Environmental Fate of Pesticides

Destino Ambiental de Pesticidas

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Environmental Monitoring Branch
California Department of Pesticide Regulation
Environmental chemistry and fate

I. Introduction
   - my background
   - what is environmental fate?

II. General environmental chemistry principles
    *pesticide registration/risk assessment perspective*

    - available data & how to interpret
      - partitioning
      - degradation
      - aquatic toxicity, bioconcentration
    - caveats:
      - “ideal” conditions vs reality
      - variability and uncertainty
    - effect of use practices on fate
    - data sources
Environmental chemistry and fate (tomorrow)

III. Case Histories/Current Issues
- organochlorines and other halogenated problem chemicals
- diazinon/chlorpyrifos in surface water
- synthetic pyrethroids and sediment toxicity
- VOCs, NOx and ozone formation
  reactivity, product emission speciation
- mitigation of rice herbicide toxicity
- probabilistic transport modeling in SJV/CFC age-dating
- examples of new chemistries
My Background

BS 1976..... 10+ yrs working in California Ag:
       truck driver, mechanic, tractor driver, etc.

MS 88      Hydrologic Sciences,
PhD 92     Ag & Environ Chem, UCD
       emphasis: soil physics, physical chemistry, transport modeling

2.5 yrs post-graduate research at UCD

Environmental Monitoring Branch, DPR, 1994 - present
       -Ground Water, Surface Water and Air Groups
What is environmental fate?

After pesticide application:

1. where does the pesticide go?
2. how long does it take to get there?
3. how long does it stay?
4. what are the degradation products?
What is environmental fate?

After pesticide application:

1. where does the pesticide go?
2. how long does it take to get there?
3. how long does it stay?
4. what are the degradation products?
   a. where do they go?
   b. how long do they take to get there?
   b. how long do they stay?
   c. what are their degradation products?
Comment on DEGRADATES

1. Terminology
   “degradates”, “breakdown products” ..... appropriate

   “metabolites” ..... often misused

2. Typically limited data ............ BUT

3. THEY CAN BE IMPORTANT!!!!!!
**N-dealkylation of simazine**
(6-Chloro-\(N,N'\)-diethyl-1,3,5-triazine-2,4-diamine)

![Chemical structures showing the process of N-dealkylation from simazine to deethyl simazine (DES) and diamino chlorotriazine (DACT).]

**N-dealkylated degradates DES and DACT:**
- toxicity is comparable to parent
- more frequent, higher concs than parent
distribution of s-chlorotriazine degradates in 51 SJV wells
- combined study 146 and ciba giegy monitoring data -

![Graph showing the distribution of s-chlorotriazine degradates in 51 SJV wells. The y-axis represents concentration in ug/L, and the x-axis represents different compounds: SIMAZINE, DES, DACT, and their sum. The MCL = 3 line is indicated on the graph.]
Environmental Fate

1. Pesticide physicochemical properties

- distribution
  a. where does a pesticide “tend” to go?
  -- "distribution" or **partition coefficients**

```
water

air  soil

biota
```

**environmental “compartments”**
1. Pesticide physicochemical properties

- distribution
  a. where does a pesticide "want" to go?
    -- EQUILIBRIUM distribution or \textit{partition coefficients}

\textbf{EXAMPLE:}

soil/water partition coefficient =

$$K_D = \frac{\text{concentration in soil}}{\text{concentration in water}}$$
1. Pesticide physicochemical properties

- **Distribution**
  a. **EQUILIBRIUM**: where does a pesticide tend to go?
  b. **KINETICS**: how fast does it get there?

- mass transfer coefficients *

<table>
<thead>
<tr>
<th>water</th>
<th>air</th>
<th>soil</th>
<th>biota</th>
</tr>
</thead>
</table>

Environmental Fate
Environmental Fate

1. Pesticide physicochemical properties distribution
   a. where does a pesticide want to be?
   b. how fast does it get there?

   ➔ degradation
   c. how fast does it breakdown?
   d. what are the degradation products?
Environmental Fate

1. Pesticide physicochemical properties distribution
   a. where does a pesticide want to be?
   b. how fast does it get there?
   ➔ degradation
   c. how fast does it breakdown?
   d. what are the degradation products?

