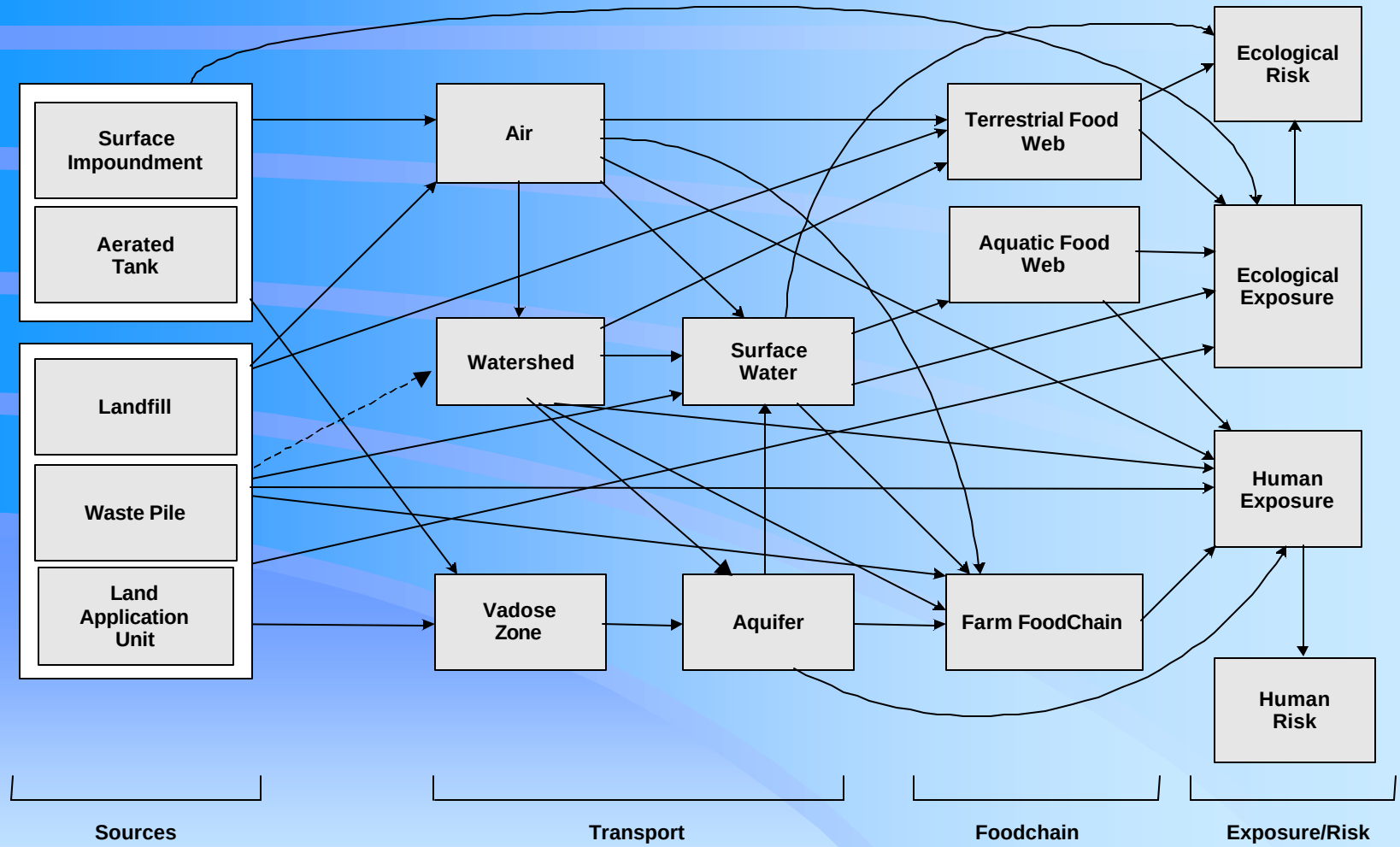
3MRA Site-Based Modeling Approach

Keith W. Little
Robert B. Ambrose, Jr.
David A. Cozzie

August 26, 2003

3MRA Science Modules and Connectivity

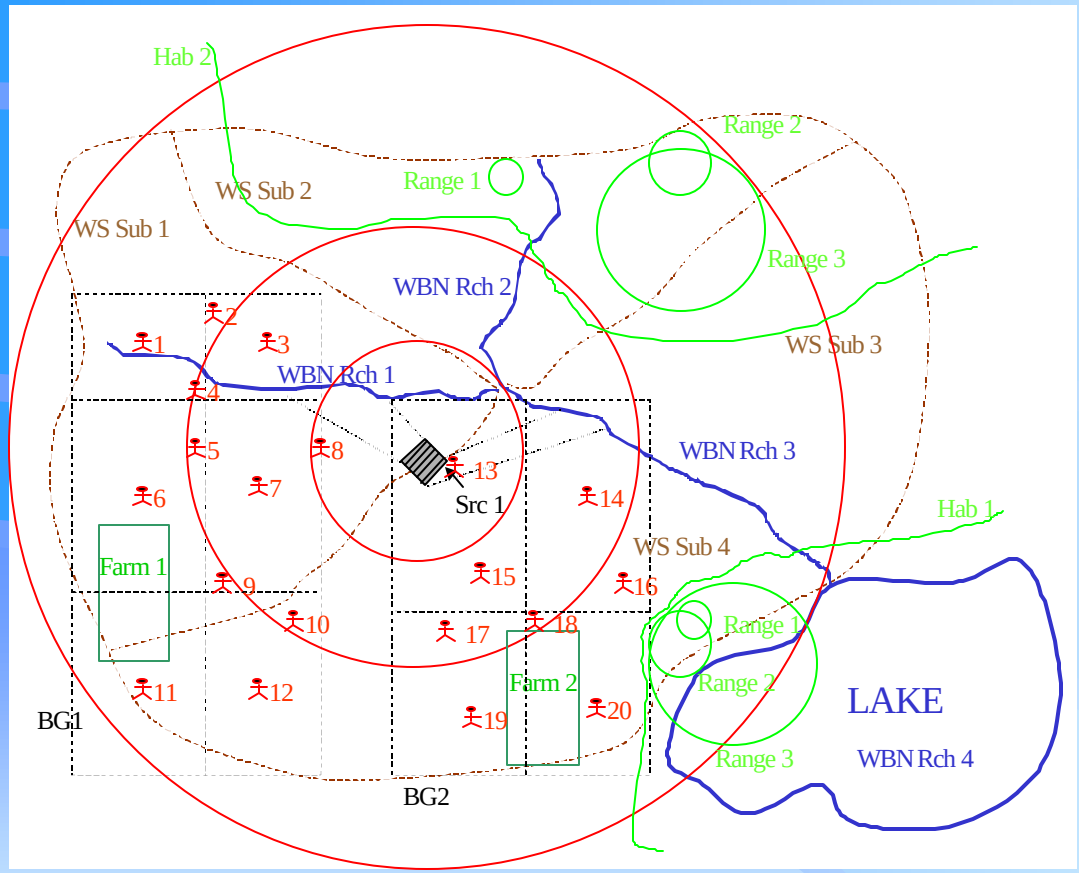


Keith Little

Robert Ambrose

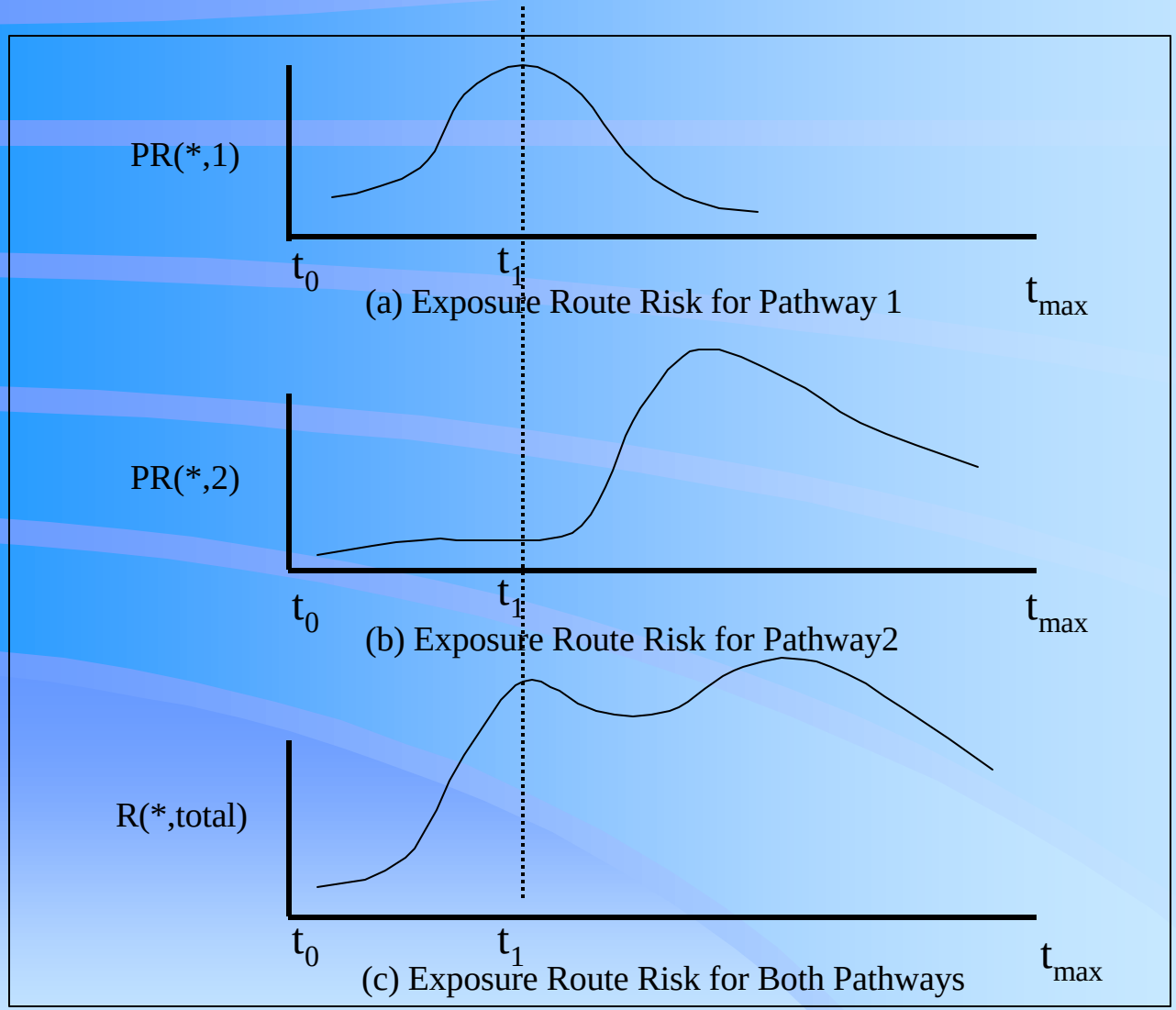
David Cozzie

Conceptual Layout of Typical 3MRA Modeling Site



Watershed
Surface Water
Habitat
Ring
Farm
Human Receptor
Source

3MRA Site-based Risk Output



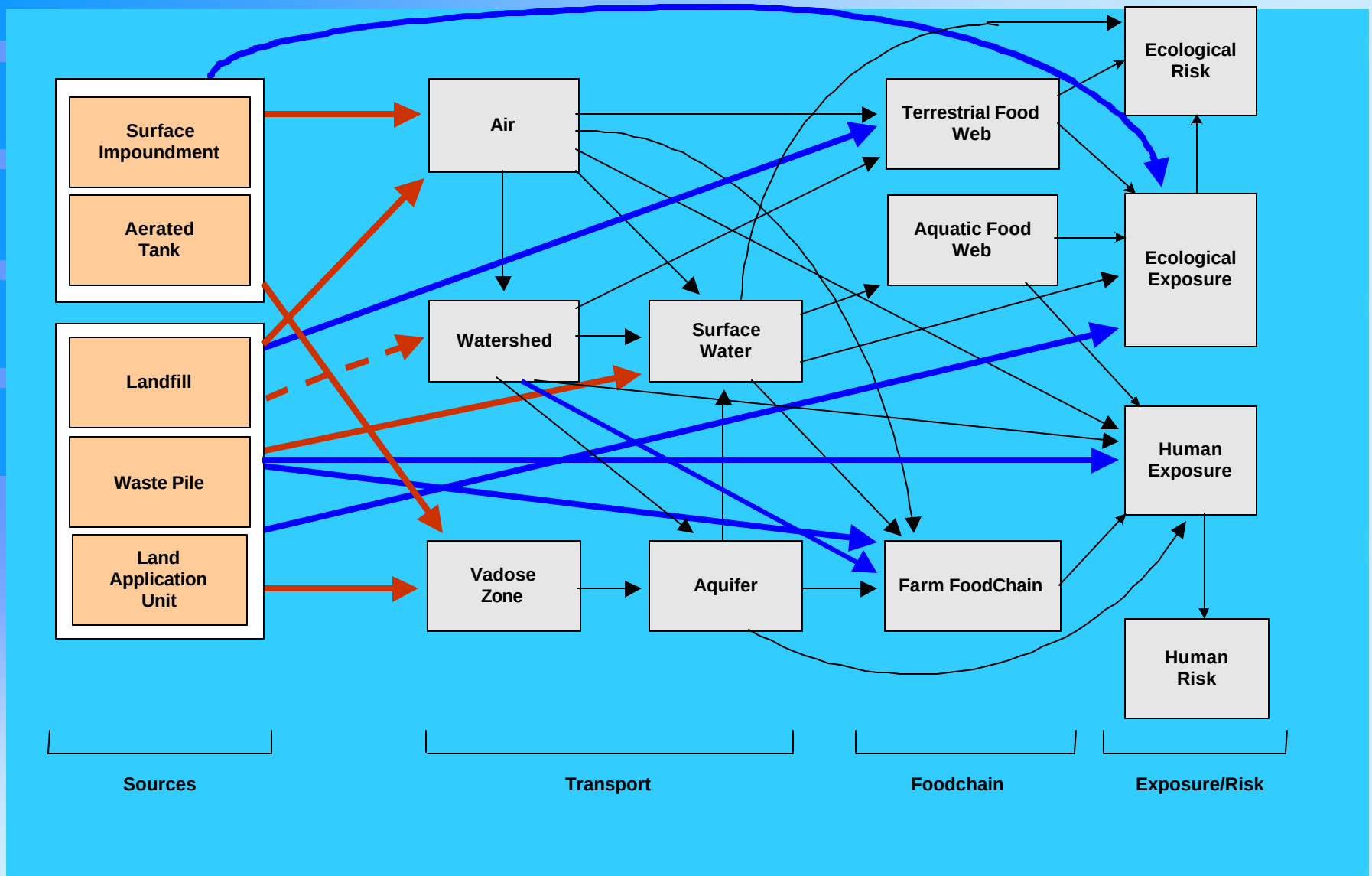
(*)
Receptor
Cohort
Exposure route
Contact medium
Chemical
Site
WMU

