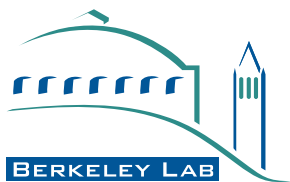# Modeling Personal and Population Exposures to Environmental chemicals

Thomas E. McKone

University of California, Berkeley

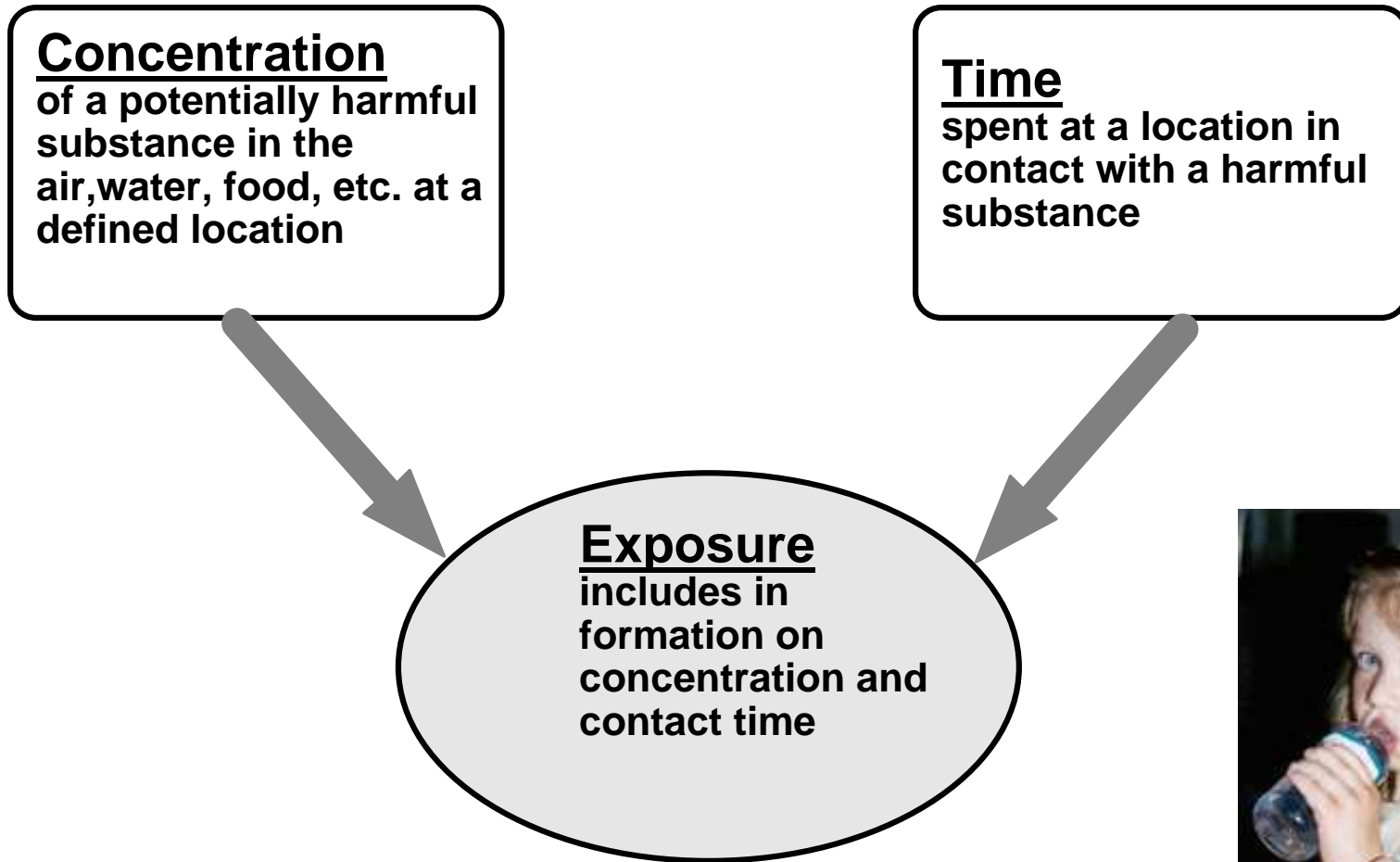**Lawrence Berkeley National Laboratory**

Overview

- **Exposure modeling questions**

- **Exposure modeling approaches**

  - **Time average concentration**

  - **Time series simulation**

  - **Cumulative contact/cumulative intake**

- **Model output**

- **Model evaluation**
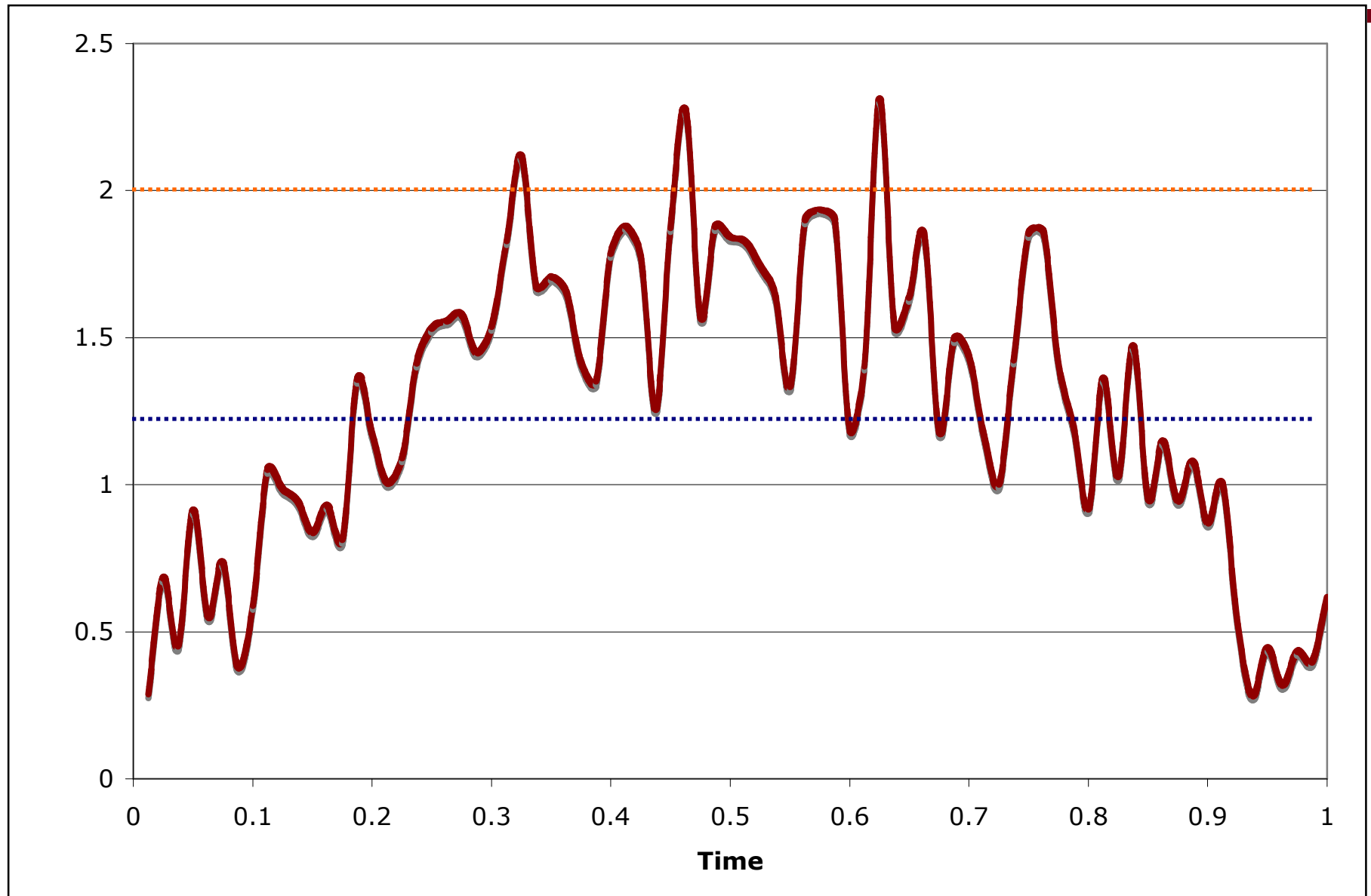
Exposure Definitions