- degradation experiments to determine:
  - rate constants or "half-lives"
  - and breakdown products

hydrolysis

biodegradation

photolysis
Basic environmental chemical data -
“physico-chemical properties”

- solubility
- octanol/water partition coefficient $K_{OW}$
- soil sorption coefficients $K_D$, $K_{OC}$
- vapor pressure
- Henry's law constant $H'$
- aerobic soil half-life
- anaerobic soil half-life
- hydrolysis half-life
- soil photolysis half-life
- aqueous photolysis half-life
- field dissipation half-life

} distribution or partition coefficients

} degradation data
Partition coefficients

- solubility pure chemical $\leftrightarrow$ water
- soil sorption coefficient $K_{OC}$ water $\leftrightarrow$ soil
- octanol/water partition coefficient $K_{OW}$ water $\leftrightarrow$ n-octanol
- Henry's law constant $H'$ water $\leftrightarrow$ air
- vapor pressure pure chemical $\leftrightarrow$ air

@ EQUILIBRIUM !!!
organochlorines - chlordane

pyrethroids - cypermethrin

organophosphates - parathion

soil applied herbicide - diuron

carbamates - carbaryl

fumigants - MITC
Solubility ranges of various pesticide classes

![Graph showing solubility ranges for different pesticide classes.](image)
UNDERSTANDING SOLUBILITY

Polar vs. Nonpolar Solvents

- High electron density
- Symmetrical, no charge separation or dipole

- Low electron density
- Symmetrical, no charge separation or dipole
Water and Hydrogen Bonding

Effect of H-bonds:
- water molecules strongly associated in solution
- high surface tension
- elevated boiling point
- excellent solvent for:
  - ionic solutes (e.g. salts such as Na\(^+\) Cl\(^-\))
  - polar solutes (charge separation, dipole moment)
  - solutes capable of H-bonding

- alcohols
- amines
- carbonyls
## Factors affecting water solubility of nonionic organic compounds

<table>
<thead>
<tr>
<th>I. polarity</th>
<th>II. size</th>
<th>halogenation</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="H" /> 67000 mg/l</td>
<td><img src="image" alt="H" /> 1800</td>
<td><img src="image" alt="H" /> 1800 H – 1.2Å</td>
</tr>
<tr>
<td><img src="image" alt="O" />CH₃ 2000</td>
<td><img src="image" alt="O" /> 34</td>
<td><img src="image" alt="O" />Cl 470 Cl – 1.8Å</td>
</tr>
<tr>
<td><img src="image" alt="H" /> 1800</td>
<td></td>
<td><img src="image" alt="H" />Br 410 Br – 1.95Å (≈ CH₃)</td>
</tr>
<tr>
<td><img src="image" alt="O" />CH₃ 520</td>
<td><img src="image" alt="O" /> 1.2</td>
<td></td>
</tr>
</tbody>
</table>

### Pauling electronegativities

ability of an atom to attract electrons

<table>
<thead>
<tr>
<th>Element</th>
<th>Electronegativity</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>2.2</td>
</tr>
<tr>
<td>O</td>
<td>3.4</td>
</tr>
<tr>
<td>C</td>
<td>2.6</td>
</tr>
<tr>
<td>Cl</td>
<td>3.2</td>
</tr>
</tbody>
</table>

*Note: Electronegativity values are approximate and for illustrative purposes.*
pyrethroids
- cypermethrin
- 340 cm$^3$/mol
- 0.004 mg/l

organophosphates
- parathion
- 230 cm$^3$/mol
- 11 mg/l

organochlorines
- chlordane
- 260 cm$^3$/mol
- 0.05 mg/l

soil applied herbicide
- diuron
- 190 cm$^3$/mol
- 42 mg/l

carbamates
- carbaryl
- 160 cm$^3$/mol
- 110 mg/l
Sorption of diuron to a sandy loam soil

[diuron] in solution (ug/ml) vs [diuron] in soil (ug/gram soil)

Graph shows a linear relationship.
Sorption of diuron to a sandy loam soil

soil/water partition coefficient = \( K_d \) (or \( K_P \))

\[
= \frac{\text{conc in soil}}{\text{conc in water}}
\]
What is sorption (partitioning to soil)?
What is sorption (partitioning to soil)?

- Water
- Soil organic matter – humic material
What is sorption (partitioning to soil)?

