



INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
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UNITED NATIONS INDUSTRIAL DEVELOPMENT ORGANIZATION



INTERNATIONAL CENTRE FOR SCIENCE AND HIGH TECHNOLOGY

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SMR.648 - 10

SECOND AUTUMN WORKSHOP ON MATHEMATICAL ECOLOGY

(2 - 20 November 1992)

"Water Quality Modeling and Government Regulations"

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These are preliminary lecture notes, intended only for distribution to participants.

Water Quality Modeling and Government Regulations

Introduction

1. Clean Water Act - 1972

Fishable - Swimmable Waters

**Technology based approach - Secondary Treatment
or its equivalent**

2. Amendments - 1978

Water Quality Based Approach

Receiving water concentrations

Water Quality Criteria

3. Presently being considered

Sediment Quality Based Approach

**Sediment concentrations - observed and
computed**

Sediment Quality Criteria

Water Quality Criteria

1. Acute Toxicity

Acute toxicity = 96hr LC50 = Concentration that causes 50% mortality in 96hr.

5th percentile of the acute toxicities for all species tested / 2 = Final Acute Value (FAV)

2. Chronic Toxicity

Chronic toxicity - long term, life or partial life cycle tests. Acute to chronic ratio

Median acute to chronic ratio = ACR

3. Chronic Criteria

Final Chronic Value = Final Acute Value / Median Acute to Chronic Ratio

FCV = FAV / ACR

SEDIMENT QUALITY CRITERIA

*** What are they?**

Chemical concentration in a sediment that is protective of aquatic life.

Applies to all sediments.

Analogous to Water Quality Criteria.

*** What units should be used?**

Traditional units for sediments:

ug chemical / g dry weight sediment

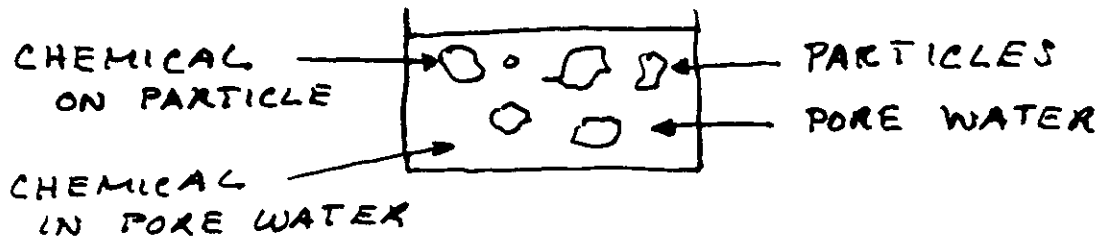
What about:

ug chemical / g WET weight sediment

The issue is:

What concentration correlates to biological effects?

DEFINITIONS : SEDIMENTS



PARTICLE CONCENTRATION:

$$m = \text{g particles} / \text{L sediment} \quad (\sim 500 \text{ g/L})$$

POROSITY

$$\phi = \text{VOLUME PORE WATER} / \text{VOLUME SEDIMENT}$$

~ 50 - 90 %

CHEMICAL CONCENTRATION

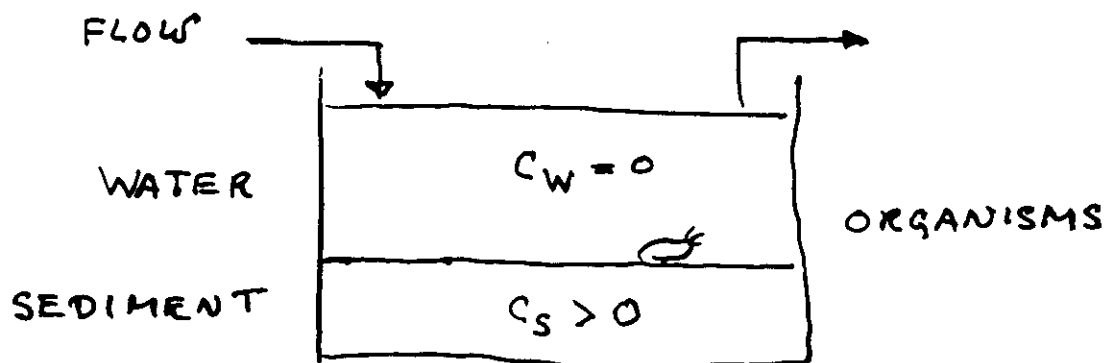
1. BULK
WET WEIGHT $C_{\text{BULK}} = \frac{\text{ug TOTAL CHEMICAL}}{\text{g TOTAL SEDIMENT}}$
2. DRY WEIGHT
(PARTICULATE) $C_s = \frac{\text{ug TOTAL CHEMICAL}}{\text{g PARTICLES}}$
3. PORE WATER
(DISSOLVED) $C_d = \frac{\text{ug DISSOLVED CHEMICAL}}{\text{L PORE WATER}}$