Exposure refers generally to the physical contact of an organism with a substance present in a liquid, solid, or a gas.

Concentration
of a potentially harmful substance in the air,water, food, etc. at a defined location

Time
spent at a location in contact with a harmful substance

Exposure
includes in formation on concentration and contact time

A profile of exposure in time

Exposure Modeling Questions

- **Compare populations**

- **Time-weighted average concentration**

- **Time-weighted average above a threshold**

- **Peak exposure**

- **Number, duration of peak exposures**

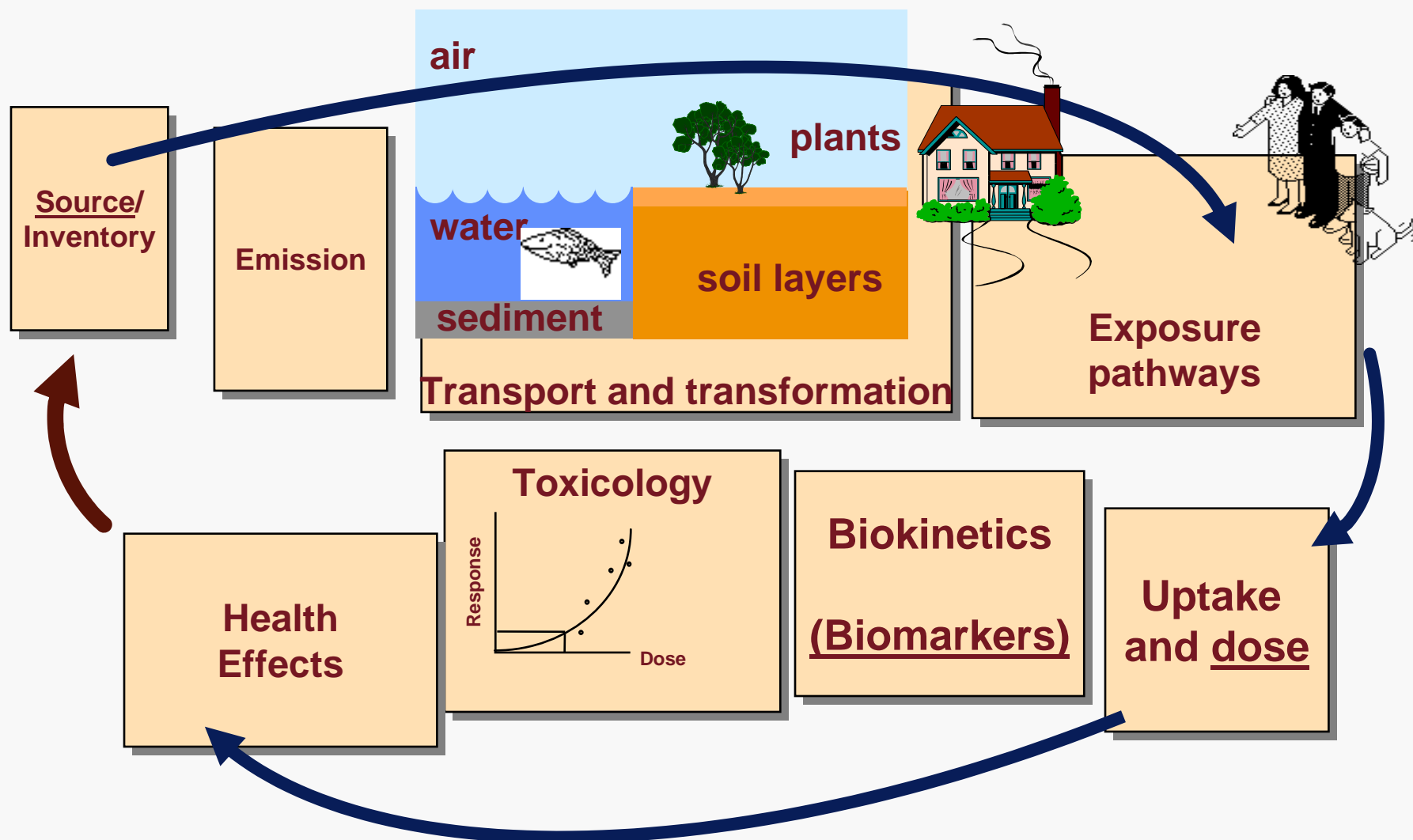- **Cumulative contact**

- **Cumulative intake**

Exposure Models

- **Time series/exposure event simulation**

- **Time average concentration**

- **Cumulative contact and cumulative intake**

- **Biomarker**

Source to Dose Assessment

Source to Dose (Terminology)

Source (power plant, auto, water, cooking, smoking)

Emission (kg/d)

↓

Environmental concentrations (mg/m^3, mg/kg)

Pathways ↓ ↓ ↓

Exposure media concentrations (mg/m^3, mg/kg)

