

# LECTURE #13

AGCHEM
PROCESSES, PARAMETERS
AND CALIBRATION





## PERLND STRUCTURE CHART

#### **PERLND**

Simulate a pervious land segment

ATEMP

Correct air temperature

**SNOW** 

Simulate snow and ice

**PWATER** 

Simulate water budget

**SEDMNT** 

Simulate sediment

**PSTEMP** 

Estimate soil temperature(s)

**PWTGAS** 

Estimate water temperature and gas concentrations

**POUAL** 

Simulate general quality constituents

**AGCHEM** 

**MSTLAY** 

Estimate solute transport

**PEST** 

**Simulate pesticides** 

**NITR** 

Simulate nitrogen

**PHOS** 

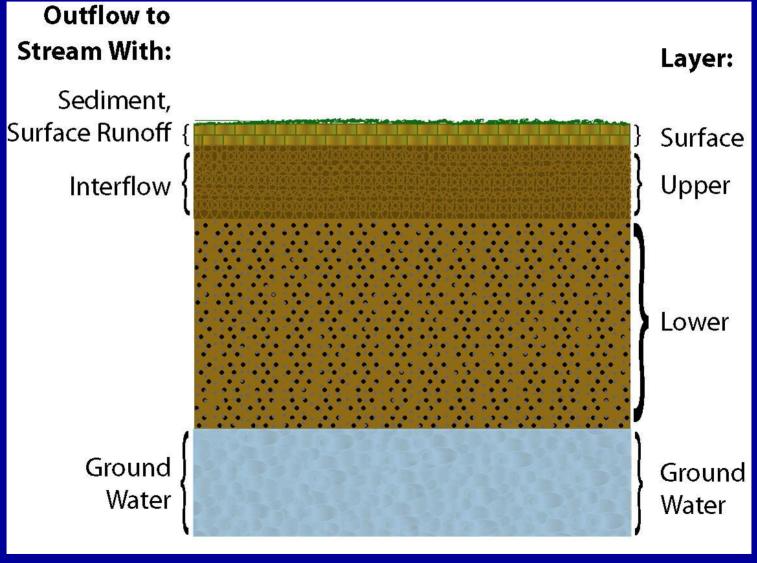
Simulate phosphorus

TRACER

Simulate a conservative tracer

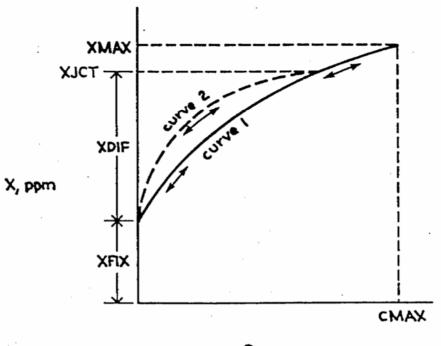
#### PESTICIDE CYCLING IN THE ENVIRONMENT APPLIED PESTICIDE Sprays, granules, pellets, fumigants Direct fall Drift **Volatility** AT MOSPHERE Wet and dry Injection **Volatilization Volatilization** Wet and dry Injection deposition soil deposition pellets, incorporation etc. Leaching WATER → Decay, exudation → PLANTS - Decay, exudation → SOIL -Absorption- Absorption,Irrigotion --- Irrigation, overflow, etc -Surface runoff, erosion, leaching, groundwater flow-

# SOIL PROFILE REPRESENTATION BY THE AGCHEM MODULE





### FREUNDLICH ISOTHERM CALCULATIONS



C, ppm

 $X = KF1 * C^{1/N1} + XFIX$ 

#### Where

X = Chemical Adsorbed to the Soil

C = Chemical in Solution

XFIX = Chemical Permanently Adsorbed to the Soil

N1 = Freundlich Exponent

KF1 = Freundlich Coefficient





# THEORETICAL DEGRADATION CURVE

Pesticide Concentration in Soil

**Application losses** Volatilization Leaching, volatilization, chemical breakdown, adsorption Enzymatic degradation, leaching and volatilization

