Waterborne Chemical Agent Transport Modeling Capability

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Presentation Overview

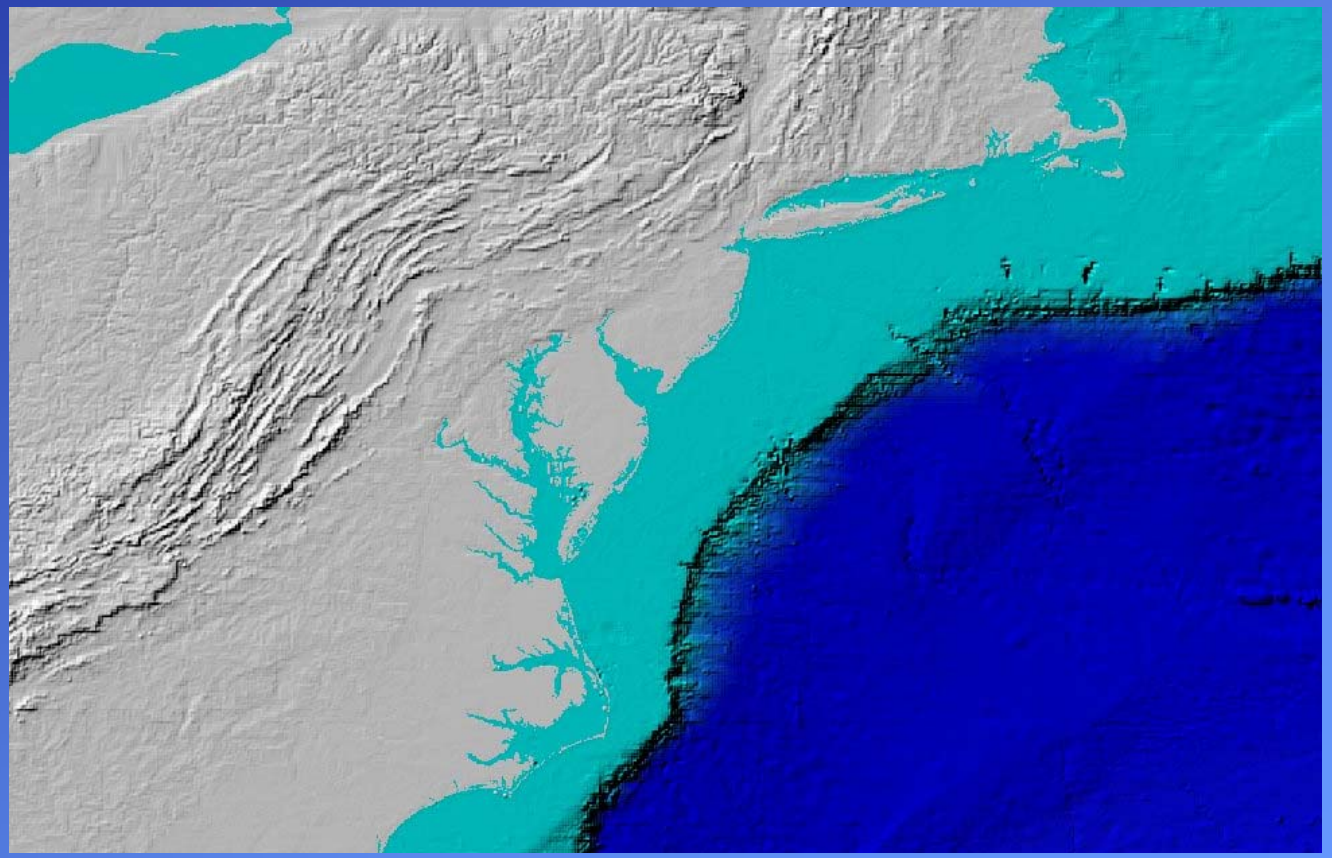
- Background
  - Why waterborne transport
  - Waterborne modeling data requirements
  - Data Availability
- Phase I SBIR
  - Objective
  - ASA Waterborne Chemical Transport Model
  - Integration Architecture
  - Results
- Phase II SBIR

Why Waterborne Transport

- Interdiction at sea
- Active Defense
- Deposition from an atmospheric chemical plume to a water body
- Intentional or accidental release of a chemical agent into a water body
- **Implications of such events can involve**
  - Impedance of expeditionary forces into theater
  - Special operators mission effectiveness
  - Contamination of combatant vessels
  - Impact to drinking water supplies

Environmental Data Requirements

- **Land-Water delineation**
- Bathymetry
- Currents
- Temperature
- Salinity
- Winds



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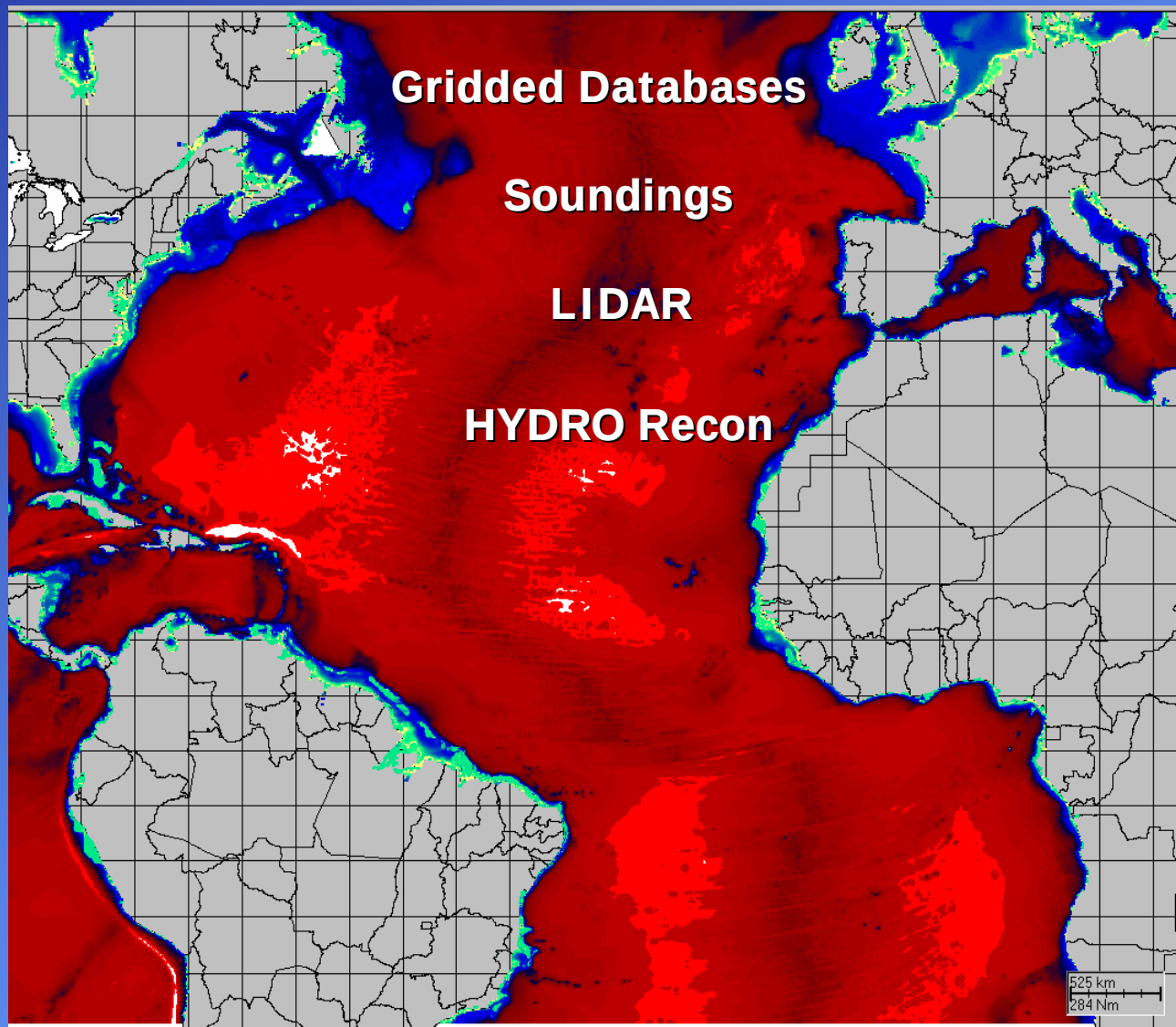

