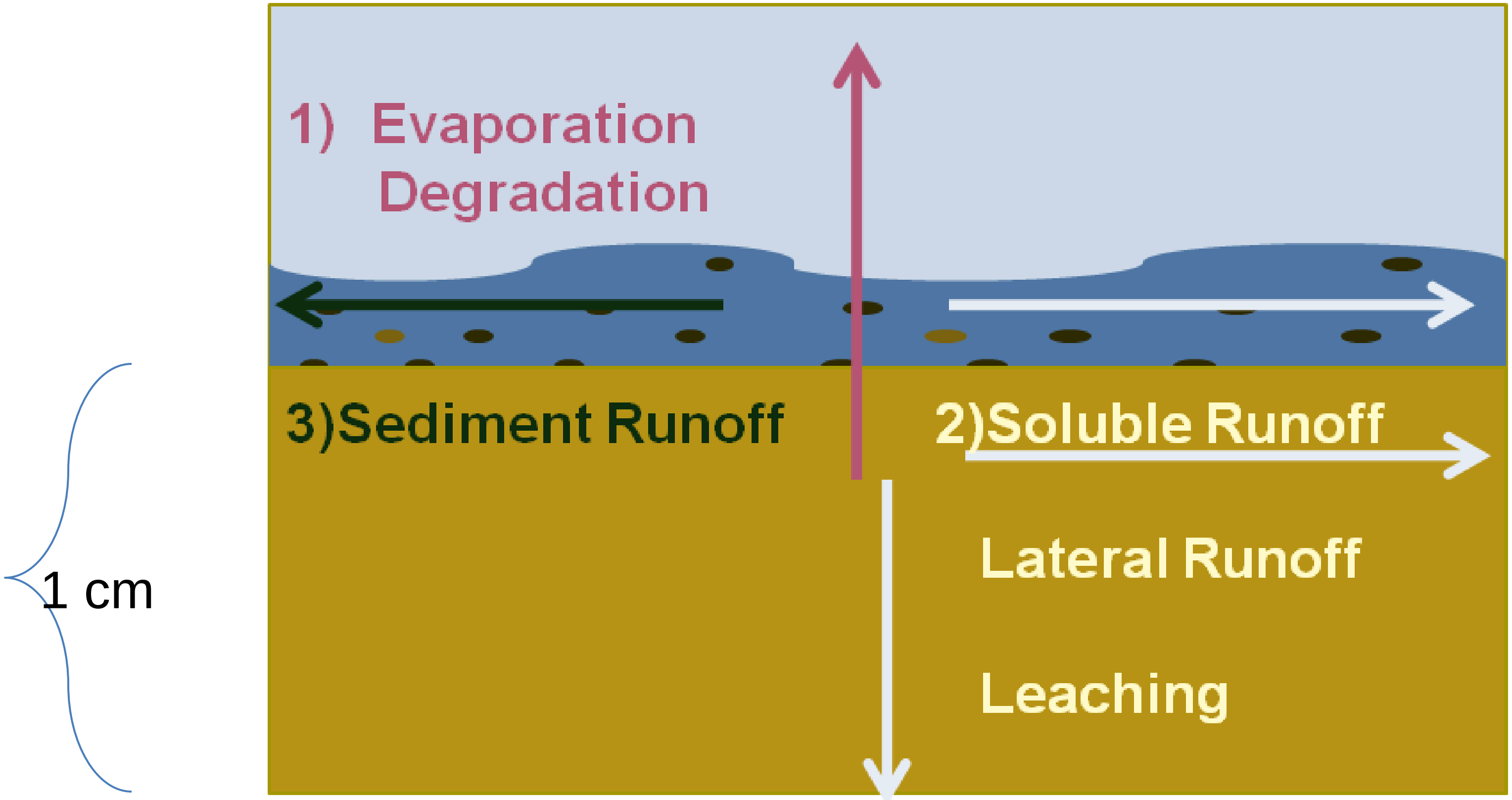
Modeling based on Hydraulic Response Unit (HRU) [SWAT Theoretical Documentation, 2005]

- Similar Soil types

•HRU- lumped land areas within the sub-basin with unique land cover, soil, management combinations [SWAT Theoretical Documentation 2005].

