Development of a generic method for hazard analysis of substances: Addressing metal speciation, fate and ecotoxicity issues

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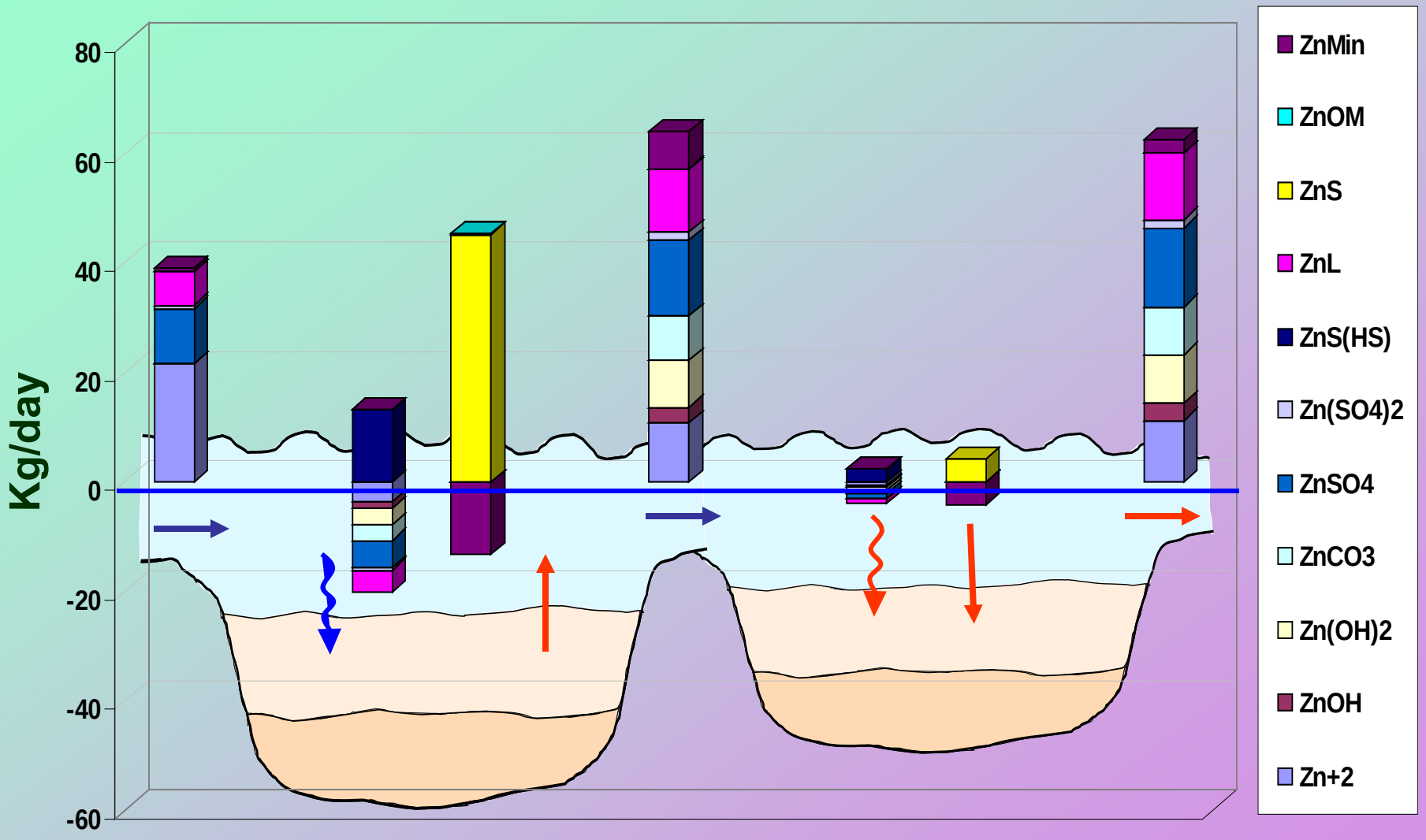
Current Practice

