Scientific workshops for Interspill 2012 - Understanding Chemicals:

Evaluating Spill Consequences – Use of Modeling

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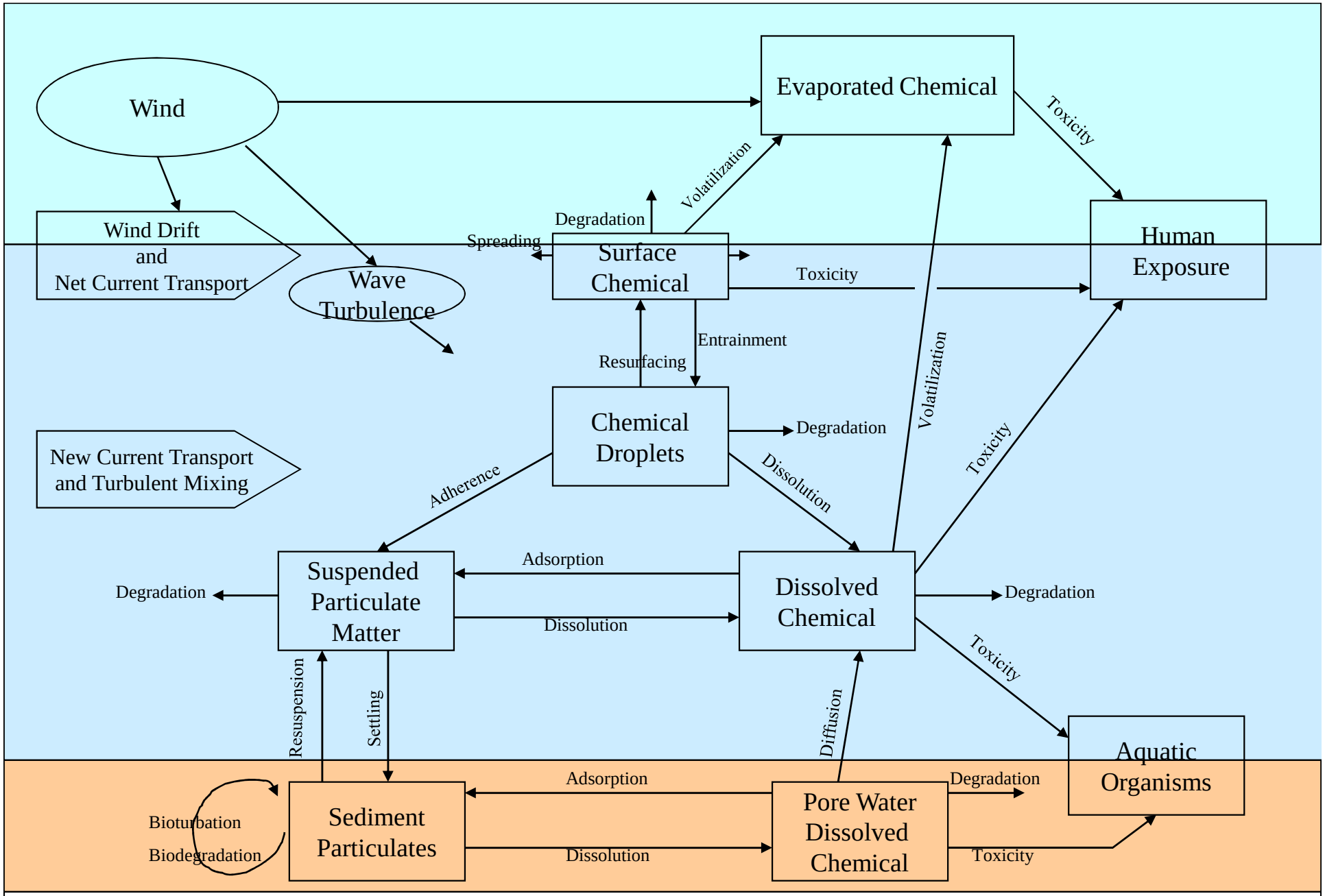
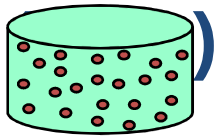
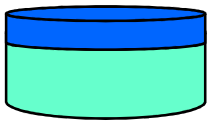
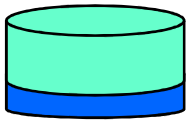


