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Monitoring and Modeling Strategies



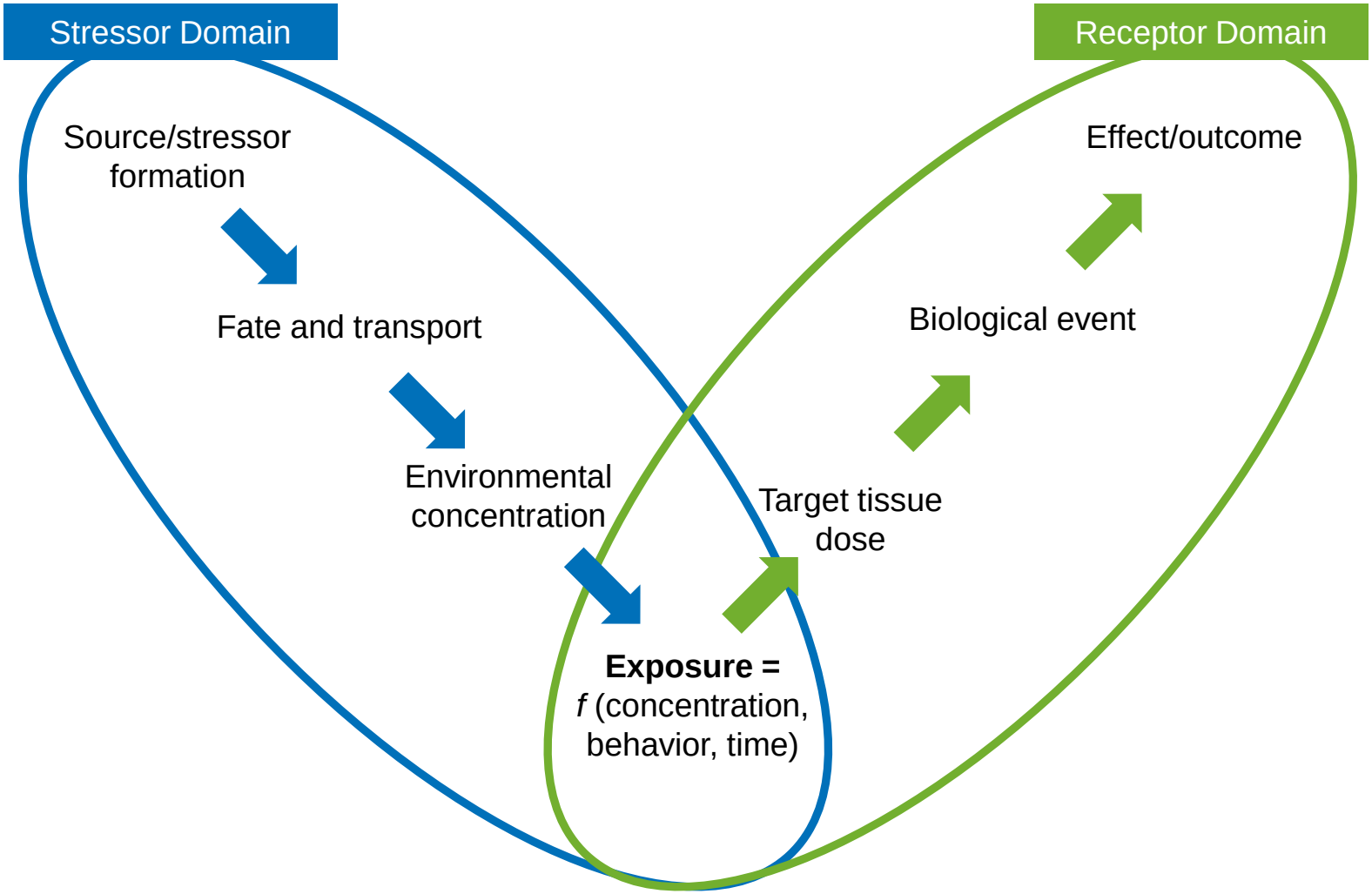
RISK ASSESSMENT TRAINING AND EXPERIENCE
Exposure Assessment Course Series – EXA 405

Office of Research and Development
National Center for Environmental Assessment

What You Can Expect to Learn from This Course

- How to evaluate the design and results of a monitoring study and use these results in exposure assessment, including considerations of:
  - Study design
  - Quality control
  - Background concentrations
  - Data interpretation
- How to select, apply, and evaluate an environmental model
  - Selecting and running a model
  - Model evaluation
  - Model types

Source to Effect Continuum



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MONITORING STUDY DESIGN AND DATA GATHERING APPROACHES

Why Monitor?

For exposure assessment, we monitor to:

- Obtain concentration terms to calculate exposure and dose
- Identify and fill data gaps

Study Design Considerations

Purpose – Why is the study being conducted? What is the question we are trying to answer?

Scope – Where does the study area begin and end?

Level of Detail – How accurate must the estimate be and what is the most effective use of resources?

Approach – How will concentration of the contaminant in the media of interest be measured?

Components of a Monitoring Plan

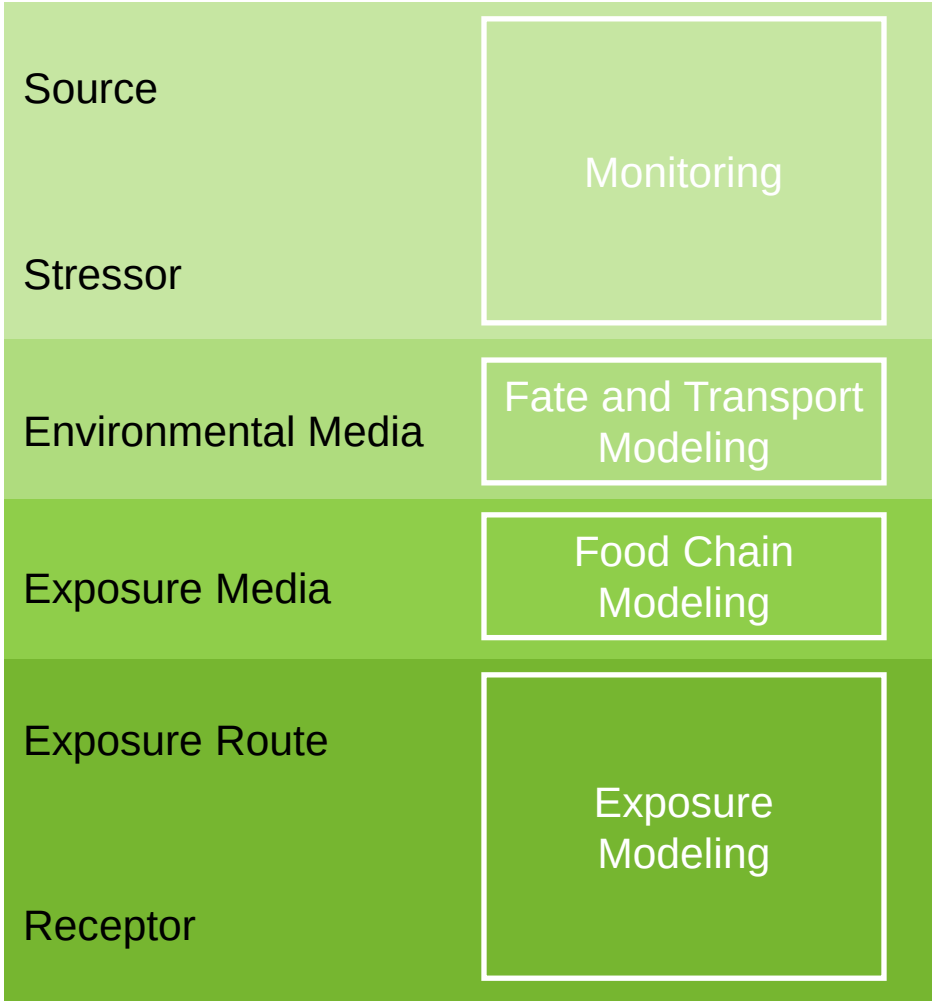
- Scenario information
  - Geographic domain
  - Site/area history
  - Previous assessment
  - Operational history
- Conceptual model
- Data quality objectives
- Sampling rationale
- Data evaluation methods

Conceptual Model

A conceptual model of exposure identifies:

- all potential or suspected sources of contamination
- types and concentrations of contaminants detected at the location
- potentially contaminated media
- potential exposure pathways, including receptors

(EPA RAGS 1989, page 4-4)



Sample Size and Locations

- Sample size
  - Consider statistical analyses
  - Variability, power, and certainty
  - Practical concerns
- Sampling location
  - Purposive
  - Random
  - Systematic

Types of Samples

WHERE?

