Comprehensive and Fully Integrated Research Program

SERF

(Shoreline Environmental Research Facility)

Texas A&M University

Temitope O. Ojo
Asst. Research Scientist
James Bonner
Director

Introduction

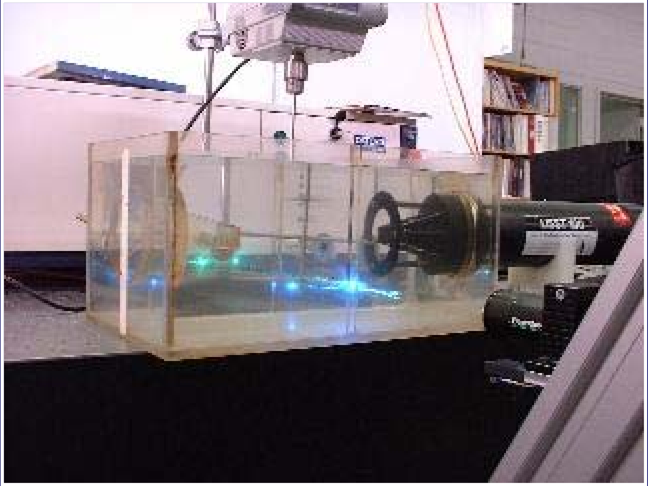
- 3-Dimensional models may be needed to describe plume transport and sediment deposition.
- Droplet coalescence is not typically incorporated in 3-D models
- Process may be important in systems with low dilution rates or large volume spills
- Transport Modeling consists of two parts:
  - Particle transport
    - Advection-Dispersion equation
  - Droplet-sediment coagulation
    - Particle Coagulation kinetic equation
      - Based on Smoluchowski's equation
      - Coagulation efficiency functions related to environmental chemical characteristics (pH, ionic strength, dispersant concentration, oil viscosity, etc.)
- Previous Research
  - Vertical transport model was developed and validated for sediment transport (Bonner et al., 1994; Ernest et al., 1995).
  - Batch studies demonstrated that dispersed oil has aggregation behavior similar to that of suspended cohesive sediment (Sterling et al., 2002)

Experimental-Laboratory

- How does chemically-dispersed oil behave when interacting with ambient particles?
- Very pertinent to coastal waters: high levels of silt, plankton and other biological particles, and are more-likely locations for oil spills.
- Oil droplet fate depends on type of ambient particle interaction
- Determining RPM vs. G_m curve
  - Power calculated from measured values

    $P = T\omega$
  - Mean shear velocity G_m calculated from power

    $G_m = (P/\mu V)^{1/2}$



Experimental-Mesoscale

- Tank Characterization
  - Impact of Oscillation Frequency on Dispersion Coefficients & Steady-state eddy distributions
  - Impact of Wave Height on Vertical Dispersion
- Investigating effects of water temperature and wave energy
- Wave Tank Scaling



Wave Tank Scaling

- Testbed = Corpus Christi Bay ---- $Fr_{testbed}$
- Model system = SERF wave tank -Fr_{model}
- Scaling factor
  - *Fr=[inertial force]/[gravity force]$^{0.5}$ = V/(g* L)$^{0.5}$ where g gravity, L is the wave length, V is the velocity or wave celerity*
- Wave length for linear waves
- Wave velocity
- Shear rate
- Power Dissipation

$$L = \frac{gT^2}{2\pi}$$

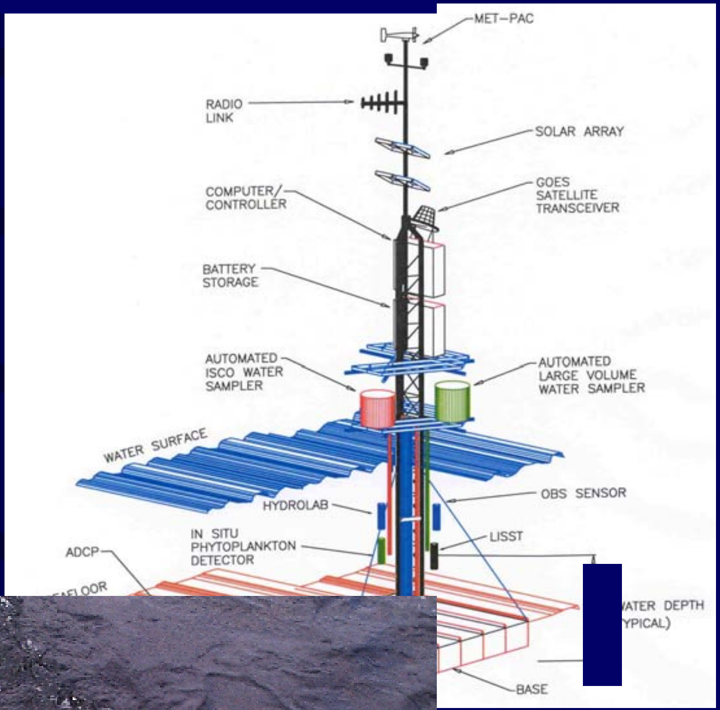
$$V = \frac{L}{T} = \frac{gT^2}{2\pi T} = \frac{gT}{2\pi}$$