•Control Volume for chemical fate model

HRU Surface Soil Layer



3 SWAT Processes

1. Combined 1st order rate constant
2. Combined 1st order rate constant
3. Constant rate parameter

SWAT Soil Surface Pesticide Algorithm

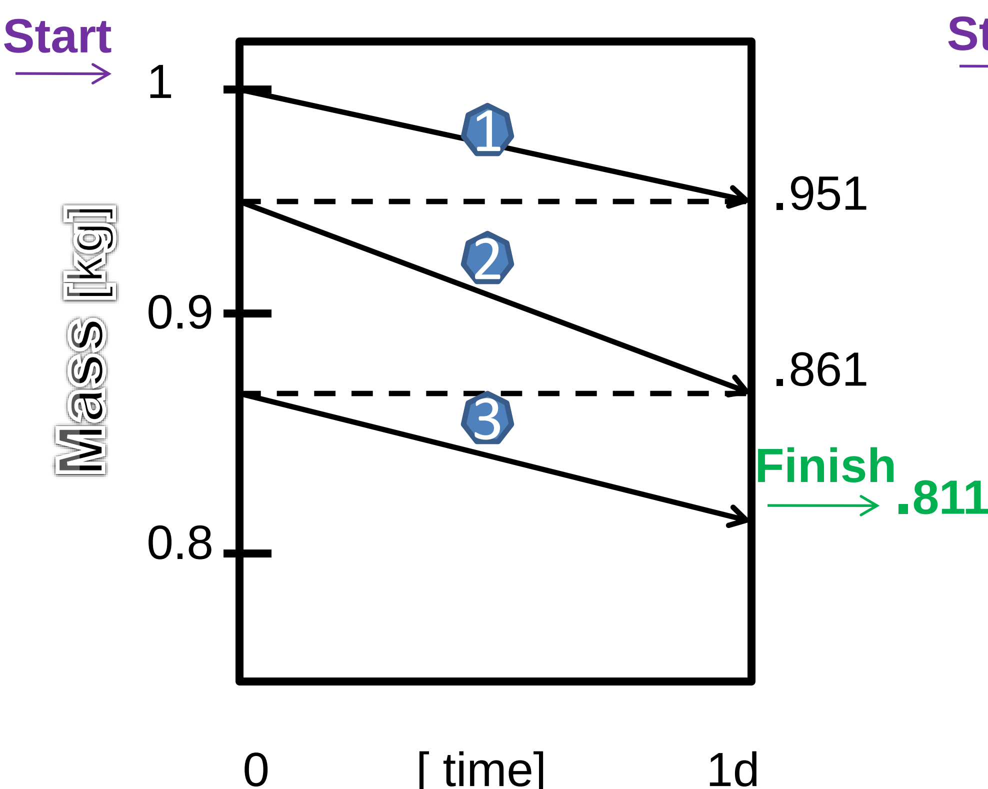
1. $Pst = Pst_0 e^{-(K_{rxn})t}$
   - ❑ Evaporation
   - ❑ Degradation
2. $P_{st} = P_{sto} e^{-(K_{sol})t}$
   - ❑ Soluble Runoff
   - ❑ Lateral Runoff
   - ❑ Leaching
3. $P_{st} = P_{sto} - tK_{ero}$
   - ❑ Sediment Runoff

Variable	Definition	Unit
P_{st}	Pesticide remaining in layer at time t	kg/ha
P_{sto}	Initial pesticide concentration loading	kg/ha
K_{rxn}	rate constant for degradation, evaporation and removal of pesticide in soil	1/day
K_{ero}	Constant rate of Pesticide sorbed into lateral runoff	kg/ha*da y
K_{sol}	rate constant for soluble transport in runoff	1/day
t	time	day