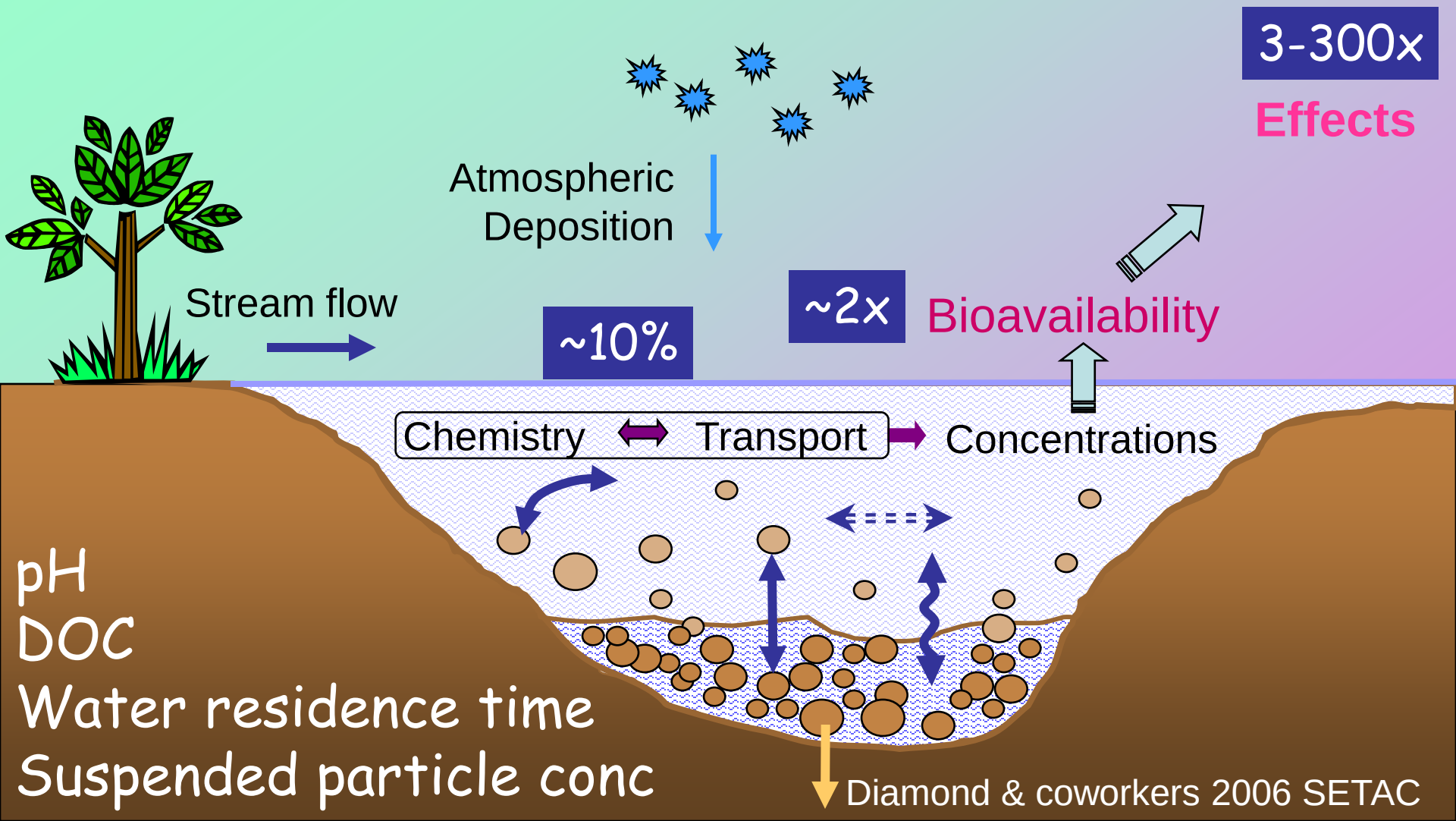
- PBT Approach
- Treatment of metal as a single species
- Lack of metal-specific fate pathways
- Missing environmental compartments
- Model parameterization
- Effects assessment – bioavailability → speciation
- BCF ⇩ as $[Me]_{biota}$ ⇧ (McGeer et al. 2003)

TRANsport-SPECiation Model



Bhavsar et al. 2004a,b ET&C

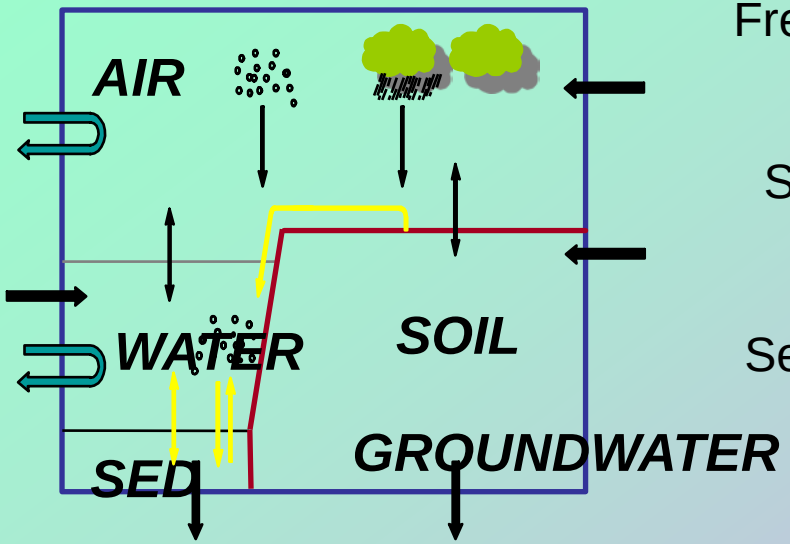
Importance of metal chemistry



Goal

- Develop a generic method to calculate metal Characterization Factors (CFs)
  - Accounts for effects of ambient chemistry on speciation & ecotoxicity
  - Compatible with methods for organic chemicals
- Analyze sensitivity of CFs to environmental chemistry and fate parameters

Proposed Method



Freshwater
Saltwater
Sediment

WHAM

Compartments
Archetypal Environ
pH, Eh, DOC, etc.