↓

Exposure (mg/m3, mg/kg)
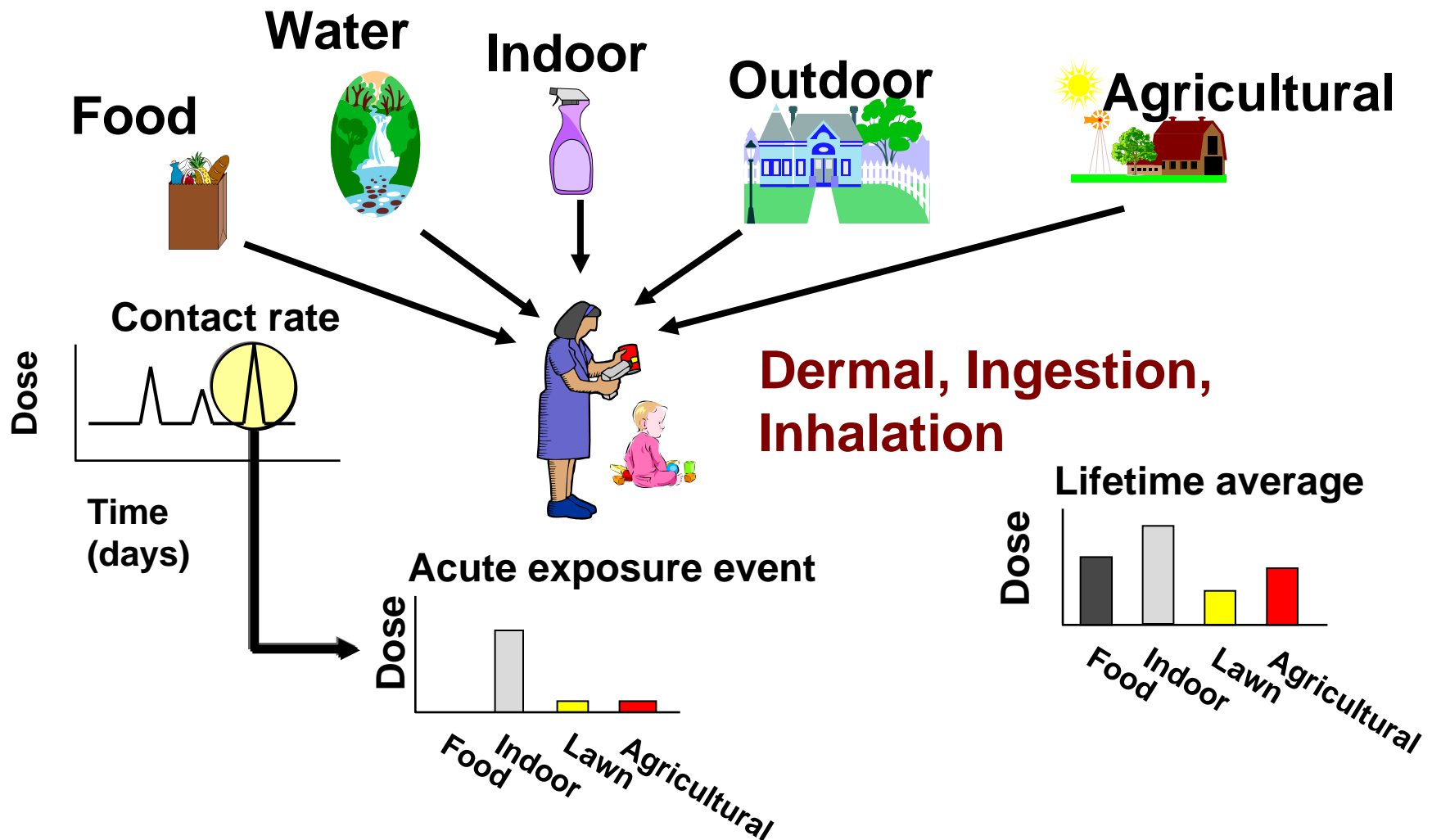
↓ ↓ ↓ **Routes**

Intake ====> Dose mg/kg-d

Activity Patterns and Time Series

- An activity pattern is simply a time budget of an individual's activities over some period of time.

- The activities can be described in terms of type (e.g., recreational, personal care, etc.), temporal variation, and location.

- Data on activity patterns can be derived from diaries that participants in time-activity surveys complete and from telephone surveys that request respondents to recall time–activity behaviors.

Indoors at home	Indoors away from home
Outdoors at home	Outdoors away from home

Pesticide intake depends on release location, transport and fate, and human intake through competing exposure pathways

Food

Water

Indoor

**Outdoor**

Agricultural

Contact rate

Dose

Time (days)