***Sequence is not fixed**

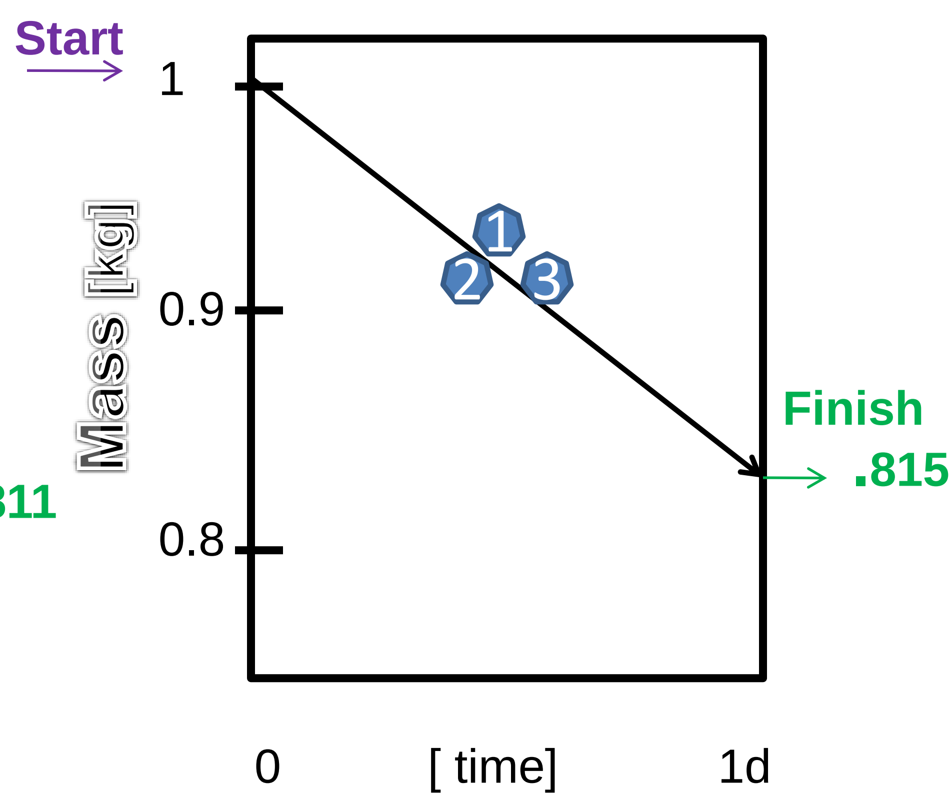
SWAT

- Computation procedure within SWAT is performed sequentially since there are three equations.



LAVOISIER MASS BALANCE

- The computation algorithm is a single equation reflecting the overall processes which occur simultaneous.



Lavoisier Mass Balance(LVM)

- ❑Mass Balance on 1cm soil surface layer
  - Simultaneous Vs. sequencing in SWAT
- ❑ Integrated Mass Balance for comparison

$$\boxed{P_{st} = [P_{sto} - \frac{K_{ero}}{K}]e^{-(Kt)} + \frac{K_{ero}}{K}}$$

$$\text{where; } K = \left(K_{evap} + K_{rxn} + K_{sol}\right)$$

$$; K_{rxn} = K_{bio} + K_{photo} + K_{hyd}$$

- Evaluated using glyphosate, trendbolone, methoxychlor, melathion, dibromochloropropane

Model Parameters

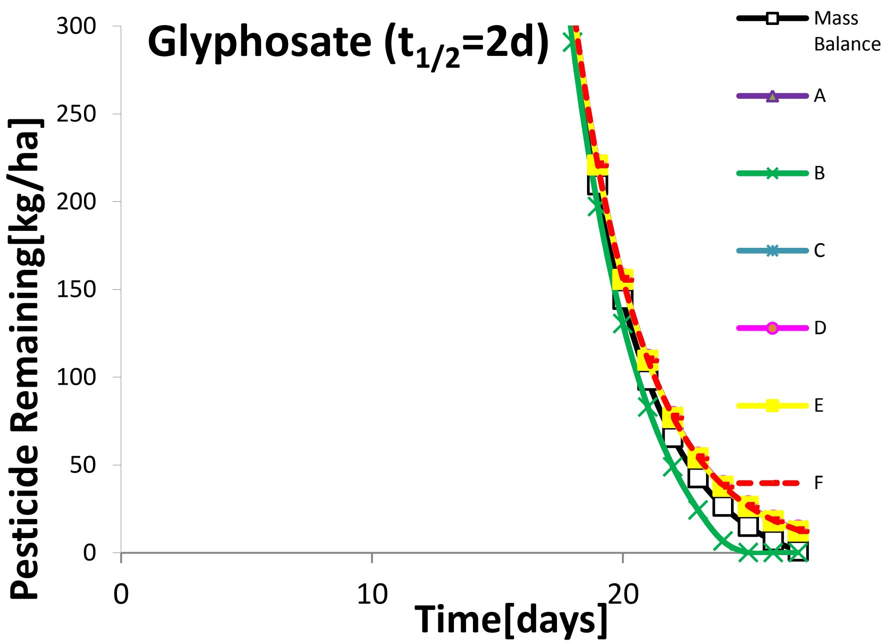
Chemical=A	$t_{1/2}$[d]	Koc [m^3/kg]	Hp	MW	K_{rxn} [d^{-1}]	K_{evap} [d^{-1}]	K_{sol} [d^{-1}]	K_{ero} [mgA/d*m]
Glyphosate	2	2.072	5.76E-9	169	0.3465	5.37E-9	4.17E-4	0.444
Glyphosate	197	2.072	5.76E-9	169	0.0035	5.37E-9	5.37E-9	0.444
Trenbolone	4	0.589	7.77E-8	270	0.173	2.53E-3	1.05E-3	4.44E-5
DiBrClpropane	45	0.04	1.0E-2	202	0.015	3.78	9.35E-2	0.444
Malathion	1	0.23	4.9E-6	330	0.693	2.64E-4	1.83E-2	0.444
Methoxychlor	100,360	80	3.0E-5	346	0.00693	4.56E-6	5.40E-5	0.444