Freshwater
Saltwater
Sediment

BLM, PAF

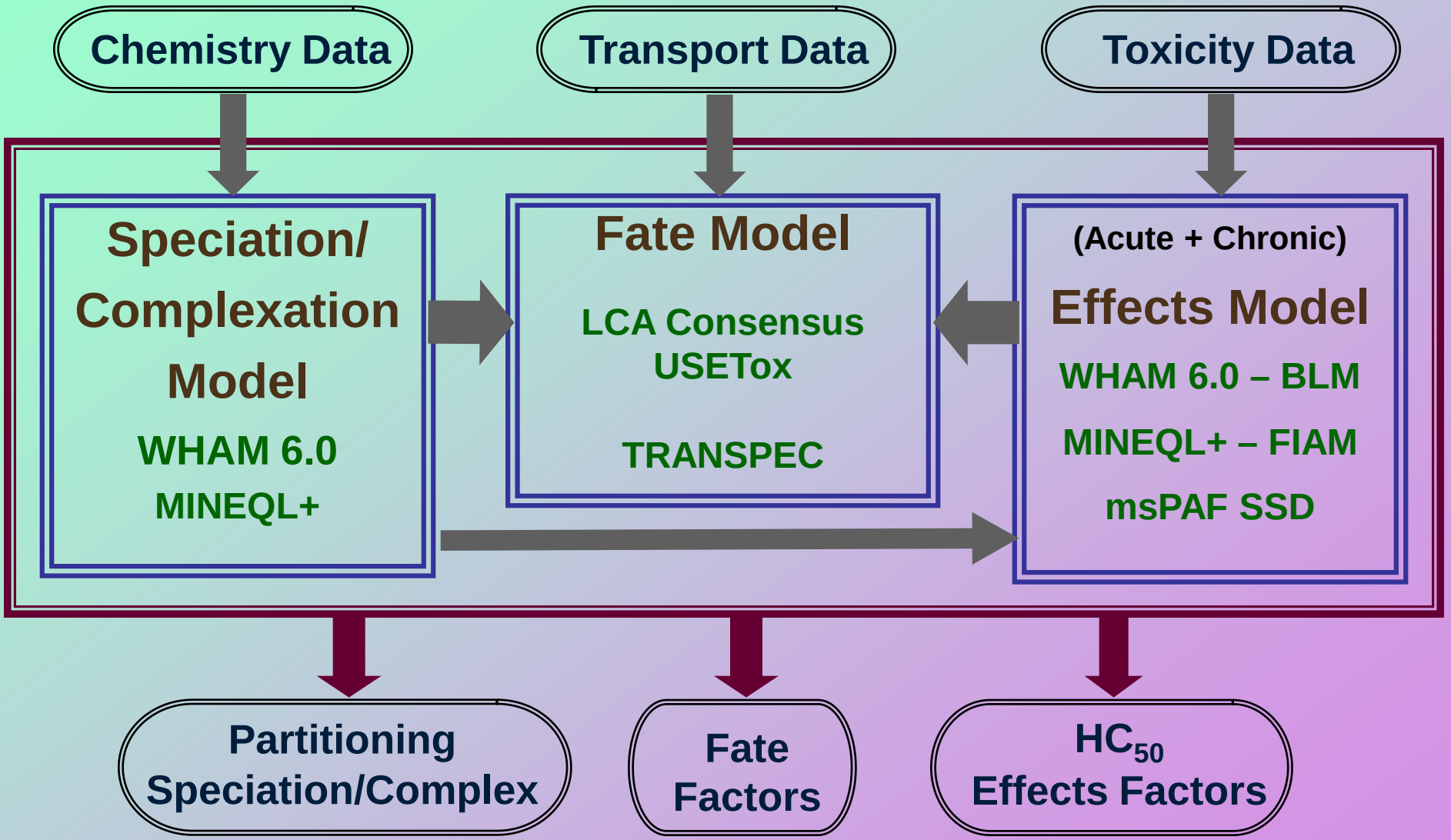
Compartments
Archetypal Environ
pH, Eh, DOC, etc.