PARTICLE COMPOSITION

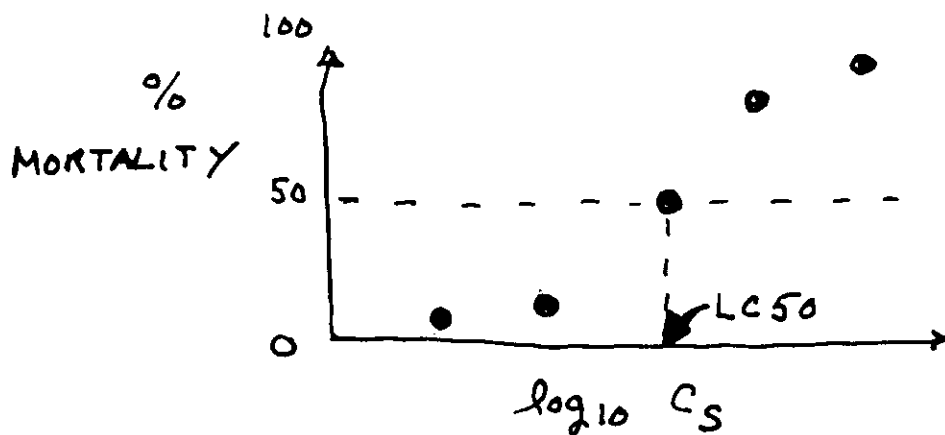
A diagram of a particle, represented as an irregular shape with a thick, textured outer layer. An arrow points from the label 'ORGANIC CARBON (HUMUS)' to this outer layer. Below the diagram, the text 'FRACTION ORGANIC CARBON' is written. To the right of the diagram, the equation for the fraction of organic carbon is given: $f_{\text{oc}} = \frac{\text{g ORGANIC C}}{\text{g PARTICLE}}$. Below this equation, the typical range is noted: $(\sim < 0.1\% - 40\%)$.