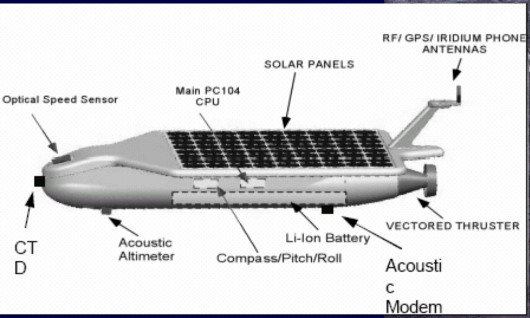
$$G_m = \left(\frac{P}{V\mu}\right)^{0.5}$$

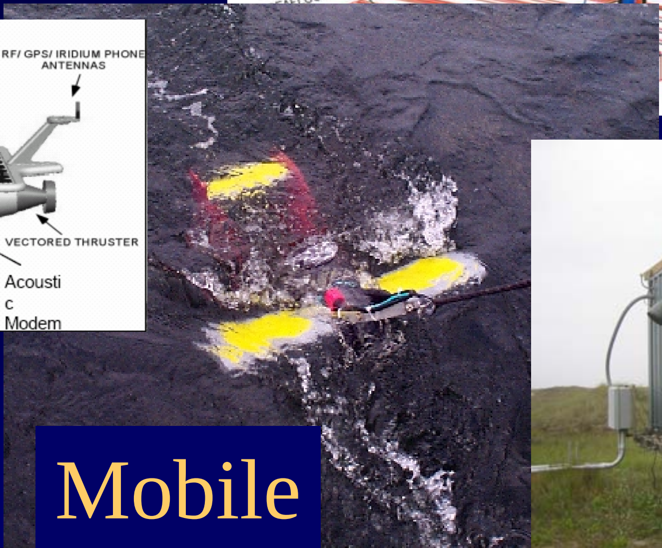
$$P = [\tau o] = G_m^2 V\mu, = E_{area} C_g, = E_{area} C_g (1m_{crestwidth}), \left[\frac{kgm^2}{s^3}\right]$$

Experimental-Field

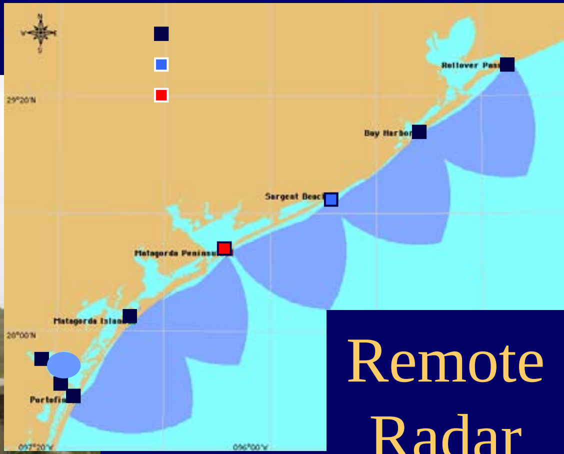
Fixed







Mobile



Remote Radar

Points to Note

- "Colloidal Oil"
  - TGLO Research Group Pioneered This Important Concept
  - Oil-in-Water Studies
    - Dissolved (soluble) component of oil
    - Colloidal component of oil
    - Oil-particle aggregation
- Mean shear rate (vertical dispersion) had the greatest impact on oil resurfacing
- Oil specific gravity and collision efficiency have comparable influence in oil resurfacing.
- Above a threshold value (3 ppm), initial oil concentration became the least significant influential factor impacting dispersed oil resurfacing.
- Mixing Energy
  - $G_m \sim 10^1$, similar to estuarine conditions
- Tracer Study
  - Near uniform mixing occurs between 8-15 min.