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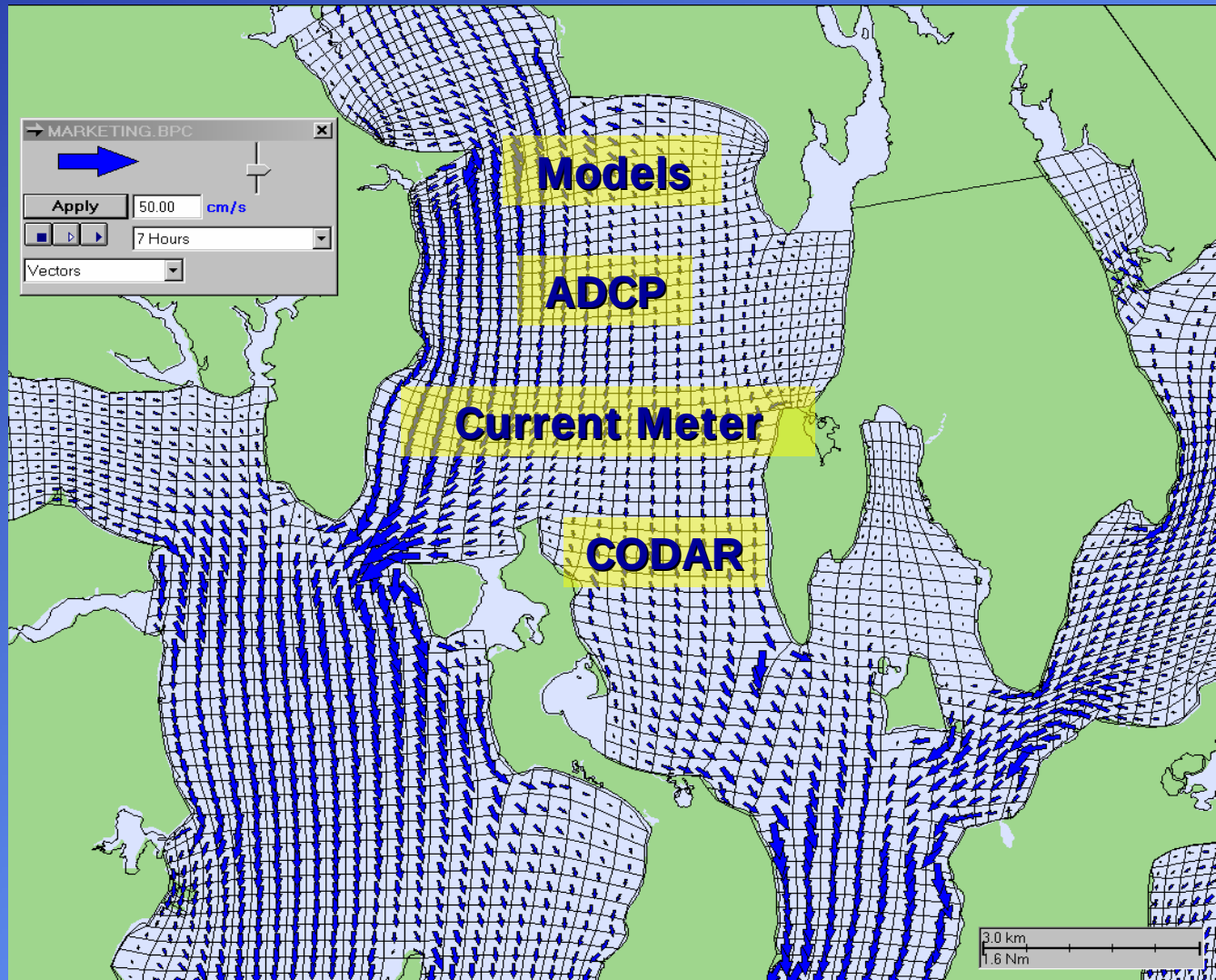

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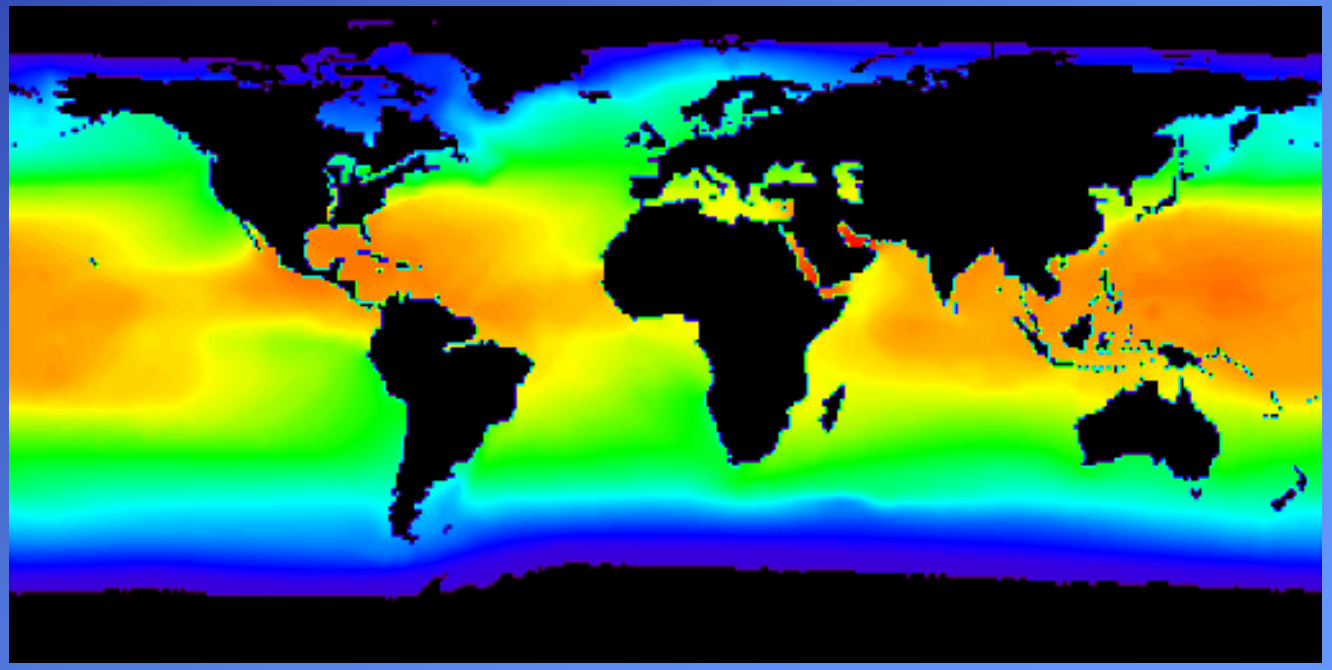