Fate Factor

Effect Factor

Characterization Factor

Modelling Framework

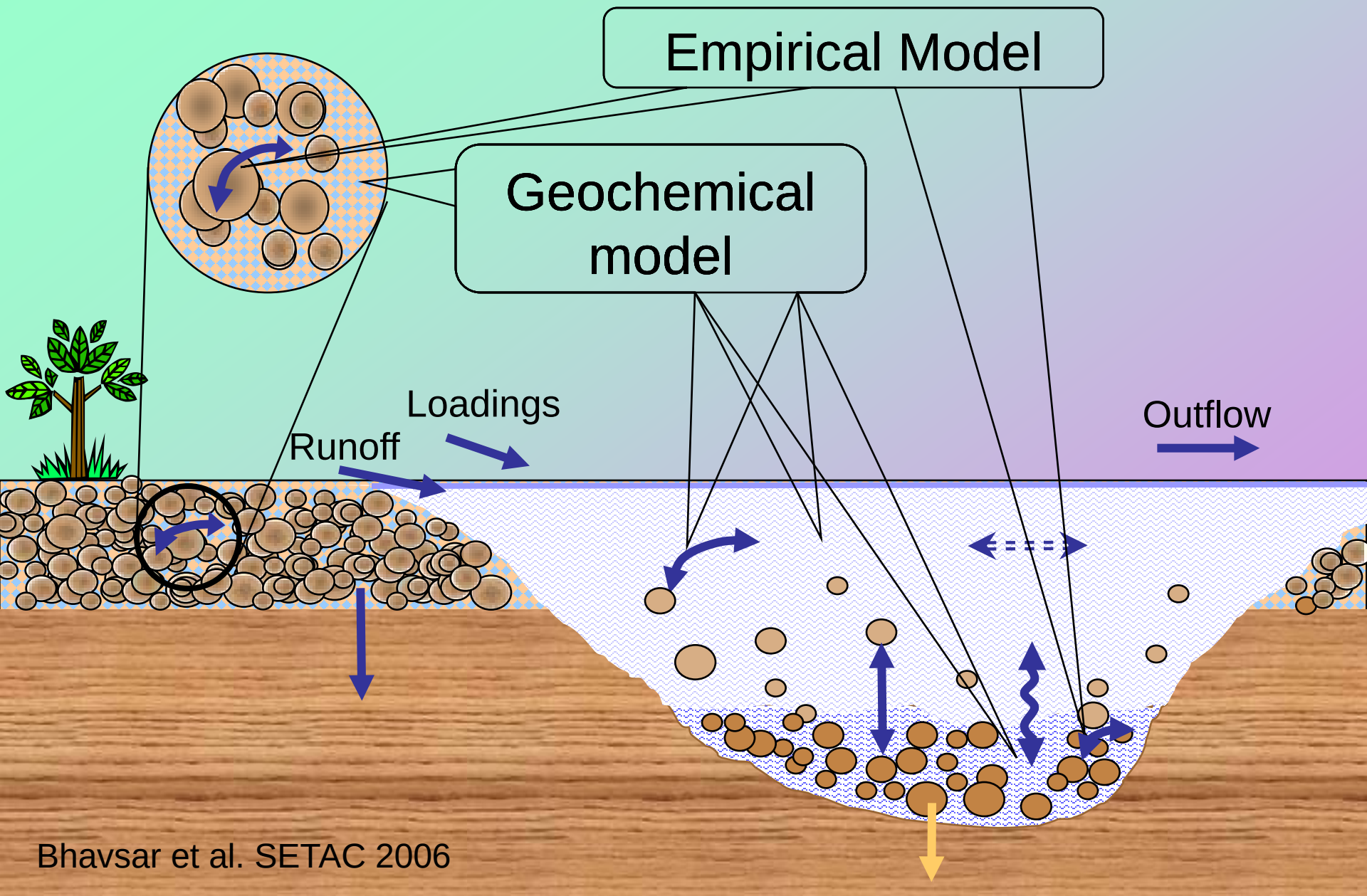


Tiered Approach

For Cu, Ni & Zn

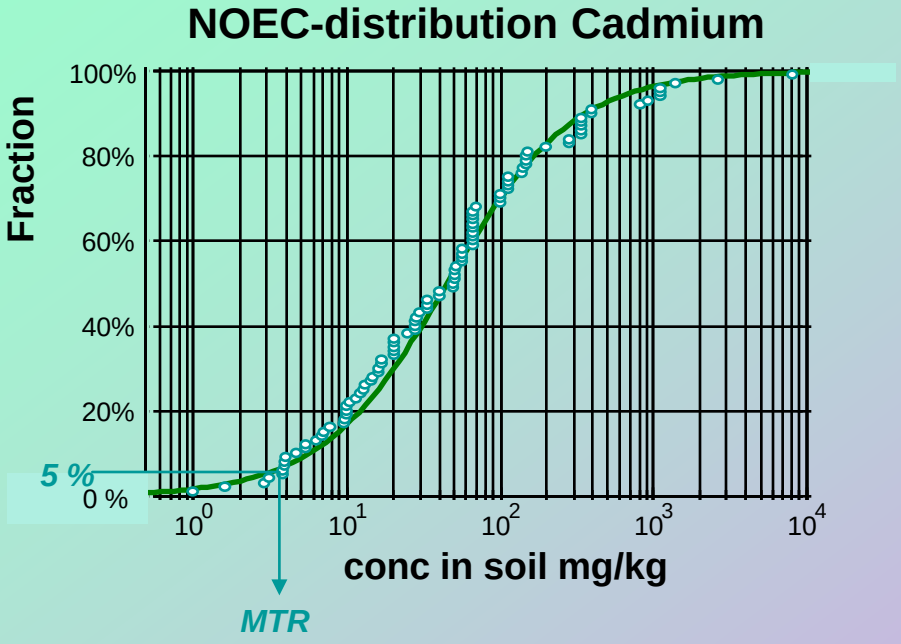
1. Fate - Calculate speciation/complexation using WHAM 6.0 & fate Model
2. Effects – FIAM and BLM for acute + chronic endpoints
3. Compare FF obtained with empirical K_d vs #1
4. Compare EF of dissolved, FIAM and BLM
5. Develop a generic method for all metals