Time →





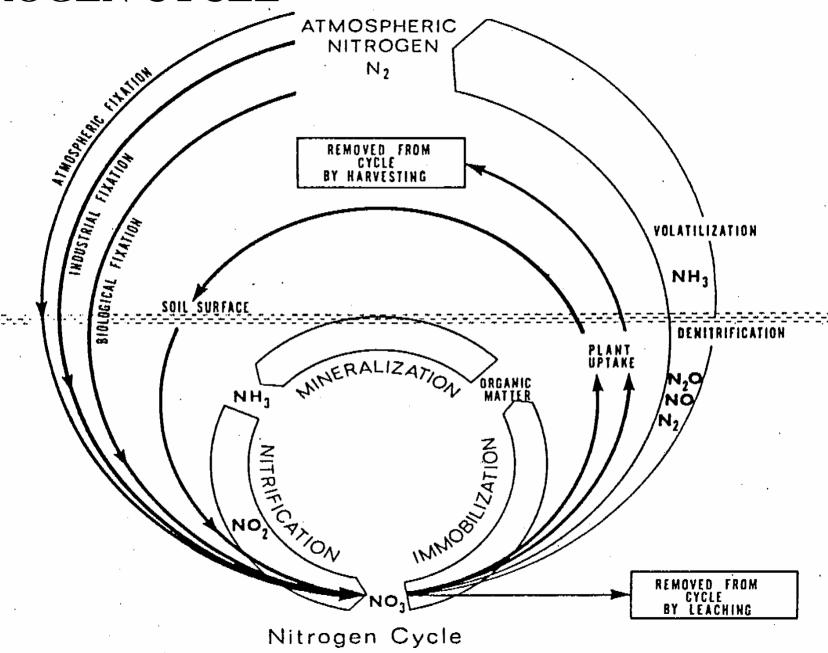
# PESTICIDE (PEST) CALIBRATION

- 1. Estimate All Pesticide (PEST) and Solute Leaching (MSTLAY)

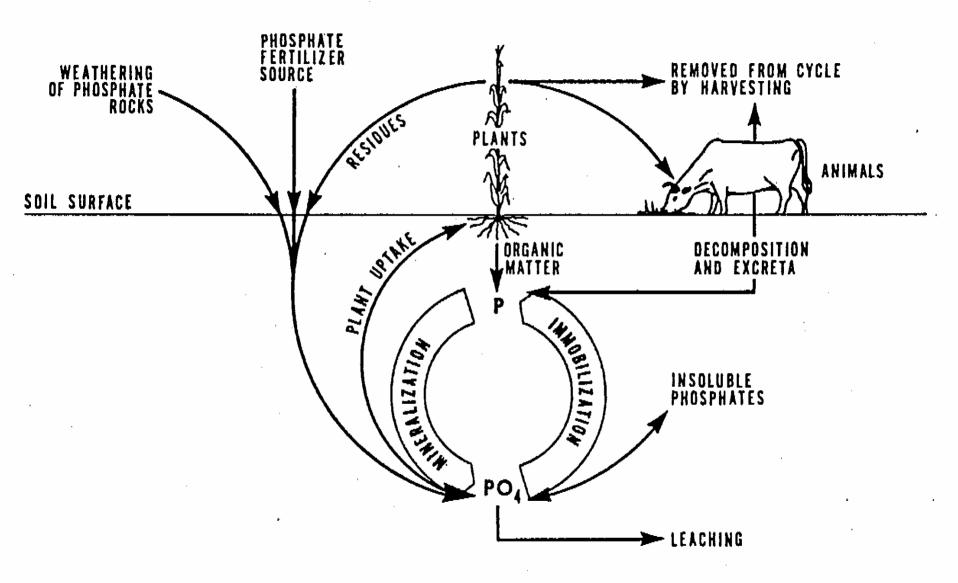
  Parameters and Application Rates
- 2. Adjust Pesticide Decay Rates (Primary Surface and Upper Soil Zones)
- 3. Adjust Solute Leaching Parameters to Reflect the Pesticide Distribution between the Surface and Upper Zones
- 4. Adjust Adsorption/Desorption Parameters to Reflect the Proper Distribution between Solution and Adsorbed Forms
- 5. Compare/Evaluate Storm Event Pesticide Losses and Make Further Parameter Adjustments as Discussed above