Dermal, Ingestion, Inhalation

Acute exposure event

Dose

Food Indoor Lawn Agricultural

Lifetime average

Dose

Food Indoor Lawn Agricultural

Exposure (Concentration) Model

$$E = \frac{\sum\limits_{i} C_i t_i}{\sum\limits_{i} t_i}$$

E = average exposure in mg/m³ over the period T = $\sum t_i$

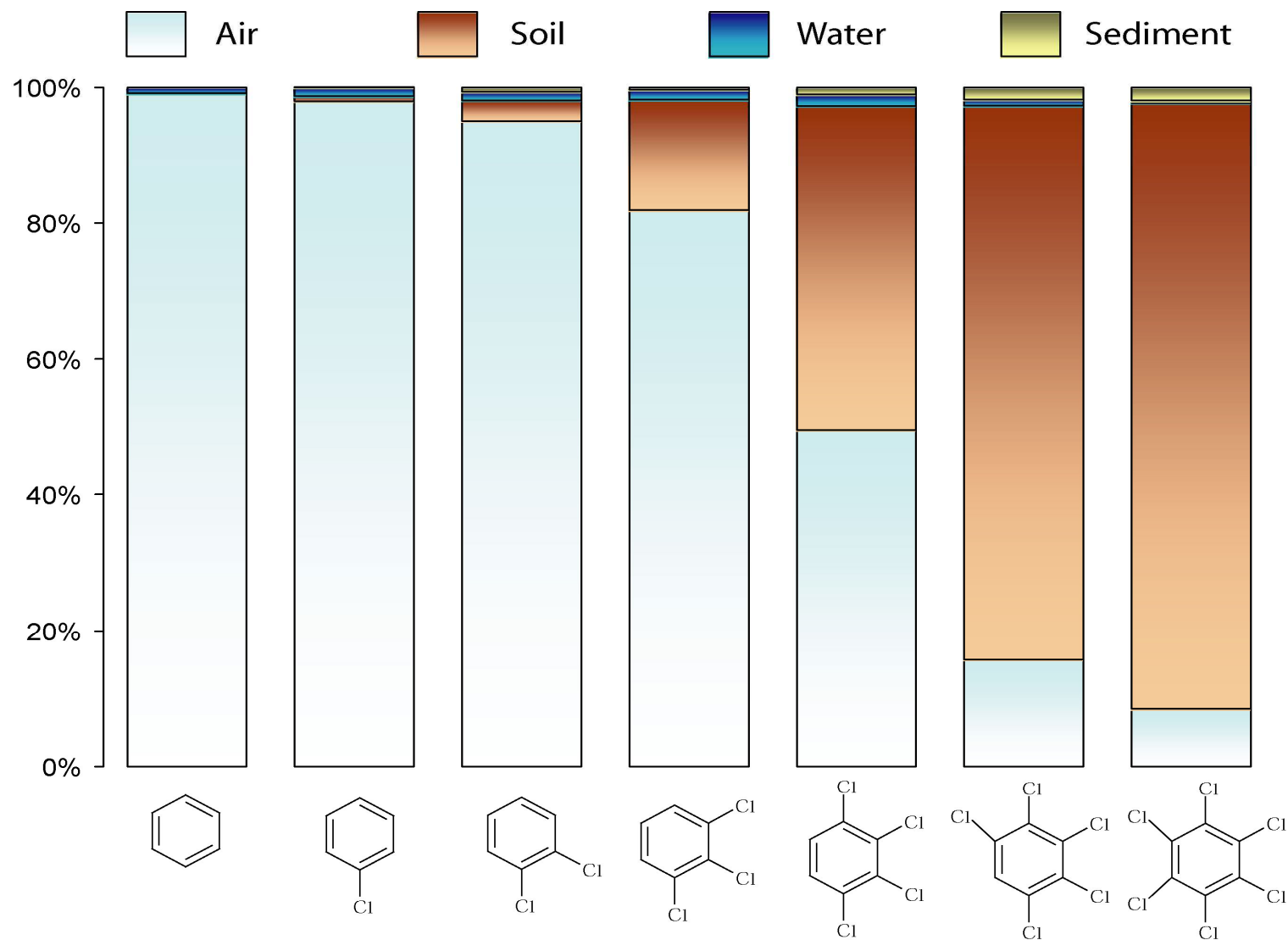C_i = concentration in mg/m³ in microenvironment i
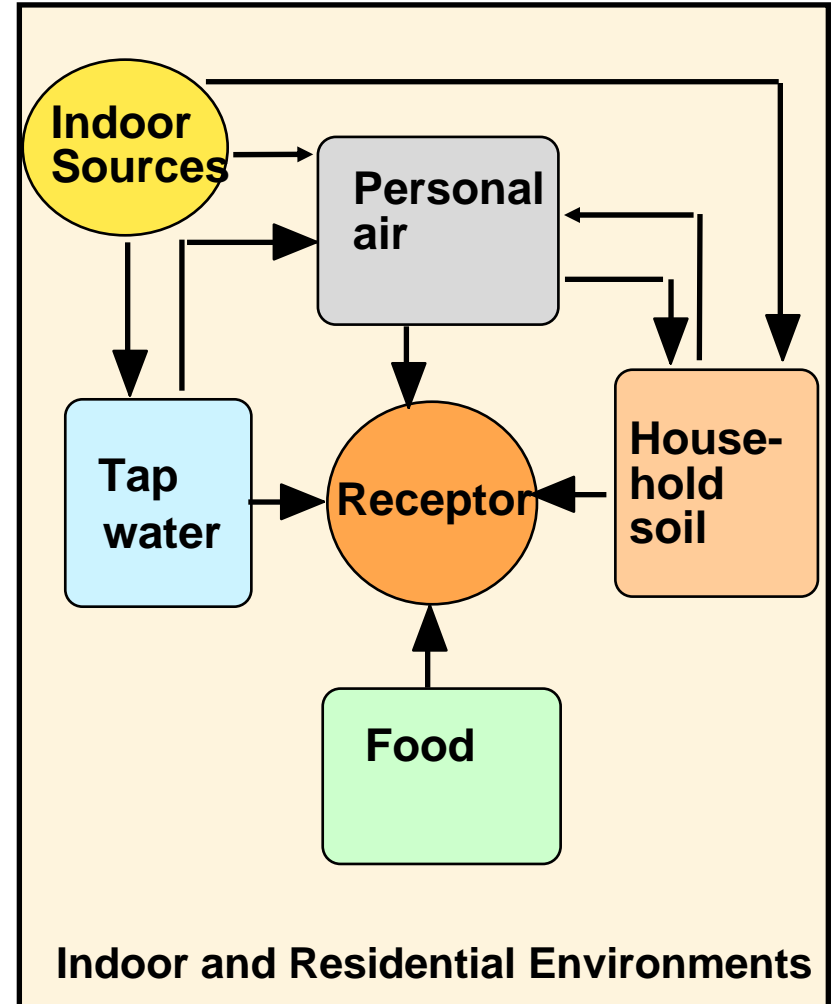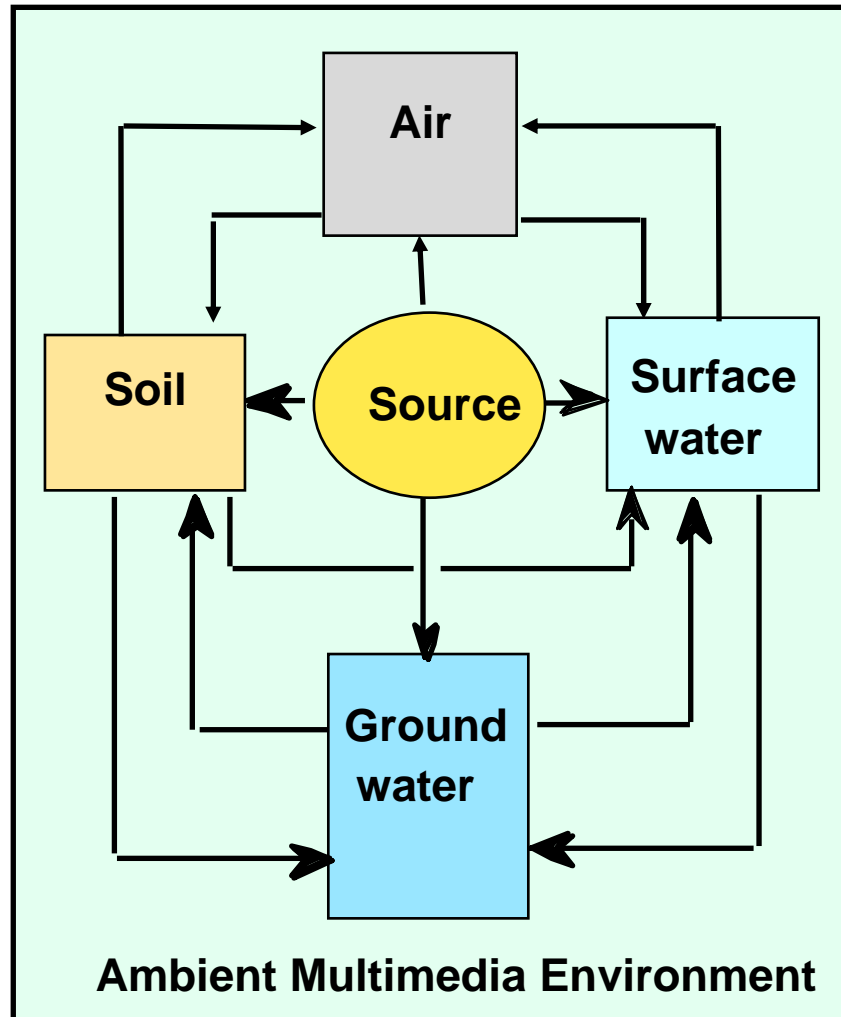
t_i = time spent in microenvironment i