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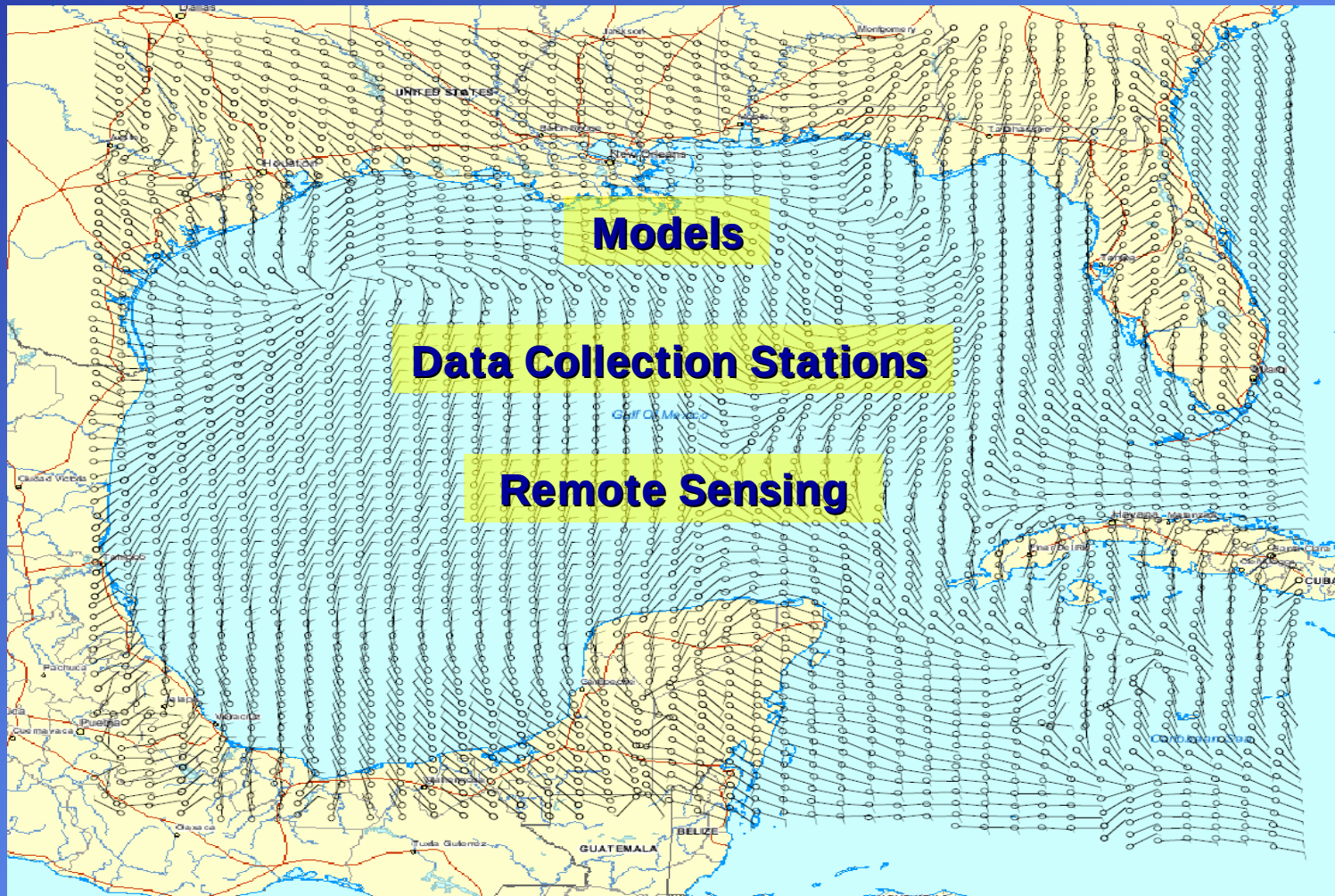
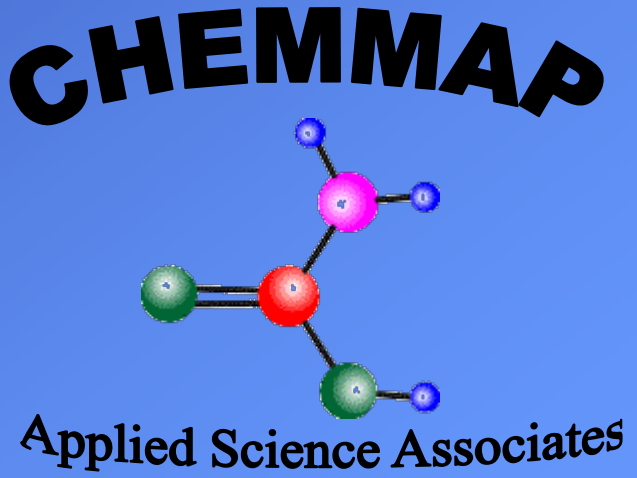


Data Availability

- A truly operational system requires rapid if not immediate availability of datasets ranging in scale from global to potentially 10's of meters
- Global scale datasets are readily available and local datasets are typically available within the Continental United States (CONUS). However, these datasets are not usually integrated.
- Outside CONUS regions mid and local scale datasets are often difficult to obtain
  - Intelligence Assets
  - Environmental Reconnaissance
  - Dedicated reach back cells