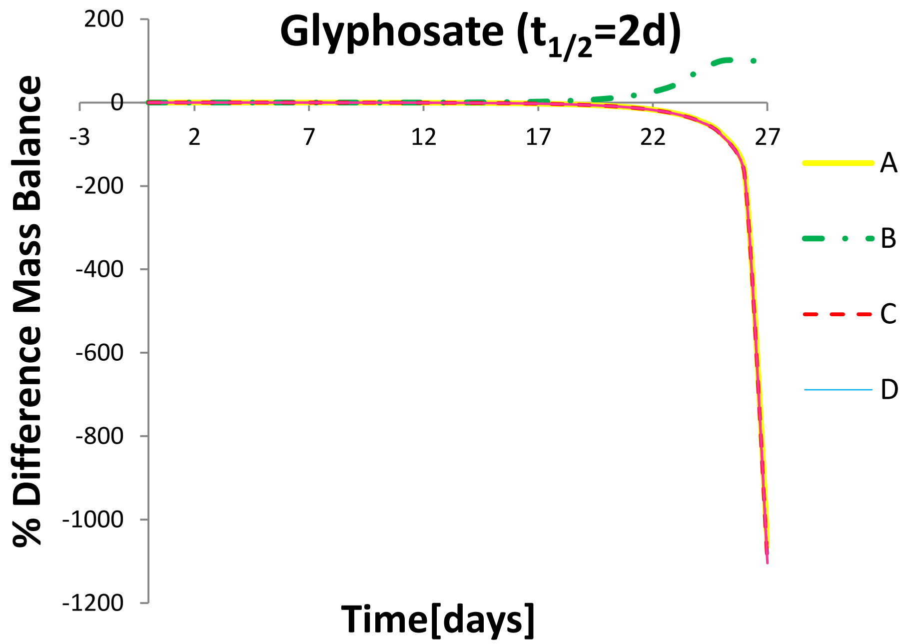
SWAT Sequencing

A	B	C	D	E	F
1→2→3	1→3→2	2→3→1	3→1→2	2→1→3	3→2→1

1) Reaction
2) Solute Transport
3) Pesticide in Runoff

Results : Glyphosate





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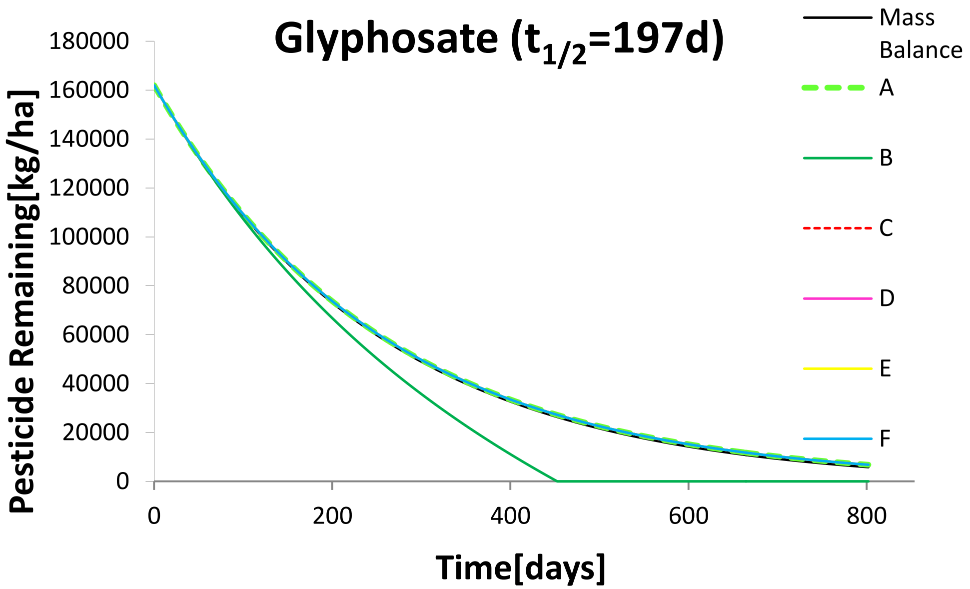

