

LECTURE #13

AGCHEM PROCESSES, PARAMETERS AND CALIBRATION







PERLND STRUCTURE CHART





adapted from EPA BASINS workshop

SOIL PROFILE REPRESENTATION BY THE AGCHEM MODULE



FREUNDLICH ISOTHERM CALCULATIONS



C, ppm

 $X = KF1 \star C^{1/N1} \star XFIX$

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 \rightarrow







PESTICIDE (PEST) CALIBRATION

- 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
- Compare/Evaluate Storm Event Pesticide Losses and Make Further Parameter Adjustments as Discussed above





PHOSPHORUS CYCLE



NUTRIENT STORAGES AND TRANSPORT MODELED BY AGCHEM



NITROGEN TRANSFORMATIONS SIMULATED BY AGCHEM



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_4/PO_4 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 NO₃ and NH₄, and PO₄
- 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. 13 of 31

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

DAYS AFTER EMERGENCE

NUTRIENT (NITR, PHOS) CALIBRATION

- 1. Estimate expected nutrient balances for each landuse and model segment (PLS)
- 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
- 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
OUTPUTS:							
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 7 of 31	-6 to -17	-2 to -9	-2 to -6

TYPICAL PHOSPHORUS BALANCE FOR MAJOR CROPS

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

	Corn	Soybeans	Grains	Hay	Forest	Pasture	Urban
INPUTS:		Ŭ					
Fertilizer/Manure	20-40	10-30	10-30	10-30		5-30	10-30
Atmos. Deposition	0-1	0-1	0-1	0-1		0-1	0-1
Mineralization	2-5	2-5	2-5	2-5		2-5	2-5
Totals	22-46	12-36	12-36	12-36		7-37	12-36
OUTPUTS:							
Plant Uptake	20-30	12-20	12-22	12-25		5-20	8-15
Surface Runoff	1-2	0-1	0-1	0-1		0-2	0-2
Leaching & Subsur Runoff	f. 0-1	0-1	0-1	0-1		0-1	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		2 to 14	4 to 18
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TYPICAL NITROGEN BALANCE AND STORAGES FOR FORESTED CONDITIONS

FLUXES:		lb/ac/yr	Comment/Source*
INPUTS:			
Atmospheric Deposition		7 - 10	
N-Fixation, Fertilization		0	
Mineralization		40 - 140	ORNL Report
Mineral Soil N		20 - 80	(2% - 7% of Labile Soil N/yr)
Forest Floor		20 - 60	
OUTPUTS:			
Runoff, includin	g erosion	Conc (mg/l)	
NO3	< 1 - 2	< 0.5 - 1.0	ORNL report
NH3	< 0.2	< 0.01 - 0.1	about 10x less than NO3
Org N	1 - 2	< 0.2 - 1.0	same magnitude as NO3
Total	<2 - 4	< 0.5 - 2.0	
Denitrification	< 1 - 5		
Leaching	< 1 – 5		
*ORNI Report – Hupsaker et al. 1004		19 of 31	

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%)	