- Media
  - Air
  - Water
  - Soil
  - Household

HOW?

- Method
  - Grab
  - Composite
- Timing
  - One-time
  - Longitudinal or continuous
- Design
  - Systematic
  - Random
  - Field screening

Other Considerations for Sampling Strategy

- Temporal and meteorological factors
- Time and cost
- Area accessibility
- How much data are enough to estimate exposure and risk?
  - Depends on how much uncertainty is acceptable

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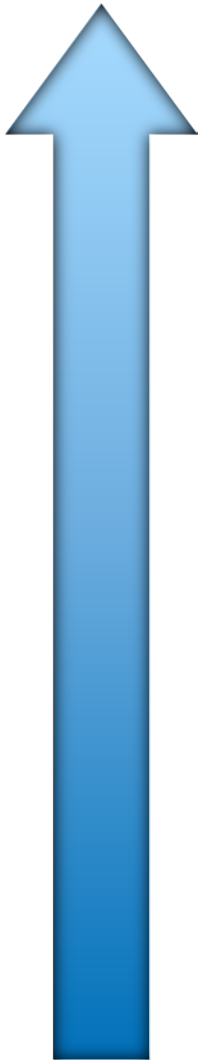
DATA EVALUATION

Data Evaluation Steps

- Gather and organize the data
- Evaluate data with respect to:
  - Quantitation limits, data qualifiers, and blanks
  - Background
- Assemble data set

Quantitation Limits



- **Quantitation limit (QL) → *Trusted***

  "Lowest level at which a chemical may be accurately and reproducibly quantitated."

  - Adjusted based on sample characteristics, preparation, and analytical methods

- **Trace → *Observed but not quantified***

  Amounts confirmed to be present, but not quantifiable

- **Detection limit → *Seen***

  "Lowest amount of a chemical that can be 'seen' above the normal random noise of an analytical instrument or method."

  - Chemical specific, instrument specific, and method specific

- **Not detected → *Not seen***

Data Qualifiers

Tetrachloroethene Concentration (µg/L)				
	Sample 1	**Sample 2**	**Sample 3**	**Sample 4**
Site 1	**40U**	40	**30U**	20
Site 2	**<30**	45	**TR**	40
Site 3	**ND**	35	40	40
Site 4	50	**BDL**	50	**0**

#U → Undetected where the # value is the detection limit

<30 → Less than detection limit of 30

BDL → below detection limit

ND → Non-detect

BMDL → below minimum detection limit

0 → ???

TR → Trace

Treatment of Non-Detects and Trace Measurements

Non-Detects

- ND = DL
- ND = ½ * DL
- ND = DL/√2
- ND = 0

Traces

- TR = DL
- TR = ½ * (QL + DL)
- TR = QL

Treatment of Non-Detects and Traces – Class Activity

How does the substitution approach affect the range of calculated average chemical concentrations?

Tetrachloroethene Concentration (µg/L)				
	Sample 1	**Sample 2**	**Sample 3**	**Sample 4**
Area 1	**40U**	40	**30U**	20
Area 2	**<30**	45	**TR**	40
Area 3	**ND**	35	40	40
Area 4	50	**BDL**	50	**0**

Note: DL = 30 µg/L; QL = 40 µg//L

Non-detects:

ND = DL

ND = DL/2

ND = 0

Traces:

TL = QL

TL = (DL + QL)/2

TL = DL

Treatment of Non-Detects and Traces – Results

How does the substitution approach change the calculated average chemical concentration?

Calculating *Highest* Possible Average TCE Concentration (µg/L)				
	Sample 1	**Sample 2**	**Sample 3**	**Sample 4**
Area 1	40U / 40	40	30U / 30	20
Area 2	0 / 30	45	TR / 40	40
Area 3	ND / 30	35	40	40
Area 4	50	BDL / 30	50	0 / 30

Note: DL = 30 µg/L; QL = 40 µg//L

Minimum:

ND = 0

TL = DL

Average Concentration: 24.4

Maximum:

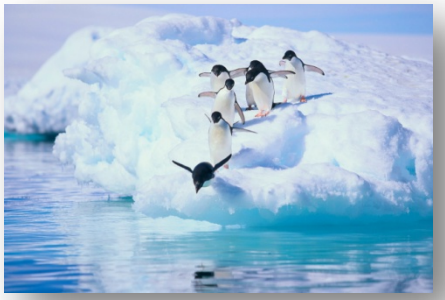
ND = DL

TL = QL

Average Concentration: 36.9

Background Concentrations

- **Background** can be defined as:
  - Contributions from natural sources
  - Contributions from regional (but not local) sources
  - Any concentration resulting from a source other than the source of interest



Assurance of Analytical Data Quality

- **Demonstration of capabilities**
  - Involves controlled analyses of known chemical standards
  - Conducted independent of a particular study

- **Standards**: Samples incorporated into array of samples for a study
  - **Chemical standards:** Check accuracy, instrument performance
  - **Duplicate/split samples:** Measure reproducibility
  - **Lab blanks:** Check for contamination
  - **Recovery standards:** Estimate recovery of the analytes