SEDIMENT TOXICITY EXPERIMENT

PURPOSE : MEASURE EFFECT OF A
CHEMICAL IN A SEDIMENT
ON AN ORGANISM

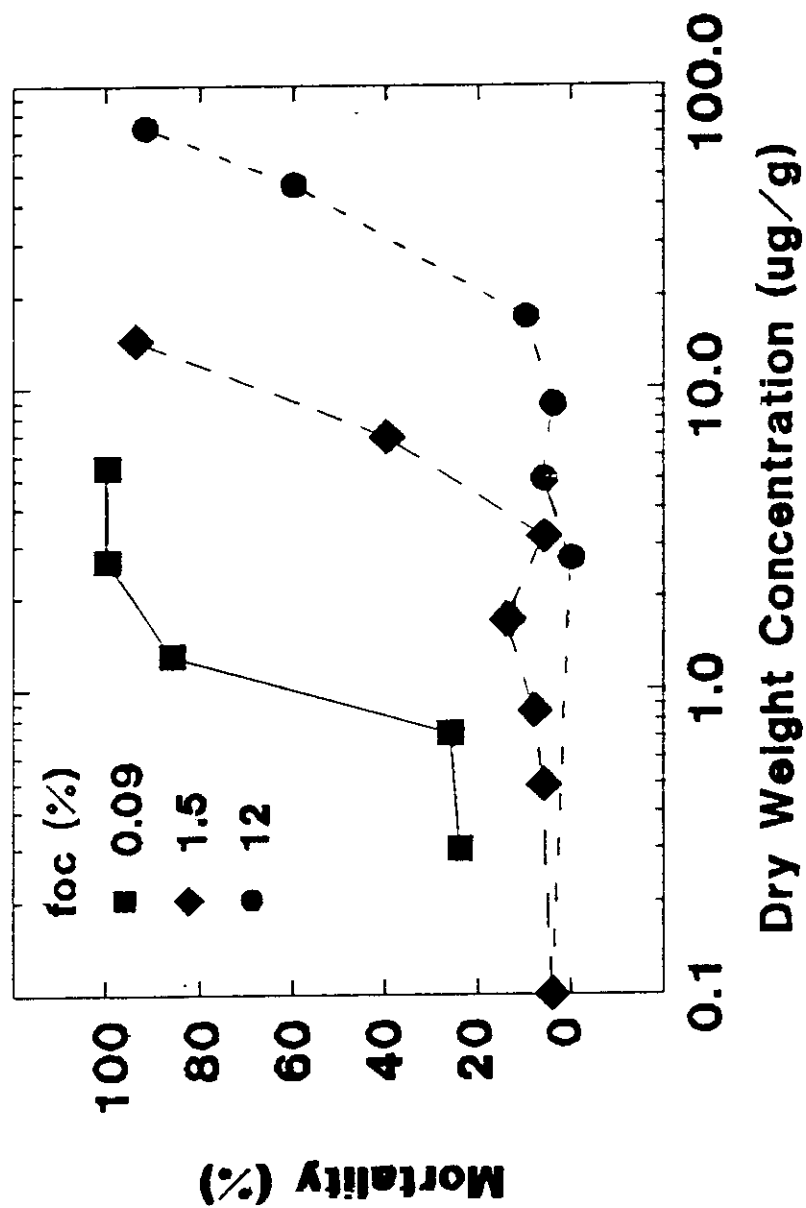


TYPICALLY : 5 CONCENTRATIONS , C_S