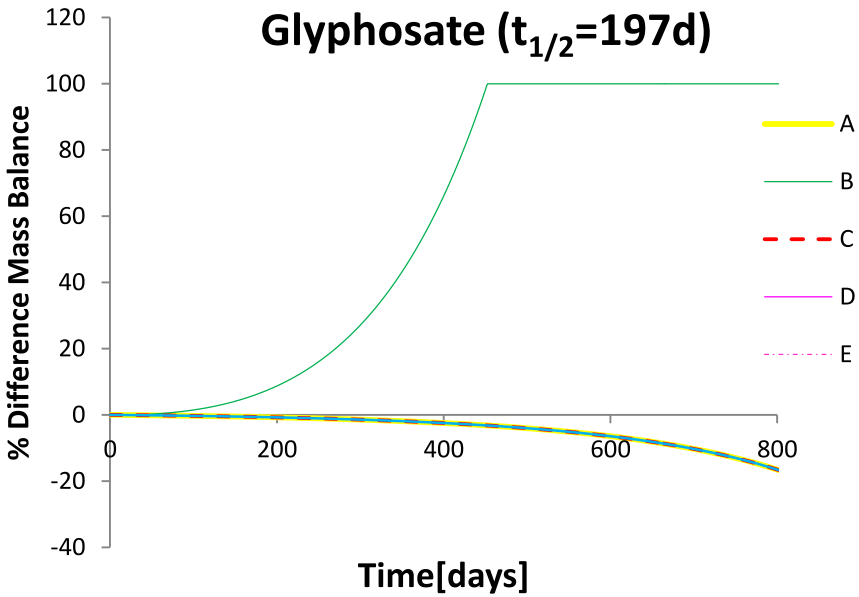

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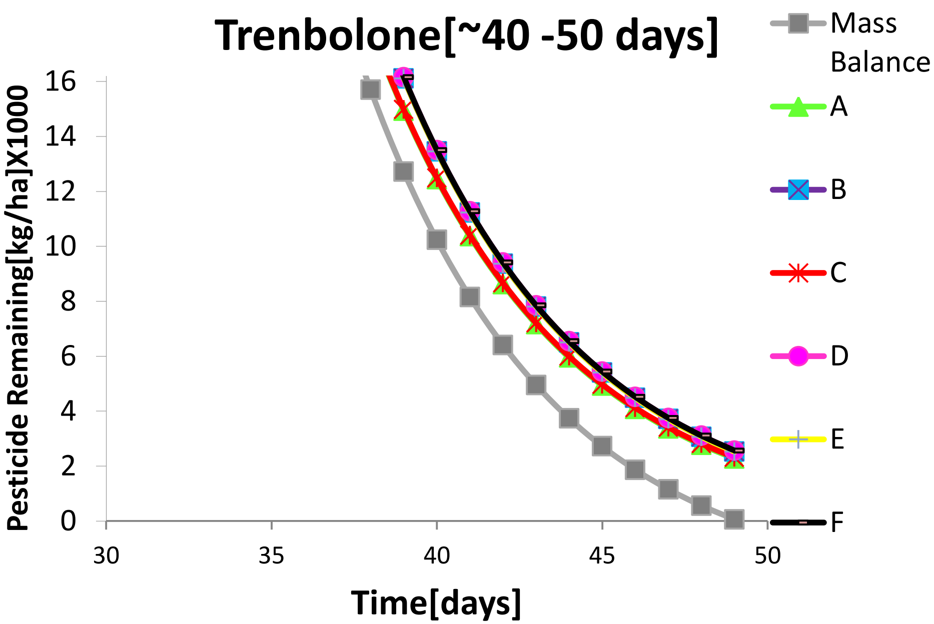
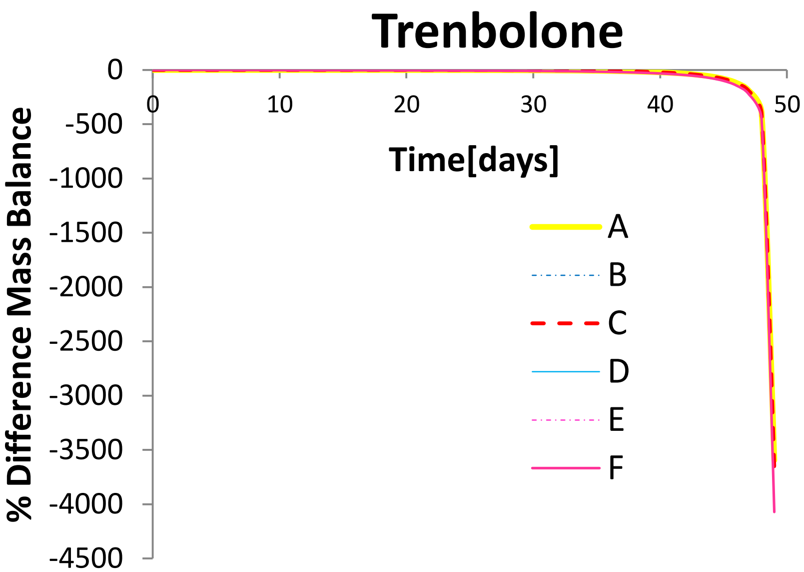
1→2→3	1→3→2	2→3→1	3→1→2	2→1→3	3→2→1