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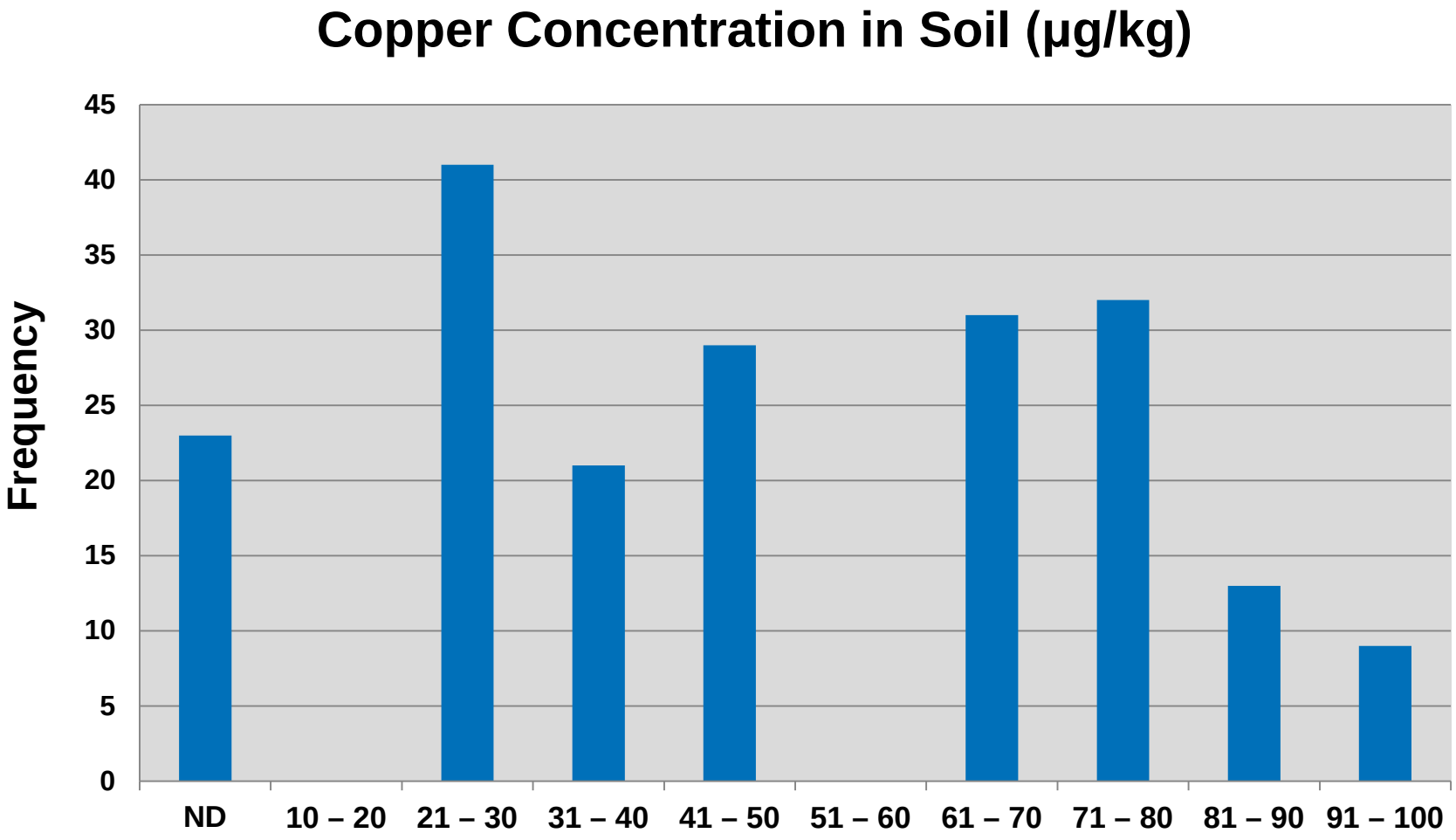
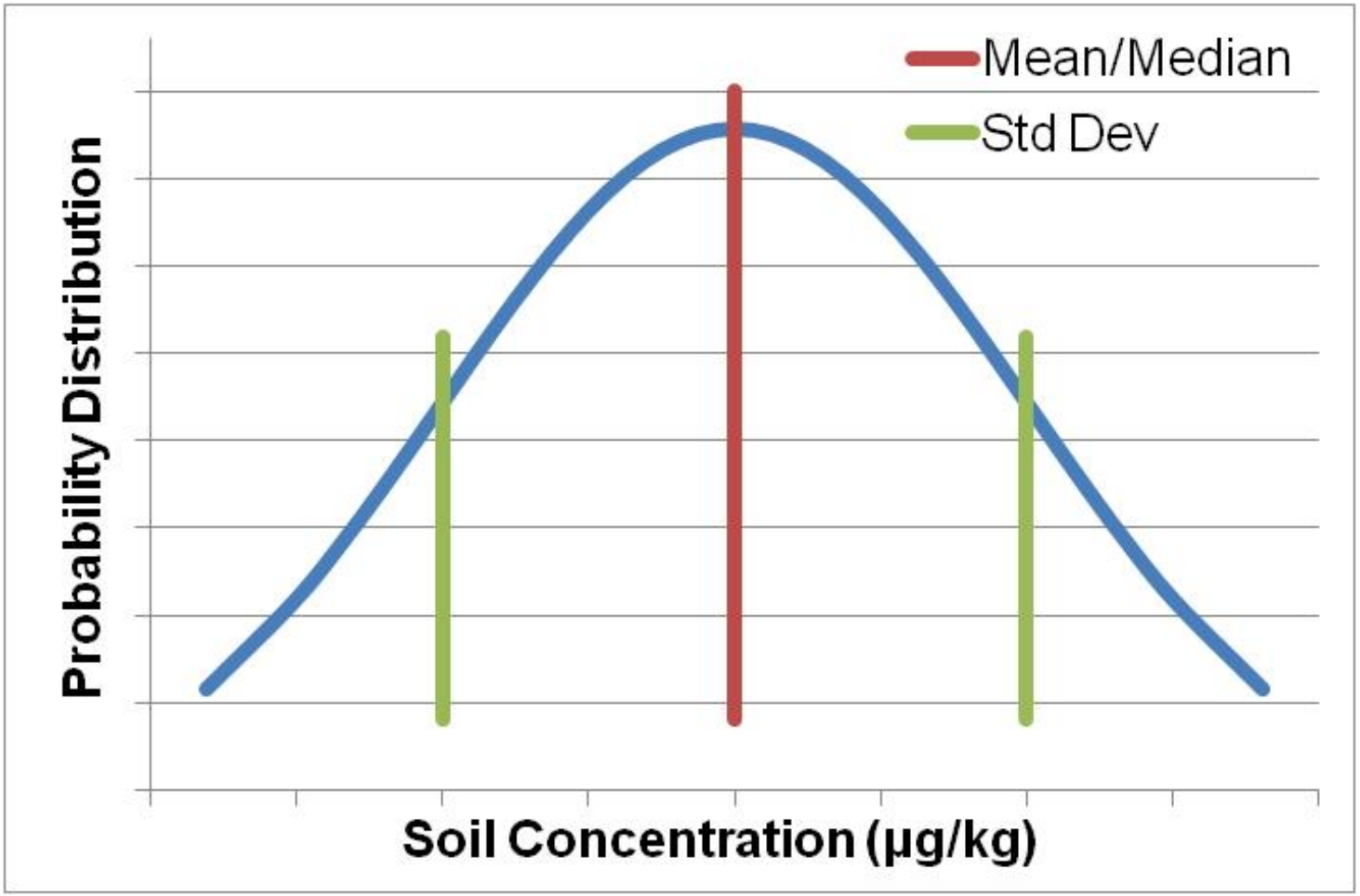
ASSEMBLING AND INTERPRETING DATA