Phase I Objective

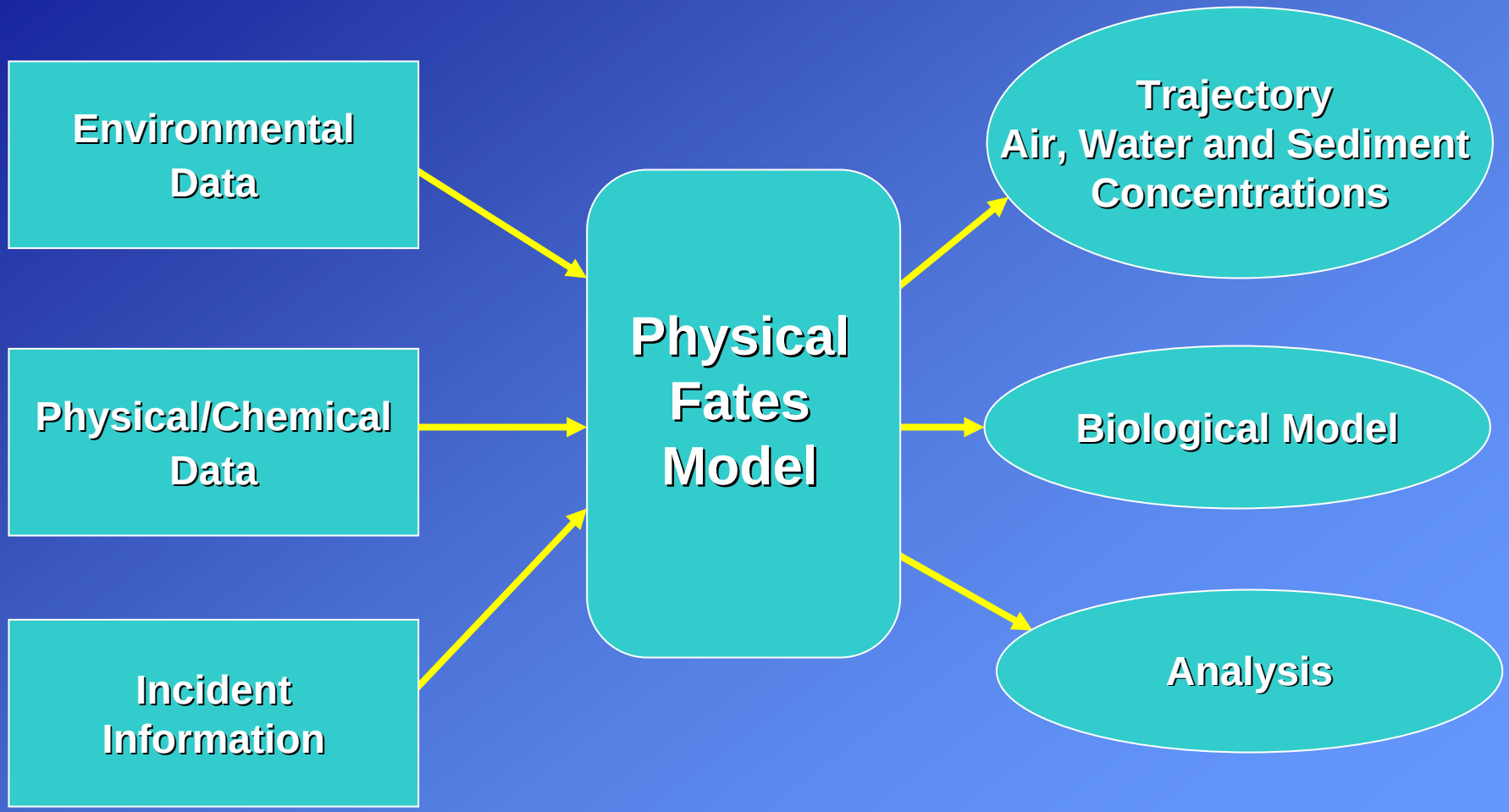
- Couple ASA's waterborne chemical transport and dispersion model with the HPAC system as a feasibility assessment for future complete integration

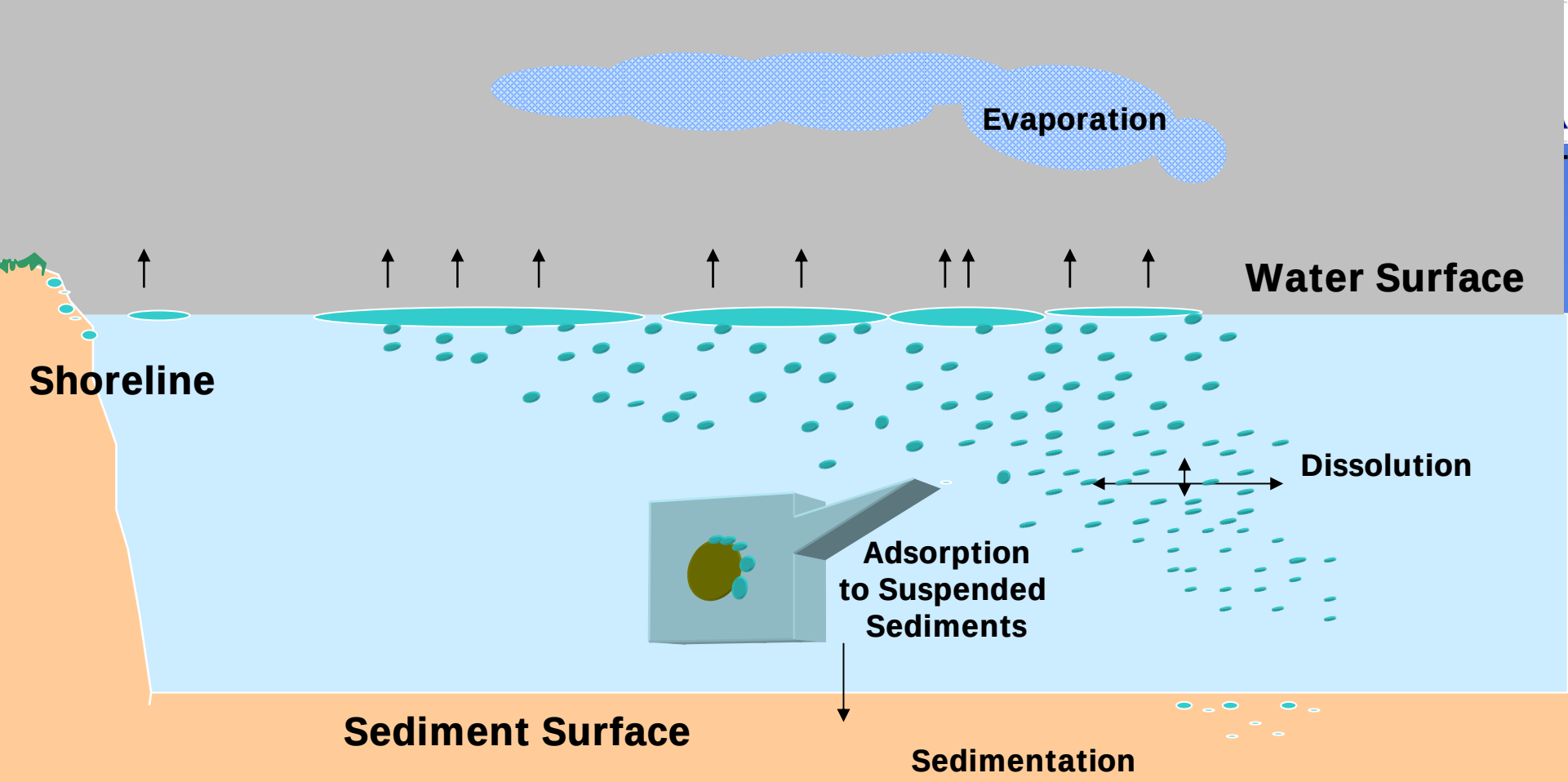


CHEMMAP

- Integrated modeling system designed to predict the trajectory, fate and effects of Toxic Industrial Chemicals and Materials
- Developed as a Natural Resource Damage Assessment Model for US Government Regulations
- Expanded commercial development
  - SIMAP (Oil Spill Impact Model Application Package)
  - CHEMMAP (Chemical Model Application Package)
- **Continued DoD development to predict transport and fate of weaponized chemical agents and refinement of TIC/TIM algorithms for military utility in waterborne environments**