3MRA Waste Management Unit Modules

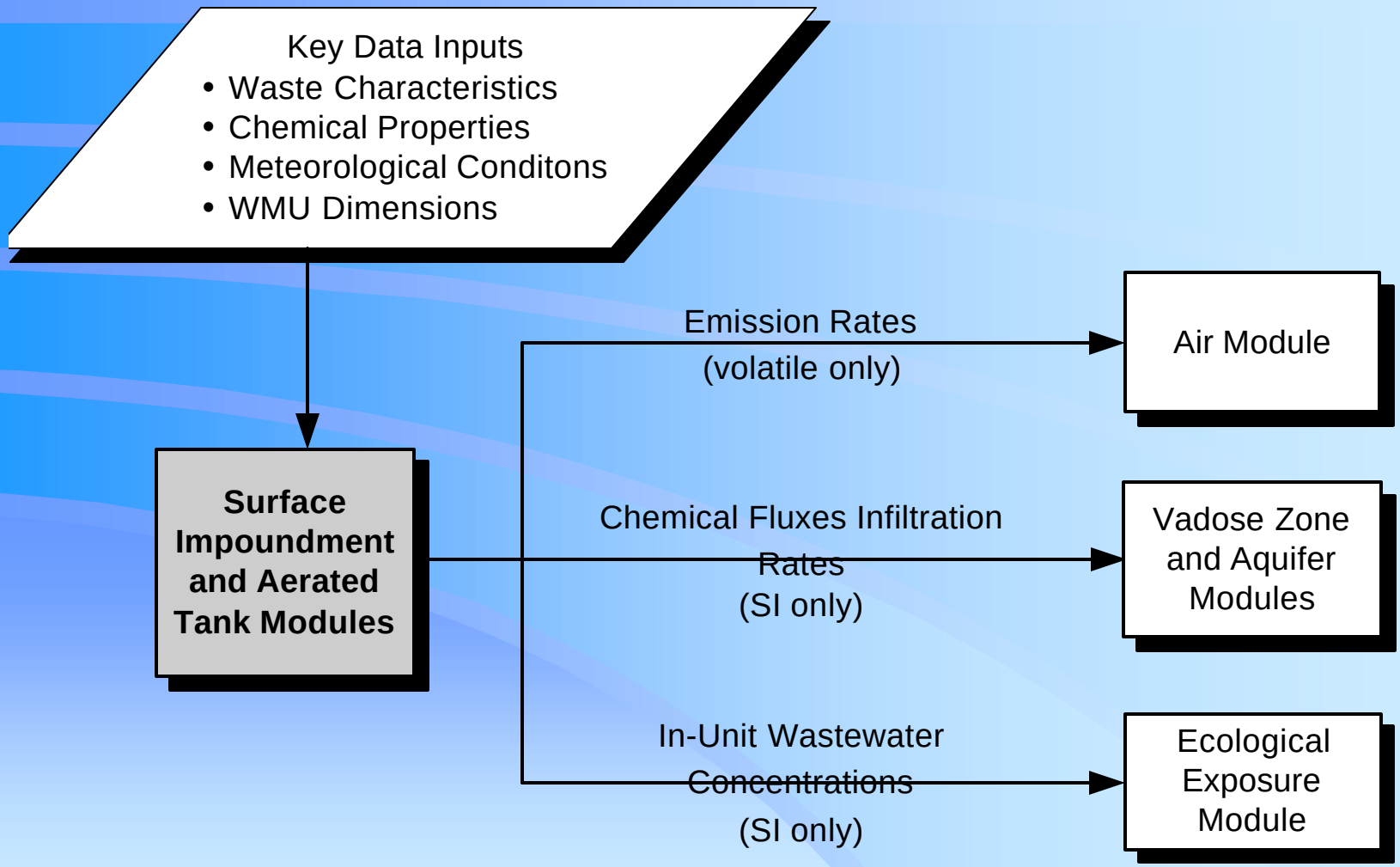
Presented by Keith W. Little

RTI International

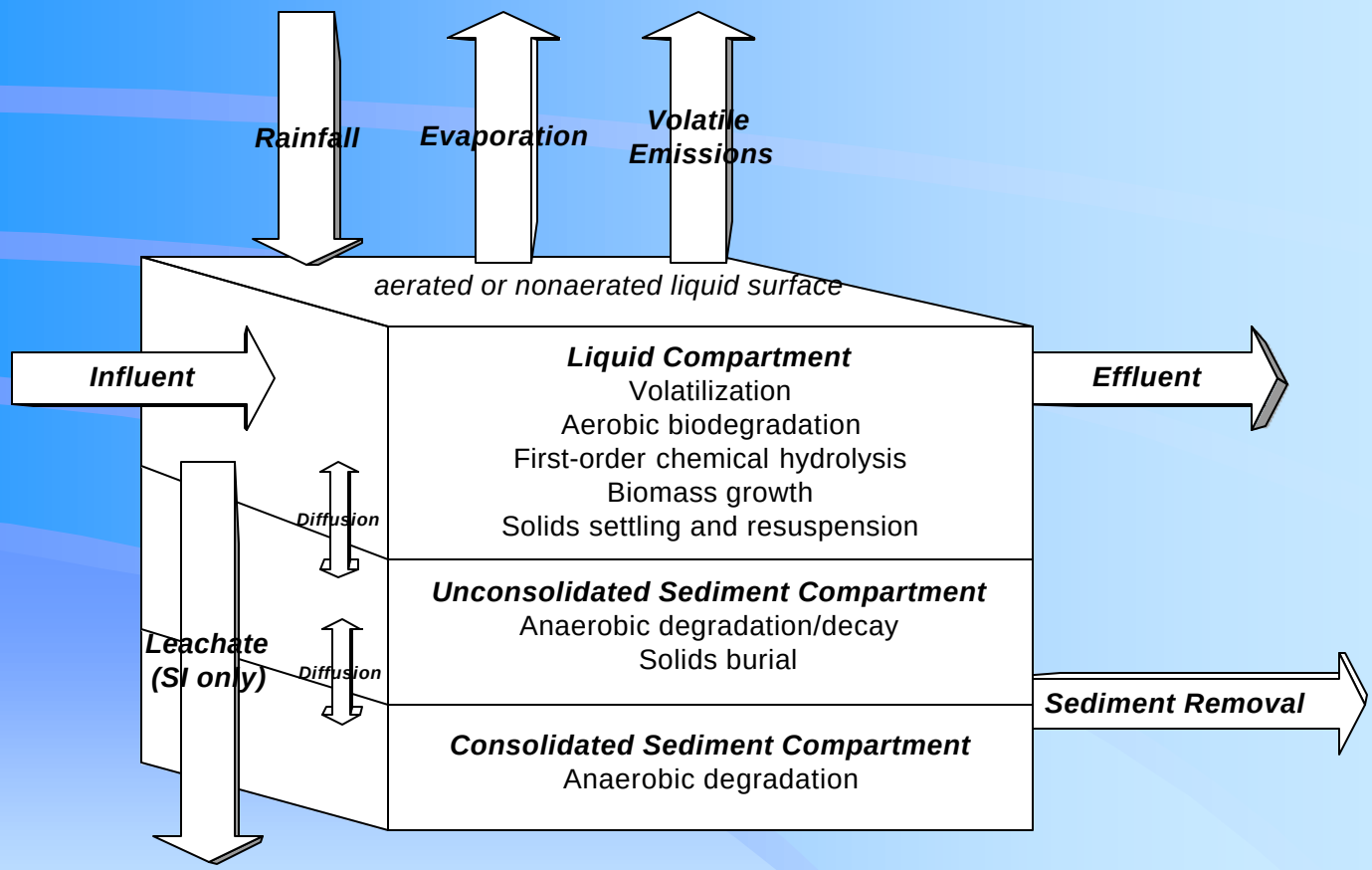
Connectivity of Waste Management Unit Modules