Multimedia Mass Balance Models
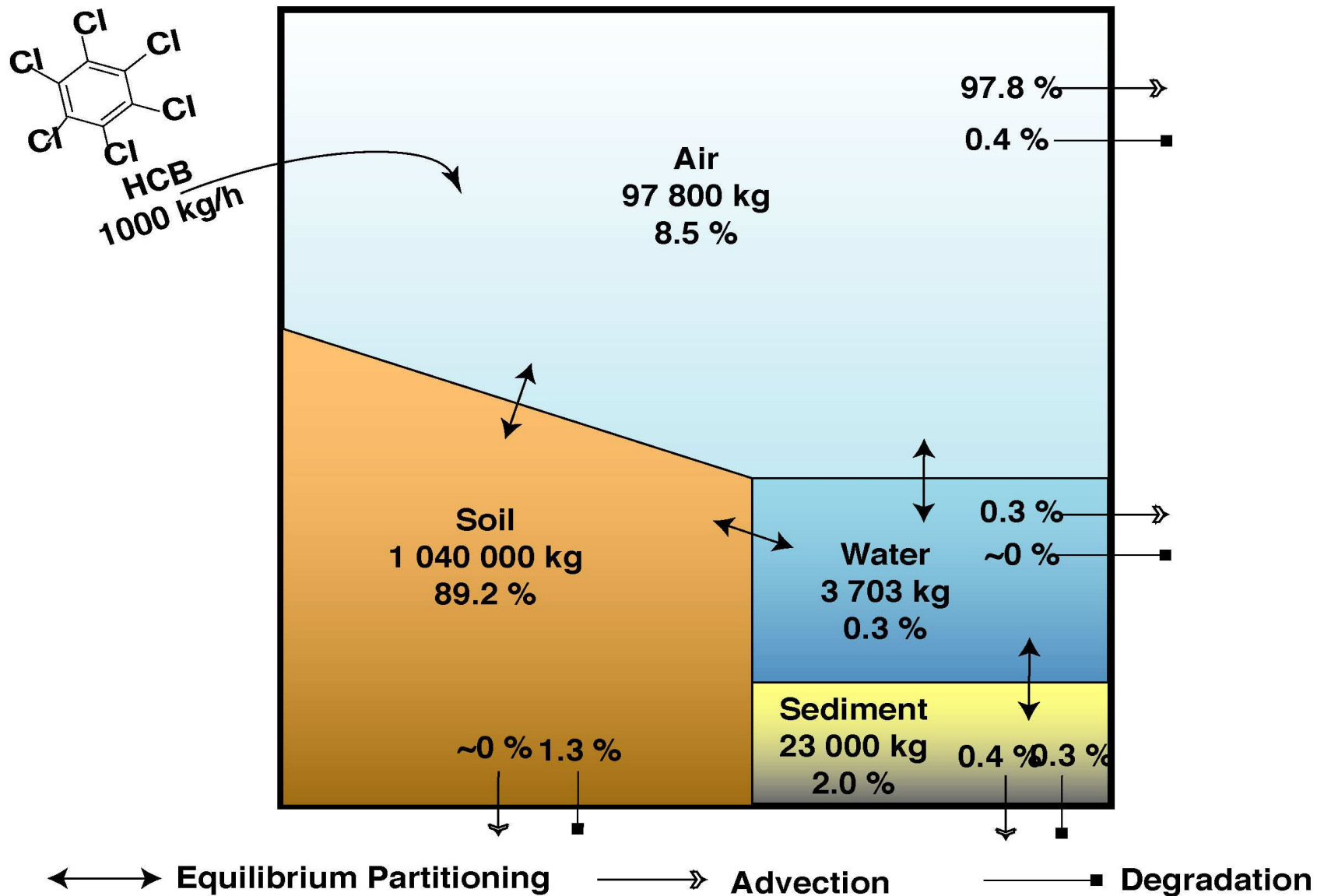
Chlorinated Benzene Series

Multimedia to Multipathway Exposure

Basic Intake/Uptake Model

Unit Dose Factor (UDF)

$$\text{ADD} = \left[\frac{C_i}{C_k}\right] \times \left[\frac{IU_i}{BW}\right] \times \frac{EF \times ED}{AT} \times C_k$$

|				
Average daily dose in mg/kg-d from exposure medium **i** and environmental medium **k**.	Inter-media transfer factor expressing the concentration ratio of the exposure medium **i** to the environmental medium **k**.	The intake or uptake factor per unit body weight associated with exposure medium **i**.	Exposure frequency, exposure duration and averaging time	Contaminant concentration in the environmental medium that provides a source to the exposure medium