= pesticide molecule

adsorption? partitioning? ........sorption.....
What if we repeat on different soils?

- $K_d = 2.8$
- $K_d = 21$
- $K_d = 10$
- $K_d = 46$
What if we compare different soils?

diuron sorption to soils of different organic carbon content

\[ K_d = \frac{K_{OC}}{OC} \]

\( K_{OC} \sim \) relatively independent of soil type
What is sorption (partitioning to soil)?

$K_{OC} =$

(Concentration in soil organic carbon)

(Concentration in water)

Dynamic reversible equilibrium
Organic carbon-normalized soil sorption coefficient $K_{OC}$
sorption and pesticide leaching

bromacil $K_{OC} = 32$

norflurazon $K_{OC} = 600$

oxyfluorfen $K_{OC} = 18,000$

Why is KOC important???

NOTE: computer modeled solute distributions
KOC and estimated dissolved fraction of pesticides in surface water

**MIREX**
- $K_{OC} = 1,000,000$
- Fraction dissolved = 0.003

**METHOXYCHLOR**
- $K_{OC} = 76,000$
- Dissolved = 0.04

**PARATHION**
- $K_{OC} = 7,700$
- Dissolved = 0.3

**SIMAZINE**
- $K_{OC} = 140$
- Dissolved = 0.96

**METHYL BROMIDE**
- $K_{OC} = 22$
- Dissolved = 0.99+

Assumes $[Sediment] = 0.01 \, g \, L^{-1}, f_{OC} \sim 0.03$
$K_{OC}$ & solubility are inversely correlated
Octanol/water partitioning

1-octanol
CH₃CH₂CH₂CH₂CH₂CH₂CH₂CH₂CH₂OH

+ pesticide

water
H₂O
Octanol/water partitioning

1-octanol

\[
\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}
\]

+ pesticide

\[
K_{OW} = \frac{\text{(pesticide concentration in octanol)}}{\text{(pesticide concentration in water)}}
\]
$K_{ow}$ & solubility are inversely correlated

$K_{ow}$ & solubility are inversely correlated.

Hydrophilic

Lipophilic
**BIOCONCENTRATION FACTOR**

\[
\text{BCF} = \frac{\text{equilibrium chemical concentration in organism (wet weight)}}{\text{chemical concentration in surrounding water}}
\]

Generally assumes that nondietary uptake across external membranes is primary source of contaminant in organisms.

- **rainbow trout**
- **fathead minnow**
- **bluegill sunfish**
<table>
<thead>
<tr>
<th>Pesticide</th>
<th>octanol/water partition coefficient - $K_{OW}$</th>
<th>bioconcentration factor - BCF</th>
</tr>
</thead>
<tbody>
<tr>
<td>simazine</td>
<td>130</td>
<td>1</td>
</tr>
<tr>
<td>atrazine</td>
<td>430</td>
<td>8</td>
</tr>
<tr>
<td>diazinon</td>
<td>2,000</td>
<td>35</td>
</tr>
<tr>
<td>methoxychlor</td>
<td>20,000</td>
<td>185</td>
</tr>
<tr>
<td>chlorpyrifos</td>
<td>100,000</td>
<td>470</td>
</tr>
<tr>
<td>trifluralin</td>
<td>130,000</td>
<td>4600</td>
</tr>
<tr>
<td>heptachlor</td>
<td>280,000</td>
<td>17000</td>
</tr>
<tr>
<td>DDT</td>
<td>560,000</td>
<td>62000</td>
</tr>
<tr>
<td>chlordane</td>
<td>1,000,000</td>
<td>38000</td>
</tr>
</tbody>
</table>

Many empirical relationships: $\log BCF = a \log K_{OW} + b$

e.g. Lyman, Rheel and Rosenblatt: Handbook of Chemical Property Estimation Methods
BCF of Pyrethroids?
- effect of depuration -

<table>
<thead>
<tr>
<th>Chemical</th>
<th>$K_{OW}$</th>
<th>BCF – Oncorhynchos mykiss</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cypermethrin</td>
<td>13000000</td>
<td>832</td>
</tr>
<tr>
<td>Permethrin</td>
<td>79000000</td>
<td>1940</td>
</tr>
<tr>
<td>Deltamethrin</td>
<td>63000000</td>
<td>502</td>
</tr>
<tr>
<td>Fenvalerate</td>
<td>32000000</td>
<td>403</td>
</tr>
<tr>
<td>DDT</td>
<td>13000000</td>
<td>72500</td>
</tr>
</tbody>
</table>