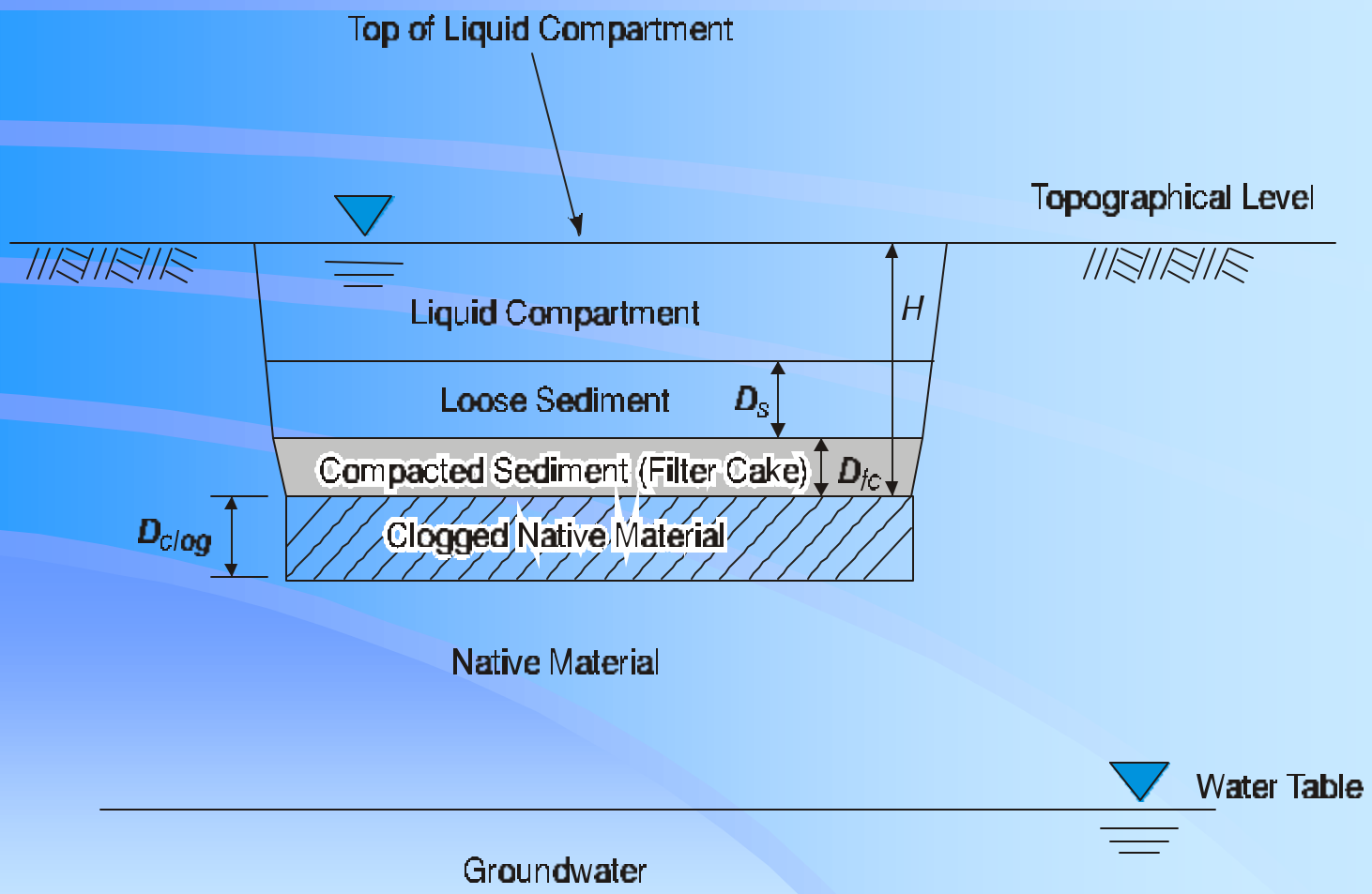
Water-Based WMU Modules



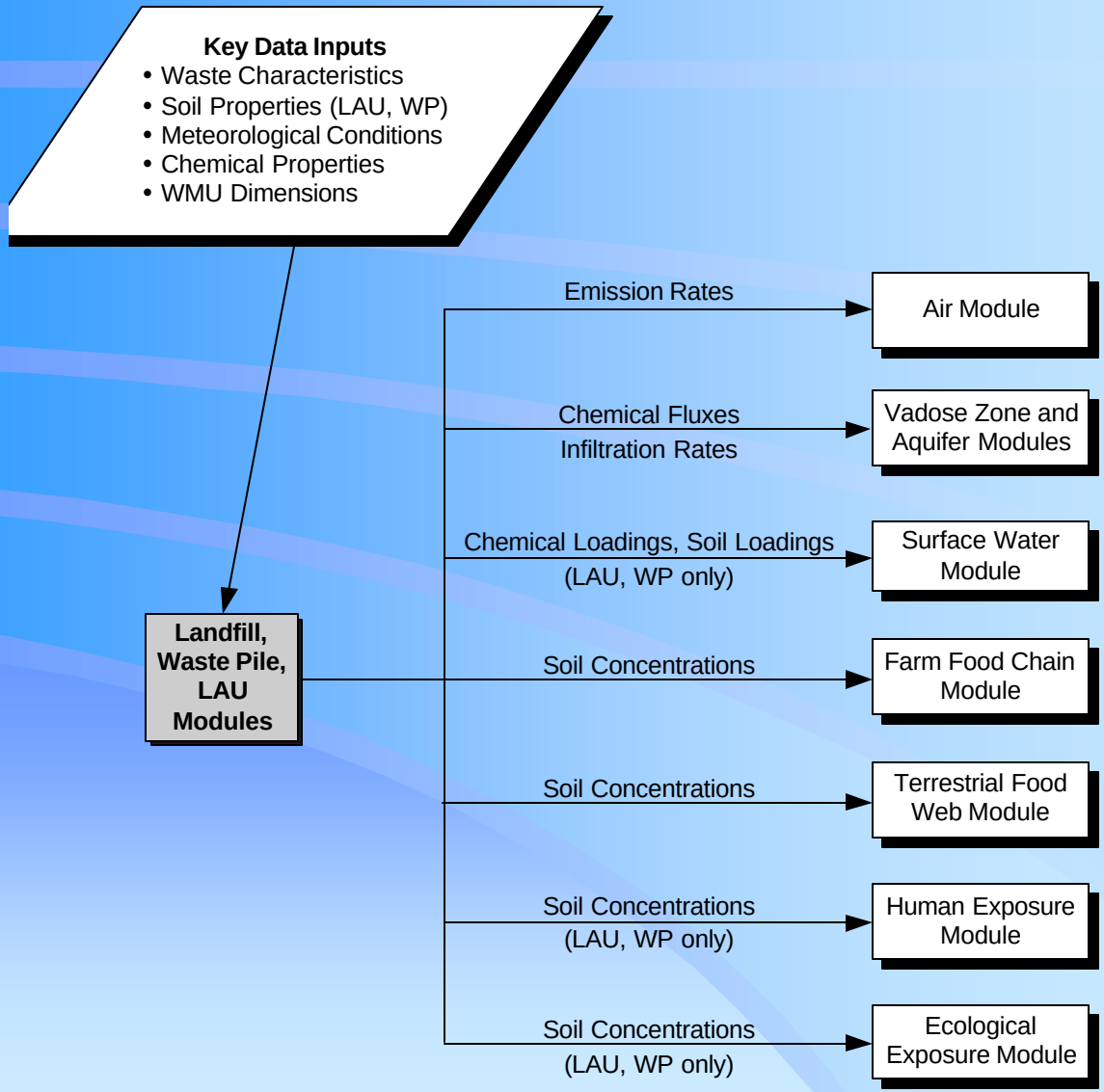
Water-Based WMU Modules



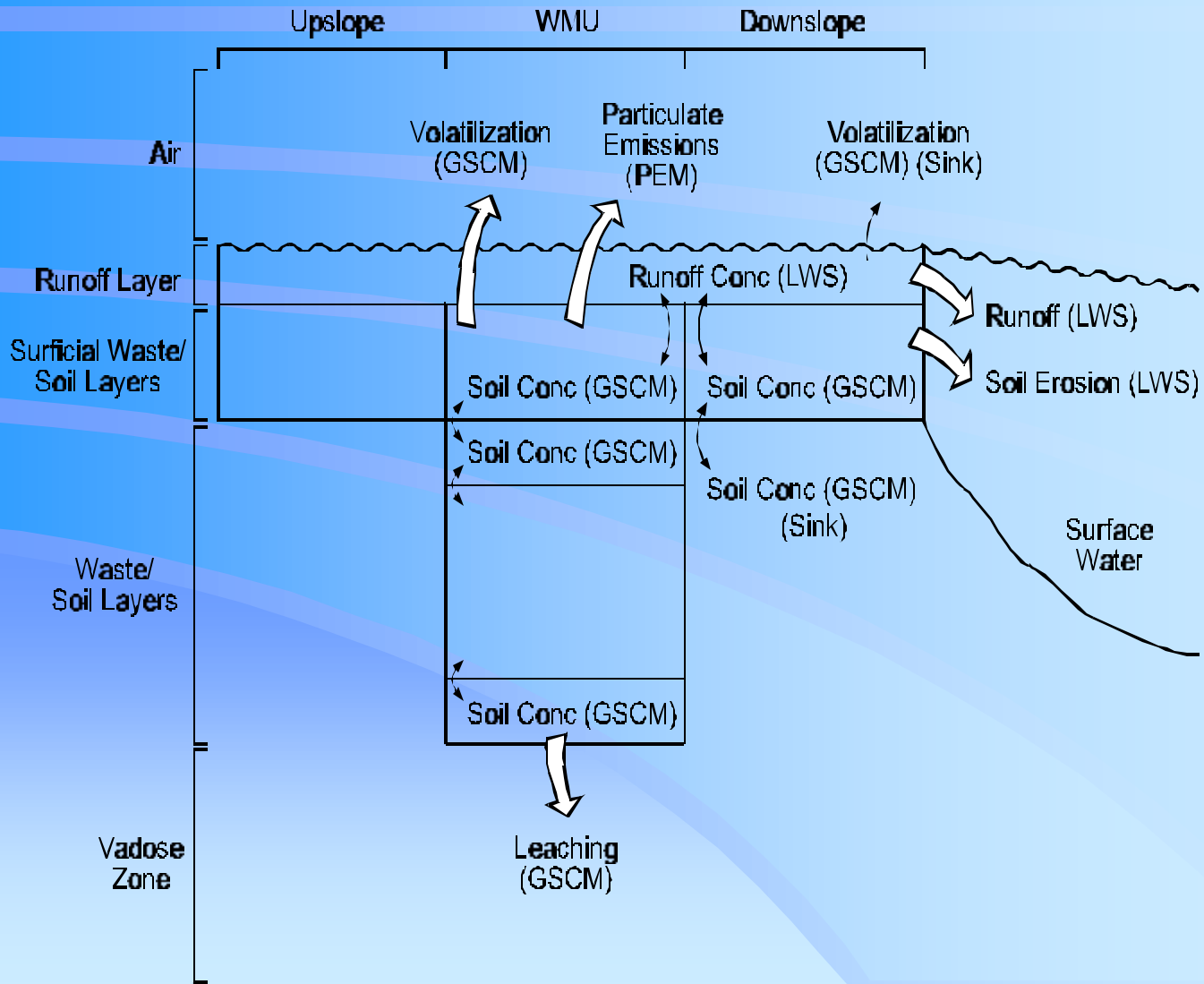
Surface Impoundment



Land-Based WMU Modules



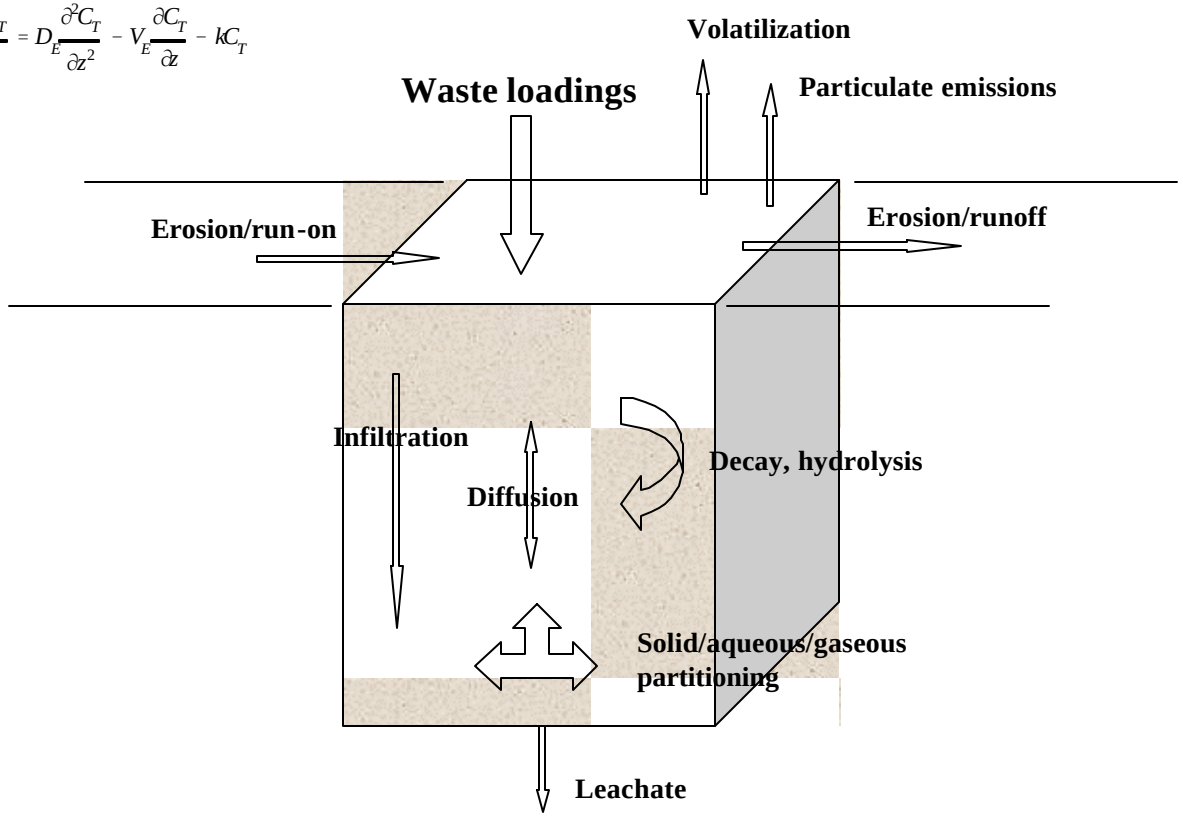
Interaction of Algorithms Comprising Land-Based WMUs



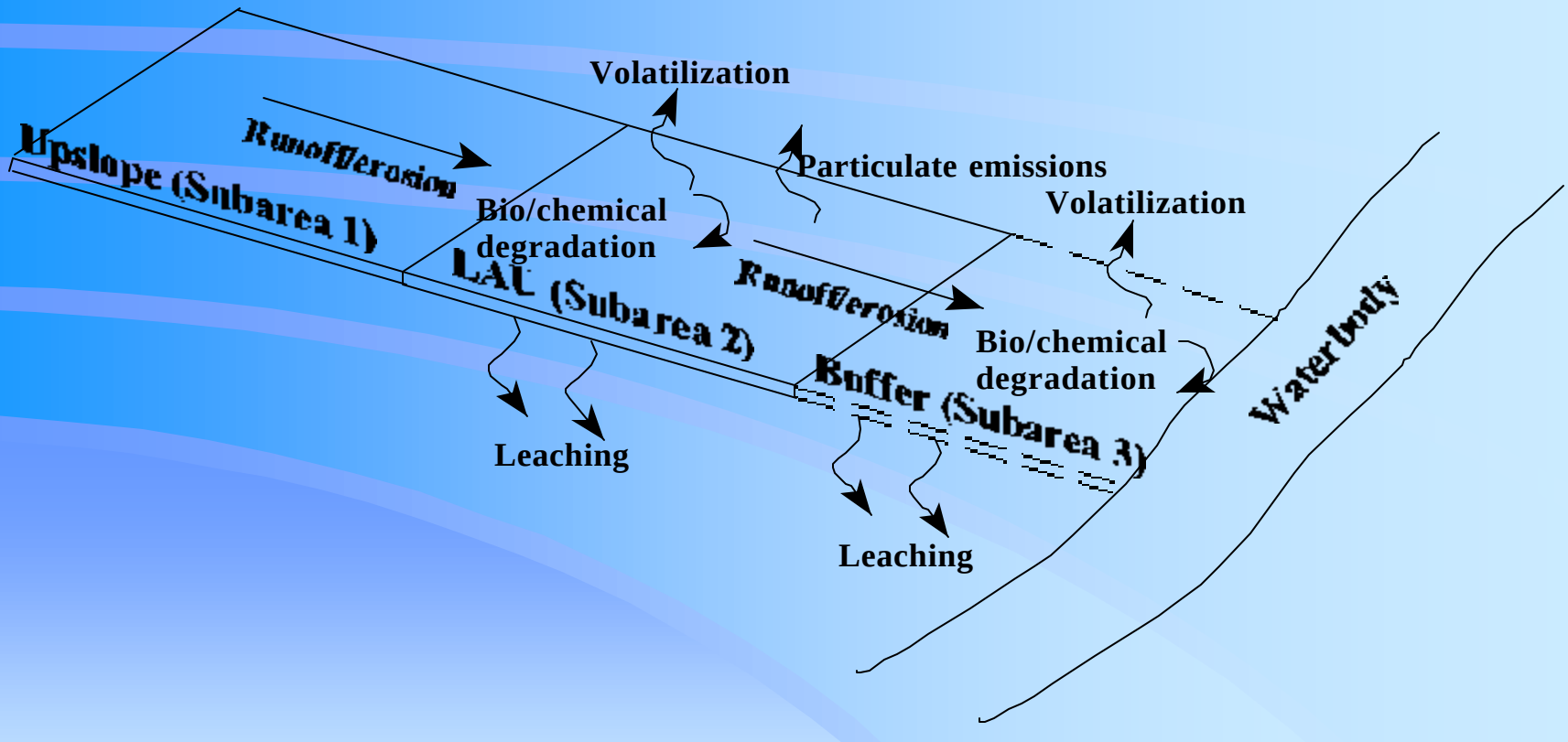
Generic Soil Column Model

Governing equation:

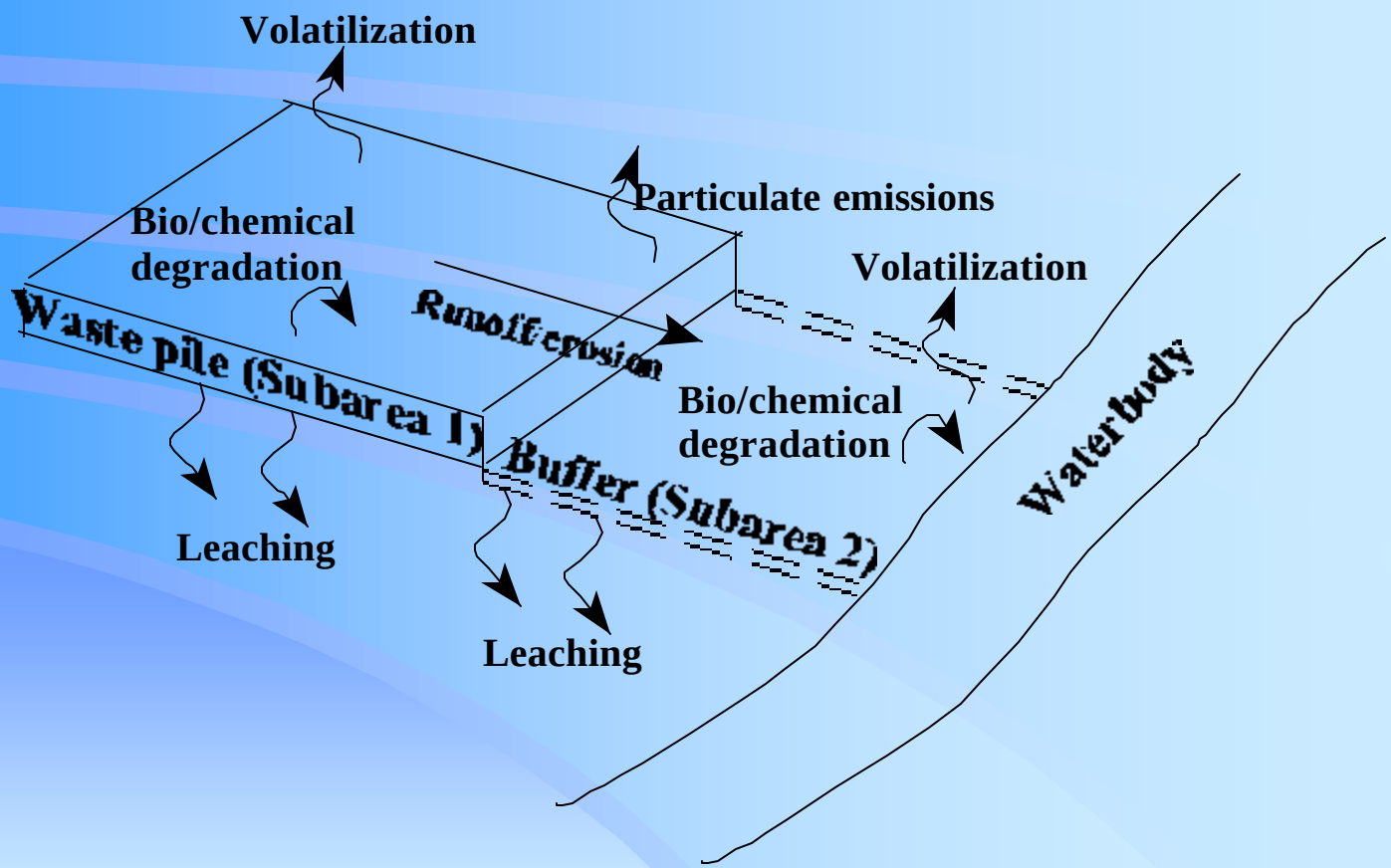
$$\frac{\partial C_T}{\partial t} = D_E \frac{\partial^2 C_T}{\partial z^2} - V_E \frac{\partial C_T}{\partial z} - kC_T$$