Exposure Histogram (HCB)
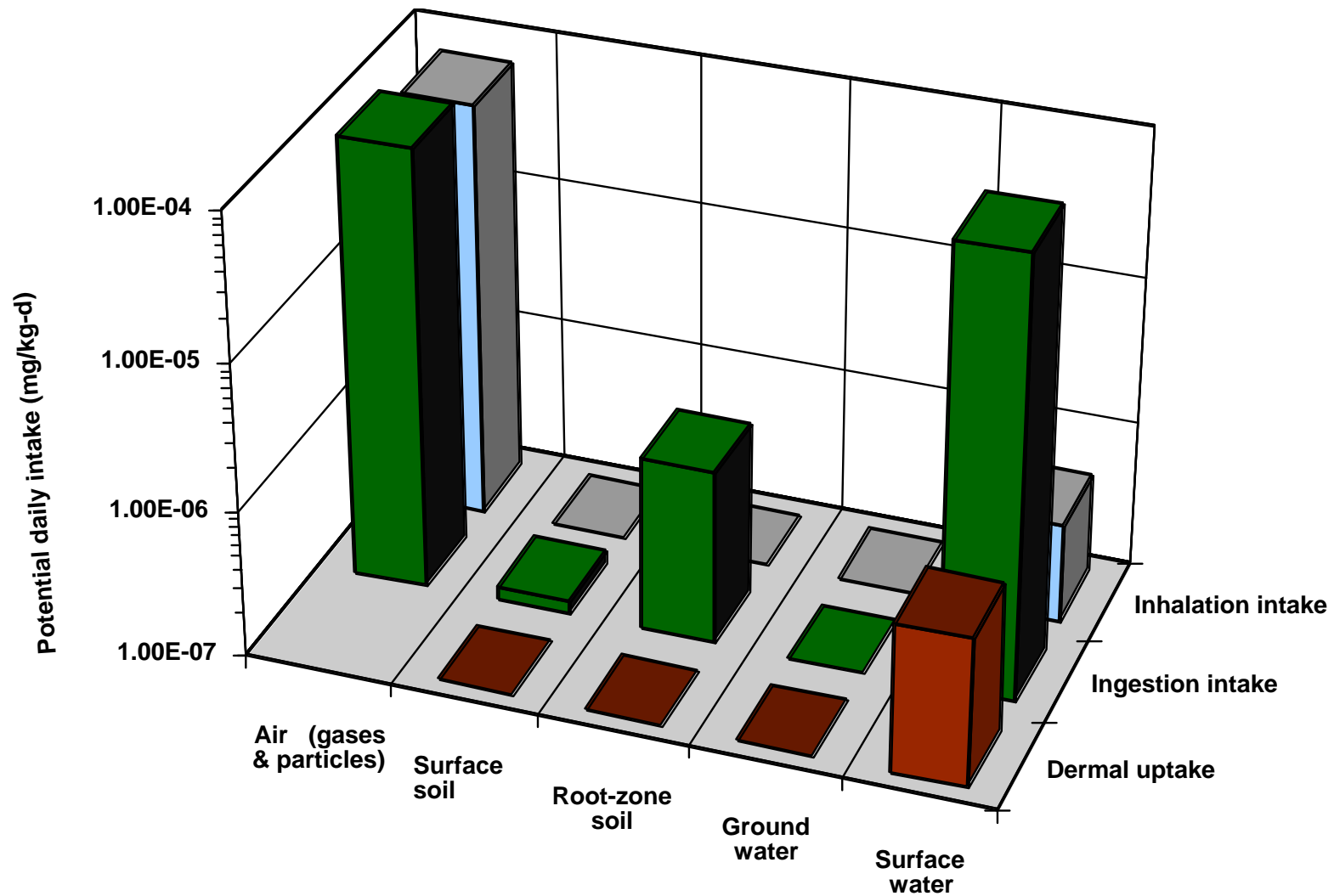
Biomarkers/Biomonitoring

- ## Biomarkers
  - ❖ **Susceptibility**
  - ❖ **Exposure**
  - ❖ **Effect**

- ## Biological media
  - ❖ **Breath**   **Saliva**
  - ❖ **Urine**   **Blood**
  - ❖ **Other--lipid samples, biopsies**

- ## Biomonitoring
  - ❖ **Who is exposed?**
  - ❖ **How does exposure vary?**
  - ❖ **Does exposure correlate with disease?**
  - ❖ **Is exposure changing in time?**
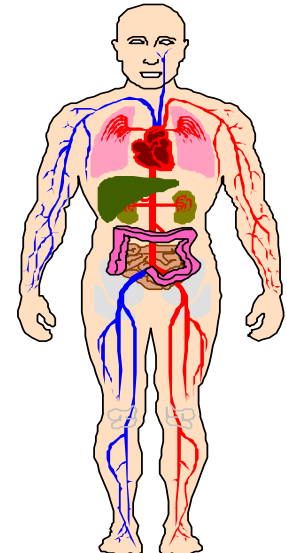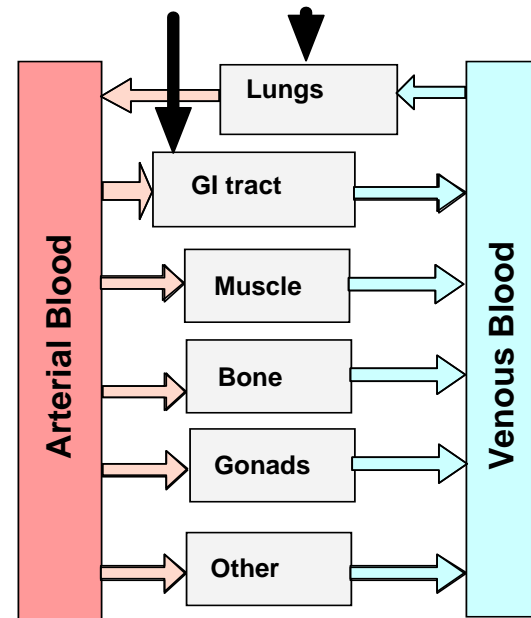
Model Outputs

- **Population/Pollutant classification**

- **Peak exposure**

- **Persistence**

- **Cumulative intake** by day, month, year, gender, age etc.