1) Reaction; 2) Solute Transport; 3) Pesticide in Runoff

Results: Trenbolone

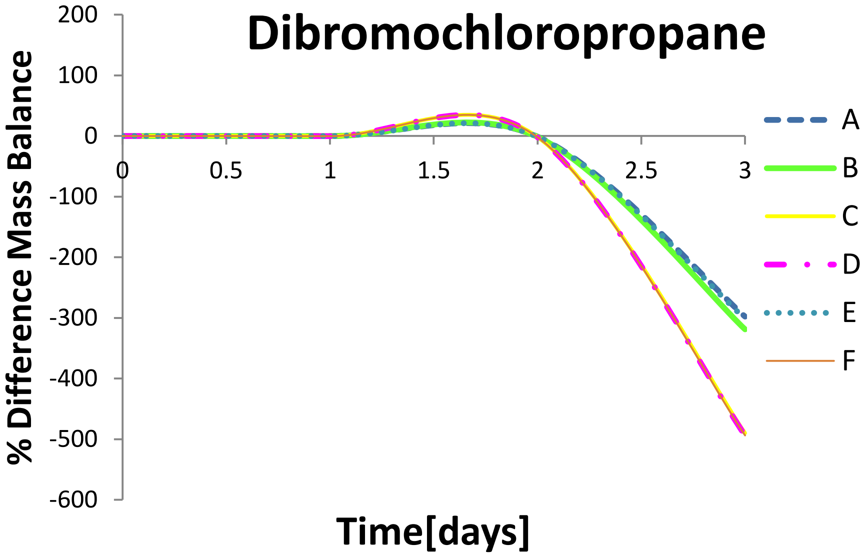


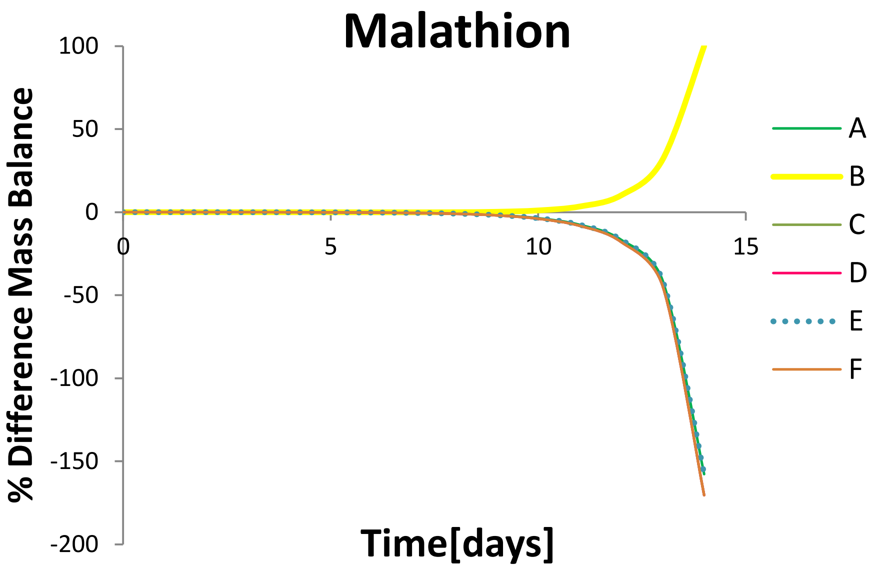


A	B	C	D	E	F
1→2→3	1→3→2	2→3→1	3→1→2	2→1→3	3→2→1

1) Reaction; 2) Solute Transport; 3) Pesticide in Runoff

Results





A	B	C	D	E	F
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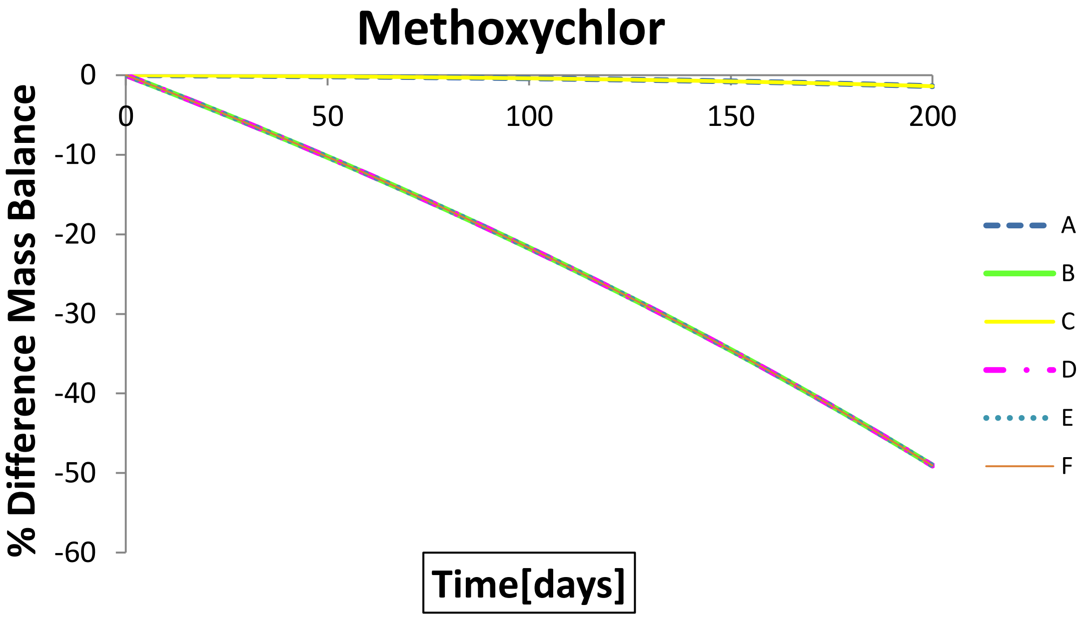
1) Reaction; 2) Solute Transport; 3) Pesticide in Runoff