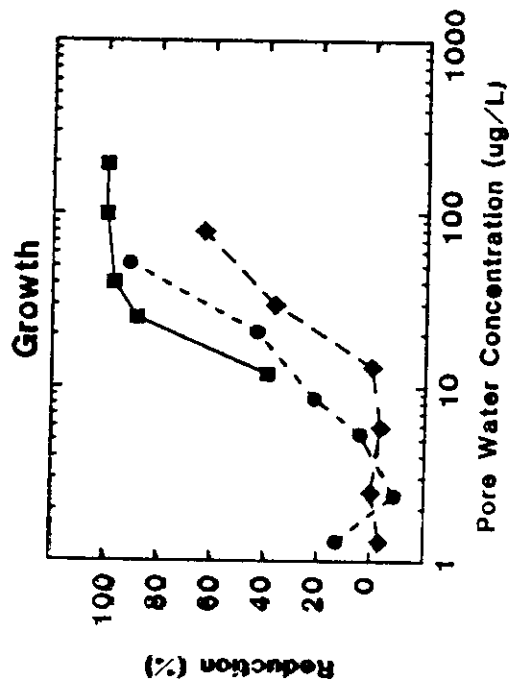
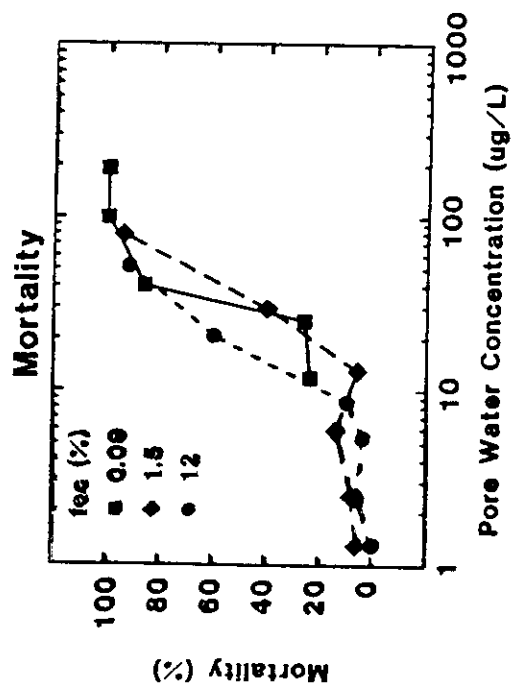
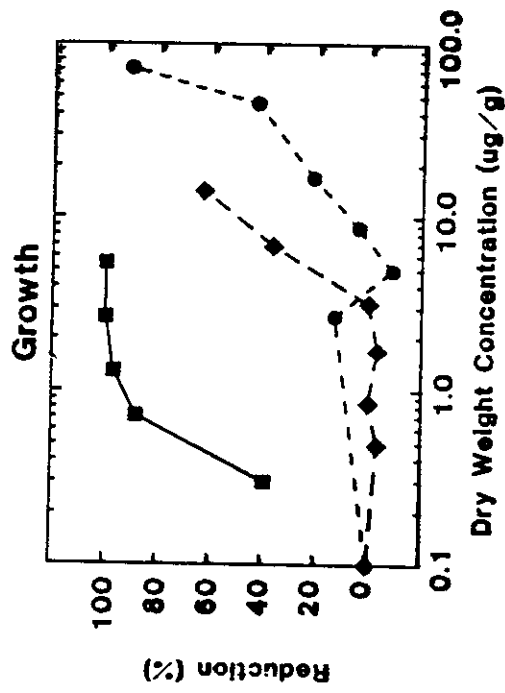
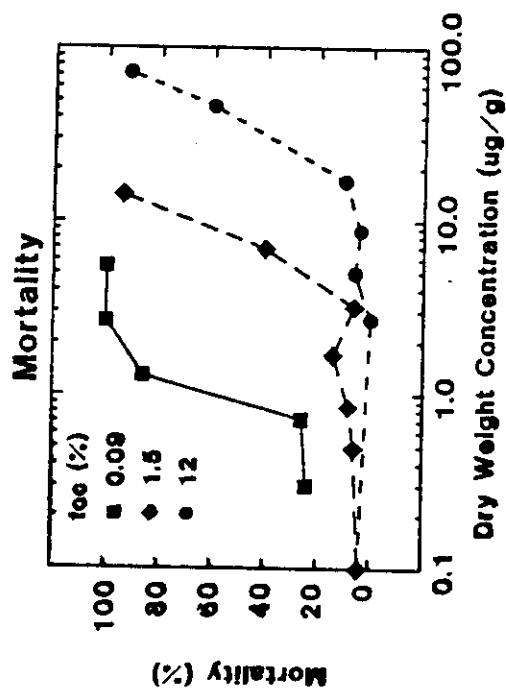
Acute Toxicity of Kepone