- **Time-weighted concentration**

- **Source-intake ratios (intake fraction)**

Model Performance Evaluation

Conceive model

- **Theory and assumptions**
- **Conceptual model**

- **Data selection**
- **Set parameter values**

Construct a quantitative model

- **Algorithm selection**
- **Empirical vs structural**
- **Computational model**

- **Set system boundaries**
- **Duration**
- **Interpret model results**

Apply the model
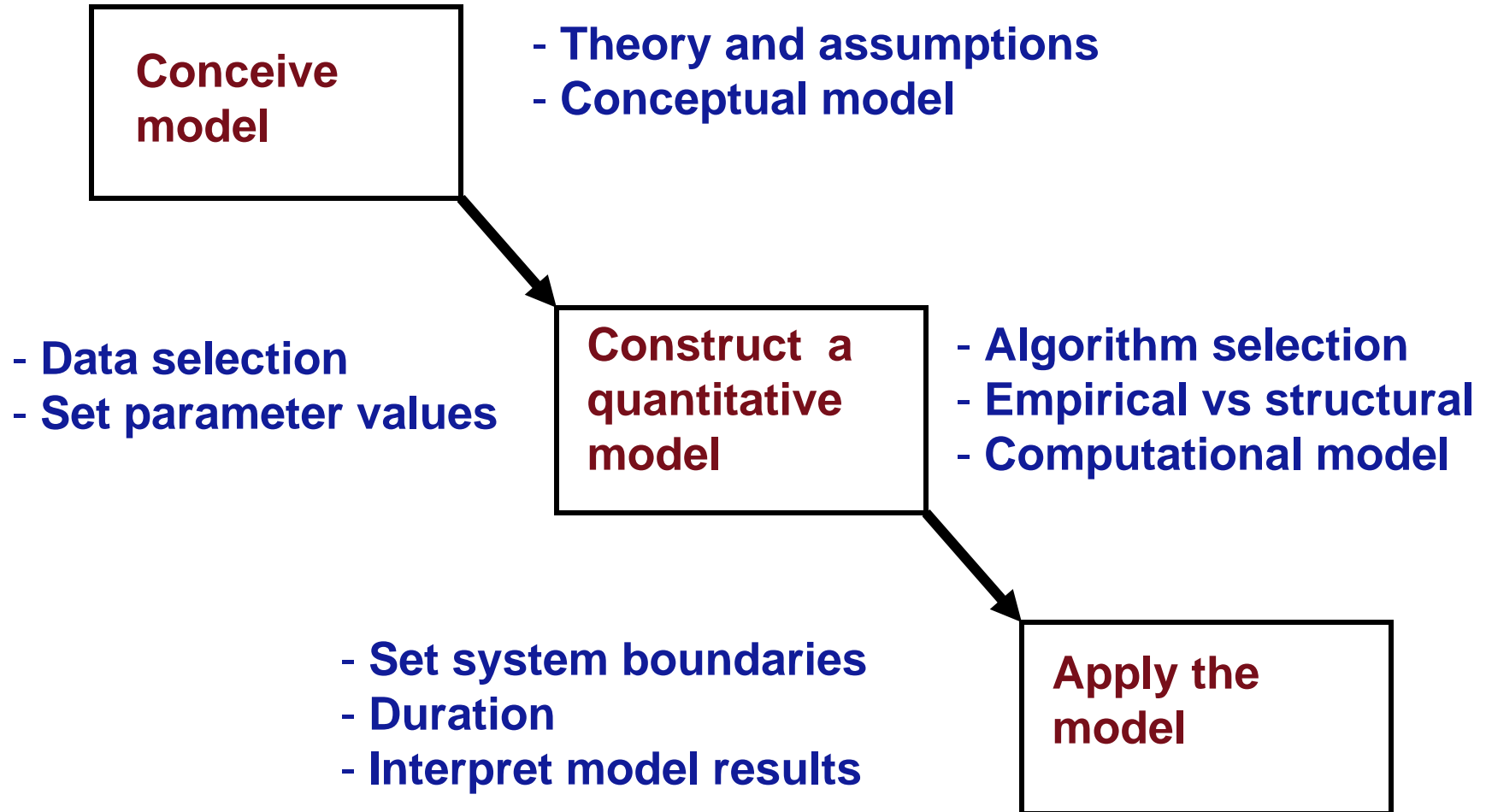
Simple vs Complex

US EPA CREM report

Uncertainty (y-axis) vs Model Complexity (x-axis)

- Total Uncertainty
- Point of Minimum Uncertainty
- Model Framework Uncertainty
- Data Uncertainty
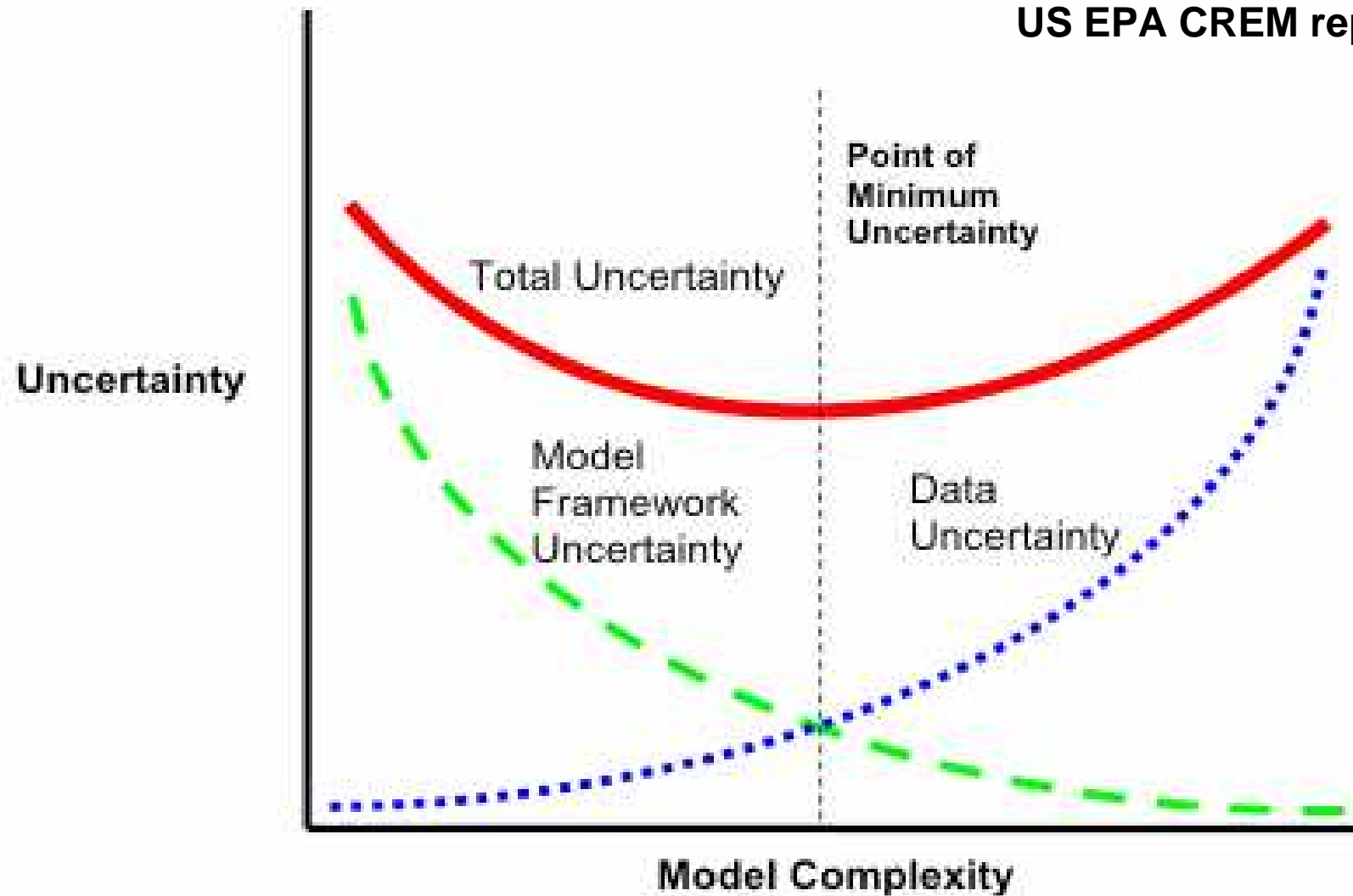
Organophosphate Pesticide Use