CHEMMAP Structure





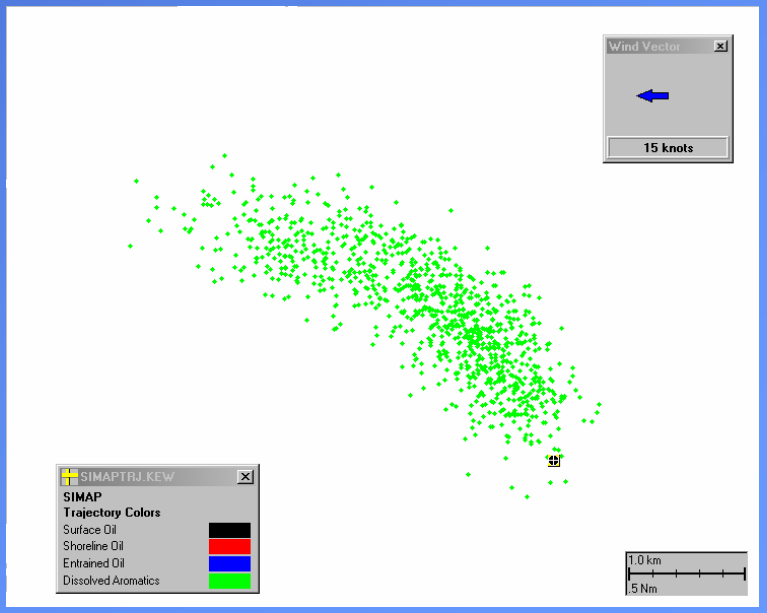
Physical / Chemical Processes

Dispersion
Spreading
Entrainment
Dissolution

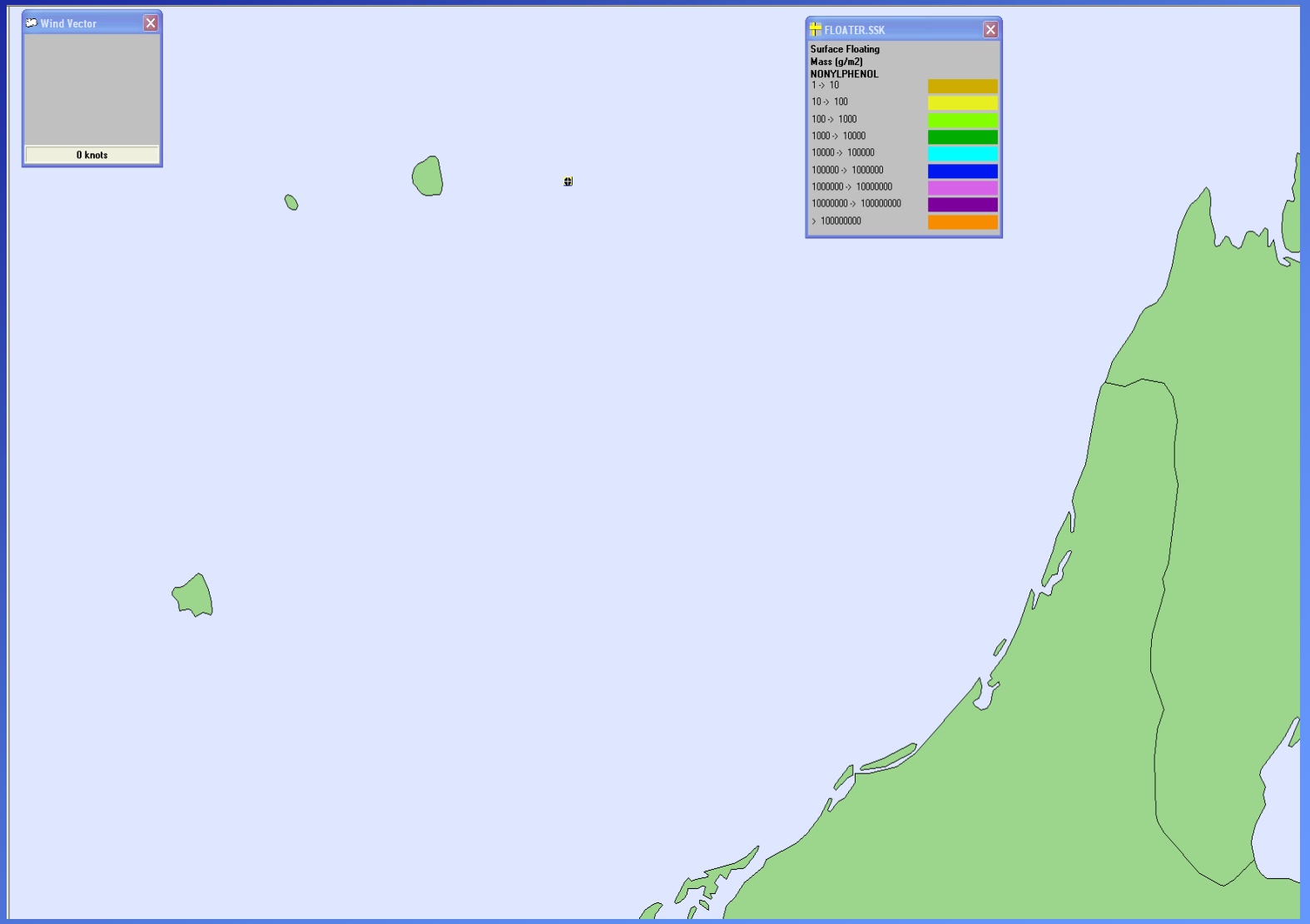
Volatization
Adsorption
Settling
Sediment Mixing
Degradation