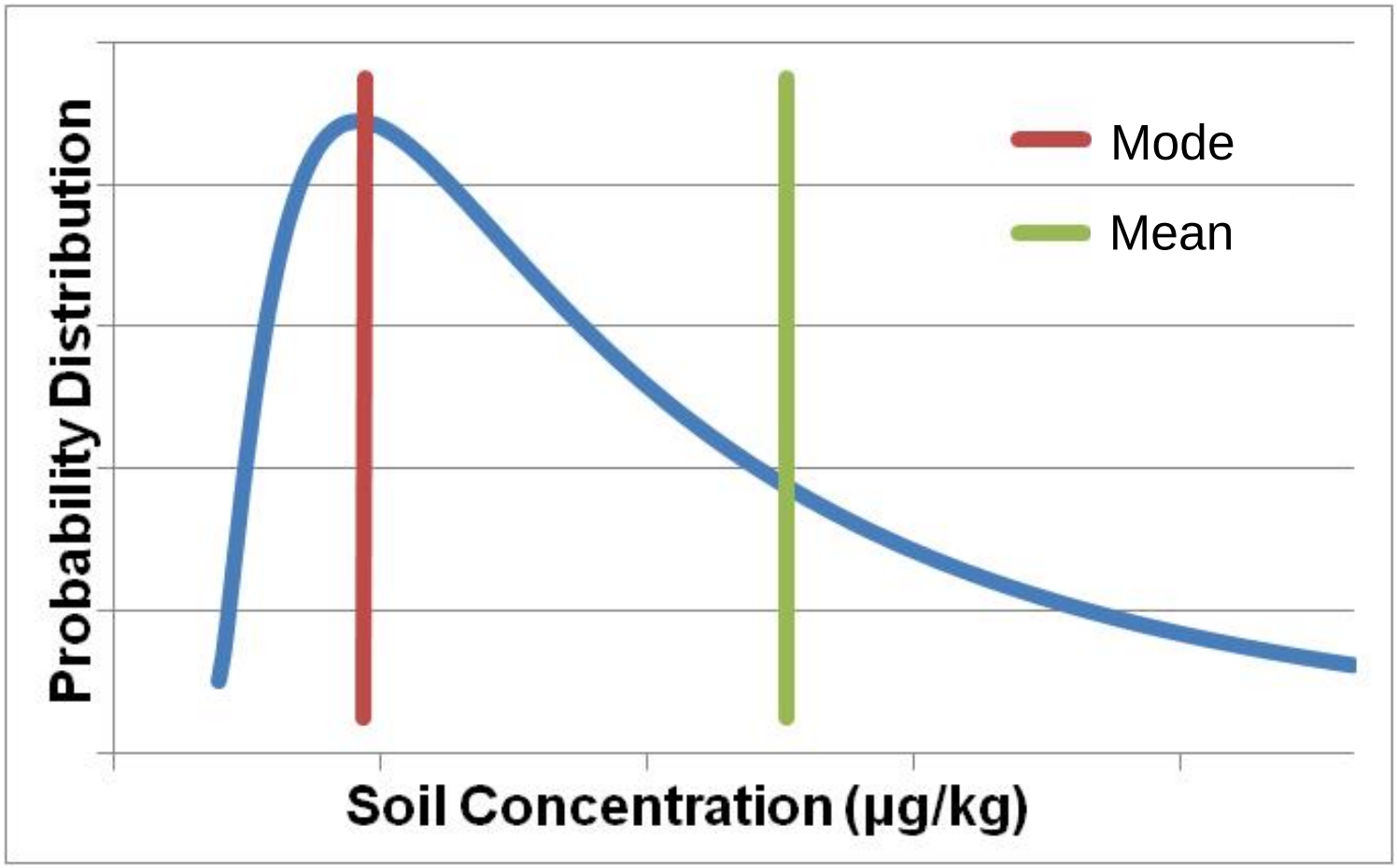
Frequency Distribution



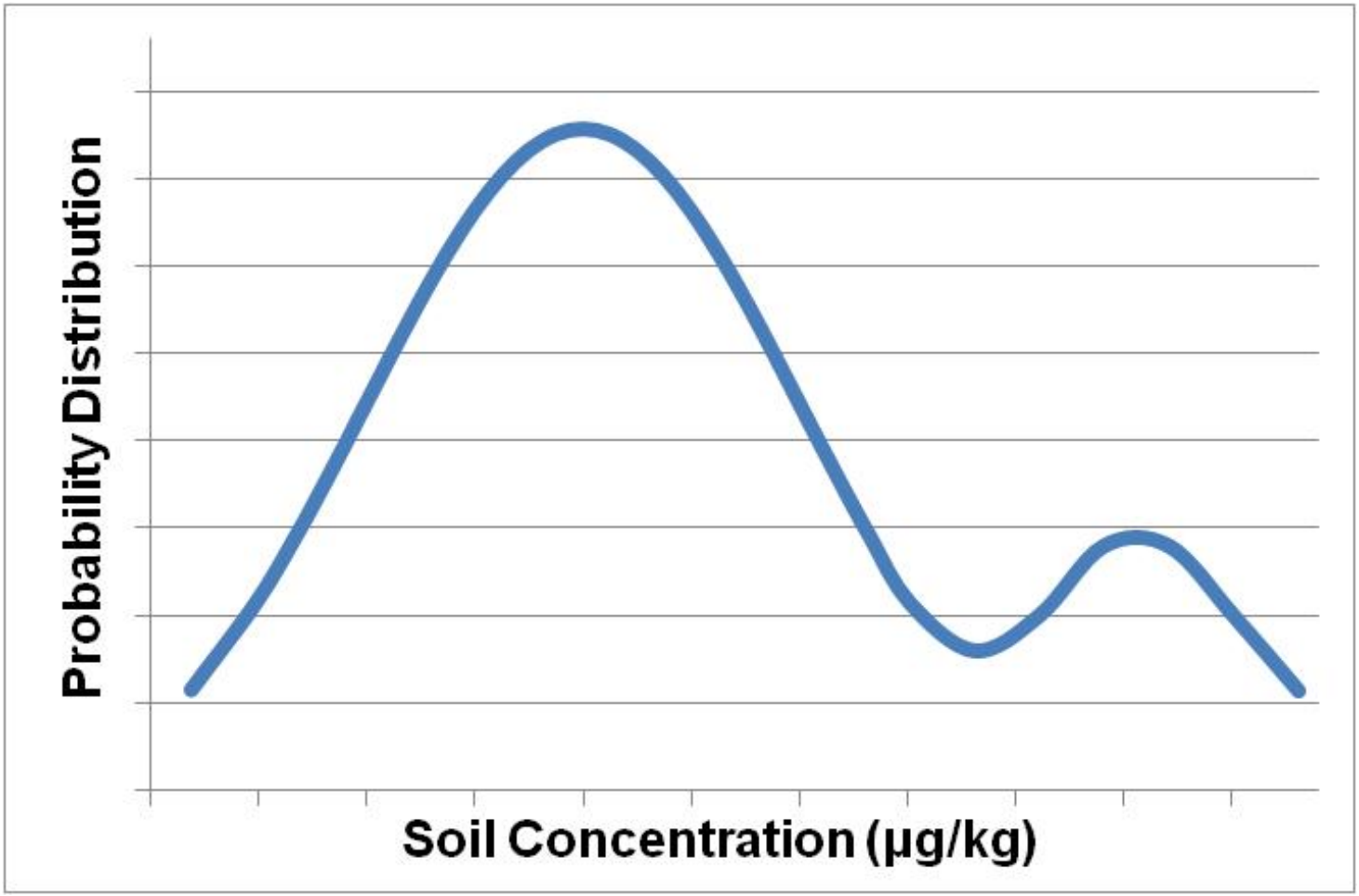
Normal Distribution



Lognormal Distribution



Bimodal Distribution



Data Interpretation

- **Acute exposures** – short-term
  - Single point measurement on distribution may be adequate
  - Health-protective uses require many measurements
  - Evaluate frequency, magnitude of high concentrations
- **Chronic exposures** – long-term
  - Mean or median of data provides “typical” exposure
  - Tail of distribution might help estimate upper bound exposure

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MODELING EXPOSURE CONCENTRATIONS

What is a Model?