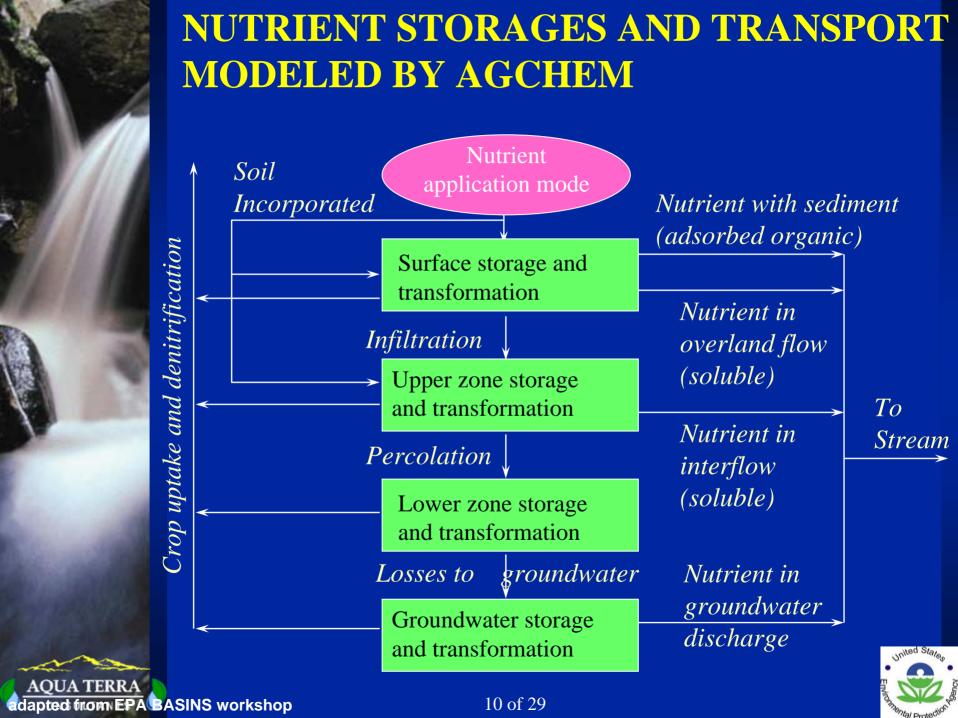
## **NITROGEN CYCLE**



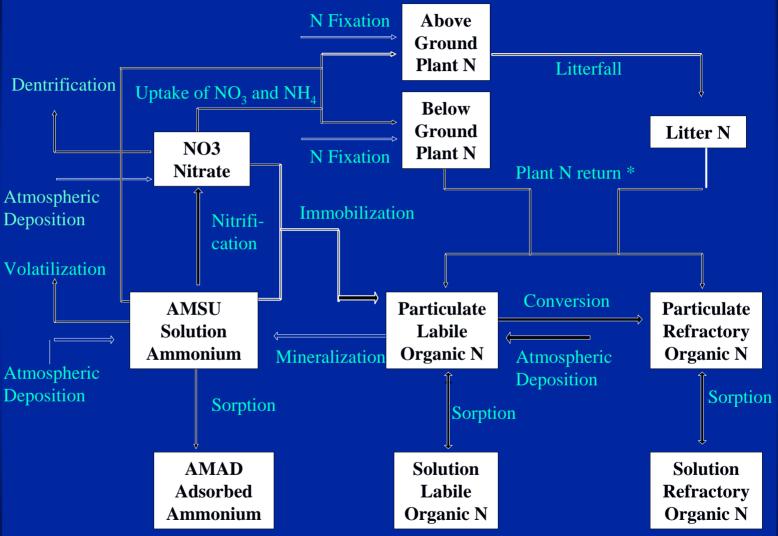
## PHOSPHORUS CYCLE



Phosphorus Cycle



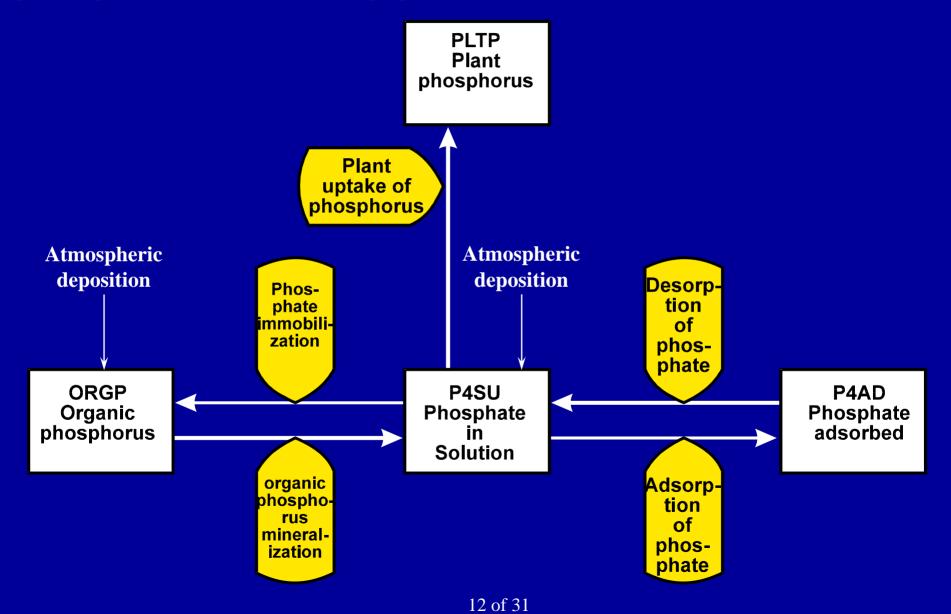
# NITROGEN TRANSFORMATIONS SIMULATED BY AGCHEM