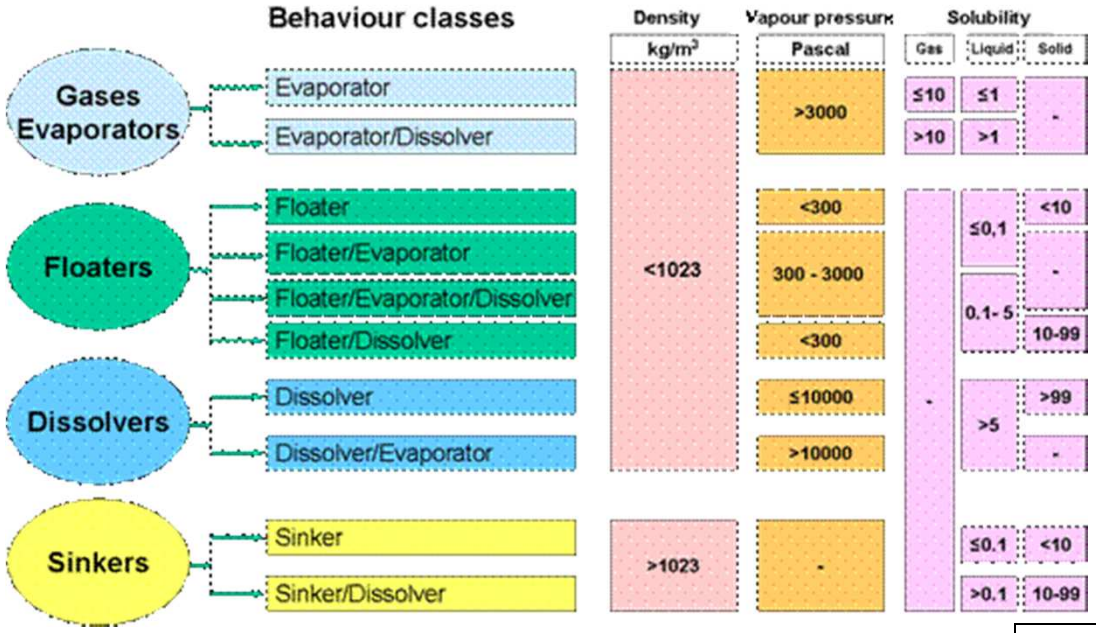
Model of Chemical Processes in Open Waters

Planning for an Emergency

- Chemical Spill Modeling – Uses for Incident Response:
  - Contingency Plans: Use stochastic modeling (analysis using 10 + years of current and wind data)
  - Drills/training and spill events: Deterministic (trajectory & fates) modeling using real-time environmental data
- Environmental Conditions – Important Data:
  - Water circulation: Contamination primarily to aquatic organisms
  - Wind and air turbulence: Affects air concentrations → human exposure
- Biological Impact Analysis
  - Identify density and types of aquatic organisms for areas of concern
  - Toxicity data/thresholds of concern for chemical(s) spilled
- Simplifying the Problem:
  - Thousands of chemicals could be spilled
  - Classification of chemicals based on physical properties (density, solubility, vapor pressure, LogKow) – Bonn Agreement

Density Relative to Water (g/cm^3)	Solubility 	Volatility – vapor pressure
Floater:  $\rho < 1.0$	Highly soluble: > 1000	Highly volatile: $> 10^{-3}$ atm
Neutral: $1.01 < \rho < 1.03$	Soluble: 100 - 1000	Semi-volatile: 10^{-7} - 10^{-3} atm
Sinker:  $\rho > 1.03$	Semi-soluble: 1 - 100	Non-volatile: $< 10^{-7}$ atm
	Insoluble: < 1	

Bonn Agreement - Classification



Potential hazards	Behaviour category *	Human health	Marine environment
Toxicity by inhalation	G/E/F	X	
Explosiveness	G/E	X	
Flammability	G/E/F	X	
Radioactivity	G/E/F/D/S	X	X
Corrosiveness	G/E/F/D/S	X	X
Carcinogenicity	G/E/F/D/S	X	X
Aquatic toxicity	D/S		X
Bioaccumulation	D/S		X
Persistence	D/S		X

*G = Gases; E = Evaporators; F = Floaters; D = Dissolvers and S = Sinkers

http://www.bonnagreement.org/eng/html/counter-pollution_manual/Chapter26_hazardous%20materials.htm

Tasks During Emergency Response

- Modeling can assist in field sampling and response activities
- Collect environmental data for input to spill model
  - Use of real-time data and models
- Perform spill forecasts; update over time
- Determine range of potential dispersion outputs:
  - Review multiple wind and hydrodynamic models (consensus modeling)
  - Vary dispersion coefficients to bound problem
- Take water column samples to calibrate dispersion calculations
- Sample aquatic organisms (for evaluation of impacts)