BIOCONCENTRATION FACTOR & BIOAVAILABILITY:
DOM Effect on Uptake of Permethrin by *D. magna*

\[ BR = \frac{BR_0}{(1 + \alpha K_{DOM}[DOM])} \]

Median lethal concentrations in surface waters and sediments

LC50 (median lethal concentration) cyfluthrin/Black Mountain sediment/ Chironomus tentans
≈ 0.009 ug L\(^{-1}\)

Effect of suspended sediment (SS) on median lethal concentrations (LC50s) of hydrophobic chemicals

Equilibrium Partitioning Theory

Henry’s law - *relative* affinity for air compared to water

$$H' \propto \left( \frac{[\text{C}_{\text{air}}]}{[\text{C}_{\text{water}}]} \right)$$

affinity for vapor phase

affinity for solution phase

describes tendency of pesticide to volatilize from water or moist soil
Hydrophilic vs Lipophilic “balance”

“high” water solubility

low $K_{OW}$
→ low bioconcentration tendency

low KOC
→ mobile in soil
→ in surface water is dissolved – not bound to sediment

“low” water solubility

high $K_{OW}$
→ high bioconcentration tendency

high KOC
→ immobile in soil
→ surface water: sorbed to sediment

filtration
→ tends to sorb to many materials – sampling containers
Hydrophilic vs Lipophilic “balance”

<table>
<thead>
<tr>
<th>“high” water solubility</th>
<th>“low” water solubility</th>
</tr>
</thead>
<tbody>
<tr>
<td>low $K_{ow}$</td>
<td>high $K_{ow}$</td>
</tr>
<tr>
<td>low bioconcentration tendency</td>
<td>high bioconcentration tendency</td>
</tr>
<tr>
<td>low KOC</td>
<td>high KOC</td>
</tr>
<tr>
<td>mobile in soil</td>
<td>immobile in soil</td>
</tr>
<tr>
<td>in surface water is dissolved – not bound to sediment</td>
<td>surface water: sorbed to sediment filtration</td>
</tr>
<tr>
<td></td>
<td>tends to sorb to many materials – sampling containers</td>
</tr>
</tbody>
</table>

**Caveats:**

Concept of hydrophilic vs lipophilic balance applies generally to many “non-ionic organic compounds” – almost NEVER applies to:

- inorganic materials
- salts or certain unusual AIs (e.g., paraquat, diquat, alkyl-amine formulations of 2,4-D and triclopyr)
Example of **non-hydrophobic** soil binding mechanism

diquat/smectite interactions
Effect of ionization

Pentachlorophenol: pKa = 4.75

\[
\text{Cl} - \text{Cl} - \text{Cl} - \text{Cl} - \text{Cl} + \text{H}^+ \rightarrow \text{Cl} - \text{Cl} - \text{Cl} - \text{Cl} - \text{O}^- 
\]

\[
\text{OH} \rightarrow \text{O}^- + \text{H}^+ 
\]

\[
\log K_{OC} = 25000 
\]

kinetic desorption experiment – effect of aging

1. incubate pesticide + water/sediment slurry for various times
2. at t=0 add tenax beads
3. at t=t₁, t₂, t₃, ...... remove tenax beads and analyze

\[
\frac{S_t}{S_0} = F_{\text{rapid}} e^{-k_{\text{rapid}} t} + F_{\text{slow}} e^{-k_{\text{slow}} t} + F_{\text{very slow}} e^{-k_{\text{very slow}} t}
\]
Kinetics: desorption of “aged” (incubated) sediments

\[ \frac{S_t}{S_0} = \text{relative fraction remaining} \]

Effect of aging on “rapid”, “slow” and “very slow” desorbing fraction of pyrethroid

Effect of aging on bioavailability?
1. Pesticide physicochemical properties distribution
   a. where does a pesticide want to be?
   b. how fast does it get there?
   ➔ degradation
   c. how fast does it breakdown?
   d. what are the degradation products?