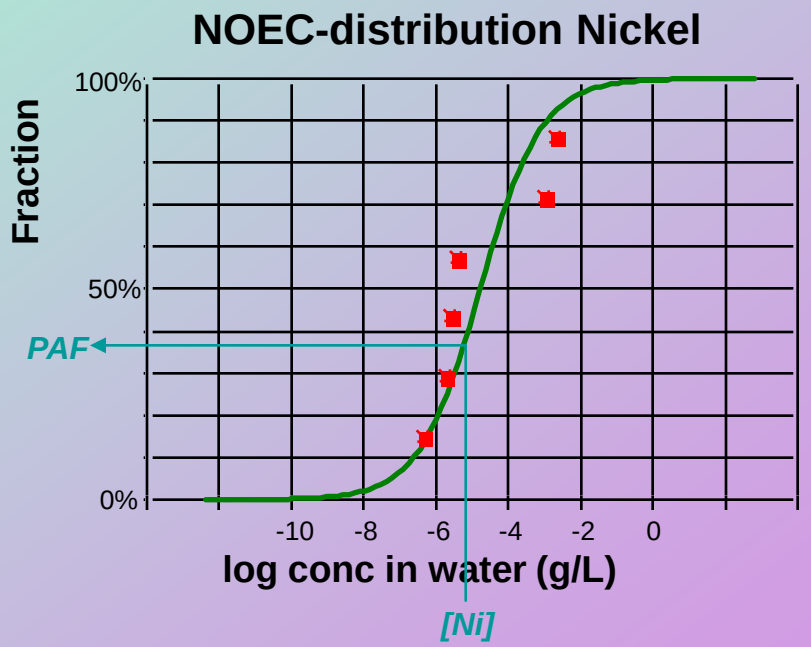
Modeling Speciation/complexation



Bhavsar et al. SETAC 2006

Species Sensitivity Distribution





Dik van de Meent, Mark Huijbreghts and Co-workers

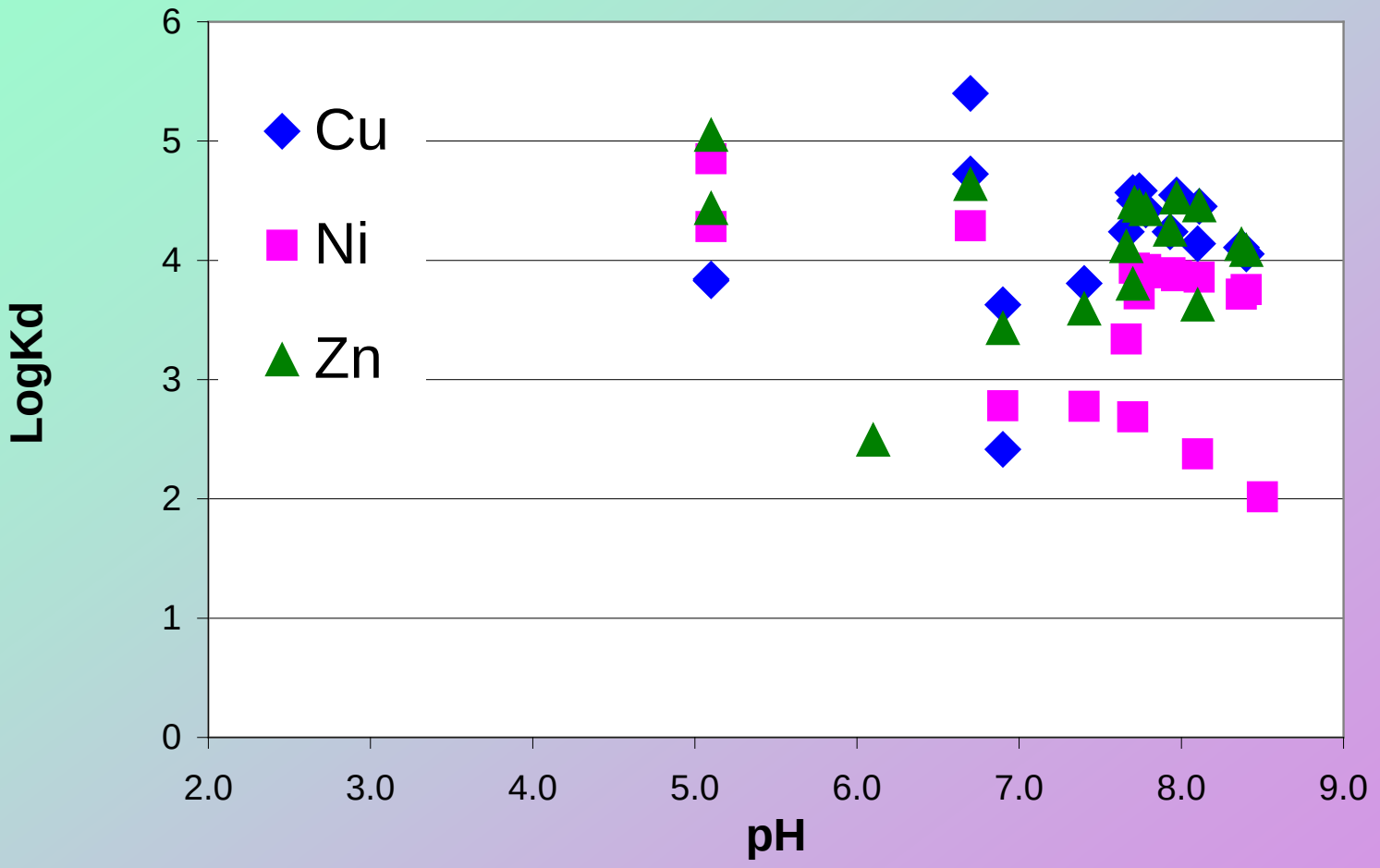
Chemistry Issues

- Explore impacts of variable water chemistry on FF & EF
- Choosing archetypes
  - Characterizing environmental variability
  - Frequency of occurrence in environment
  - Lack of consistent measured data
- Linking chemistry with environmental variability (e.g., morphology, transport rates)