Current State of Modeling

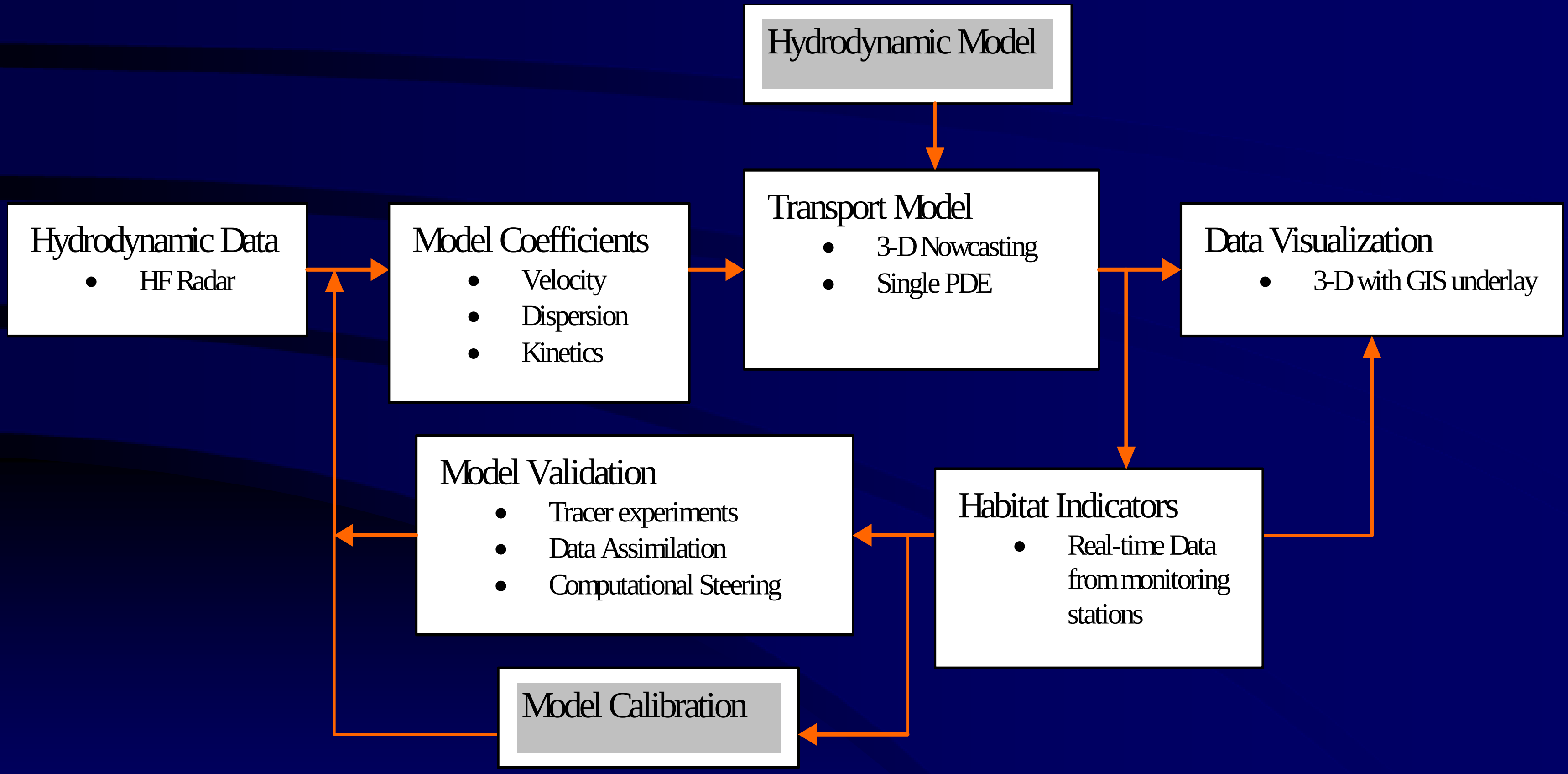
- Fraction of dispersed oil resurfacing is function of vertical dispersion rate and oil coalescence rates.
- Two methods for calculating resuspended fraction
  - Mackay et al. (1980)
  - Delvigne and Sweeney (1988)
- Both methods empirically based
- Single value for dispersion coefficient
  - Determined through dye-tracer experiments
  - Determined using nomograms
- Either method does not allow for spatial-temporal variability
  - Taylor (1921), Batchelor (1950), Ippen (1966), Fisher, List et al. (1979), Tchobanoglous & Shcroeder (1985)

Shear Augmented Diffusion

- Where shear currents are present, shear diffusivity will dominate over turbulent diffusivity Taylor's (1953 and 1954)
  - Enhanced diffusion encountered even in laminar flow
- Extension of this finding to natural systems is subject of ongoing research
- In a shallow wind-driven bay, the velocity gradients that produce shear will be more pronounced in the vertical than in the lateral (horizontal) plane, except near the shore or close to land boundaries)