\* Return of above ground N and litter N occurs with only surface and upper zones



# PHOSPHORUS TRANSFORMATIONS SIMULATED BY AGCHEM



# NUTRIENT (NITR, PHOS) SIMULATION IN AGCHEM #1

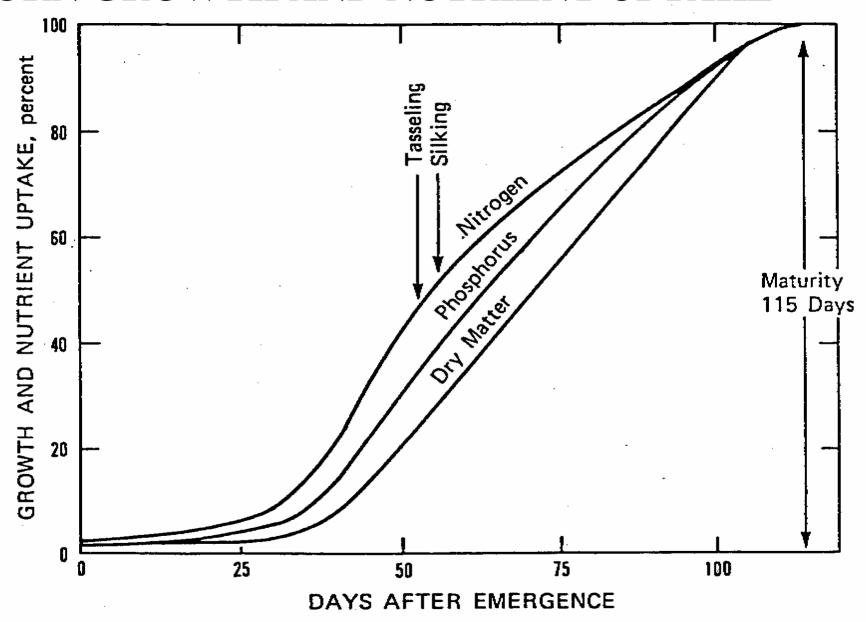
- First-order reaction rates for all biological processes; other options available for selected nitrogen processes
- Input optimum reaction @ 35°C are adjusted for lower soil temperatures using Arrhenius formulation; reactions are considered optimum above 35°C, and stopped below 4°C
- NH<sub>4</sub>/PO<sub>4</sub> adsorption/desorption can be either kinetic, with first-order rates, or equilibrium with either Freundlich or linear partitioning
- Reactions performed, and parameters specified in each soil layer
- Timesteps: chemical and biological can be different, specified as multiples of hydrologic timestep (usually 1 to 6 hours)
- Plant uptake allowed from each soil layer with monthly variable uptake rates; uptake allowed for both NO<sub>3</sub> and NH<sub>4</sub>, and PO<sub>4</sub>
- First-order and Yield-Based plant uptake options for N and P
- No distinction between above and below ground Plant P, multiple compartments for Plant N
- HSPF SPECIAL ACTIONS capability used for chemical applications, harvesting, tillage/disruption activities, etc.

# NUTRIENT (NITR, PHOS) SIMULATION IN AGCHEM #2

RECENT NITROGEN MODELING ENHANCEMENTS (HSPF V.11) TO AGCHEM FOR FORESTED WATERSHEDS

- Multiple Organic N state variables particulate and soluble forms of both Labile and refractory Organic N (4 state variables)
- Conversion of Labile Organic N to Refractory form by first-order rate
- 'Saturation kinetics' available for immobilization and plant N uptake
- Pathway for Plant N to return to the soil Organic N form
- Total Plant N separated into Above Ground and Below Ground compartments
- Litter N compartments available as an intermediate state variable between Above Ground Plant N and soil Organic N
- Volatilization of ammonia included as a loss mechanism

## CORN GROWTH AND NUTRIENT UPTAKE





# **NUTRIENT (NITR, PHOS) CALIBRATION**

- 1. Estimate expected nutrient balances for each landuse and model segment (PLS)
- 2. Evaluate initial Soil Nutrient Parameters and Include Fertilizer/Animal Waste and Atmospheric Deposition Sources
- 3. Calibrate Initial Mineralization Rates
- 4. Evaluate and Adjust Leaching Factors, as needed
- 5. Adjust Plant Uptake Rates and Timing to Develop the Expected Nutrient Uptake Distribution and Amount during the Growing Season
- 6. Adjust Nutrient Partition Coefficients
- 7. Refine the Leaching, Uptake, and Partition Parameters Based on Observed or Expected Runoff Data, Associated Sources (i.e., Surface Interflow, Ground-water) and Expected Nutrient Balances