Results Continued



A	B	C	D	E	F
1→2→3	1→3→2	2→3→1	3→1→2	2→1→3	3→2→1

1) Reaction; 2) Solute Transport; 3) Pesticide in Runoff

Conclusion

- The present SWAT pesticide module is the appropriate place for developing an EMCON module
- Transforming the sequential process code to a simultaneous process code that reflects the[Lavoisier] mass balance on the HRU is recommended
- Further research EMCON reaction, transport and thermodynamic partitioning and update pesticide algorithms
- Extend application of mass balance approach to deeper soil layers and other sub-units on the HRU


Questions?

SWAT Model Assumptions/Characteristics

- User defined Watershed divided into 2-5 sub layers
- Chemical concentration and properties assumed constant in control volume(HRU)
- Model time series
  - 1 time step=1day
  - Growing seasons
- Rain, temperature, water content, concentration in layers, etc. updated daily
- Model tracks chemodynamics in HRU
- Model computes the mass of chemical, soil in runoff ,from HRU

$$K_{rxn} = \frac{0.693}{\tau_{1/2(bio)}} + \frac{0.693}{\tau_{1/2(ph0to)}} + \frac{0.693}{\tau_{1/2(hydro)}}$$

$$K_{evap} = \frac{K'_{A13}}{K^*_{A31}\,\rho_3 h_3}$$

The evaporation half life (K'_{A13}) is the ratio of the overall mass transfer coefficient for pesticide vapor transport from the soil-–to-atmosphere (to the soil-to-air pesticide partition coefficient (, soil thickness (and bulk density of the soil (The units respectively are day^{-1}, meters/day, m^3/kg, meters, and kg/ m^3.

$$K'_{A13} = [\frac{1}{k'_{A1}} + \frac{.5h_3}{D_{A1}\epsilon_1^{4/3}}]^{-1}$$

The overall mass transport coefficient, depends on the air side mass transfer coefficient ([meters/day]), the chemical's molecular diffusivity in air ([m^2/day]) the volumetric air content of the soil (, and the soil thickness.

Round UP

- Active ingredient-glyphosate
- “inert” ingredients-Ethoxylated tallowamine, isopropylamine, Diazinon
- Leading herbicide
  - 100 million pounds applied to U.S farms and lawns every year (EPA)
- Regulated at relatively high concentrations in our drinking water
  - Toxic
  - Carcinogenic
- Roundup’s “inert” ingredients have been recently seen to have toxic effects on human cells

[1]Enviromental Health News , [2] Organicconsumers.org

EMCONS , PBT, & Emerging Toxic substances

- endocrine disrupting compounds (EDCs)
- pharmaceutical drugs
- personal care products (PPCPs)
- atrazine (herbicide)
- caffeine
- Contamination of drinking water

Development of Lavoisier Mass Balance

$$\frac{d}{dt}\iiint_V C_A\,dV = \iint_A C_A\overline{\mathbf{V}}\bullet(-\overline{\mathbf{n}})\,dA + \iint_A \left(\overline{\mathbf{j}}_{\mathbf{D}} + \overline{\mathbf{j}}_{\mathbf{V}}\right)_A \bullet(-\overline{\mathbf{n}})\,dA + \iiint_V r_A\,dV + \sum_1^n w_A$$

Accumulation	Advective Transport	Diffusive Transport	Chemical Reaction	Forced Inputs
	Particle(soils) erosion	Evaporation		Pesticides
	Solubility	Leaching		