Modeling Approach

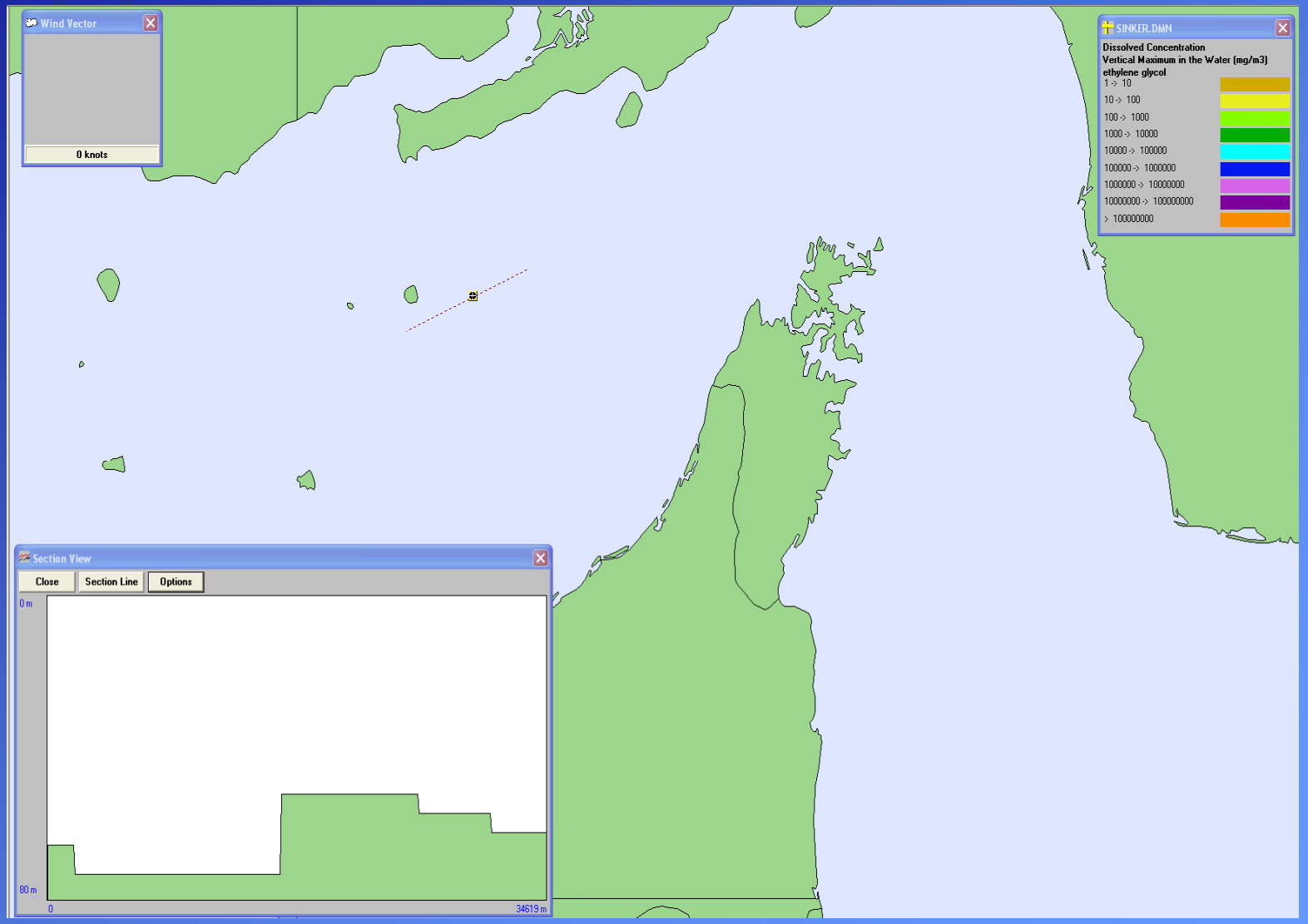
- Three-Dimensional Lagrangian Particle Model
- Each particle has an associated
  - mass (density)
  - size
  - age
- Particle classified by spill conditions and chemical properties
  - on the surface (slick)
  - particulate in the water column
  - dissolved in the water column
  - adsorbed to sediment in the water column
  - on bottom sediments
  - stranded on shoreline
- Particles transported by
  - Currents
  - Winds
  - Natural Dispersion
  - Stokes settling