### TYPICAL NITROGEN BALANCE FOR MAJOR CROPS

Typical Nitrogen Balance For Major Crops and Land Use/Land Cover Categories (lb/ac/yr)

	Corn	Soybeans	Grains	Hay	Forest	Pasture	Urban
INPUTS:							
Fertilizer/Manure	100-160	25-35	50-100	30-60	0	10-60	100-200
Atmos. Deposition	7-10	7-10	7-10	7-10	7-10	7-10	7-10
Mineralization	25-40	25-40	25-40	25-40	40-140	25-40	25-40
Totals	132-210	57-85	82-150	62-110	47-150	42-110	132-250
<b>OUTPUTS:</b>							
Plant Uptake	120-150	25-40	60-90	30-55	50-150	31-80	86-163
Surface Runoff	2-5	1-3	2-4	1-3	1-2	1-5	5-10
Leaching & Subsur Runoff	. 10-25	10-15	5-15	5-15	1-5	5-15	13-25
Volatilization & Denitrification	15-25	5-15	10-20	10-20	1-10	7-19	30-58
TOTALS:	147-205	41-73	77-129	46-91	53-167	44-119	134-256
Delta STORAGE	-15 to 5	16 to 12	5 to 21	16 to 10	-6 to -17	-2 to -9	-2 to -6

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### TYPICAL PHOSPHORUS BALANCE FOR MAJOR CROPS

Typical Phosphorus Balances For Major Crops and Land Use/Land Cover Categories (lb/ac/yr)

INPUTS:	Corn	Soybeans	Grains	Hay	Forest	Pasture	Urban
Fertilizer/Manure Atmos. Deposition	20-40 0-1	10-30 0-1	10-30 0-1	10-30 0-1	 	5-30 0-1	10-30 0-1
Mineralization Totals	2-5 22-46	2-5 12-36	2-5 12-36	2-5 12-36	 	2-5 7-37	2-5 12-36
OUTPUTS:							
Plant Uptake Surface Runoff Leaching & Subsur Runoff	20-30 1-2 f. 0-1	12-20 0-1 0-1	12-22 0-1 0-1	12-25 0-1 0-1	  	5-20 0-2 0-1	8-15 0-2 0-1
TOTALS:	21-33	12-22	12-24	12-27		5-23	8-18
Delta STORAGE	1 to 13	0 to 14	0 to12	0 to 9 8 of 31		2 to 14	4 to 18

### TYPICAL NITROGEN BALANCE AND STORAGES FOR

< 1 - 2

< 0.2

1 - 2

<2 - 4

< 1 - 5

< 1 - 5

FORESTED CONDITIONS

lb/ac/yr

7 - 10

40 - 140

20 - 80

20 - 60

Conc (mg/l)

< 0.5 - 1.0

< 0.01 - 0.1

< 0.2 - 1.0

< 0.5 - 2.0

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0

**Comment/Source\*** 

**ORNL** Report

**ORNL** report

about 10x less than NO3

same magnitude as NO3

(2% - 7% of Labile Soil N/yr)

**INPUTS:** 

**FLUXES:** 

**Atmospheric Deposition** 

N-Fixation, Fertilization

Mineralization

Mineral Soil N

Forest Floor

**OUTPUTS:** 

Runoff, including erosion

Total

Leaching

Denitrification

NO3

NH3 Org N

\*ORNL Report = Hunsaker et al., 1994

# TYPICAL NITROGEN BALANCE AND STORAGES FOR FORESTED CONDITIONS (cont.)

OTHER FLUXES:	lb/acre/yr	
Plant Uptake	50 - 150	50/50 split AG/BG, ORNL Report
Plant Return	40 - 120	80%-90% of uptake, ORNL Report
to Litter	15 - 40	
BG to Soil N	25 - 65	BG/AG ratio of 1.6; ORNL Report
STORAGES:	lb/ac	
Plant N	290 - 740	ORNL Report
Above Ground (AG)	230 - 580	
Below Ground (BG)	60 - 160	
Litter N	20 - 50	5% to 10% of AG
Soil N	2000 - 8500	ORNL Report
Surface Soils	700 - 3000 (35%)	ORNL Report
Subsurface	1300 - 5500 (65%)	