Dry Weight Normalization



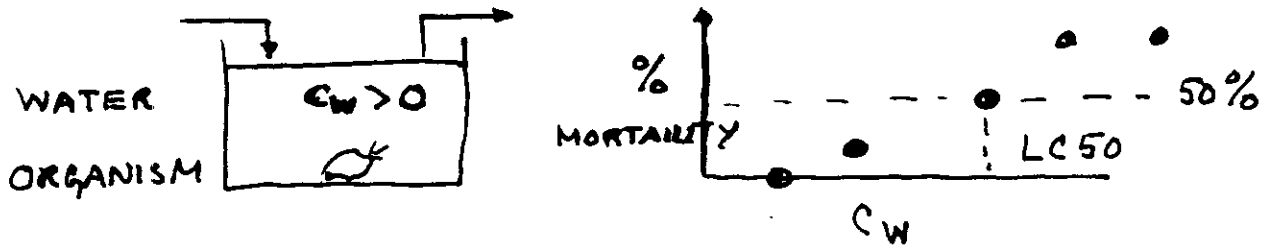
Acute and Chronic Toxicity of Kepone

Dry Weight and Pore Water Normalizations

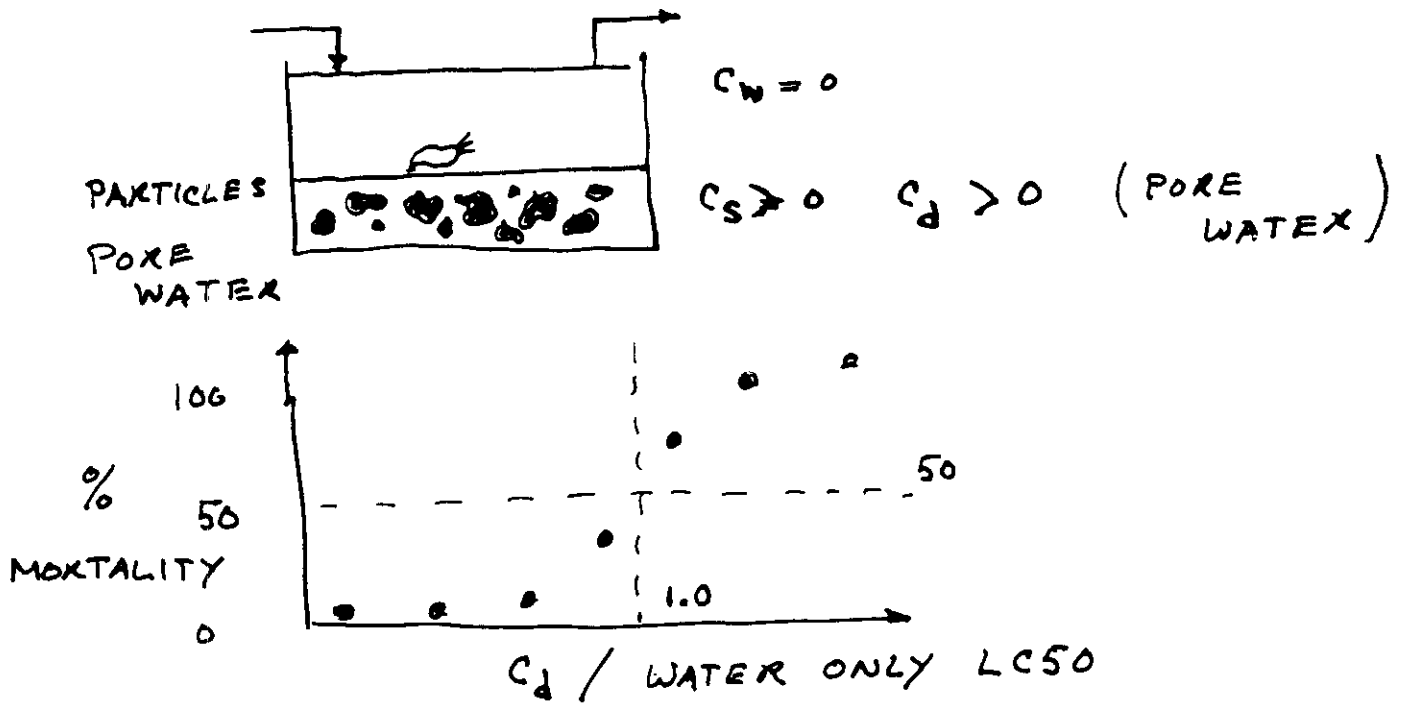


TOXICITY TESTS

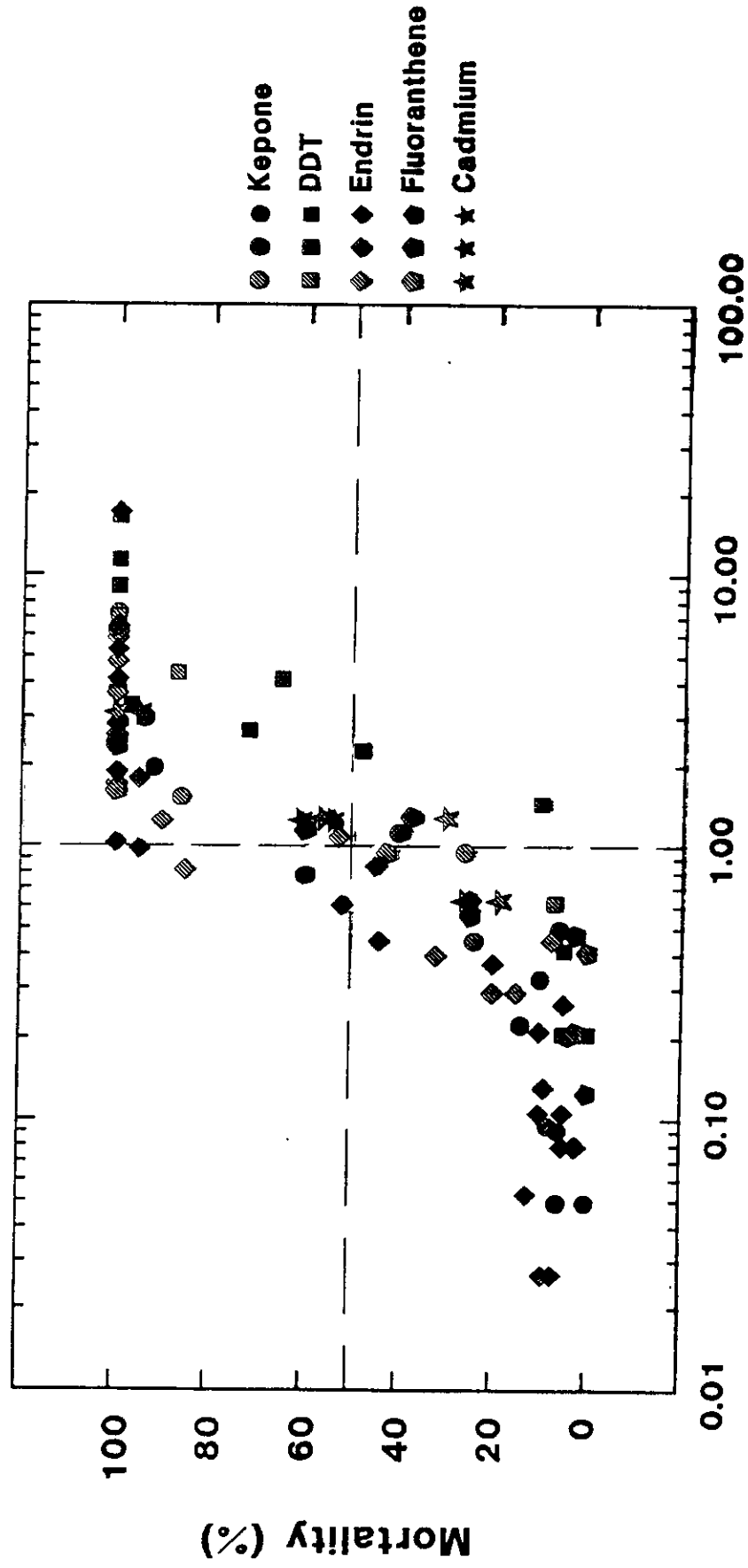
WATER ONLY EXPOSURE



SEDIMENT EXPOSURE

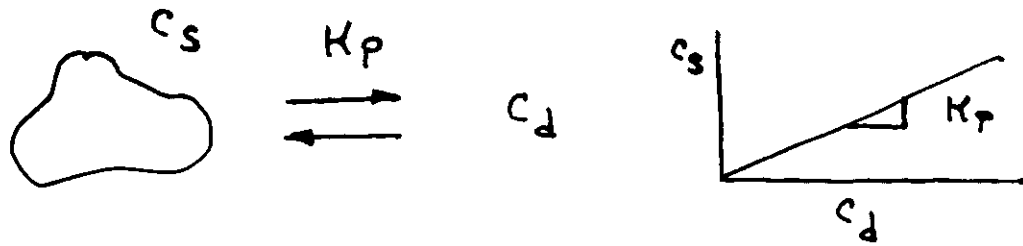


Pore Water Normalization



Predicted Pore Water Toxic Units

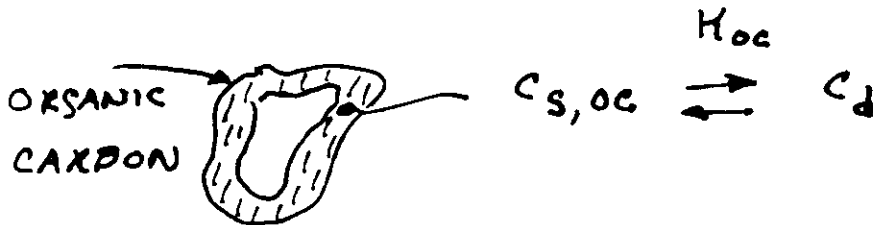
PARTITIONING BETWEEN PARTICLES AND PORE WATER



PARTITION COEFFICIENT

$$K_p = \frac{c_s \text{ (}\mu\text{g CHEMICAL/g)}}{c_d \text{ (}\mu\text{g CHEMICAL/L)}} \left(\frac{\text{L}}{\text{g}} \right)$$