Degradation experiments to determine:
- rate constants or "half-lives"
- and breakdown products
Degradation data typically available

- aerobic soil half-life
- anaerobic soil half-life
- hydrolysis half-life
- soil photolysis half-life
- aqueous photolysis half-life
* - field dissipation half-life

laboratory studies

field study that is intended to reflect net degradation from all pathways under actual use conditions
First-order degradation kinetics - "half-life"

14 day half-life

110 day half-life
First-order degradation kinetics - "half-life"

1. Half lives usually refer to disappearance of parent
2. 1st - order kinetics often an approximation

14 day half-life – $k = 0.05 \text{ day}^{-1}$

110 day half-life – $k = 0.006 \text{ day}^{-1}$
First order kinetics example

\[ \frac{d[C]}{dt} = -k[C] \]

\[ C = e^{-kt} \]

\[ \ln[C] = -kt + \ln[C_0] \]

\[ k = \text{rate constant} \]

units = (time\(^{-1}\))

\[ t_{1/2} = \frac{\ln\left(\frac{1}{2}\right)}{k} = \frac{0.693}{k} \]

\[ = \frac{0.693}{0.0112} \]

\[ \approx 62 \text{ days} \]
Sulfentrazone Example: Field Dissipation Study

Often data don’t conform to first order kinetics........
Wide Variety of Rate Laws

- **data**
- **first-order**
  - $\ln(C) vs t$
  - "biphasic"?
- **3/2-order**
  - $C^{-1/2} vs t$
- **2-order**
  - $C^{-1} vs t$
- **3-order**
  - $C^{-2} vs t$

*Others: zero-order, Monod, Michaelis-Menton, dual Monod, hyperbolic rate law etc.*
General types of biodegradation mechanisms/profiles

- cometabolism
- acclimation/degradation
- immediate degradation

Percent remaining vs. Time (days)
Acclimation........
enzyme induction?

long-term efficacy of repeat applications

hydrolysis rates often vary with pH-
Sample preservation and storage
Most reactions strongly dependent on temperature

Sample preservation and storage

Effect of temperature on parathion hydrolysis

A gross “rule of thumb” estimate: 2 – 3 fold increase per 10°C (over 10-40°C range)
Degradation: multiple simultaneous pathways
- both biotic and abiotic

hydrolysis

photolysis

reduction

oxidation
<table>
<thead>
<tr>
<th>Compound</th>
<th>Log Field Dissipation Half-life (d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbamates</td>
<td>1.3</td>
</tr>
<tr>
<td>OC</td>
<td>1.0</td>
</tr>
<tr>
<td>OPs</td>
<td>1.5</td>
</tr>
<tr>
<td>Pyrethroids</td>
<td>3.3</td>
</tr>
<tr>
<td>Soilherbs</td>
<td>6.3</td>
</tr>
</tbody>
</table>

**Field dissipation half-lives**

The diagram above illustrates the field dissipation half-lives for various compounds, with the x-axis representing different chemical classes and the y-axis showing the log field dissipation half-life in days. The values are as follows:

- Carbamates: 1.3 days
- OC: 1.0 days
- OPs: 1.5 days
- Pyrethroids: 3.3 days
- Soilherbs: 6.3 days
Aerobic soil half-lives

- Carbamates: 7 days
- OC: 2000 days
- OPs: 7 days
- Pyrethroids: 23 days
- Soilherbs: 70 days
Variability in Environmental Fate Data

- **CV = 52%** for simazine KOC 97-440
- **62%** for nicosulfuron TFD 20-103
- **61%** for mesosulfuron aerobic 8-73
- **46%** for chlorpyrifos aerobic 57-179

Variability in Environmental Fate Data CV = 52%
Variability in Environmental Fate Data

% coefficient of variation = standard deviation/mean

%CV = \frac{\sigma}{\mu} \times 100

rule of thumb for environmental data: CV>30% often reflect non-normal data (log-normal or other distributions)