Floater Example

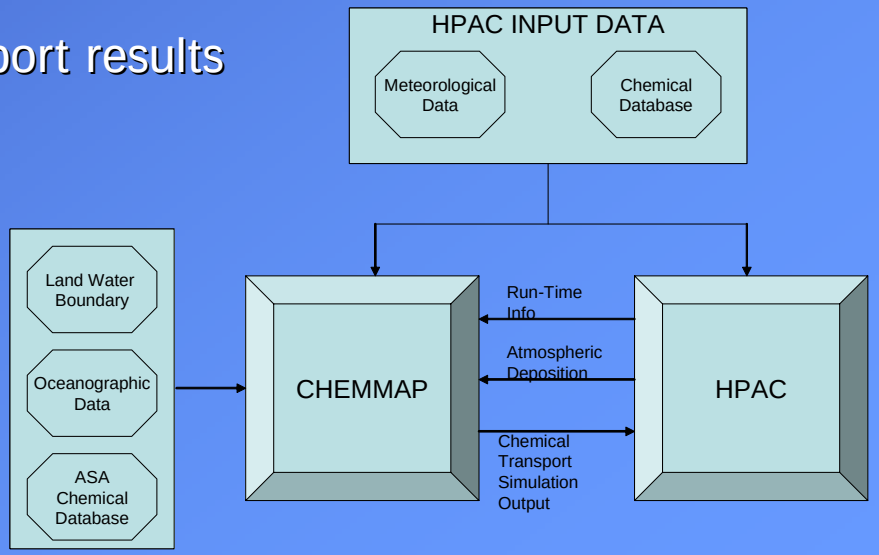


Dissolved Example

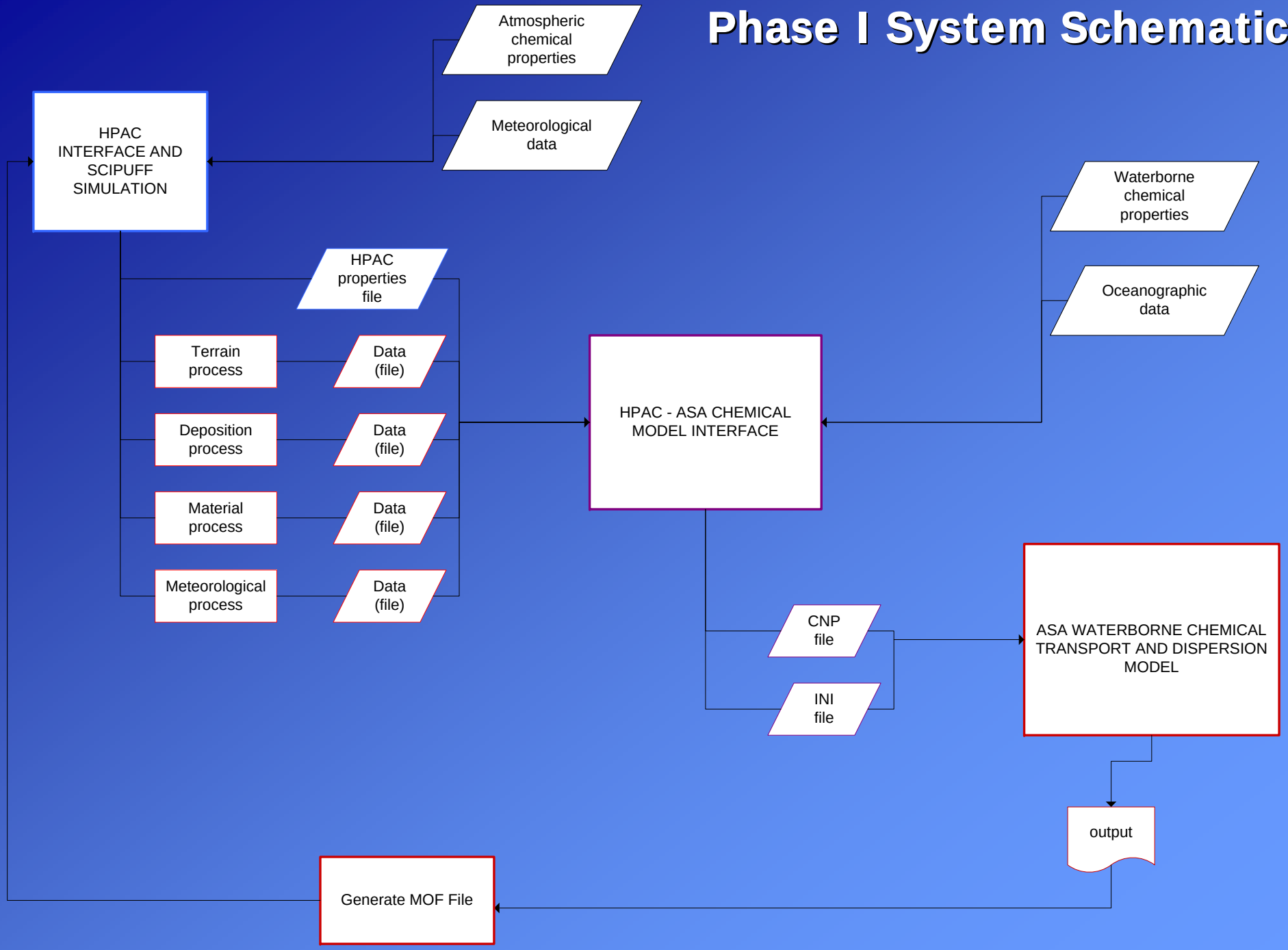


Phase I Integration

- Link HPAC meteorological files to ASA model
- Link HPAC chemical database to ASA model
- Link HPAC run-time files to ASA model
- Utilize HPAC terrain data to develop land-water grids
- Utilize SCIPUFF atmospheric deposition results as waterborne source
- HPAC readable waterborne chemical transport results

