# Integrated Modeling: A New Approach to Improved Spill Response Modeling

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I. Trajectory models II. Coagulation models

## Overall Themes

- Not one size fits all—scale dominates the choice of 'best' model
- Tension between development and practicality
- Moore's law extended



Moore's Law

### Not one size fits all-scale dominates

0-12 hours post-spill

- Oil Slick Location Spreading Drifting
- Oil Slick Mass Loss and Compositional Changes Evaporation Dispersion Emulsification
- Toxicity
  acute oiling

## Not one size fits all-scale dominates

12 hours – few days post-spill

- Oil Slick Location
  Drifting
  Interaction with shoreline
- Oil Slick Mass Loss and Compositional Changes Dispersion Emulsification/vertical mixing Dissolution

• Toxicity acute toxicity of mixture Not one size fits all-scale dominates

Days to months to years post-spill

- Oil Slick Location
  Remobilization from oiled shoreline
- Oil Slick Mass Loss and Compositional Changes Reaction/Biolysis Coagulation/Sinking Tar Ball Formation
- Toxicity

chronic toxicity of weathered mixtures altered bioavailability altered habitats, trophic structure, *etc.*  Part I. Trajectory Models On-Site Hydrodynamically-Integrated Trajectory (O-SHIT) models

### Operational criteria

- Always up
- Always fast
- Data lean
- Conservative
- Easily understood output

### Examples

### General NOAA Oil Modeling Environment (GNOME; NOAA Hazmat)

### DISPRO

### SIMAP

MEDSLICK (European Commission V Framework Program Energy, Environment and Sustainable Development)

### Strengths

- Operational
- Fast
- Minimal data requirements

### Weaknesses

- Often 1 D in the vertical
- Often no chemical weathering
- Averaged hydrodynamics
- Often poorly documented in accessible peer-reviewed literature

An inherent characteristic (limitation?)

The operational requirements of reliability and constant availability work against rapid assimilation of 'new' information.

The criticism that these models are 'out of date' or 'too simple' must be tempered against their operational requirements.

However, shortening the 'product development cycle', especially to take advantage of faster/cheaper hardware, is possible.

- Three operational strategies
  - Use current surface winds and tabulated local currents and tides to predict surface flows at the time of the spill
  - Prior to event, model the most-likely currents by running climatologies run through 3-D models
  - Integration of real-time data

### Climatology-driven scenario runs



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# Current data assimilation modelling for oil spill contingency planning

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Copeland and Thiam-Yew (2006)

- Brunei shelf sea (375 x 100 km)
- 3 ADCP current profilers and met. towers deployed for 1 year



- 209 'typical flow fields' identified were used as the 'library' of hydrodynamic conditions encountered (5.4 days on a 1.7 GHz P4!)
- Year-long simulations of a variety of spills run to generate probability of land-fall



Fig. 7. Landfall occurrences in parts per thousand of total number of 'surviving' particles.

# Part I. Trajectory Models: Integration of real time data

- Motivation: More accurate trajectories based on 'now-casting' with near-real time observations
  - Meteorology
  - Drifter deployments
  - Current profilers
    - Deployed in response to spill
    - Long-term deployments in critical areas
- Challenges: getting the real time stuff to talk to the models during a spill (hurricanes, etc.)

Tracking and Predicting the Atmospheric Dispersion of Hazardous Material Releases: Implications for Homeland Security

> Committee on the Atmospheric Dispersion of Hazardous Material Releases, National Research Council

ISBN: 0-309-08926-3, 114 pages (2003)

# Findings from NRC 2003

- ... (I)t often is difficult to obtain the data from multiple observational arrays, especially in real time.
- A comprehensive survey of the capabilities and limitations of existing observational networks should be conducted, followed by action to improve these networks and access to them, especially around more vulnerable areas.
- Mobile observational platforms can provide valuable information and fulfill multiple needs in the first minutes to hours after a hazardous release.

# Findings from NRC 2003



"...(U)tilize ... instrumentation for other applications (e.g., to enhance air pollution monitoring, optimize agricultural practices, aid in severe storm forecasting and highway network safety), thus sharing the costs and ensuring that the array will be continuously used, maintained, evaluated, and quality controlled." (NRC 2003)



### Chesapeake Bay Operational Forecast System (CBOFS)

"It is necessary to learn how to more effectively assimilate into models an appropriate range of meteorological data ... from observing systems..., especially as the quality and availability of these data increase." (NRC, 2003)



NOAA Air Resources Laboratory

### Motivation

- Entrainment of oil below surface
- Colloidal-sized droplets
  buffer dissolved
  hydrocarbon concentrations
- Coagulation with aquatic particles drives oil settling and controls water column residence times
- Size and surface properties influence bioavailability and reactivity



Sterling *et al.* (2003) Environ. Sci. Technol. 37,4429-4434

### Physical characteristics of flocs

- Lower settling velocity
- Lower bulk density
- Higher contact area (porosity)



http://www.water-technology.net/contractor\_images/cu\_water/flocke.jpg

Laser In-Situ Scattering Transmissometry (LISST)



Schneider and Baker, submitted



### Coagulation Kinetics

$$\frac{dn}{dt} = -\alpha\beta n^2$$

$$\beta_{Brownian\_motion} = \frac{2}{3} \frac{kT}{\mu} \frac{(D_i + D_j)^2}{D_i D_j}$$

$$\beta_{different\_velocity;i\_and\_j} = \pi \left( D_i + D_j \right)^2 \left| w_{s,i} - w_{s,j} \right|$$

$$\beta_{shear\_stress;i\_and\_j} = \frac{4}{3} \left(\frac{\varepsilon}{\nu}\right)^{0.5} \left(D_i + D_j\right)^3$$

- Chang and Baker estuarine coagulation model
  - 1000 particle sizes between 2 and 1000 μm
  - Two fundamental particles
    - Diatoms
    - Clay
  - Size-specific porosity, bulk density, organic carbon content, and settling velocity calculated dynamically at each time step



### See also

- Sterling, M.C., Bonner, J.S., Ernest, A.N.S., Page, C.A., Autenrieth, R.L., (2004) Characterizing aquatic sediment–oil aggregates using in situ instruments. Mar. Pollut. Bull. 48, 533–542.
- Sterling, M.C., Bonner, J.S., Ernest, A.N.S., Page, C.A., Autenrieth, R.L., (2005) Application of fractal flocculation and vertical transport model to aquatic sol–sediment systems. Water Research 39,1818–1830.
- Hill, P. S., A. Khelifa and K. Lee (2002). "Time scale for oil droplet stabilization by mineral particles in turbulent suspensions." Spill Science & Technology Bulletin 8(1): 73-81.
- Khelifa, A., P. Stoffyn-Egli, P. S. Hill and K. Lee (2002). "Characteristics of oil droplets stabilized by mineral particles: Effects of oil type and temperature." Spill Science & Technology Bulletin 8(1): 19-30.
- Khelifa, A., P. Stoffyn-Egli, P. S. Hill and K. Lee (2005). "Effects of salinity and clay type on oil-mineral aggregation." Marine Environmental Research 59(3): 235-254.

# Final Thoughts

### 0-12 hours post-spill

- Early weathering (volatilization/evaporation)
- Subsurface transport ( $\rho_{oil} > \rho_{seawater}$ )
- Real-time data

### 12 hours – few days post-spill

- Conversion to small droplets
- Coagulation
- Acute toxicity to sensitive targets

# Days to months to years post-spill Bioavailability!