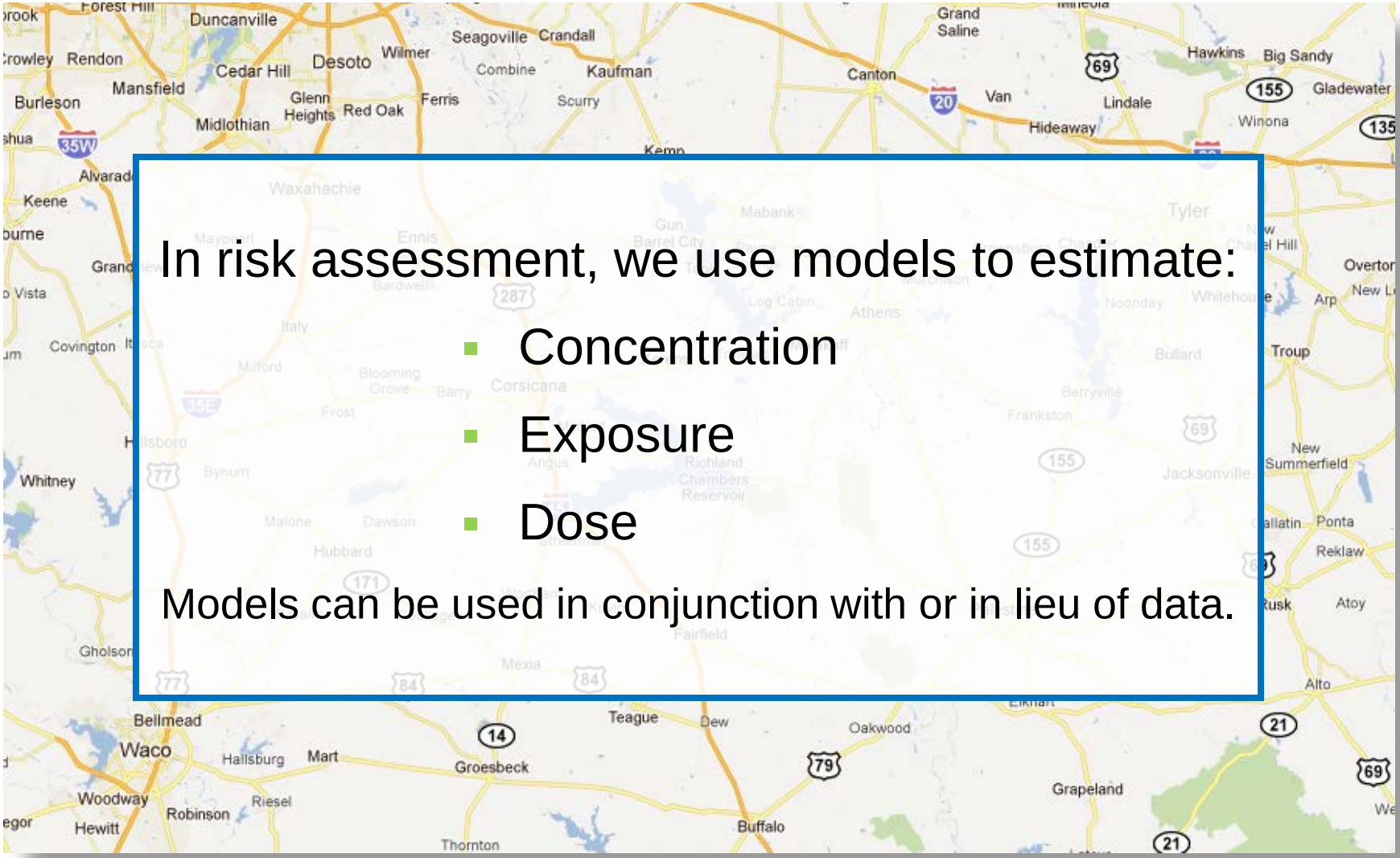
"A simplification of reality that is constructed to gain insights into select attributes of a particular physical, biological, economic, or social system."

Types of models:

- Physical
- Analogs
- Conceptual
- Empirical
- Computational

Source: National Research Council (2007). *Science and Decision.*

Why Model?


In risk assessment, we use models to estimate:
Concentration
Exposure
Dose
Models can be used in conjunction with or in lieu of data.

Environmental Concentration Models

- Estimate concentrations of chemicals in environmental media, microenvironments, and surfaces
- Consider source, emissions, transport, and transformation

Approaches	Processes	Media
Mechanistic vs. Empirical	**First principles**	**Air**
Deterministic vs. Stochastic	**Partitioning**	**Water**
Steady-State vs. Dynamic	**Mixing**	**Soil**
Screening-Level vs. Detailed	**Bioaccumulation**	**Food & Food Webs**
		Microenvironments
		Surfaces

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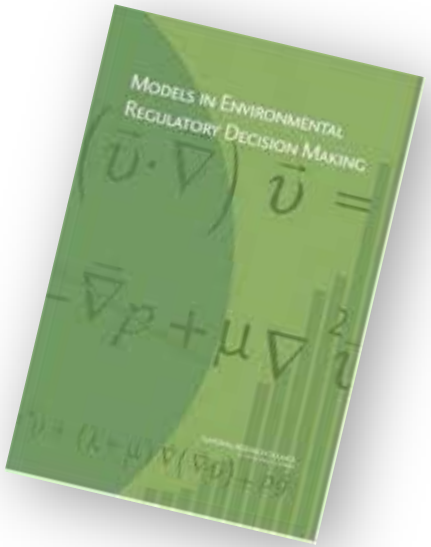
IMPLEMENTING AN ENVIRONMENTAL MODELING STRATEGY

Implementing a Modeling Strategy

- Set objectives
- Select a model
- Calibrate (if necessary) and run the computer model
- Validate and verify (i.e., evaluate)
  - Continuum of accuracy and usefulness



Setting Modeling Objectives

- Develop a clear statement
  - What information will the model help estimate?
  - How will this estimate be used?
- Consider schedule, budget, and other resource constraints

Model Selection

- Considerations:
  - Mathematical simplicity
  - Computational simplicity
  - Interpretability
  - Consistency
  - Accuracy in prediction
  - Accessibility of input variables and data

Source: WHO/IPCS (2005) *Principles of Characterizing and Applying Human Exposure Models*

Principles of Model Evaluation

How well does the model represent the processes occurring in the environment?

- Does the model get the "correct" result?
- Does the model get the correct result for the right reason?
- Is the model transparent?

Methods for Evaluation

- Verify concepts are accurately represented in the model
- Verify code is free of error
- Compare model outputs to measured values
- Compare model outputs to those from other models
- Conduct bounding analyses
- Conduct sensitivity analyses

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MODELING APPROACHES

Mechanistic Versus Empirical Models

Mechanistic models "simulate the real behavior of an agent in the environment and in target organisms as it is transported and undergoes physical and chemical transformations." (IPCS, 2005)

Empirical models "predict concentrations and exposures based on their statistical associations with concentrations in the relevant media and other independent variables that are observed in measurement studies." (IPCS, 2005)

Source: WHO/IPCS (2005) *Principles of Characterizing and Applying Human Exposure Models*

Deterministic Versus Stochastic Models

Variables in Deterministic Models:

"...are given fixed values so that the system is at any time entirely defined by the initial/boundary conditions chosen. A given set of input variables produces a fixed output."
(IPCS, 2005)

Variables in Stochastic (probabilistic) Models:

"...take into consideration the presence of some randomness in one or more of the input parameters or variables."

(IPCS, 2005)

Source: WHO/IPCS (2005) *Principles of Characterizing and Applying Human Exposure Models*

Steady-State Versus Dynamic Models

Steady-state models have constant values for all parameters, and chemical levels in modeled compartments ***do not change*** with time.

In dynamic models, the parameter values & chemical concentrations ***can*** change with time.