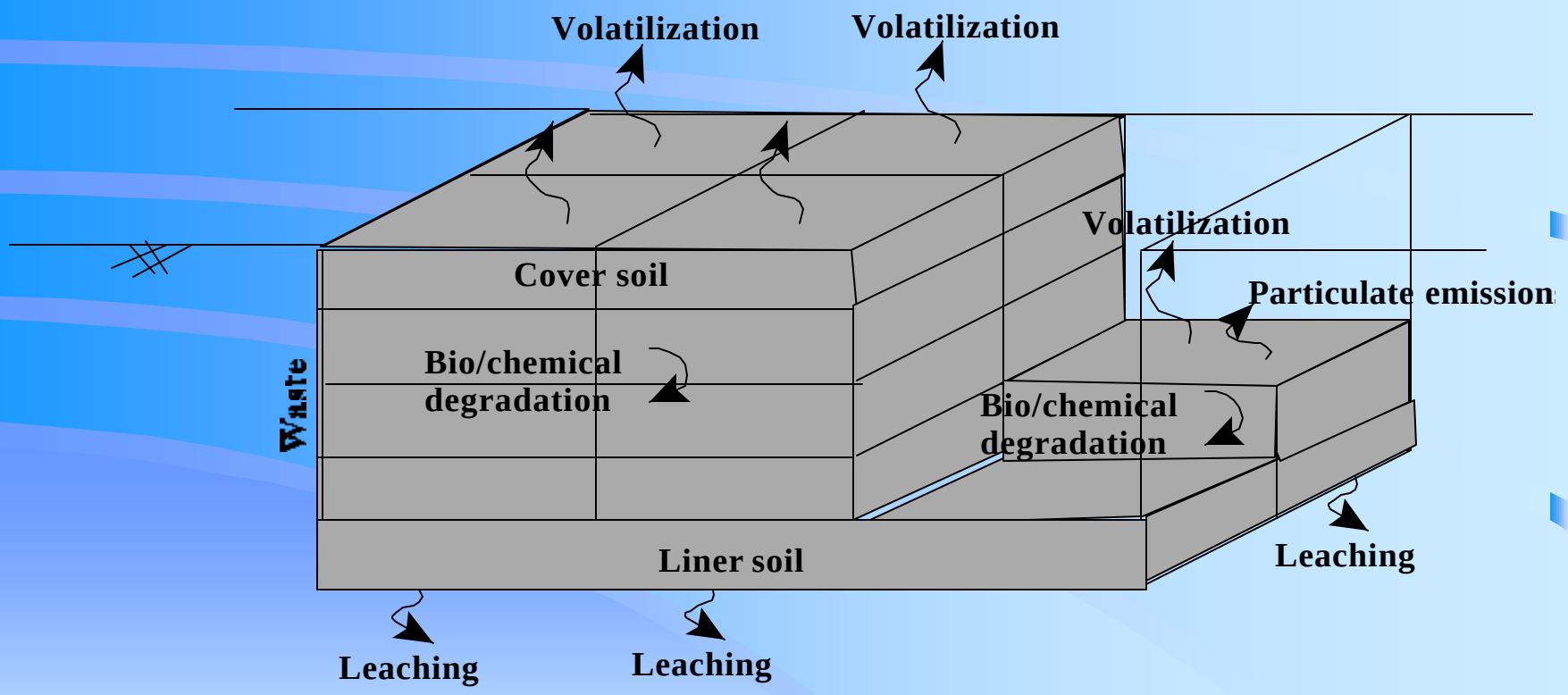
LAU Module


Volatilization
Runoff/erosion
Upslope (Subarea 1)
Particulate emissions
Volatilization
Bio/chemical degradation
LAU (Subarea 2)
Runoff/erosion
Bio/chemical degradation
Buffer (Subarea 3)
Waterbody
Leaching
Leaching

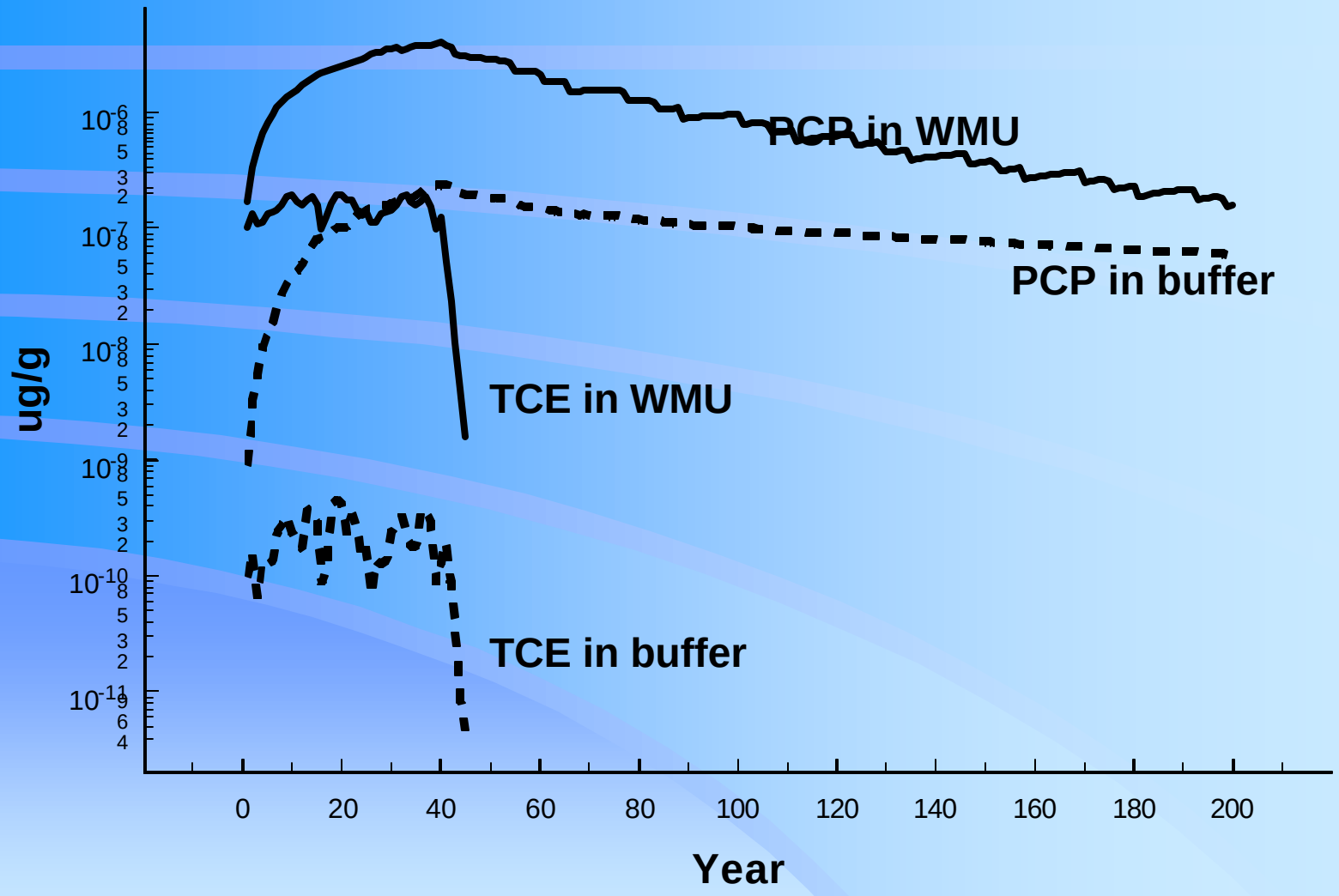
Waste Pile Module



Landfill Module



Illustrative Results (LAU at Site 0435510) Depth-Averaged Soil Concentrations (LAU vs Buffer)



3MRA Environmental Media Transport and Fate Modules

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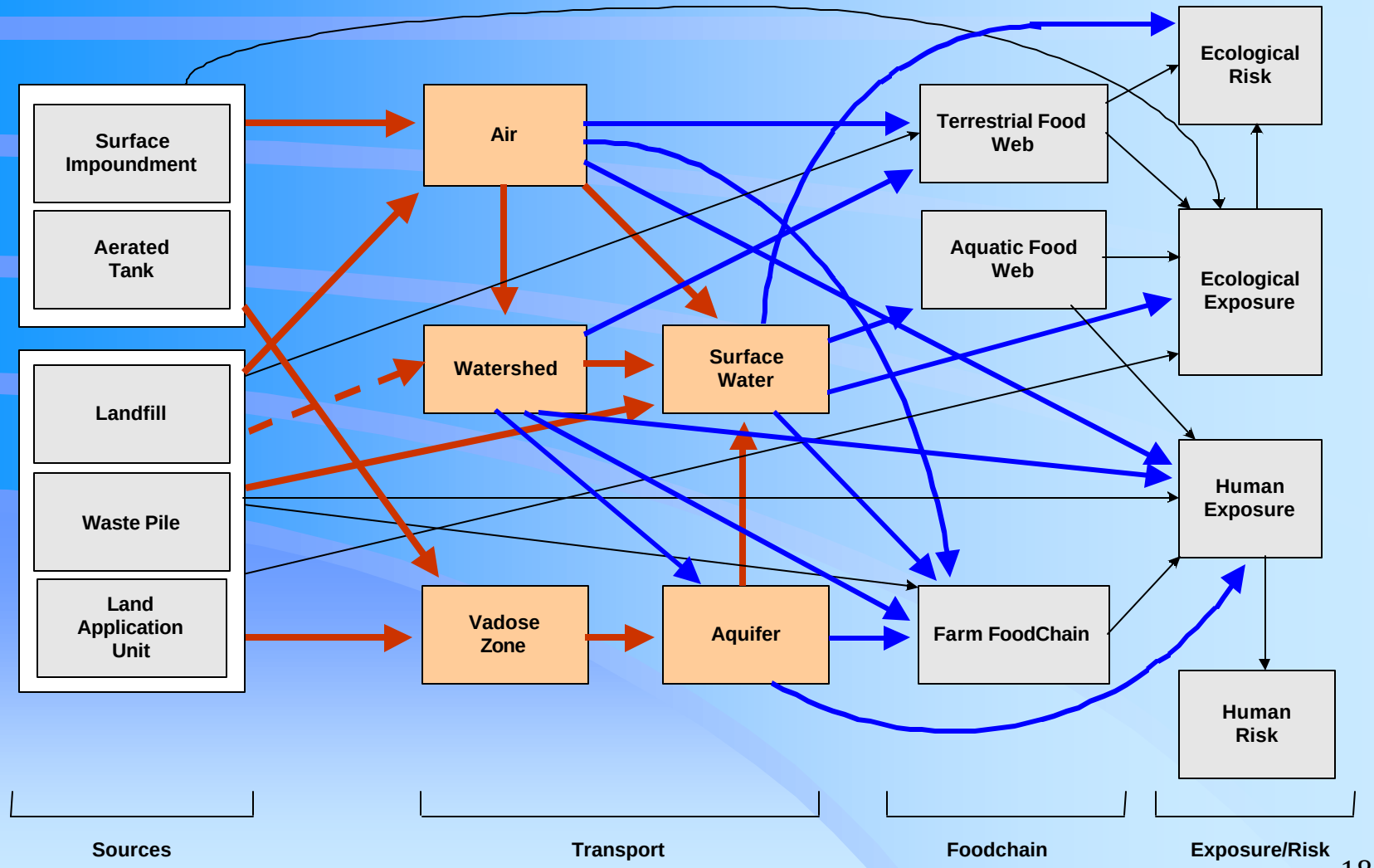
EPA/ORD

Connectivity of Environmental Media Modules



Intermedia Contaminant Fluxes

- Air to watershed soil (wet, dry deposition)
- Air to surface water (wet, dry deposition)
- Watershed soil to surface water (runoff, erosion)
- Vadose zone to saturated ground water (infiltration)
- Saturated ground water to surface water (interception)

Secondary Intermedia Contaminant Fluxes (not connected)

- Watershed soil to air (volatilization)
- Surface water to air (volatilization)
- Watershed soil to ground water (infiltration)
- Surface water to ground water (seepage)
- Ground water to watershed soil (e.g., vapor intrusion)

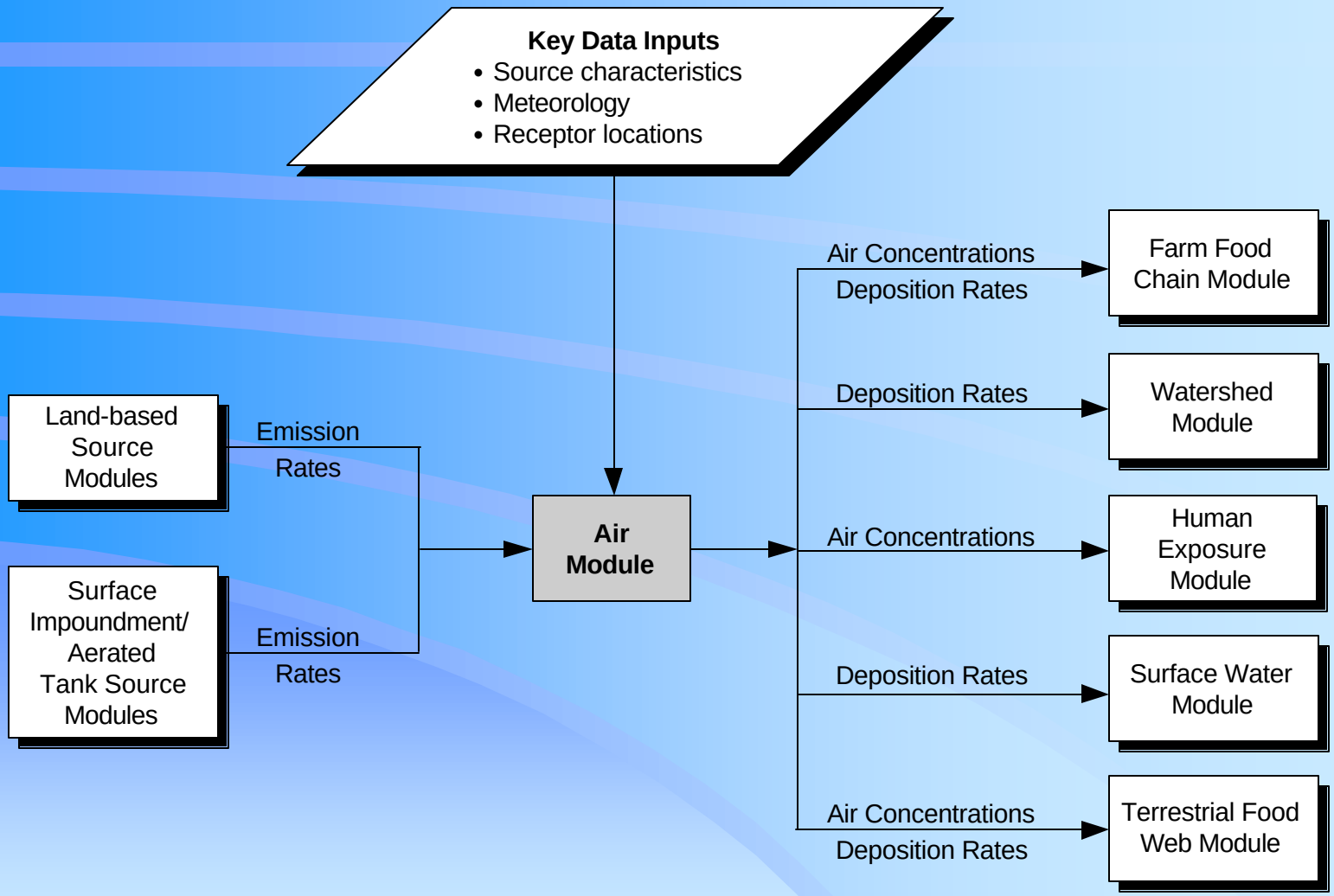
Environmental Media Contaminant Transfers to Humans and Biota