FOR NON-IONIC ORGANIC CHEMICALS



$$\begin{aligned} \text{WHERE : } c_{s,oc} &= \frac{\mu\text{g CHEMICAL}}{\text{g ORGANIC CARBON}} \\ &= c_s / f_{oc} \end{aligned}$$

$$\text{AND : } K_{oc} = K_p / f_{oc}$$

IT HAS BEEN FOUND THAT :

K_{oc} IS INDEPENDENT OF SEDIMENT PROPERTIES ($f_{oc} > 0.2\%$)

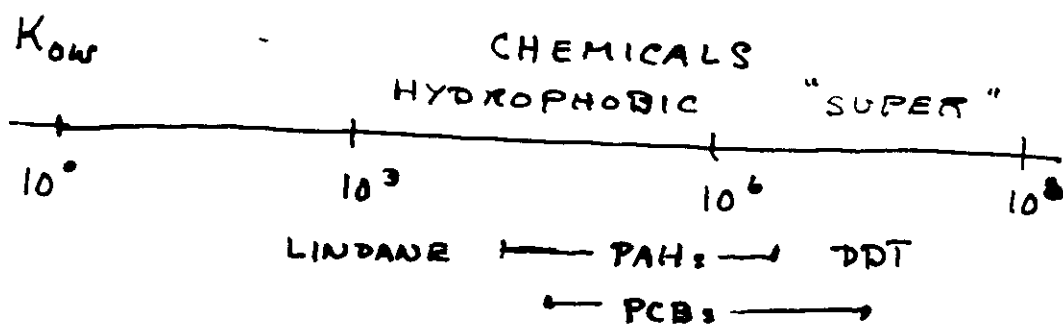
OCTANOL WATER PARTITION COEFFICIENT AND K_{oc}

C_{oct}
C_d

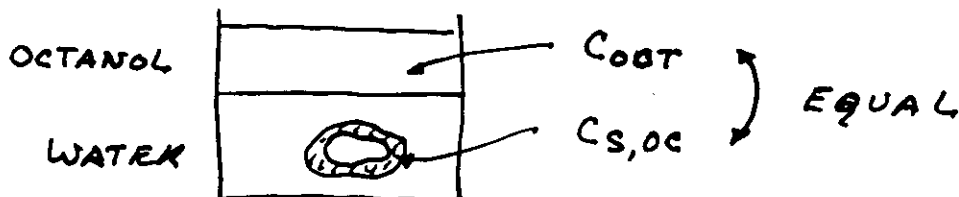
OCTANOL ($C_8H_{17}OH$)

WATER

$$K_{ow} = \frac{C_{oct}}{C_d} \frac{(\mu g \text{ CHEMICAL} / L - \text{OCTANOL})}{(\mu g \text{ CHEMICAL} / L - H_2O)}$$



OBSERVATION : $K_{oc} \approx K_{ow}$



I.E. CHEMICALS ARE ABOUT AS SOLUBLE
IN ORGANIC CARBON AS THEY ARE
IN OCTANOL

THEREFORE :