Screening-Level Versus Detailed Models

- Screening-level analysis
  - First approximation
  - Conservative

- Detailed (or Refined)
  - Area-specific
  - More complex

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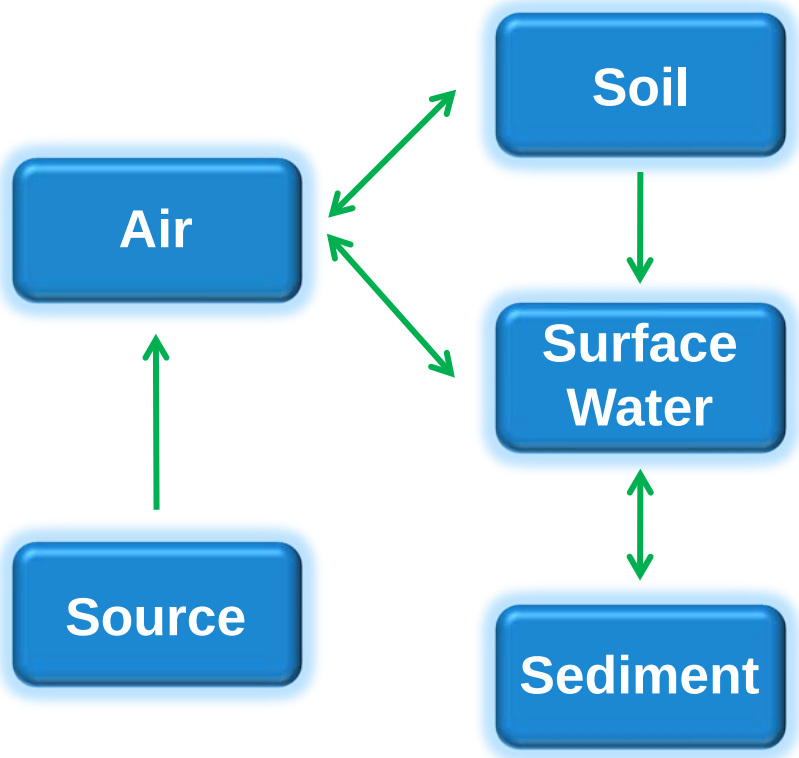
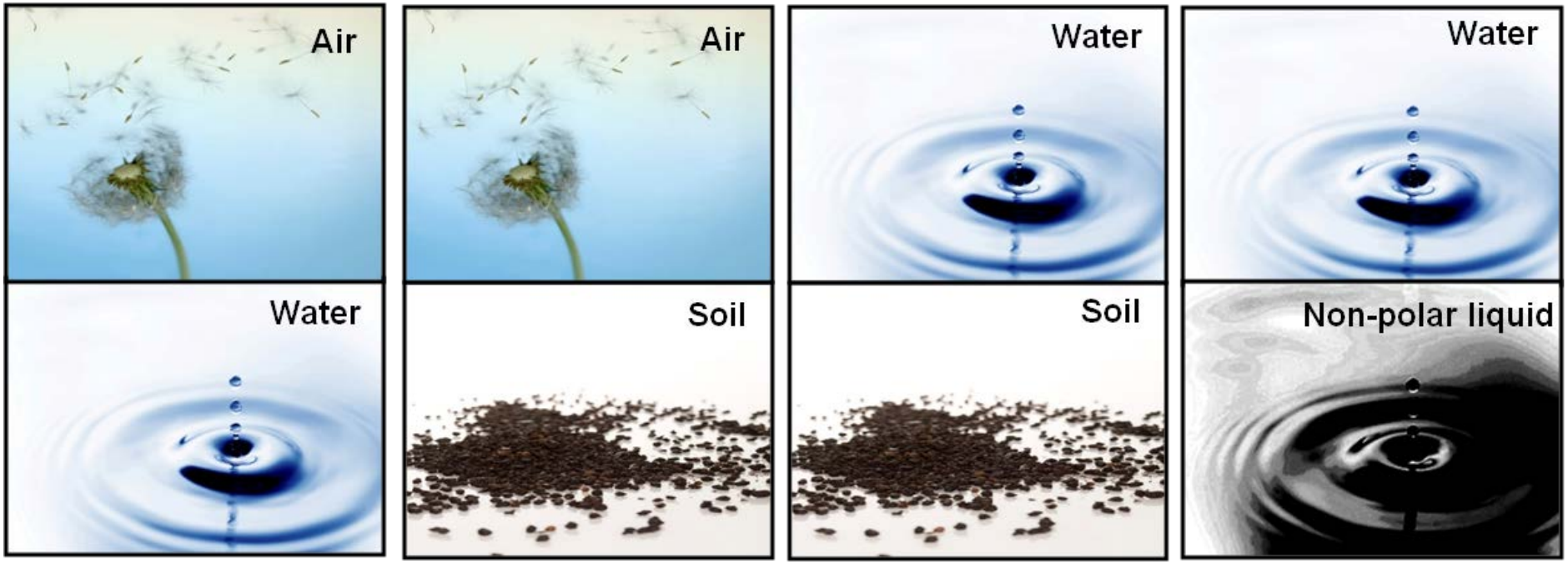
TYPES OF ENVIRONMENTAL CONCENTRATION MODELS