•HRU is the control volume

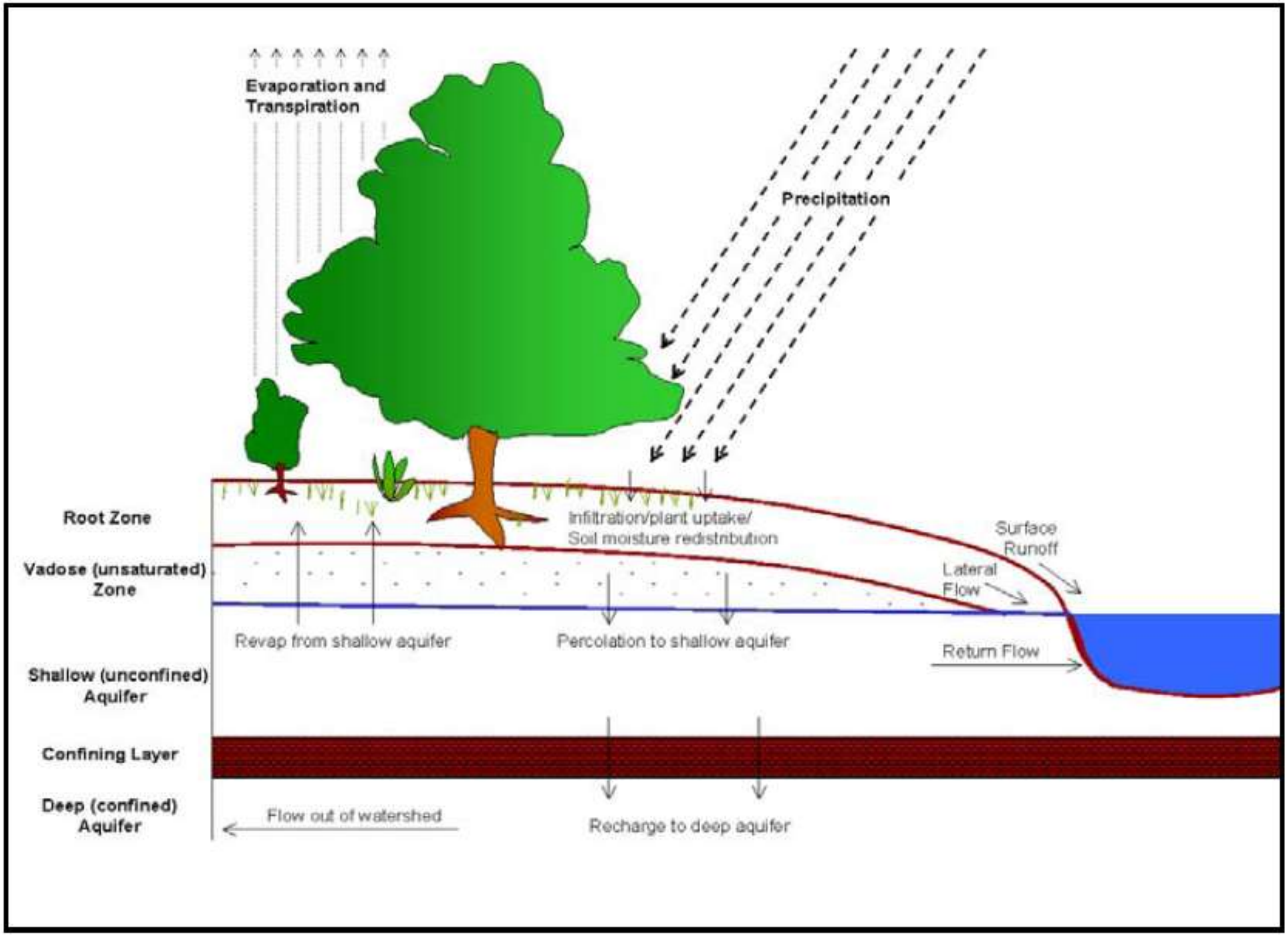


Figure 0.3: Schematic representation of the hydrologic cycle.

[Swat Theoretical Documentation, 2005]

Mass Balance continued – connecting the media boxes

Chemical flux across media boxes, examples:

Vaporization from soil to air:

$$j_D = k_a\left[C_A^* - C_A(\text{air})\right]$$

k_a = vaporization MTC

Soil particle erosion to atmosphere:

$$j_V = v_r C_A(\text{soil surface})$$

v_r = resuspension velocity

Soil-to-air partitioning:

$$C_A(\text{soil}) = K_{SA} \cdot C_A^*$$

K_{SA} = partition coefficient

Air-to-water partitioning:

$$C_A(\text{air}) = H_C \cdot C_A(\text{water})$$

H_C = Henry's constant

Transport coefficients k_a and v_r (m s^{-1}); partition coefficients K_{SA} and H_C (L kg^{-1}).