<table>
<thead>
<tr>
<th>PROPERTY</th>
<th>% coefficient of variation</th>
</tr>
</thead>
<tbody>
<tr>
<td>solubility</td>
<td>7</td>
</tr>
<tr>
<td>KOW</td>
<td>11</td>
</tr>
<tr>
<td>KOC</td>
<td>51</td>
</tr>
<tr>
<td>vapor pressure</td>
<td>40</td>
</tr>
<tr>
<td>H'</td>
<td>28</td>
</tr>
<tr>
<td>aerobic halflife</td>
<td>46</td>
</tr>
<tr>
<td>anaerobic halflife</td>
<td>50</td>
</tr>
<tr>
<td>TFD</td>
<td>58</td>
</tr>
<tr>
<td>soil Phot</td>
<td>52</td>
</tr>
<tr>
<td>aq Phot</td>
<td>51</td>
</tr>
<tr>
<td>hydrolysis</td>
<td>16</td>
</tr>
</tbody>
</table>
OVERALL STRUCTURE
Correlation Matrix/Plot for pesticide physicochemical properties (N=173 chemicals)

water application
75% of evapotranspiration

atrazine recovered:
22% of application

medium water application
125% of evapotranspiration

atrazine recovered:
45% of application

high water application
175% of evapotranspiration

atrazine recovered:
61% of application

Agronomic practices Influence actual fate

DATA SOURCES (except for pyrethroids!!)

DATABASES
1. European Pesticide Properties Database – FOOTPRINT
   http://sitem.herts.ac.uk/aeru/footprint/en/
2. USDA-ARS PPDB
   http://www.ars.usda.gov/Services/docs.htm?docid=14147
3. DPR PESTCHEM ..............................................
   on-line internally
4. EXTOXNET
   http://ace.ace.orst.edu/info/extoxnet/
5. Pesticide Handbook – Tomlinson

ESTIMATION PROGRAMS/METHODS
1. EPI Suite –outstanding program – also includes data
   http://www.epa.gov/opptintr/exposure/pubs/episuite.htm
2. Handbook of Chemical Property Estimation Methods – Lyman Rheel and Rosenblatt
3. SPARC (SPARC performs automated reasoning in Chemistry)
   http://ibmlc2.chem.uga.edu/sparc/

ALWAYS CHECK DATA FOR CONSISTENCY!!!!!!!!!!
1. **Synthetic Pyrethroids:**

   posted on EM’s internal website

2. **Suggested reading/browsing:**

   *How Reliable are Chemical Property Data in the Literature?*

   especially:


3. **Excellent text:** Environmental Organic Chemistry, R. P. Schwarzenbach, P.M. Gschwend, D. W. Imboden
Environmental Fate Summary
Resúmen de Destino Ambiental

1. Environmental fate: where, how long, what products?

   infer or understand behavior using physico-chemical properties:
   hydrophobicity
   persistence/degradation
   volatility
Environmental Fate Summary
Resúmen de Destino Ambiental

1. Environmental fate: where, how long, what products?
2. Different chemical families/classes have different "personalities"

<table>
<thead>
<tr>
<th>Chemical Class</th>
<th>solubility</th>
<th>soil sorption</th>
<th>volatilization from water</th>
<th>persistence</th>
</tr>
</thead>
<tbody>
<tr>
<td>soil-applied herbicides</td>
<td>moderate</td>
<td>low</td>
<td>low</td>
<td>medium</td>
</tr>
<tr>
<td>carbamates</td>
<td>moderate</td>
<td>low</td>
<td>low</td>
<td>low</td>
</tr>
<tr>
<td>organophosphates</td>
<td>moderate</td>
<td>low</td>
<td>medium</td>
<td>low</td>
</tr>
<tr>
<td>pyrethroids</td>
<td>low</td>
<td>high</td>
<td>medium</td>
<td>medium</td>
</tr>
<tr>
<td>organochlorines</td>
<td>low</td>
<td>high</td>
<td>medium</td>
<td>very high</td>
</tr>
</tbody>
</table>
1. Environmental fate: where, how long, what products?

2. Different chemical families/classes have different "personalities".

3. Actual fate: physicochemical properties, environmental factors, agricultural practices.

- chemigation
- season of the year
- foliar-applied
- soil-applied
- irrigation method
- rainfall
- incorporation
- irrigation amount
- soil texture
- topography
- soil organic carbon content
- soil permeability
- irrigation scheduling
1. Environmental fate: where and how long?
2. Different chemical families/classes have different "personalities"
3. Actual fate:
   - chemical properties
   - environmental factors
   - agricultural practices

No substitute for actual field data