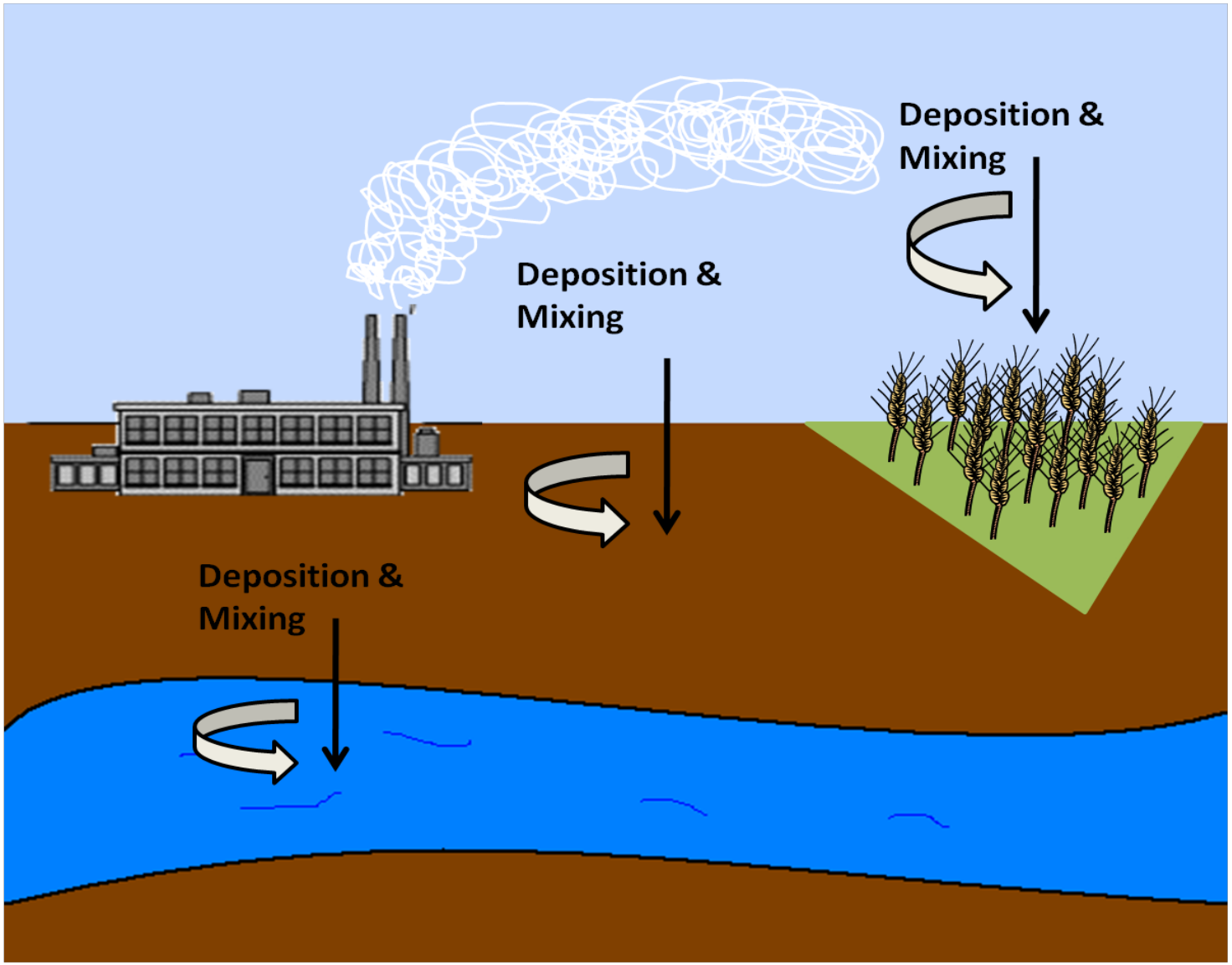
First Principles



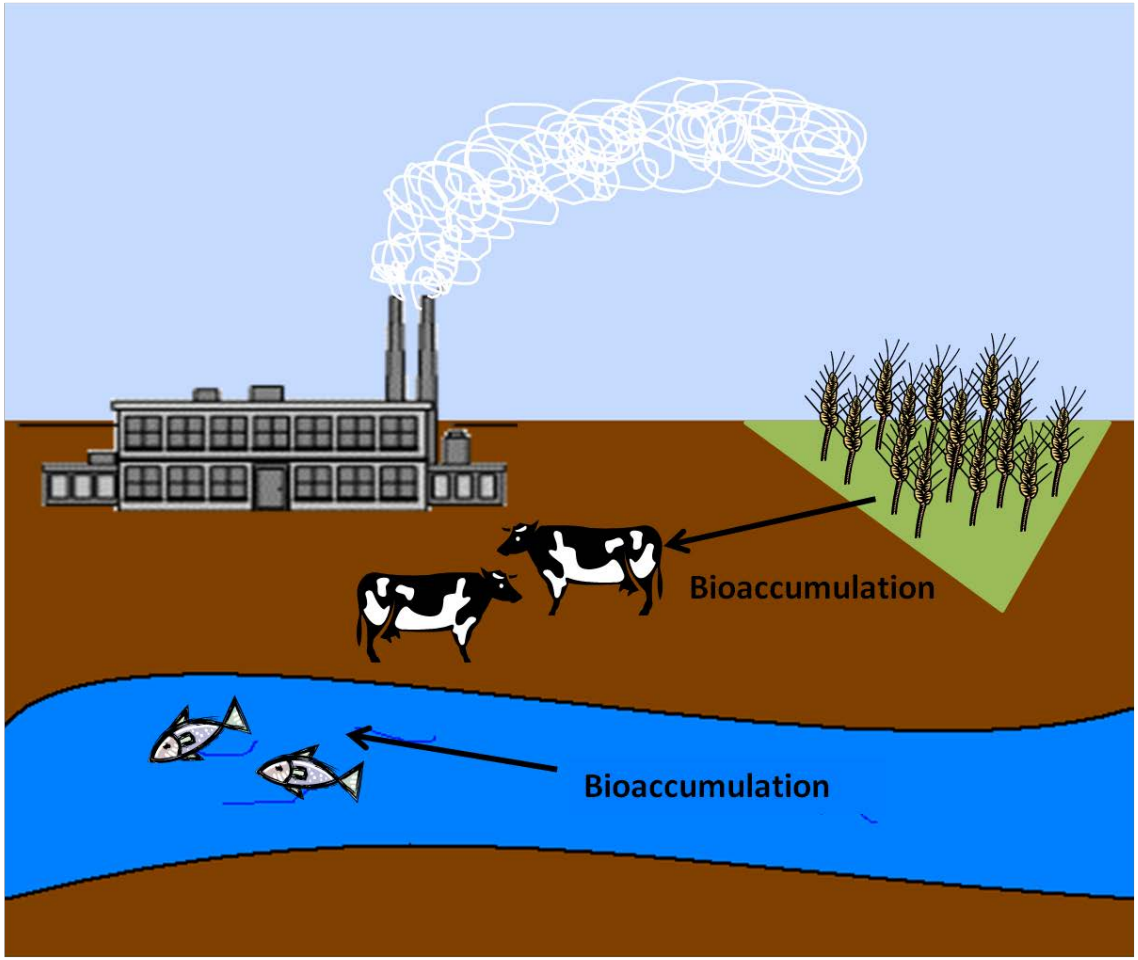
Partitioning

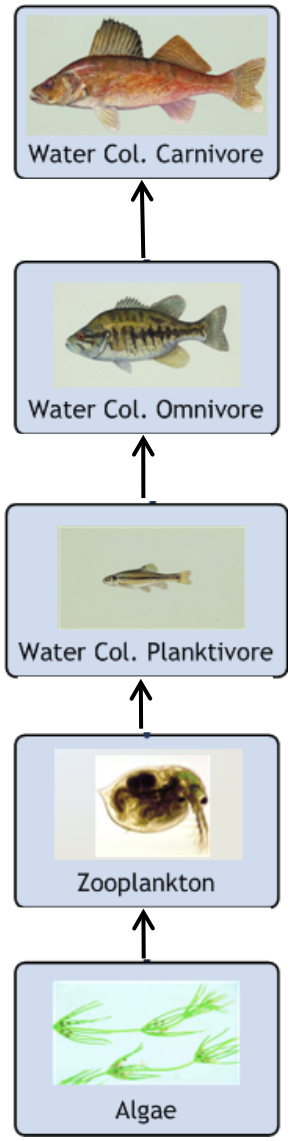


Mixing Models



Bioaccumulation Models





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EXAMPLE ENVIRONMENTAL CONCENTRATION MODELS

Universal Soil Loss Equation (USLE)

Erosion and sediment delivery:

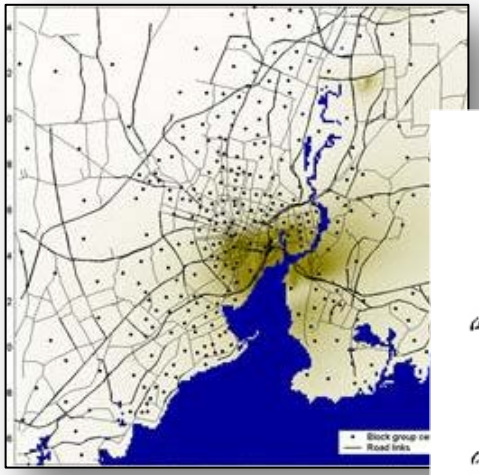
$$ER = [R \times K \times LS \times C \times P] \times SD$$