- Air to vegetation (particulate deposition, vapor diffusion)
- Watershed soil to vegetation (root uptake, translocation)
- Vegetation, watershed soil, surface water to terrestrial animals and humans (consumption)
- Surface water to aquatic organisms (uptake)
- Ground water to humans (consumption)

Environmental Media Fate Processes

- Linear partitioning (e.g., air-plant, soil-soil gas, soil water-soil solids, water-suspended solids, pore water-benthic solids)
- Nonlinear partitioning (i.e., metals in vadose zone)
- Chemical/biological reactions – decay (i.e., hydrolysis, reduction, biodegradation)
- Chemical/biological reactions – transformation (i.e., mercury in surface water)

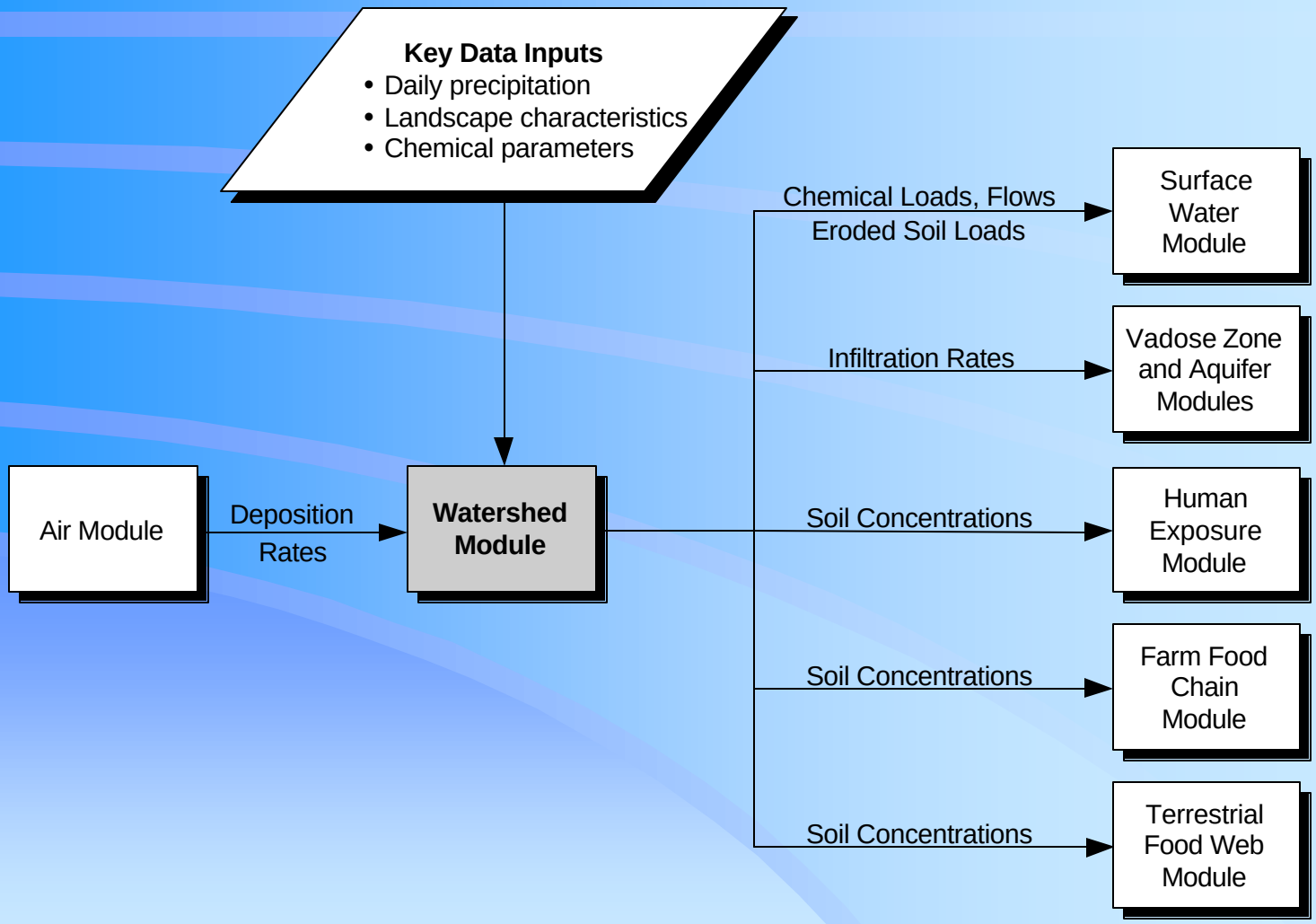
Air Module


Key Data Inputs
• Source characteristics
• Meteorology
• Receptor locations
Land-based Source Modules
Emission Rates
Surface Impoundment/ Aerated Tank Source Modules
Emission Rates
Air Module
Air Concentrations
Deposition Rates
Farm Food Chain Module
Deposition Rates
Watershed Module
Air Concentrations
Human Exposure Module
Deposition Rates
Surface Water Module
Air Concentrations
Deposition Rates
Terrestrial Food Web Module

Air Module, continued

- Uses legacy EPA regulatory model ISCST3; wrapper controls interface to modeling system
- Steady-state Gaussian plume dispersion model
- Depletion of plume due to dry and wet deposition
- Added SCIM capability – sample long-term meteorological file to reduce runtime; maintains serial correlation for precipitation events
- Annual average concentration and dry and wet deposition; 1 hour calculational time step

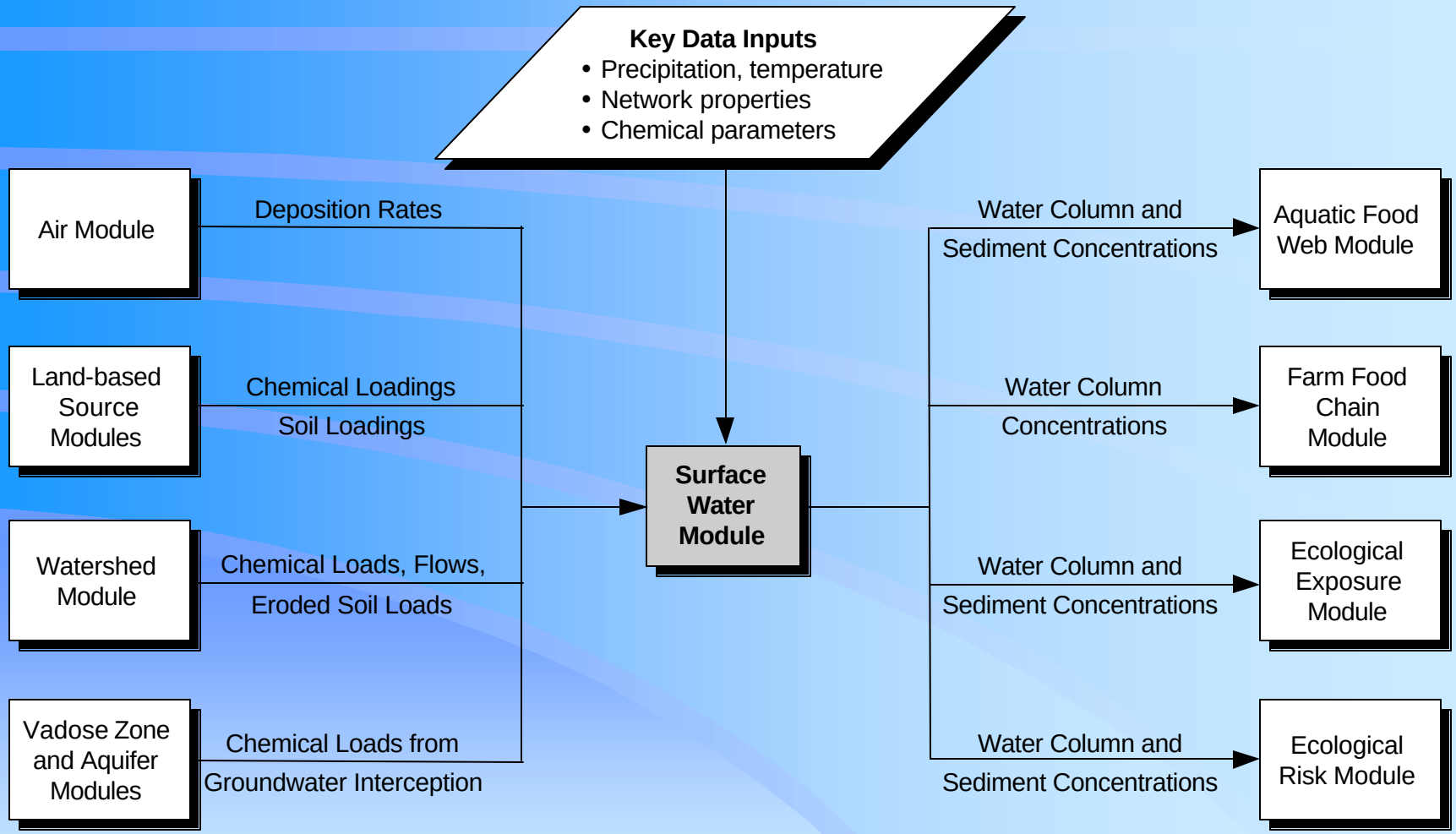
Watershed Module



Watershed Module, continued

- New model developed for 3MRA
- Based on Generic Soil Column Model, GSCM
  - Hydrology uses SCS curve number
  - Erosion uses Modified USLE
  - Transport implements modified Jury equations
  - Partitioning to soil particles, soil gas
  - Decay rates for hydrolysis, biodegradation
  - Particulate release from wind erosion
- Applied to each subwatershed in area (1 to 30)
- Calculational time steps:
  - Hydrology: day
  - Contaminant mass balance: day < Ät < year

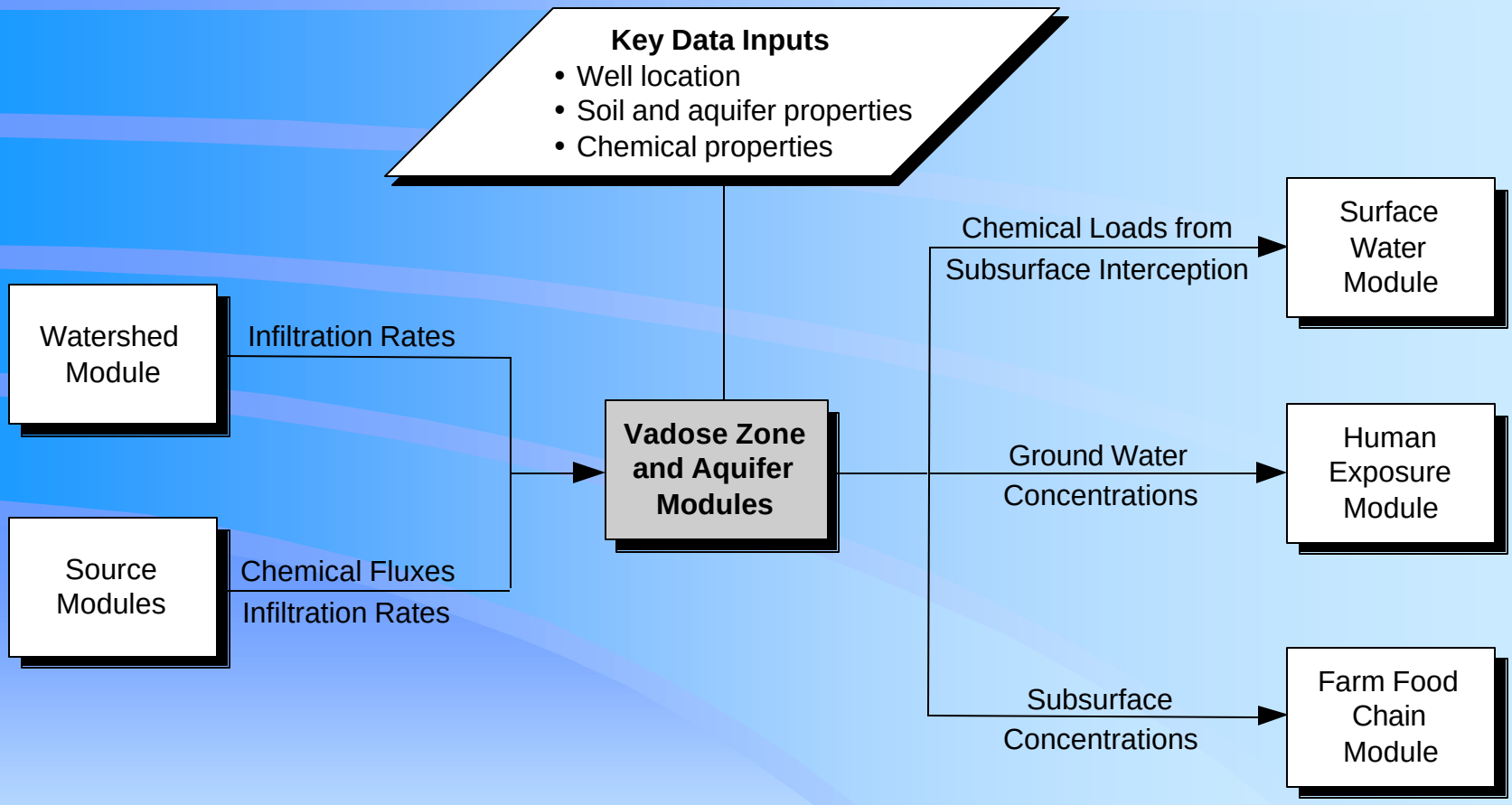
Surface Water Module



Surface Water Module, continued

- Uses legacy EPA regulatory model EXAMS-2; wrapper controls interface to modeling system
- Applied to local water network (1 to 50+ reaches)
  - Streams, rivers, wetlands, ponds, lakes, bays
  - Water column and benthic segments
- Quasi-dynamic solution mode
  - Inflows, loadings specified yearly
  - Simple flow and solids balances performed
- Contaminant concentrations calculated over time
  - Partitioning to dissolved, particle sorbed, biosorbed phases
  - Decay rates for hydrolysis, biodegradation, reduction
  - Predicted concentrations averaged yearly
  - Calculational time step < 1 day