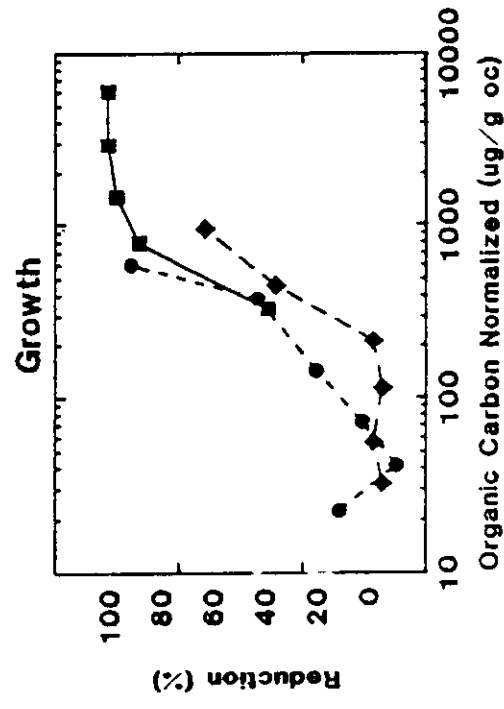
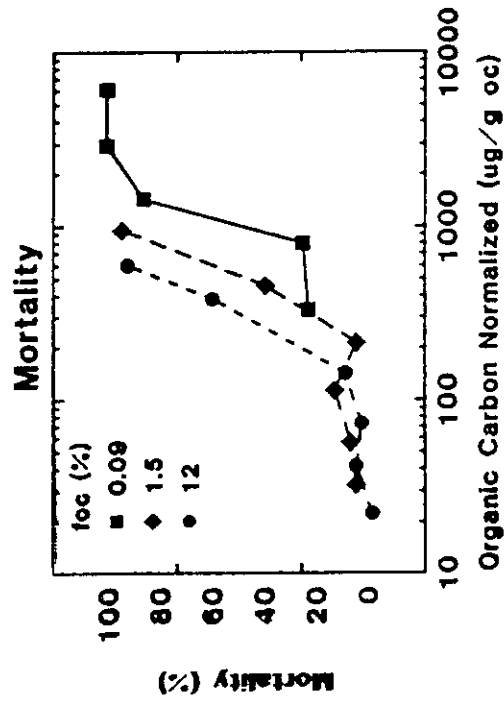
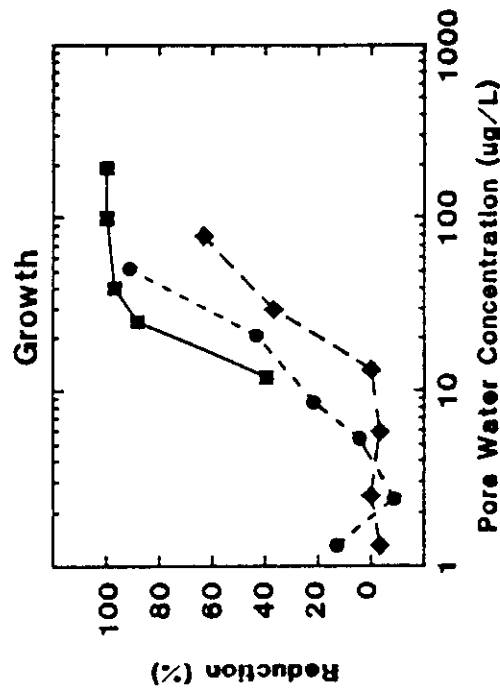
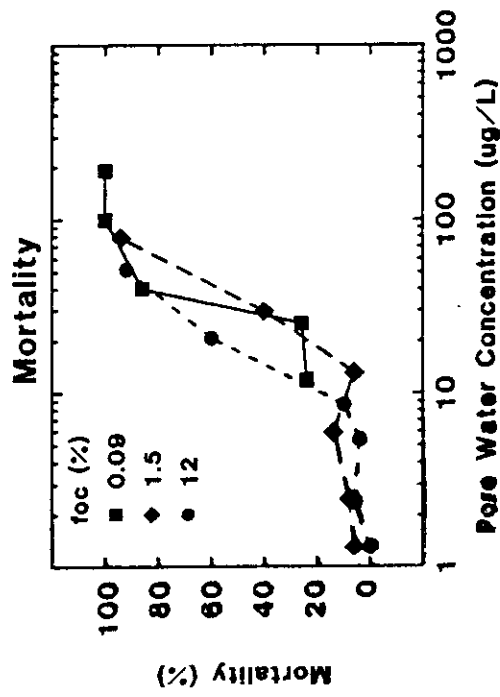
$$C_{s,oc} = \frac{C_s}{f_{oc}} = K_{oc} C_d \approx K_{ow} C_d$$

CHEMICAL PROPERTY

SEDIMENT PROPERTY

Acute and Chronic Toxicity of Kepone

Pore Water and Organic Carbon Normalizations



MORTP2A

3-58

Definition

Sediment Toxic Units: STU

$$PTU = \frac{\text{Sediment Concentration}}{\text{Sediment LC50}}$$

Predicted Sediment Toxic Units: STU

Predict the sediment LC50

from the water only LC50 and K_{oc} .

$$STU = \frac{[\text{Sediment Concentration}]_{oc}}{K_{oc}[\text{Water Only LC50}]}$$

Organic Carbon Normalization