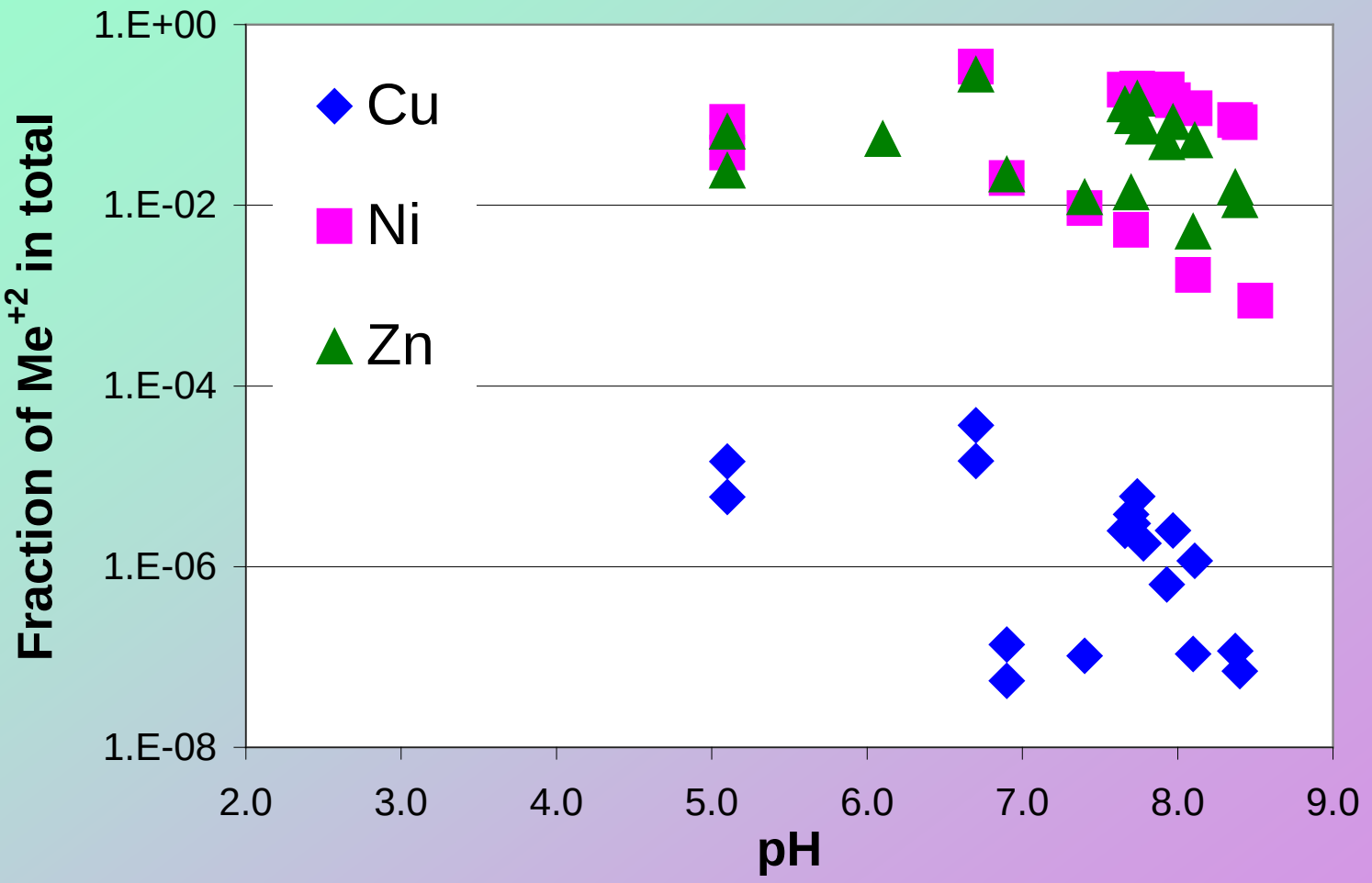
Selected Sudbury Lakes

- Surface water measurements from Sudbury
  - MOE monitoring data between 1990 & 2003
  - Categorized according to chemistry
- 16 measured water chemistries
  - pH: 4.3 → 9.0
  - DOC: 0.5 → 10.8 mg/L
  - alkalinity 0.9 → 65 mg $CaCO_3$/L
  - hardness 7 (soft) → 865 mg/L (very hard)