Vadose Zone and Aquifer Module



Vadose Zone Module

- Extracted from EPA regulatory model EPACMTP
- Simulates vadose zone below waste unit
- Steady-state, 1-D analytical and numerical flow
- 1-D analytical transport driven by long-term average infiltration rate
- Infiltration calculated using Richard's equation using Van Genuchten parameters
- Calculates annual-average leachate concentrations
- Linear partitioning for organics; nonlinear for metals
- Decay rates for hydrolysis and anaerobic degradation
- Infiltration flux passed to aquifer module

Aquifer Module

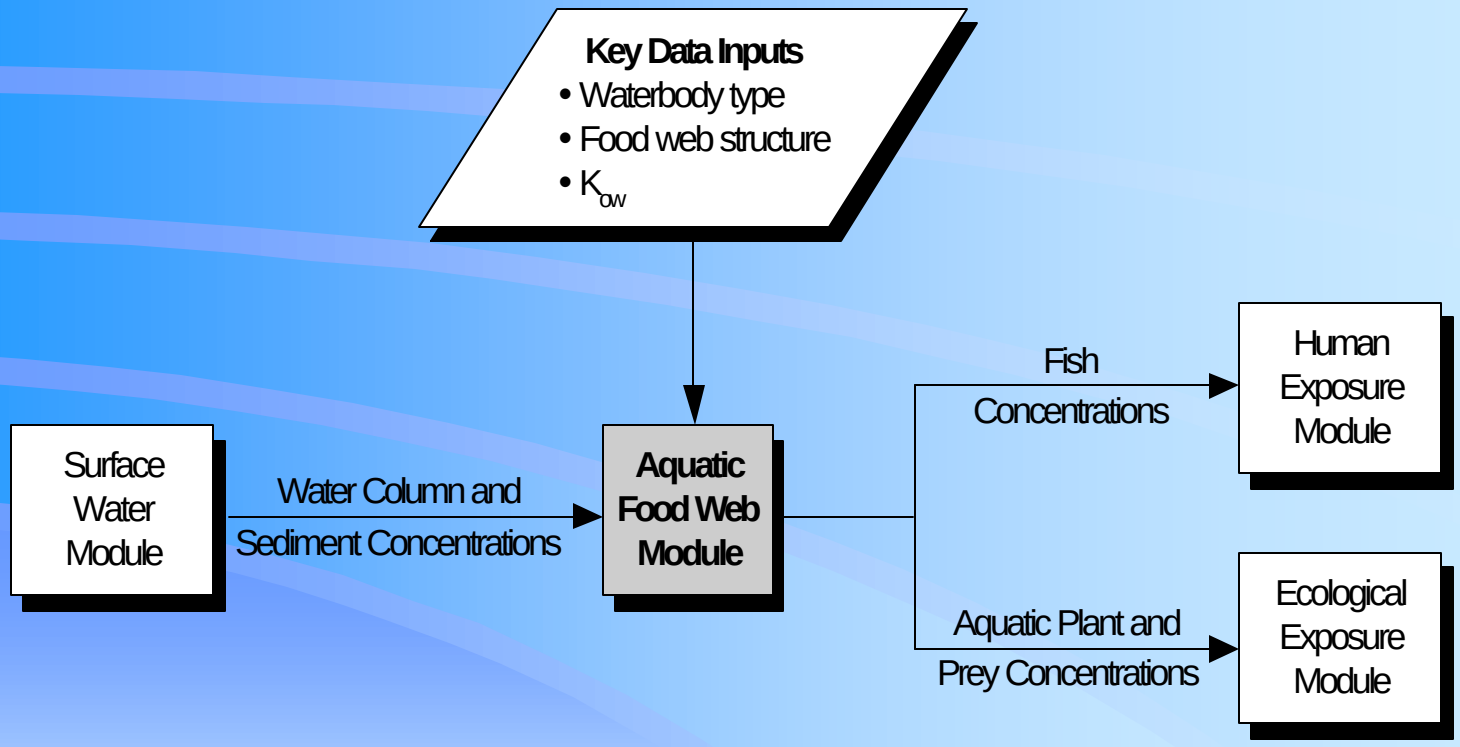
- Extracted from EPA regulatory model EPACMTP
- 1-D steady state ground water flow, pseudo 3-D contaminant transport
- Flow follows Darcy's Law applied to unconfined aquifer with constant thickness
- Contaminant transport driven by infiltration flux from vadose zone module
- Effects of uniform regional recharge
- Linear partitioning for organics and for metals
- Decay rates for hydrolysis and anaerobic degradation
- Fracture flow uses equivalent porous media approach
- Stochastic correction for heterogeneity

Foodchain, Exposure and Risk Modules

David A. Cozzie
EPA/OSW

3MRA Foodchain Modules

Aquatic Food Web



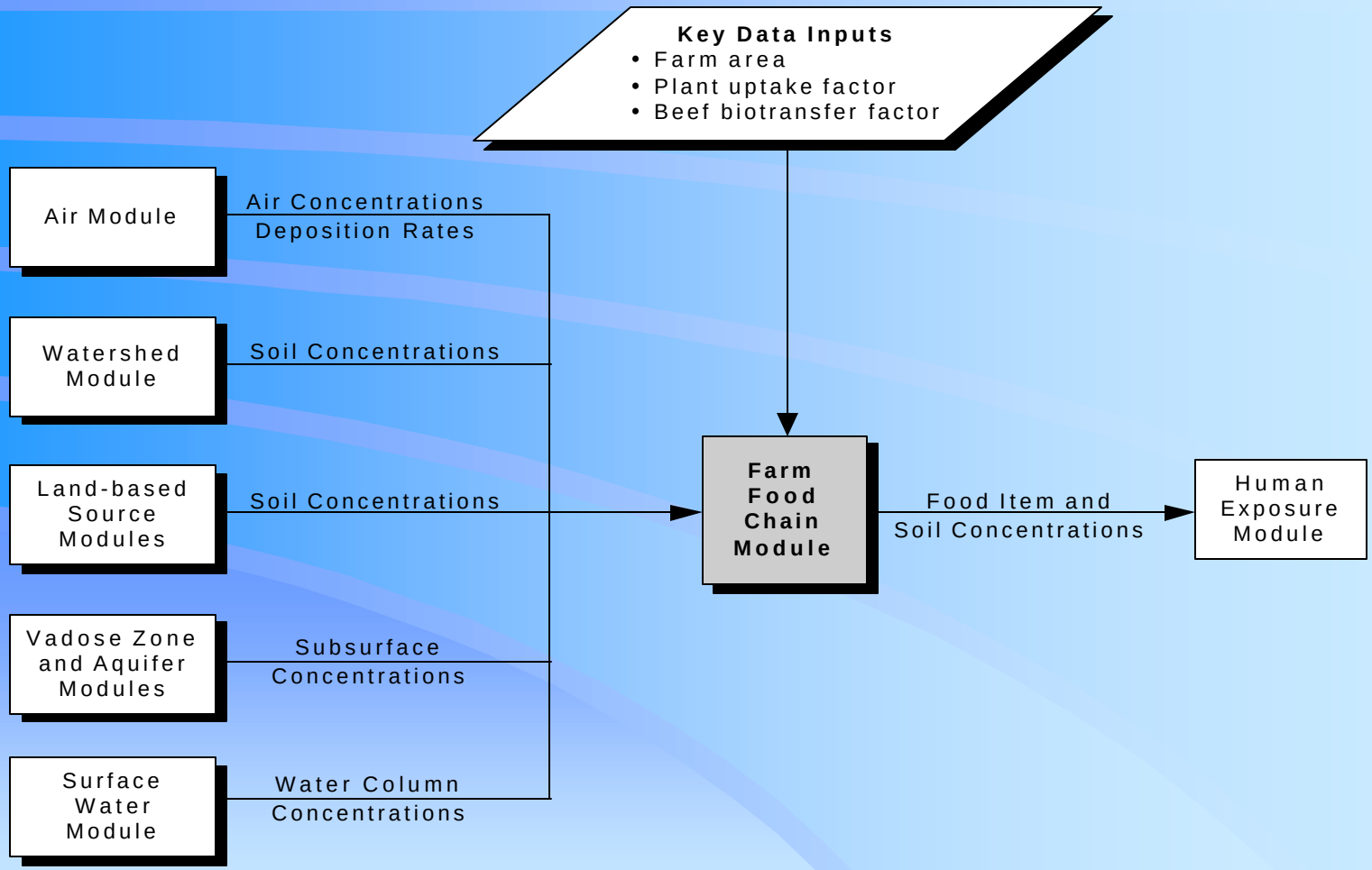
Aquatic Food Web

- Based on approach developed by Gobas et al., but for specific chemicals integrates empirical data, and other Agency approaches
- Calculates steady-state contaminant concentrations in aquatic organisms consumed by human and ecological receptors
- Develops dietary matrices based on water body type and habitat (i.e., warm or cold water)
- Uses random sampling techniques to represent dietary variability

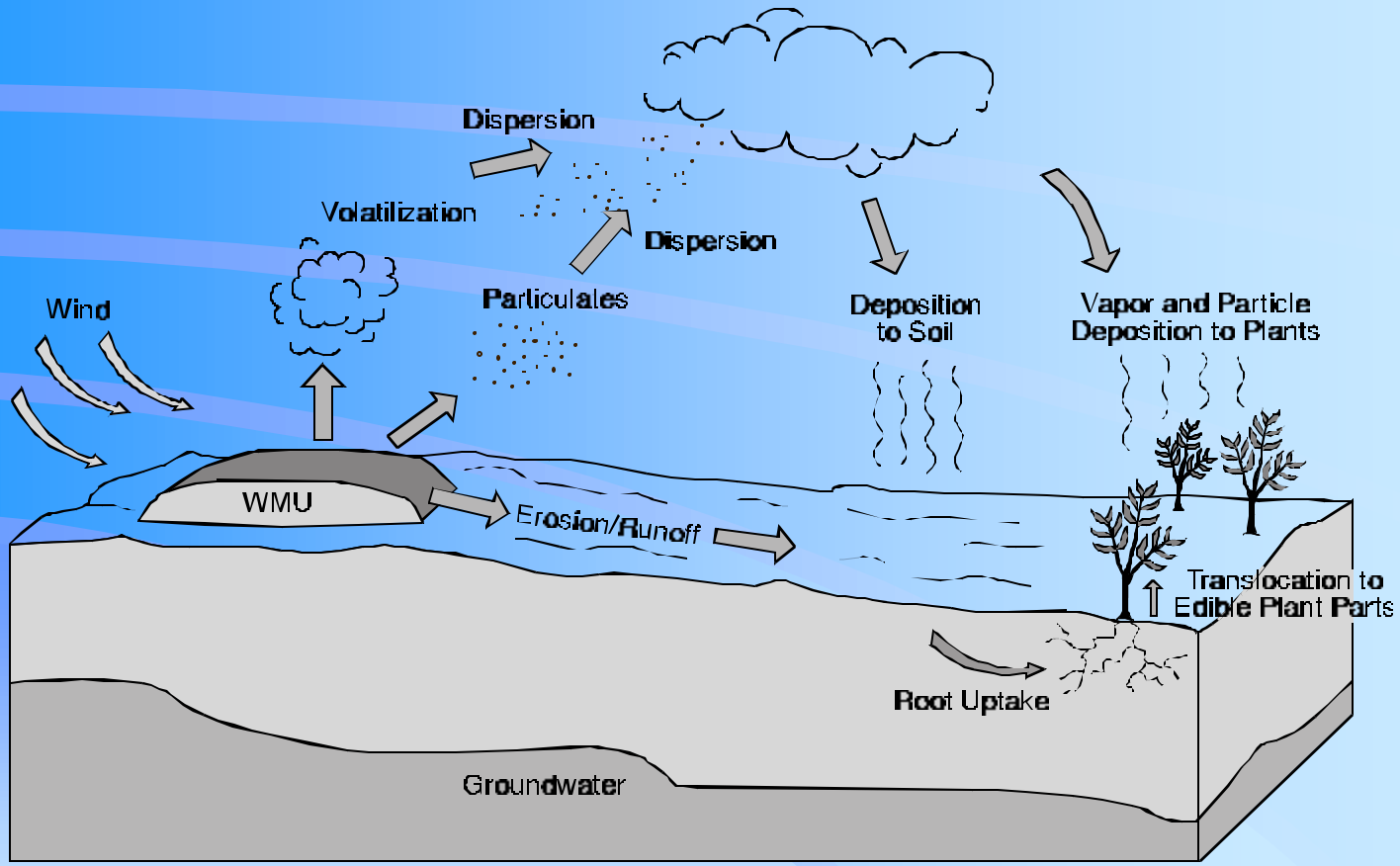
Matrix of Biota in Food Webs for Freshwater Systems in 3MRA

	Coldwater habitats				Warmwater habitats			
Biota	**Stream**	**Wetland**	**Pond**	**Lake**	**Stream**	**Wetland**	**Pond**	**Lake**
Periphyton	✔	✔	✔	✔	✔	✔	✔	✔
Phytoplankton		✔	✔	✔		✔	✔	✔
Aquatic macrophytes	✔	✔	✔	✔	✔	✔	✔	✔
Zooplankton		✔	✔	✔		✔	✔	✔
Benthic detrivores	✔	✔	✔	✔	✔	✔	✔	✔
Benthic filter feeders	✔			✔	✔			✔
TL3 benthivore (small)	✔				✔			✔
TL3 benthivore	✔	✔	✔	✔	✔	✔	✔	
TL3 benthivore (large)								✔
TL3 planktivore (small)			✔					
TL3 planktivore				✔			✔	
TL3 planktivore (large)								✔
TL3 omnivore (small)		✔	✔	✔		✔	✔	
TL3 omnivore (medium)	✔	✔	✔		✔	✔		✔
TL3 omnivore (large)				✔			✔	✔
TL4 piscivore	✔	✔	✔	✔	✔	✔		✔