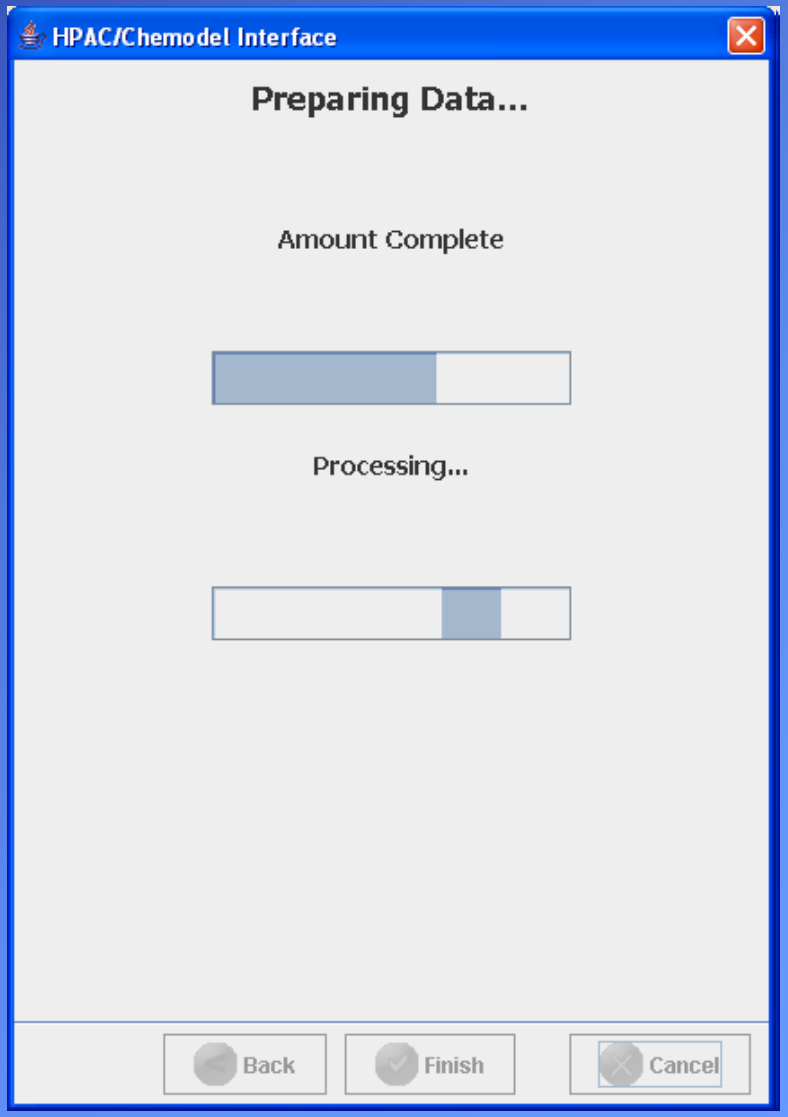


Phase I System Schematic

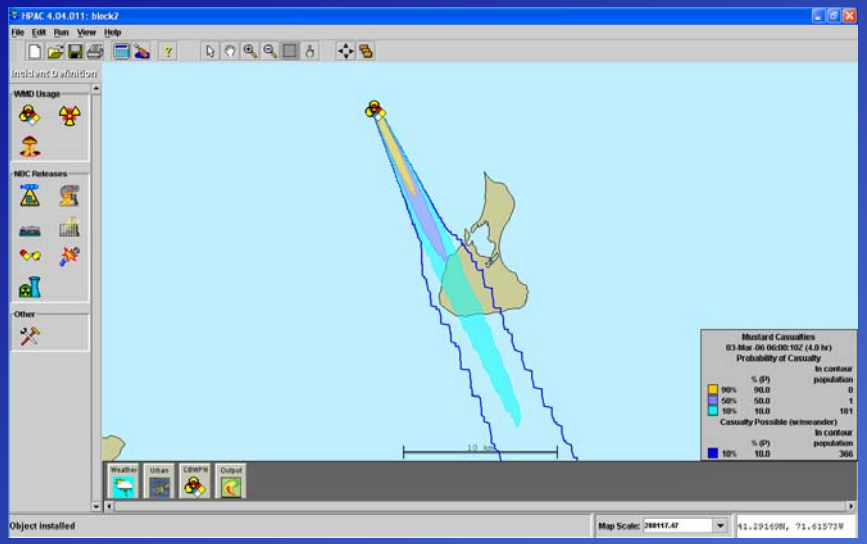


Interface

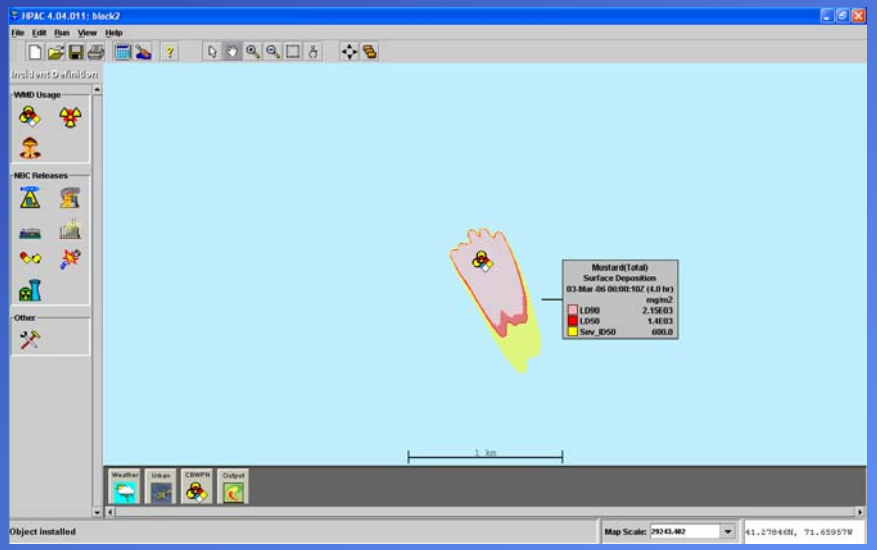
- Simplified wizard approach
- JAVA based interface and algorithms
- Consistent with HPAC development philosophy
  - Design patterns
  - Cross platform utilization
  - Re-using existing HPAC classes where possible



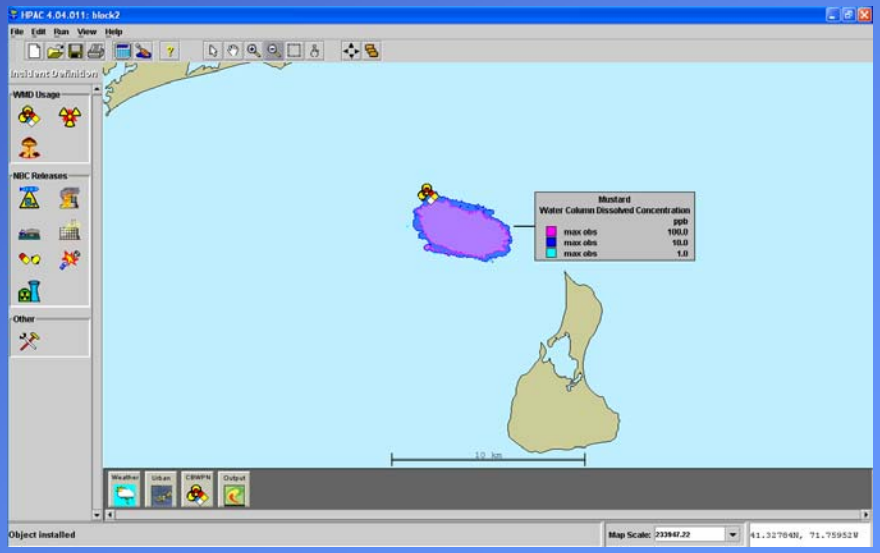
HPAC Atmospheric Results



HPAC Deposition Results



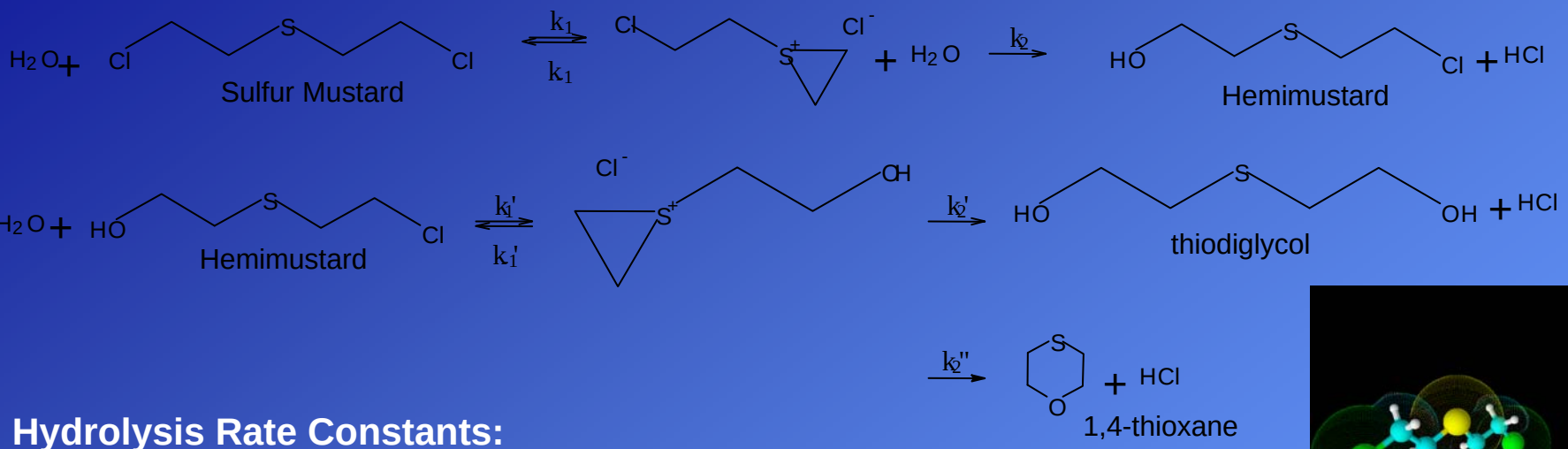
HPAC Waterborne Results

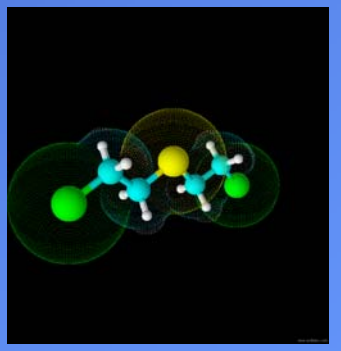


Phase II Objectives

- Investigate integration of model into JEM architecture
- Expand model's I/O architecture accommodate passing evaporated waterborne mass to SCIPUFF
- Develop analytical summary of traditional and thickened weaponized chemical agents fate and kinetics
  - Tabun
  - Sarin
  - Soman
  - Cyclosarin
  - VX
  - Distilled Sulfur Mustard
- Develop and incorporate numerical algorithms based upon analytical summary
- Develop expanded chemical agent database
- Develop advanced numerical algorithms to simplify operational user inputs
  - Adaptive time step
  - Adaptive gridding
  - Smart stochastic modeling

Mustard Kinetics





Hydrolysis Rate Constants:

Temperature	Fresh Water	Sea Water
(°C)	k_1 (min^{-1})	k_1 (min^{-1})
5	0.0124	0.0040
15	0.0390	0.0141
25	0.155	0.046

- In quiescent conditions, high concentrations of thiodiglycol result in the formation of stable sulfonium salts.
- These salts encase the remaining sulfur mustard preventing further dissolution and hydrolysis. If flow conditions remain low-energy, crusted mustard nodules can remain toxic for many years (<5).

QUESTIONS?