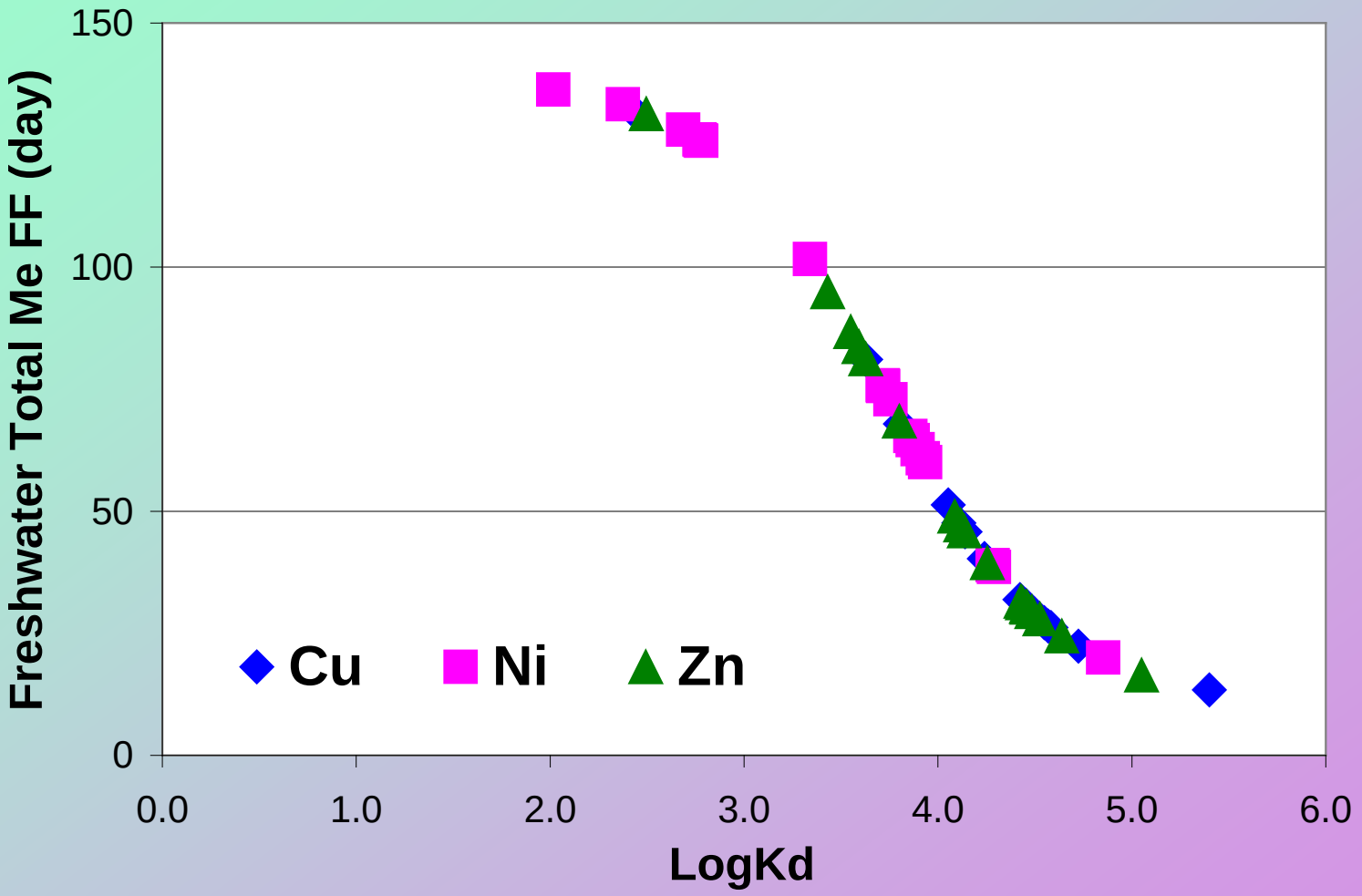
Estimated Kd – Freshwater



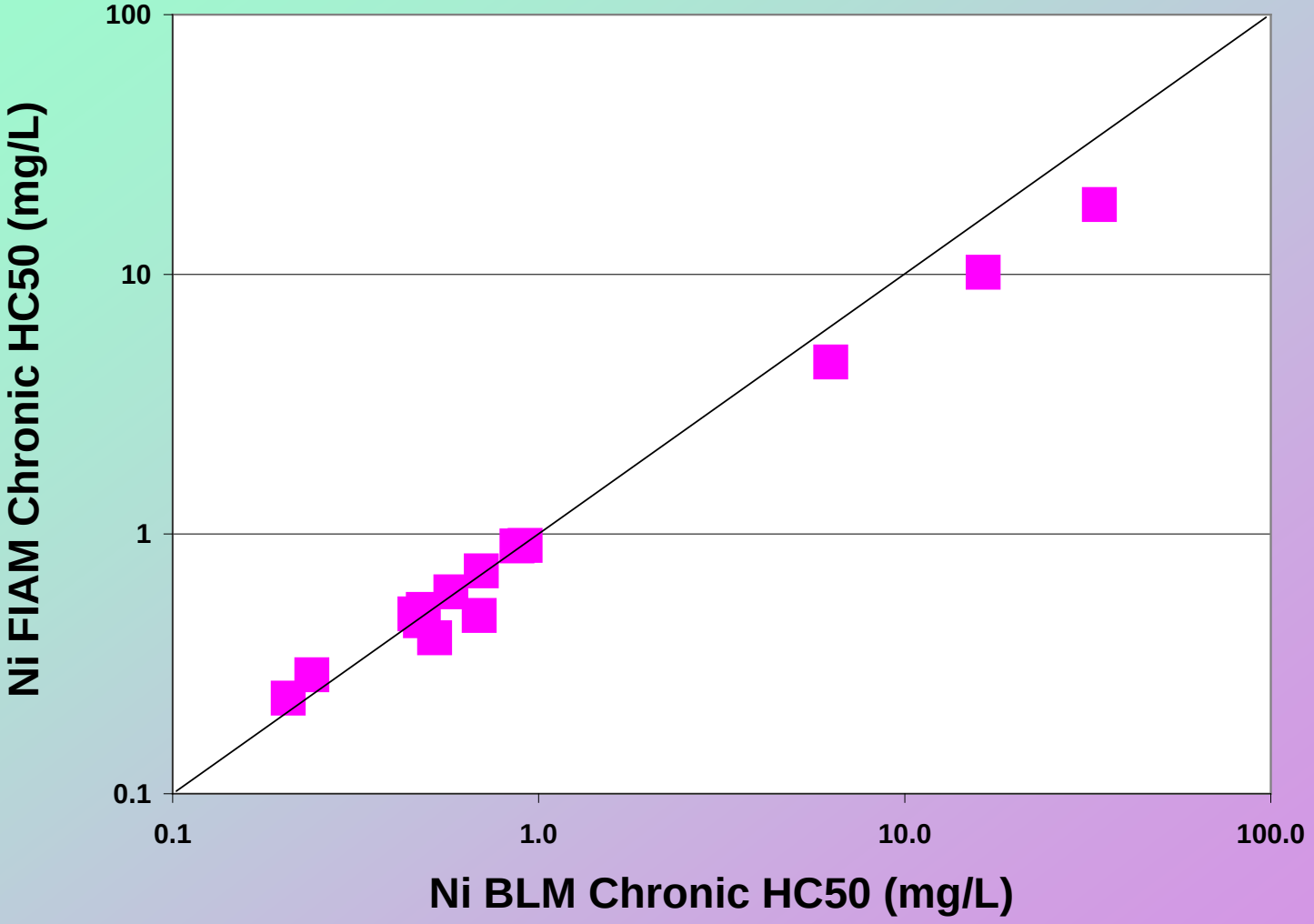
Fraction Me^{+2} – Freshwater



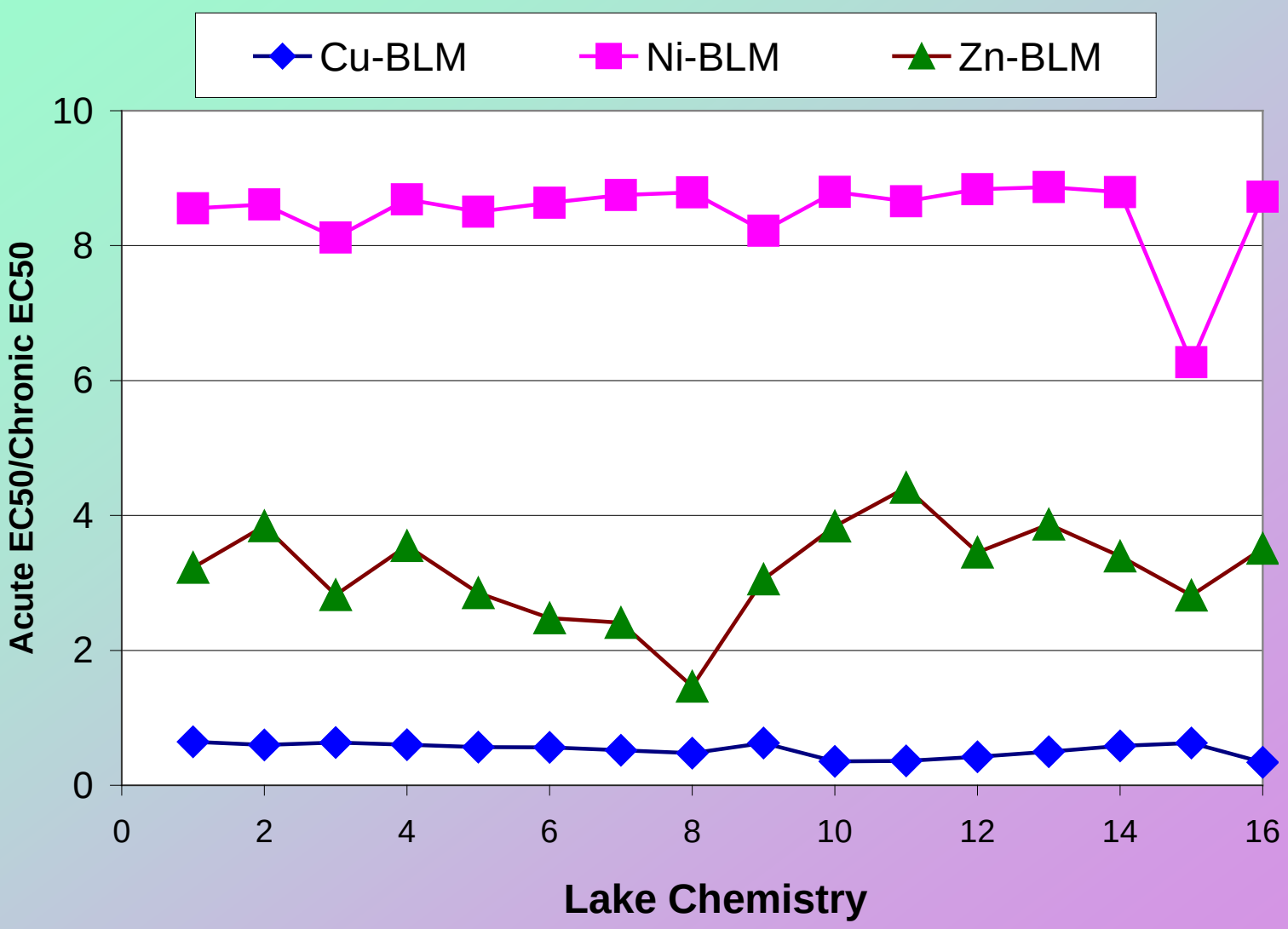
Fate Factors – Tot Me



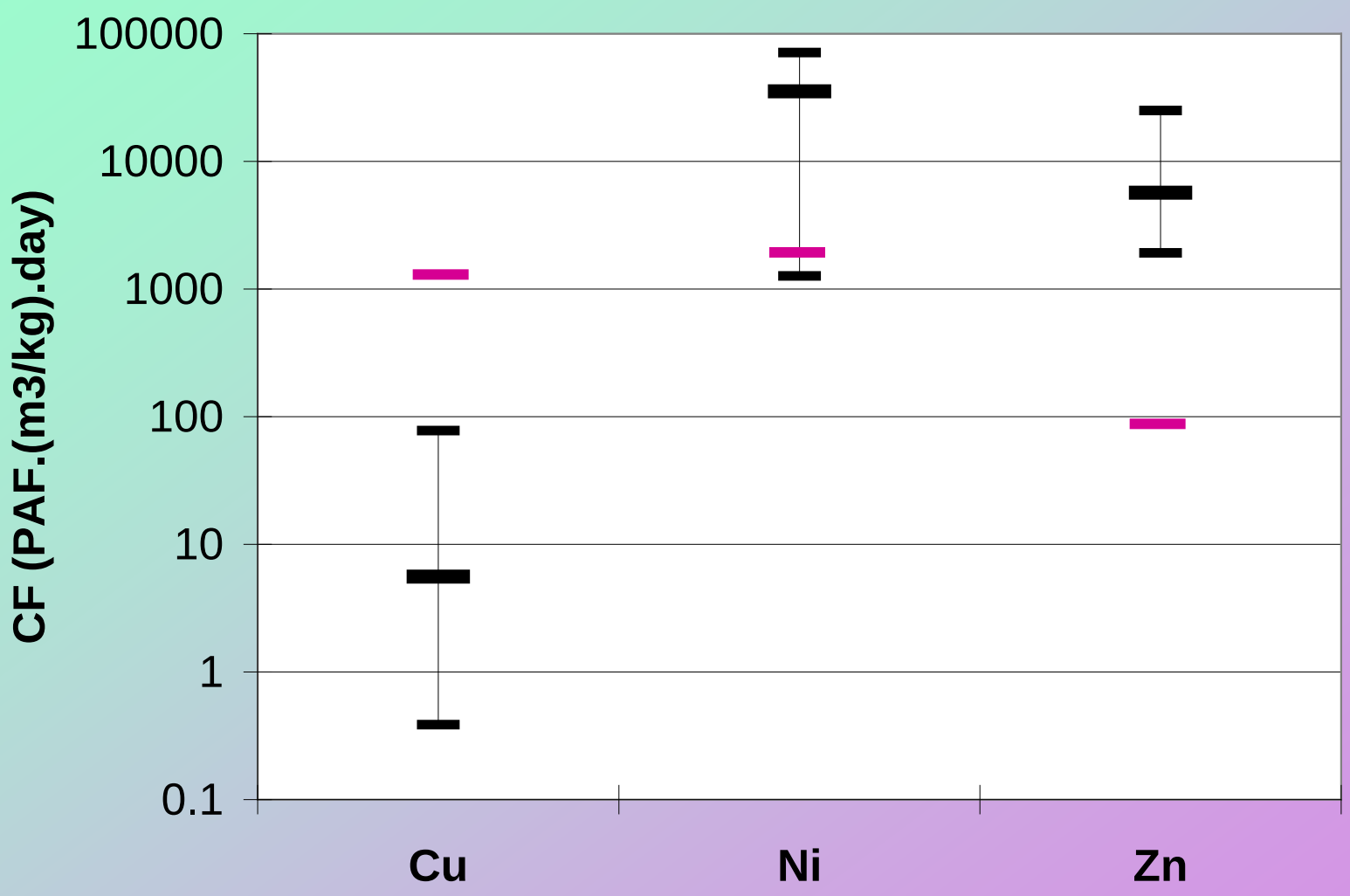
Ni Effect Factors – BLM vs FIAM



Acute vs Chronic EC_{50}



CFs – Chronic



Summary

- Development of a generic method for chemical hazard assessment
- Address metal speciation, fate & ecotoxicity
- FF – sensitive to chemistry & environment
- EF – Chemistry is more important, FIAM can be used in absence of BLM, constant ratio between toxicity endpoints
- CF – Vary over 3 orders

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