Farm Food Chain



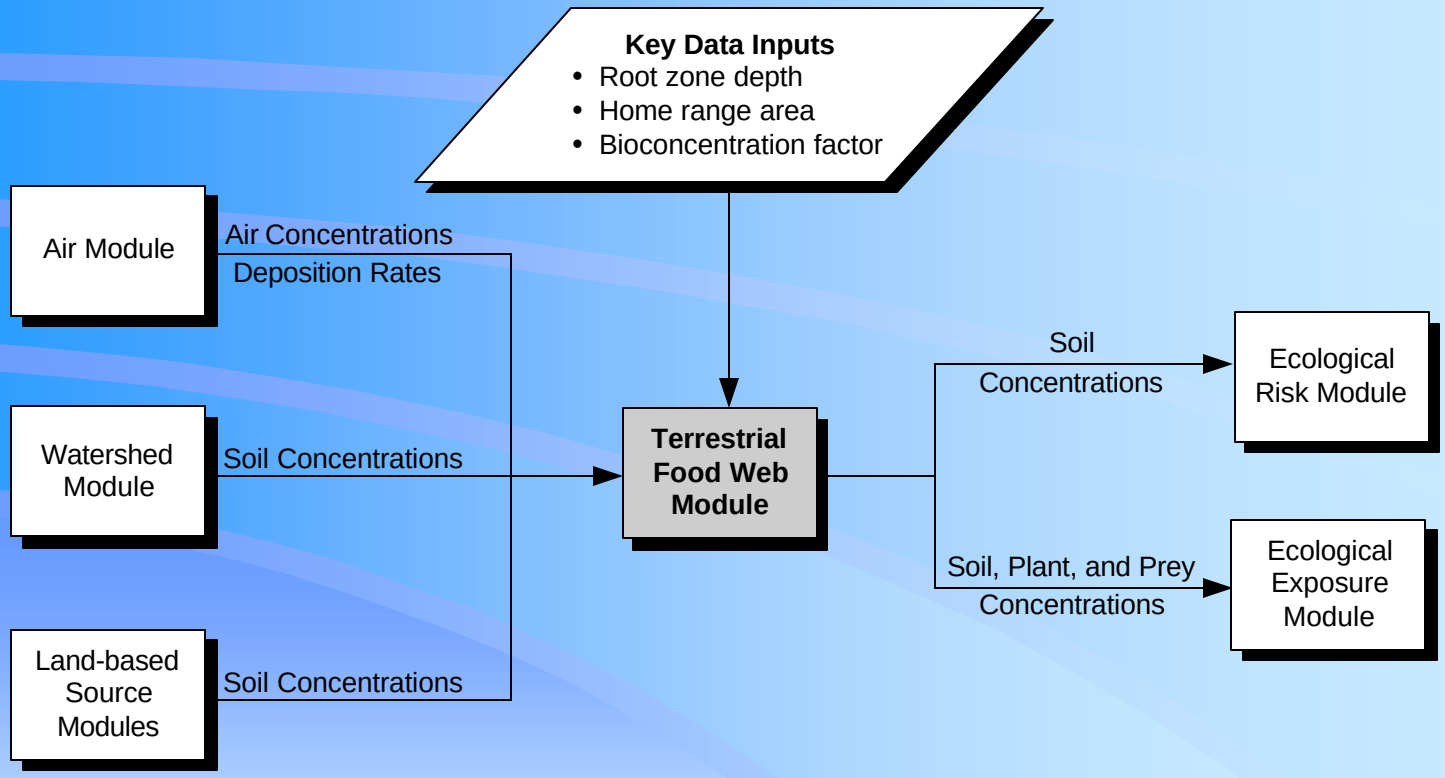
Release, Exposure, and Uptake in Plants



Farm Food Chain

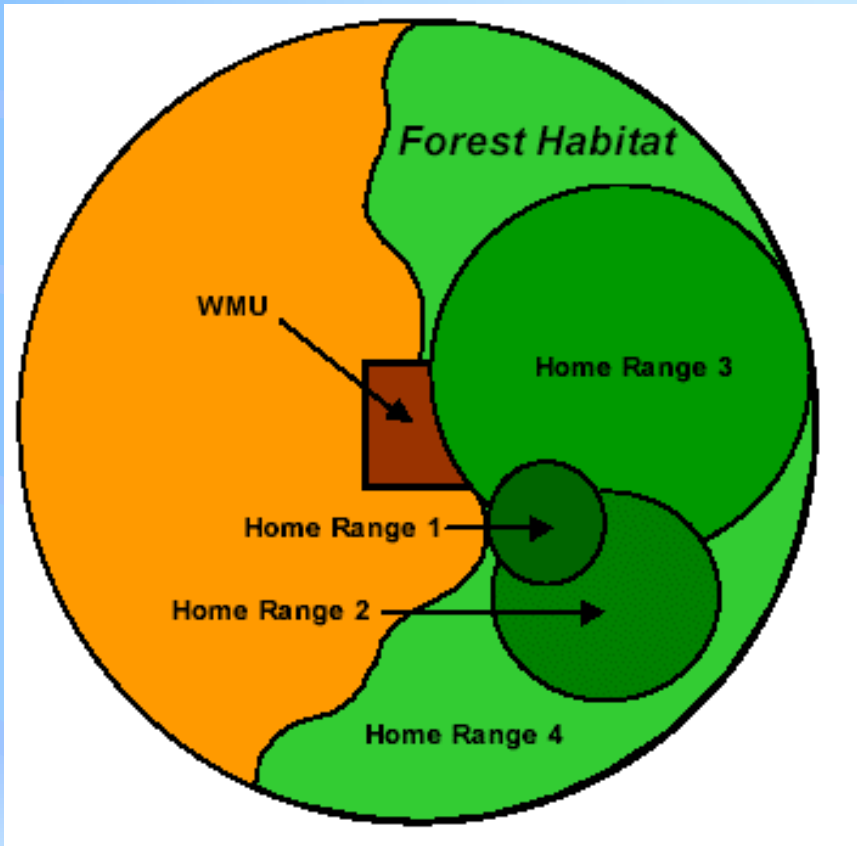
- Approach based on reviewed science, algorithms, and data and is being widely used in other EPA analyses
- Calculates point estimate constituent concentrations in produce for home gardeners and areal averaged estimates for produce, beef and milk for farmers

Terrestrial Food Web in the System



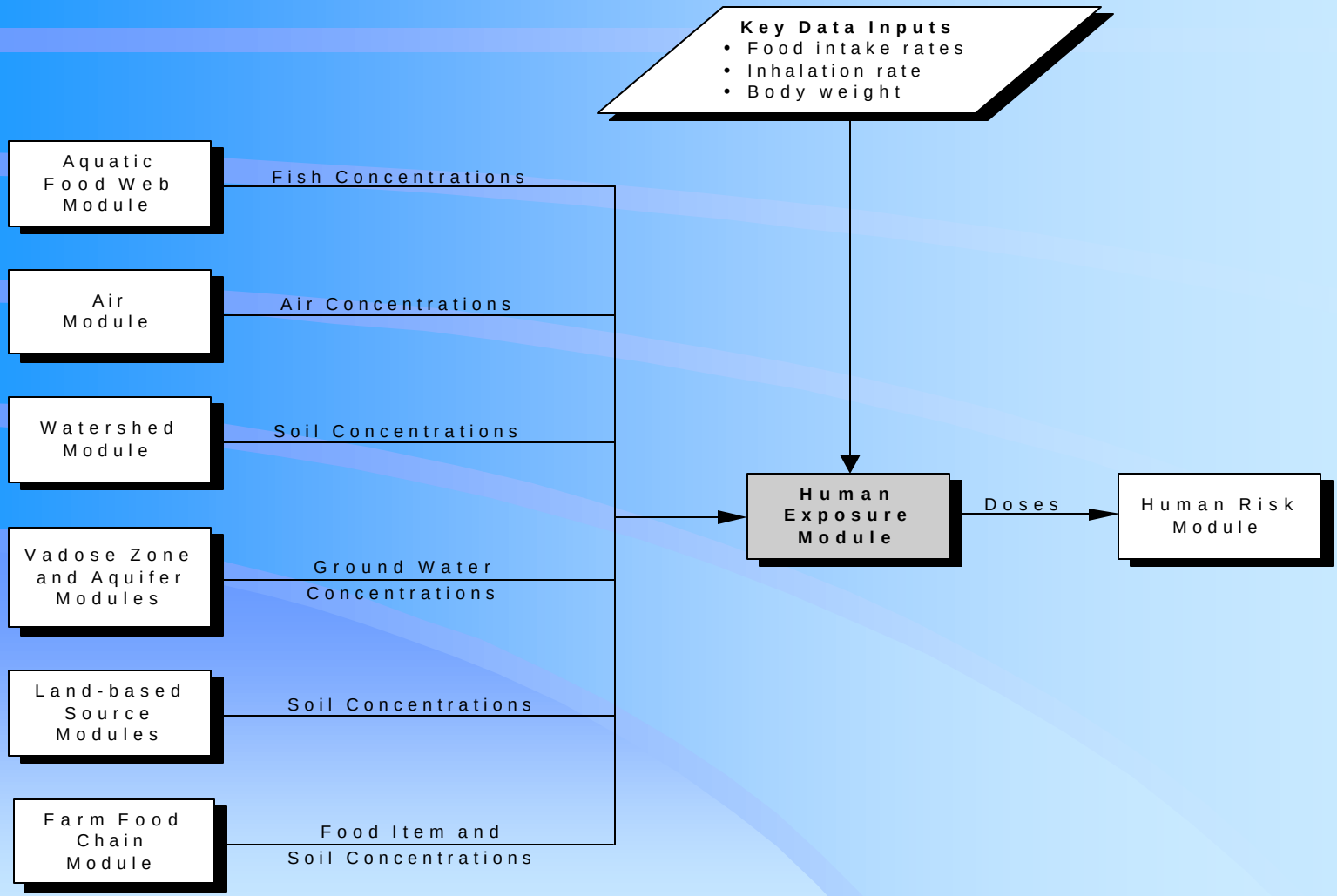
Assignment of Predator-Prey for Terrestrial Habitats

- Uses algorithms, methods, and data consistent with previous EPA analyses
- Defined, overlapping home ranges for predator-prey
- Spatially consistent contaminant concentrations in home ranges

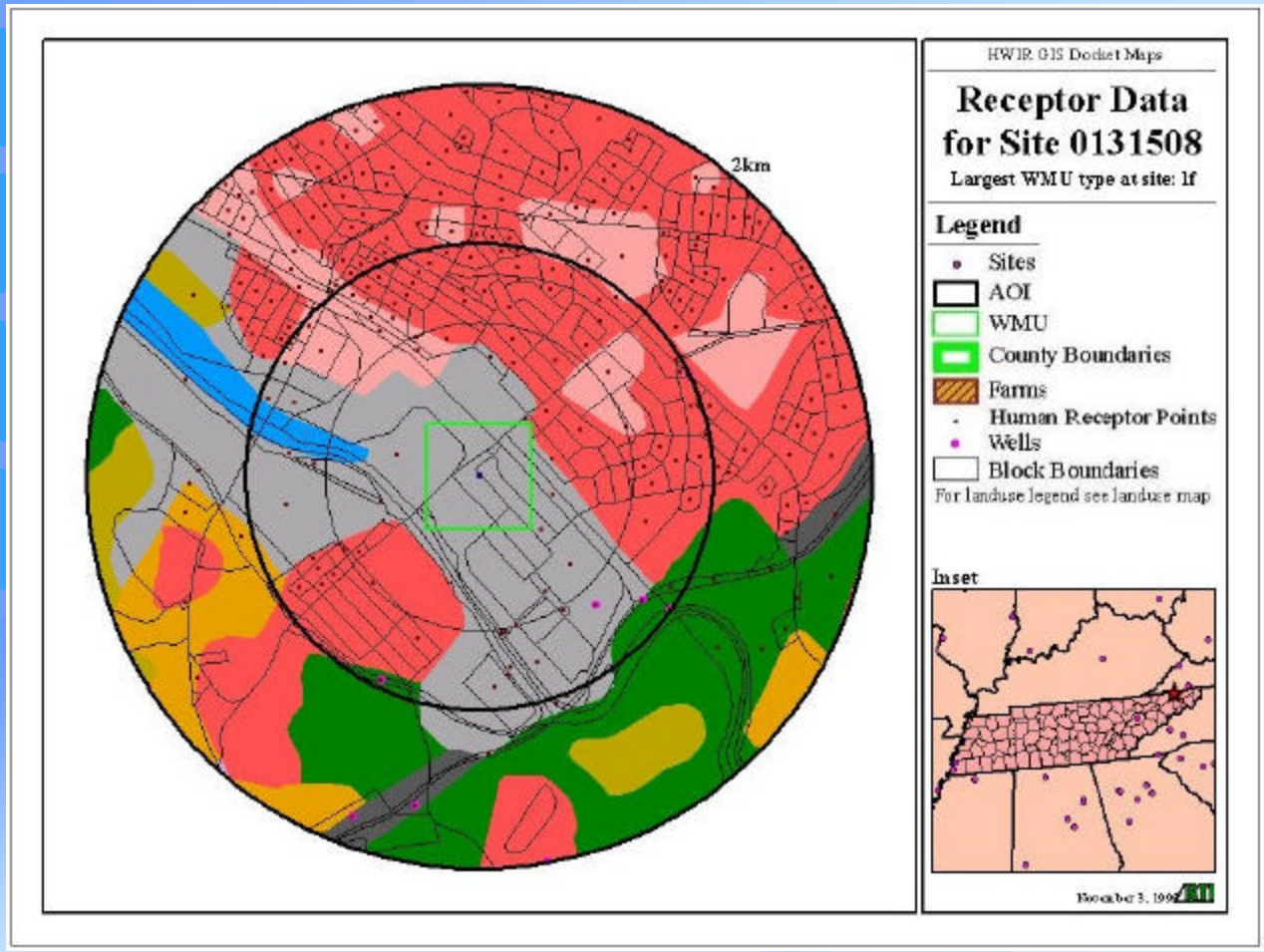


3MRA Human Exposure and Risk Modules

Human Exposure Module



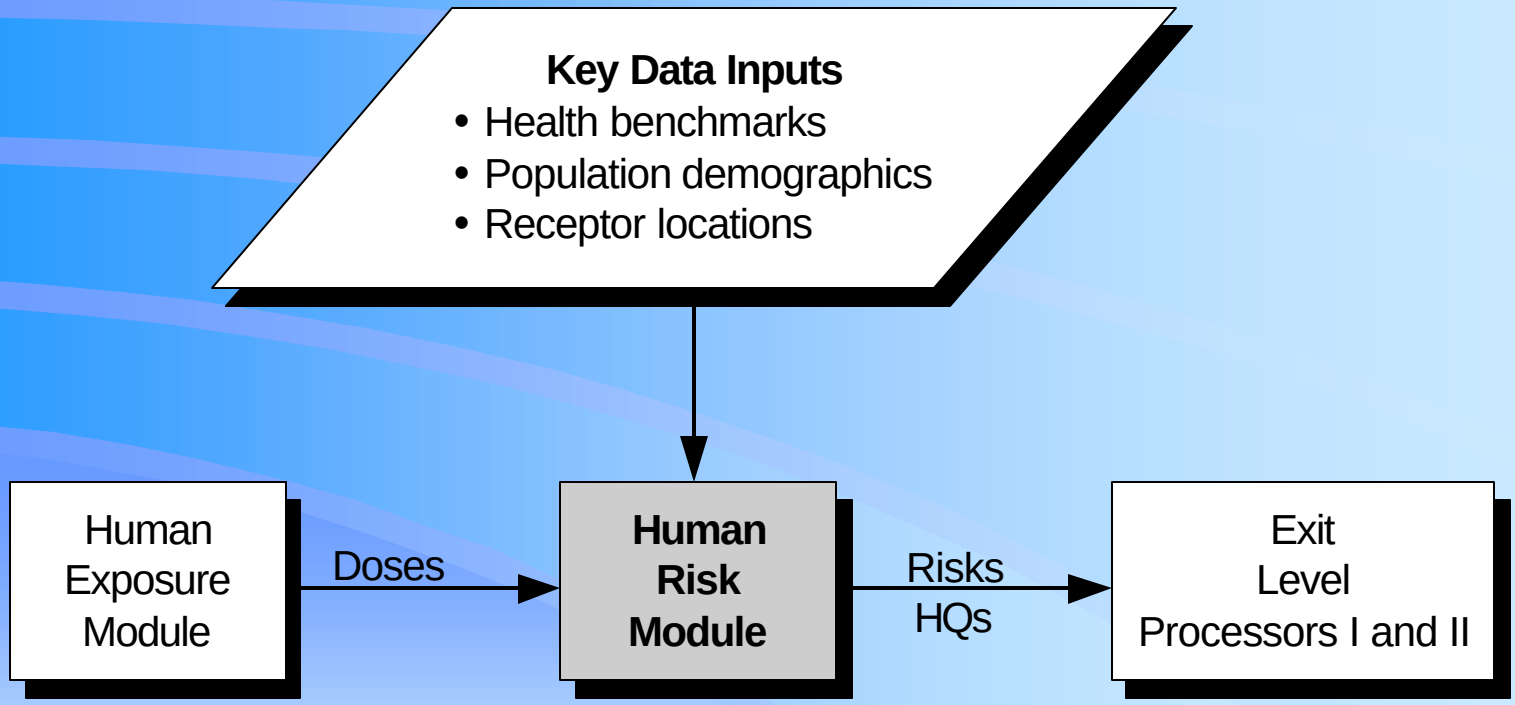
Site-receptor Layout



Receptor-Pathway Combinations

	Receptors (as output by Human Risk Module)							
	Resident	Resident Gardener	Fisher				Farmer	
	Receptors (as output by Human Exposure Module)							
Pathway	**Resident**	**Resident Gardener**	**Resident Fisher**	**Resident Gardener Fisher**	**Beef Farmer Fisher**	**Dairy Farmer Fisher**	**Beef Farmer**	**Dairy Farmer**
Air inhalation	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Shower air inhalation	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Soil ingestion	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Water ingestion	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Crop ingestion	No	Yes	No	Yes	Yes	Yes	Yes	Yes
Beef ingestion	No	No	No	No	Yes	No	Yes	No
Milk ingestion	No	No	No	No	No	Yes	No	Yes
Fish ingestion	No	No	Yes	Yes	Yes	Yes	No	No