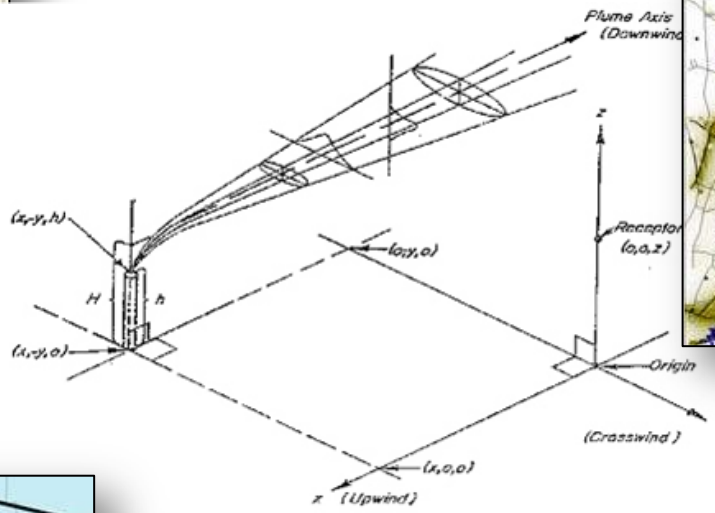
where:

ER = erosion amount (tons/acre-yr)
R = rainfall erosivity
K = soil erosivity
LS = length/slope
C = crop factor
P = support practice
SD = sediment delivery ratio

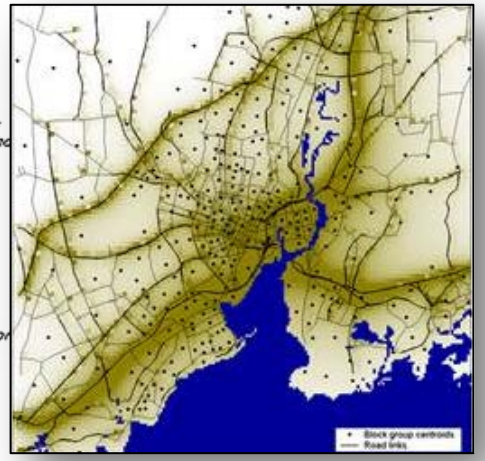
AMS/EPA Regulatory Model (AERMOD)

Local impact from stationary sources as modeled in AERMOD

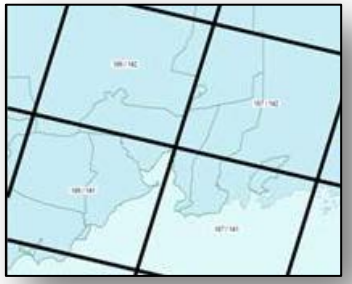




Near-road impact from mobile sources as modeled in AERMOD

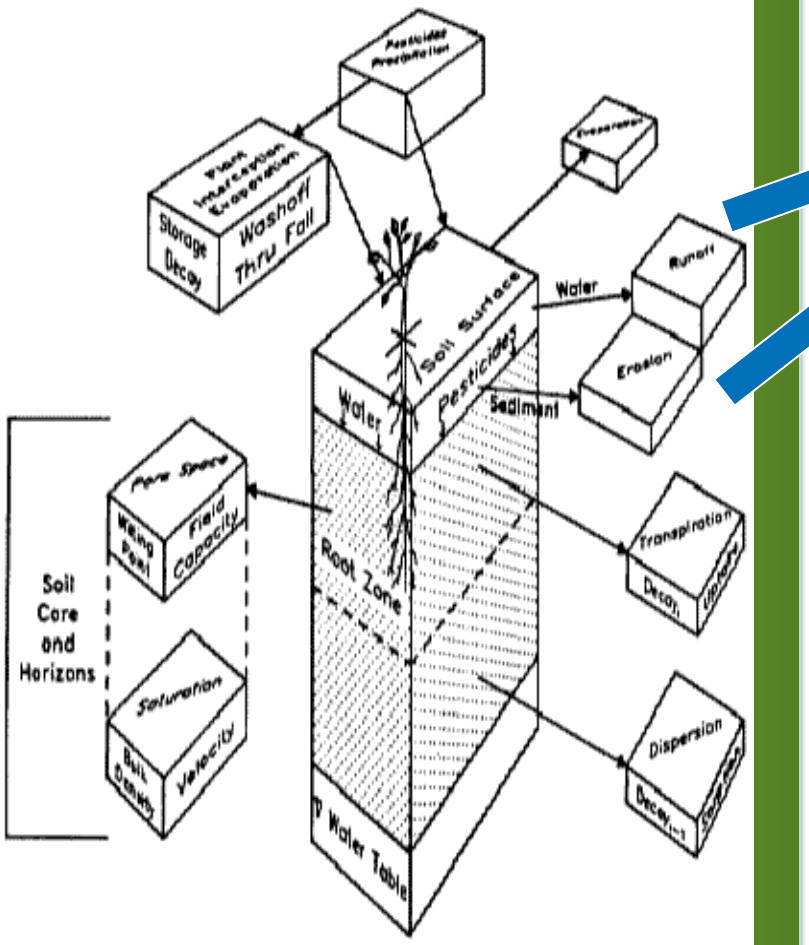


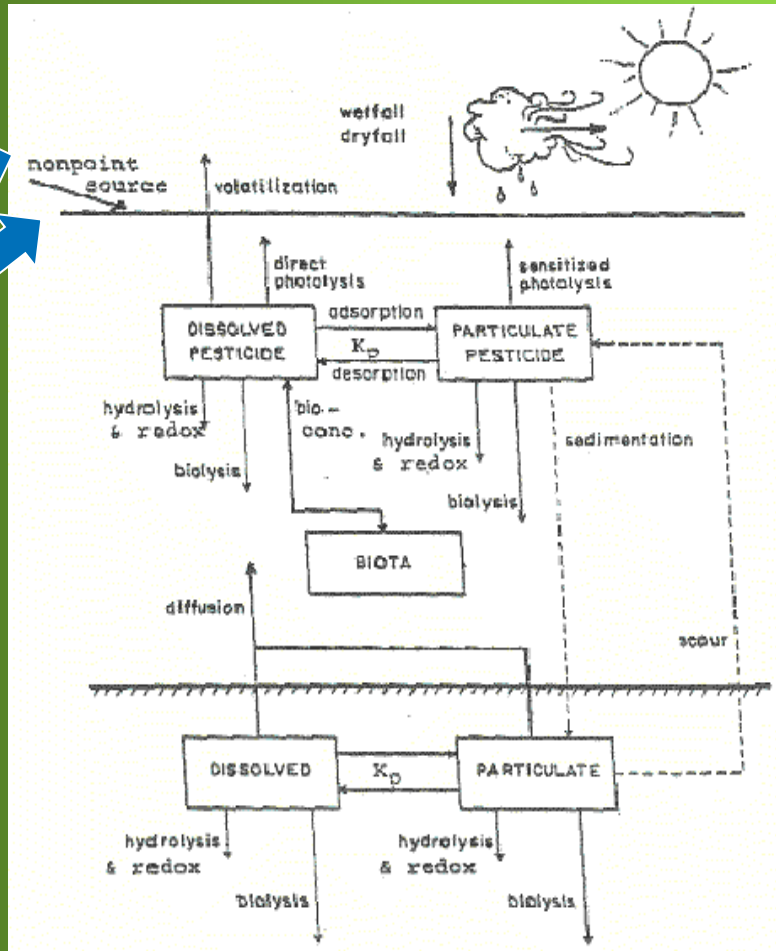
Regional background contributions modeled in CMAQ



Resulting hourly concentrations for multiple pollutants input to exposure models to estimate total exposure

Pesticide Root Zone Model (PRZM) and Exposure Analysis Modeling System (EXAMS)





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CONCLUSION

Conclusion

- Monitoring and modeling: Both can be valuable
  - Monitoring: Direct measurements of chemical concentrations
  - Modeling: Estimated chemical concentrations
- Both require careful evaluation