Salinas Valley, CA
Agriculturally Applied Organophos
Average Annual Pounds
From 1999 through 2001

Agricultural pesticide use in California is re
the Department of Pesticide Regulation per
Public Land Survey (PLS) System.

Pounds applied per PLS section (= 1 sq mi)
- Zero
- 1 to 100 lbs.
- 101 to 1000 lbs.
- 1001 to 5000+ lbs.
- Participant Residence
- County boundary
- Highway

Prepared by: Rusty Scalf, Bob McLaughlin & Martha Harnly
Environmental Health Investigations Branch
California Department of Health Services

Scale 1:450,000

Data sources: California Dept. of Pesticide Regulation, the US Geologic Survey,
and Geographic Data Technologies, Inc.   April, 2003

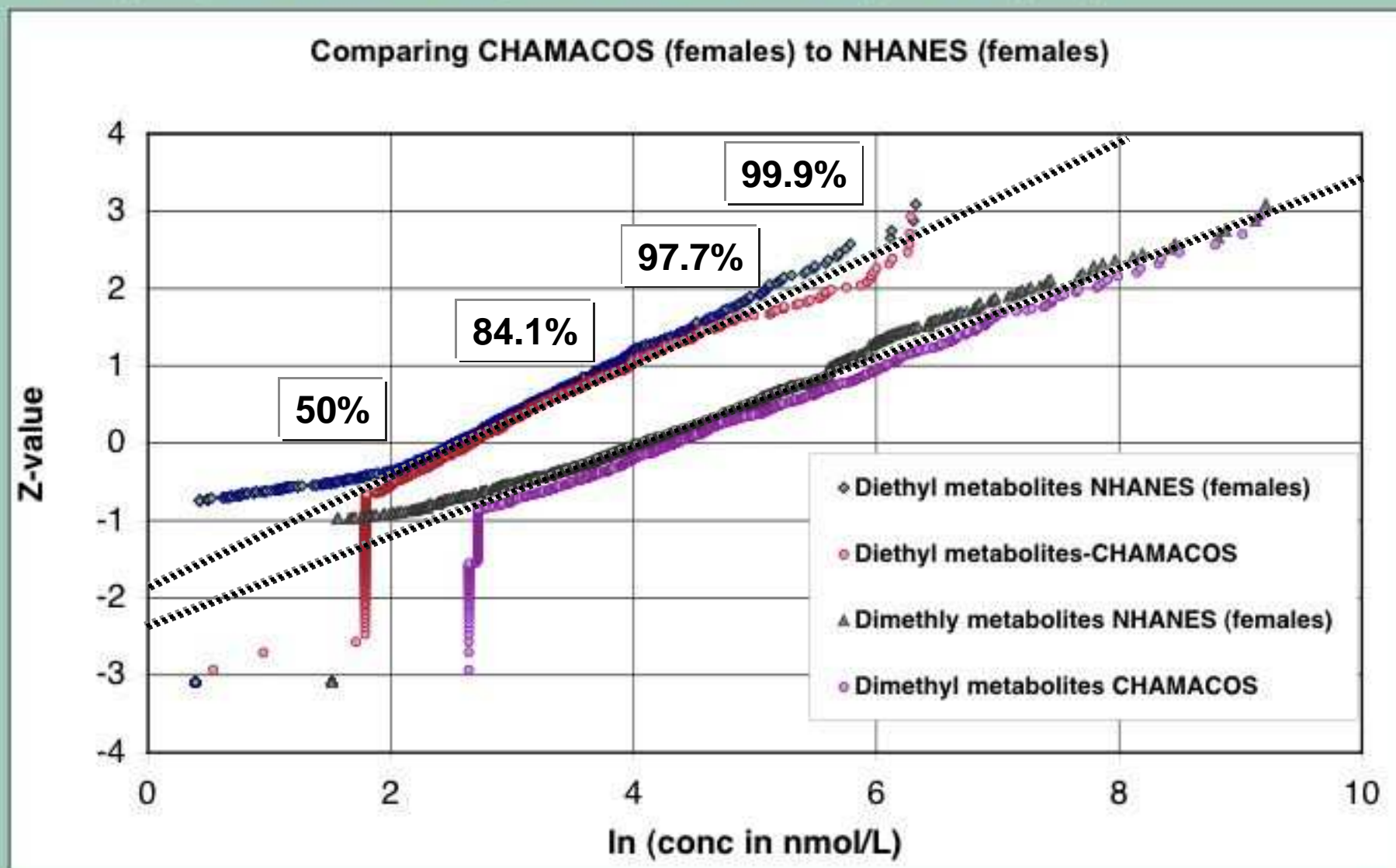**The Salinas Valley is a region of intense pesticide use**

Probability plot for the distributions of total **diethyl** and **dimethyl** phosphate concentrations the CHAMCOS mothers at baseline visit to the clinic (**585** samples) and NHANES subjects who are female (**996** samples)

Discussion/Conclusions

□ **How can we use models to support exposure assessments?**

 ➢ **Insight**

 ➢ **Repositories of existing knowledge**

 ➢ **Exploring plausible exposure pathways**

 ➢ **Integrated metrics of source/dose relationships**

 ➢ **Accurate predictions of exposure???**

□ **Evaluation--confronting model limits**

 ➢ **Relevance   Transparency   Complexity**

 ➢ **Uncertainty**

 ➢ **Do people trust the model?**

The End... Thank you

I want to acknowledge the research support our group receives from the

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and from

The Center for Disease Control

and Prevention (CDC) Health

Tracking Program