Human Risk Module



Human Exposure And Risk

Uses: standard algorithms

Inputs: estimated annual average media and food concentrations; intake rates (air and media); health benchmarks; receptor locations; population demographics

Outputs: estimates of annual average concentrations, doses, risks, and hazards from inhalation and ingestion of contaminated food and media

Output Data…

Data that are 3-dimensional:

- Location, time, receptor type

Descriptors of risk for human receptors

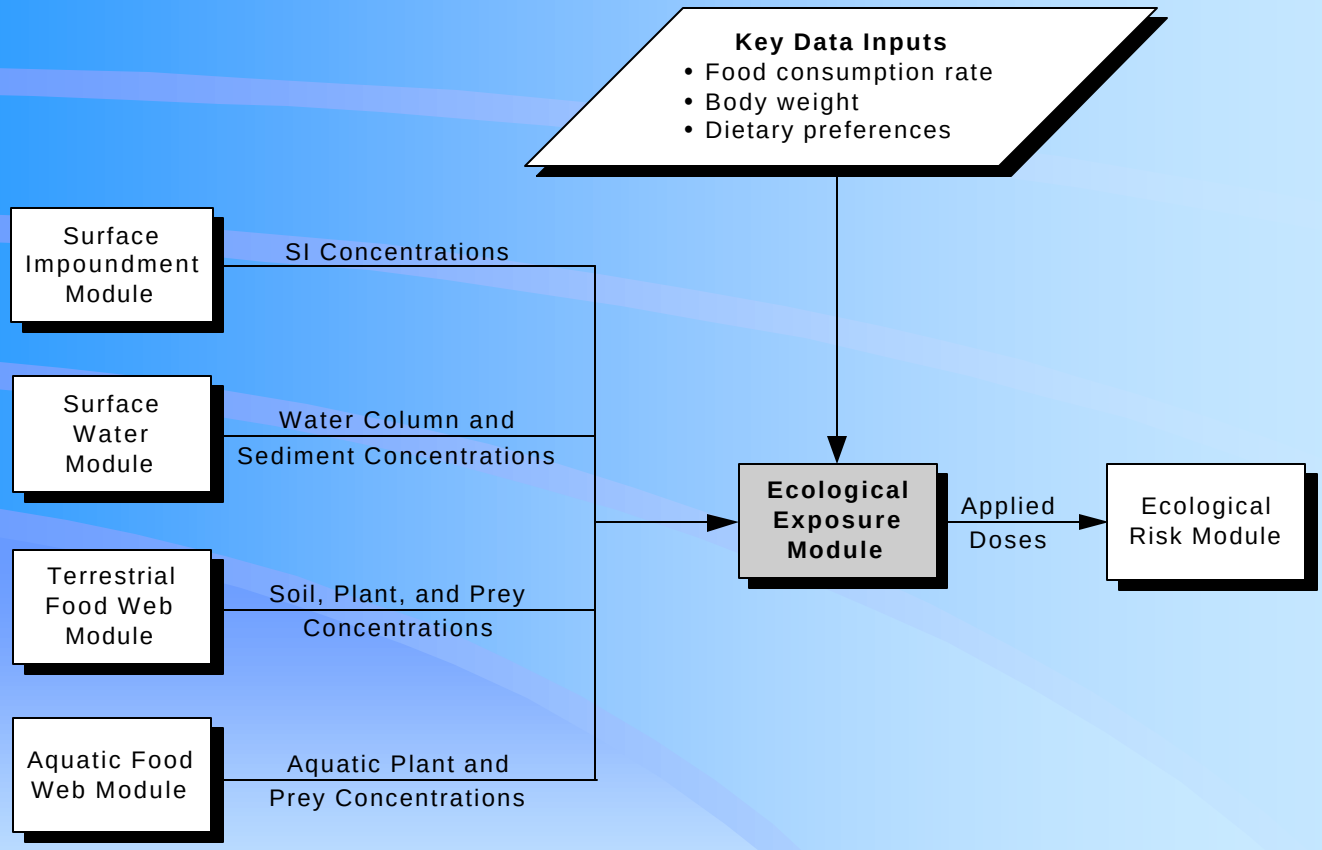
- Distribution of individual risk/hazard weighted by population at the site level

Aggregation of risk/hazard by:

- Receptor type (resident, gardener, farmer, fisher, all)
- Cohort (infant, 1 – 12 years, 13 years+, all)
- Pathways (individual (8), combined)
- Distance (500, 1000, 2000 meters)

3MRA Ecological Exposure and Risk Modules

Ecological Exposure Module



Criteria for Ecological Exposure Module

- Capture the wide variability in ecological systems with available data to characterize and evaluate ecological exposure and risk.
- Define spatial boundaries for ecological exposures at a scale that takes full advantage of the spatial resolution offered by the 3MRA
- Allow for the site-based assignment of ecological receptors that reflect the major trophic elements and feeding strategies relevant to exposure

Representative Habitats for the 3MRA Model

Terrestrial

grasslands
shrub/scrub
forests
crops/pastures
residential

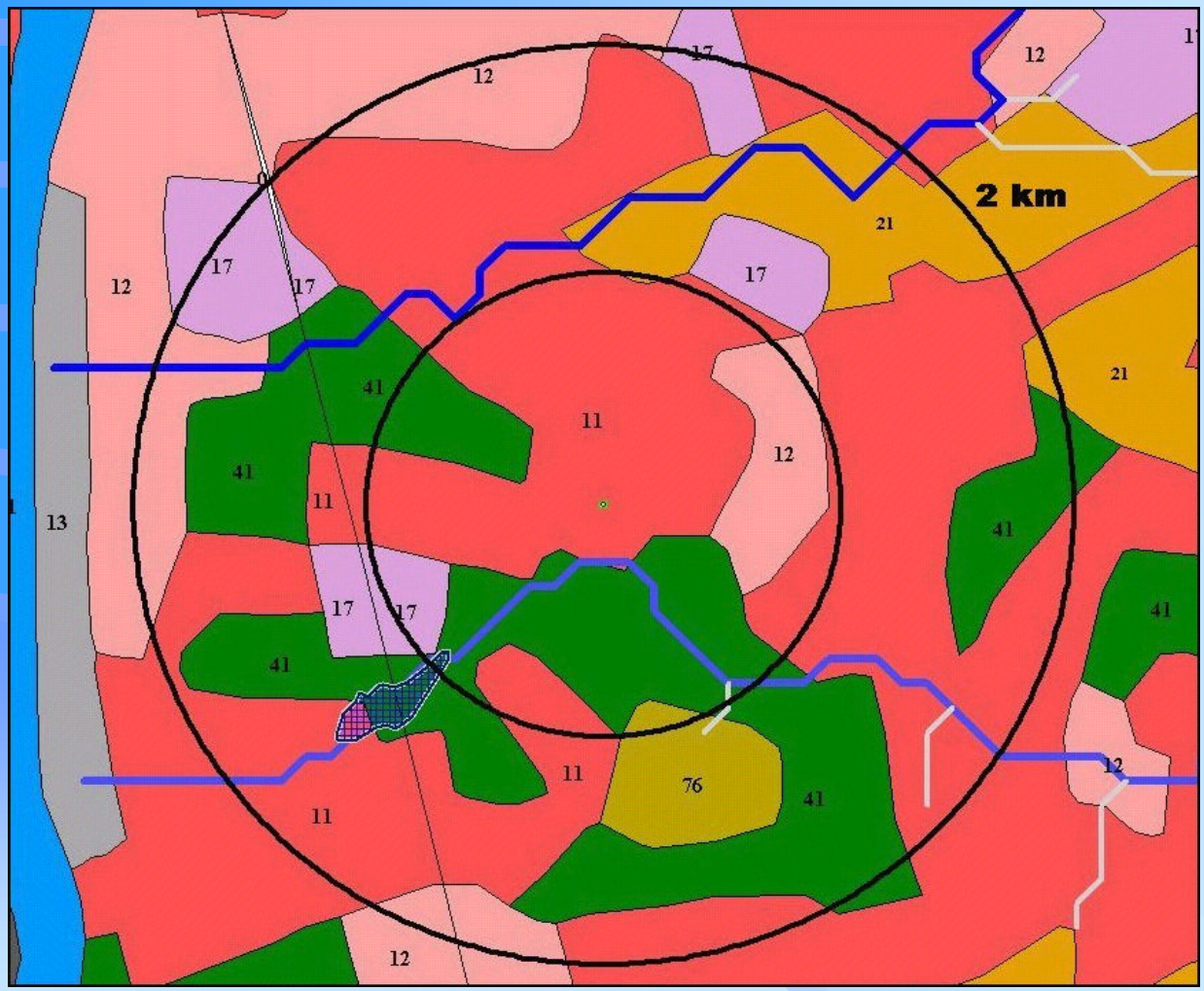
Aquatic

rivers/streams
lakes
ponds

Wetlands

PF grasslands
PF shrub/scrub
PF forests

Habitat Delineation



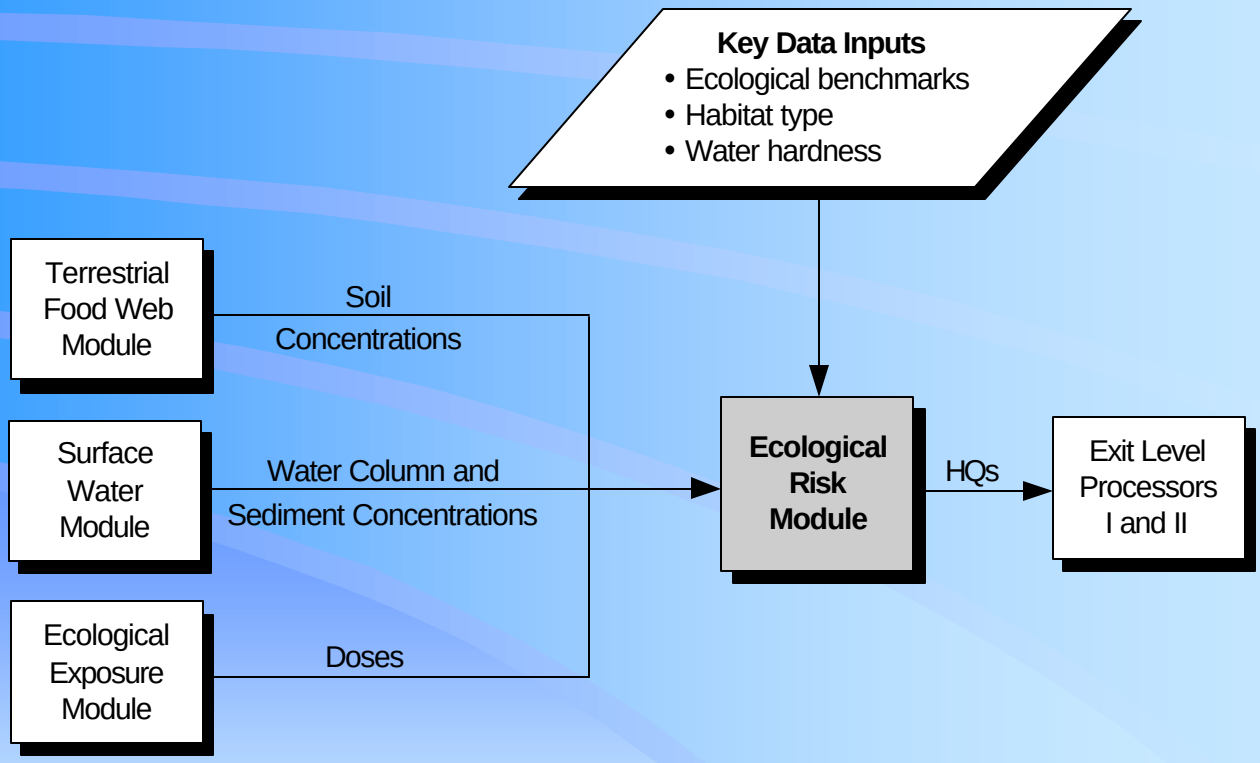
Considerations for Assigning Ecological Receptors

- Geographic distribution
- Availability of wildlife exposure factors
- Faunal class
- Functional niche

Ecological Exposure

- Consistent with Guidelines for Ecological Risk Assessment and uses equations similar to those used in other Agency and non-Agency assessments
- Calculates applied contaminant dose (in mg/kg-d) to ecological receptors that may be exposed to contaminated plants, prey, and media
- Components include representative habitat scheme; habitat-specific foodwebs; and receptors for each habitat and foodweb

Ecological Risk Module



Assessment Endpoints

- Survival and reproductive fitness of mammalian wildlife populations
- Survival and reproductive fitness of avian wildlife populations
- Survival of amphibian populations
- Reproductive success and survival of reptile populations
- Survival of species that comprise key structural and functional elements of the soil community
- Growth and survival of terrestrial plants
- Survival of species that comprise key structural and functional elements of the freshwater aquatic community
- Survival of species that comprise key structural and functional elements of the sediment community
- Growth and survival of aquatic plants and algae

Ecological Risk

- Quantifies the potential for adverse ecological effects by calculating HQs for individual receptors such as raccoons, aquatic plants, or the soil community
- Incorporates benchmarks that reflect the assessment endpoints for the national assessment
- Each HQ maintains specific attributes that allow the ecological risk to be examined in numerous ways (e.g., by habitat, by trophic level)