Modeling Framework

- Grayed out modules not implemented in this scheme



Model Description

- **Rate of change of concentration measured by aggregate sum of gradient of advective flux and gradient of dispersive flux and kinetics**

$$\frac{\partial C_k}{\partial t} = -\frac{\partial (uC_k)}{\partial x} - \frac{\partial (vC_k)}{\partial y} - \frac{\partial (wC_k)}{\partial z} + \frac{\partial}{\partial x}\left[D_x \frac{\partial C_k}{\partial x}\right] + \frac{\partial}{\partial y}\left[D_y \frac{\partial C_k}{\partial y}\right] + \frac{\partial}{\partial z}\left[D_z \frac{\partial C_k}{\partial z}\right] \pm r_k)$$

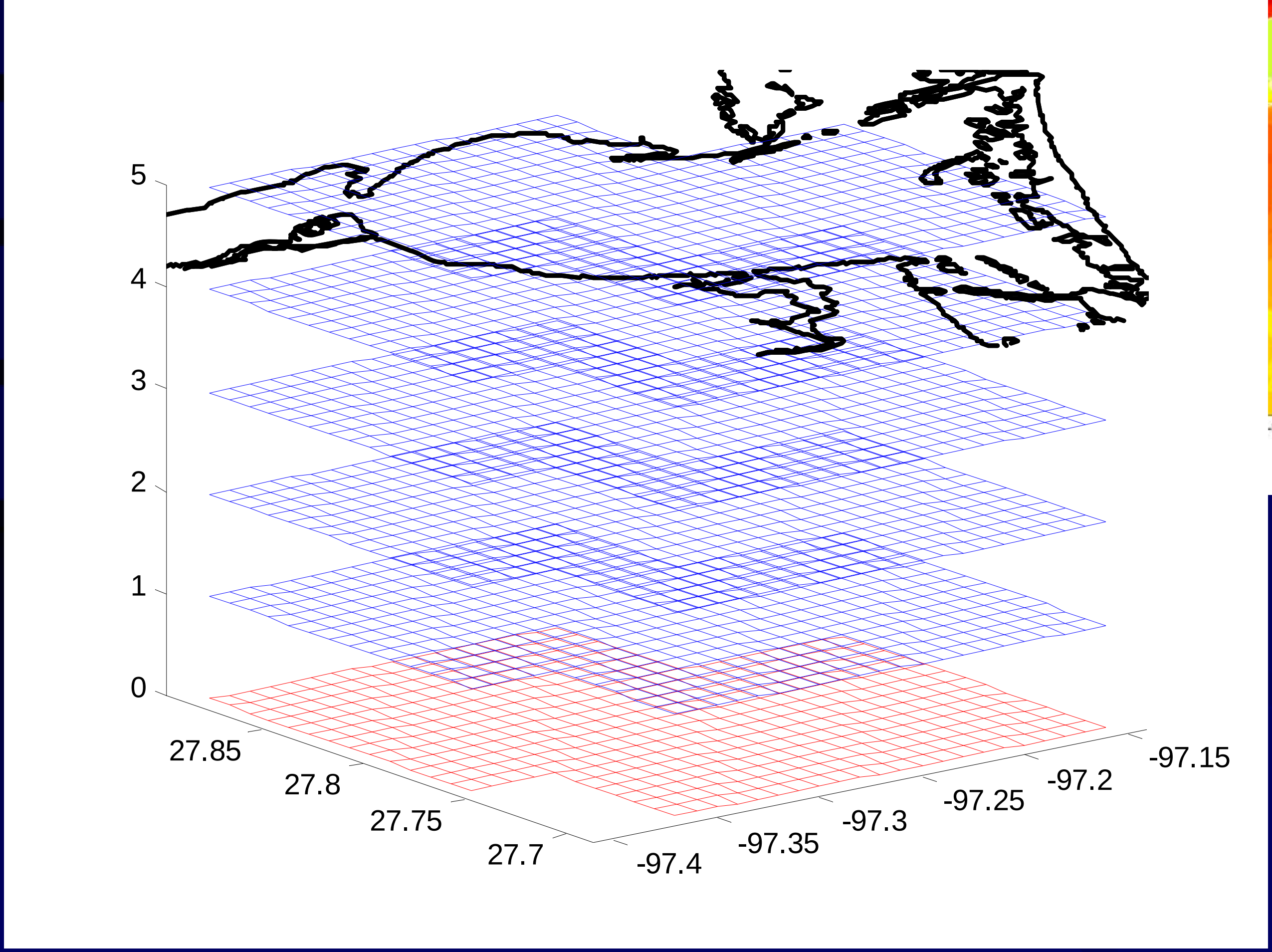
Rate of change of concentration with time = Gradient of Advective flux + Gradient of Dispersive flux + Source/ Sink

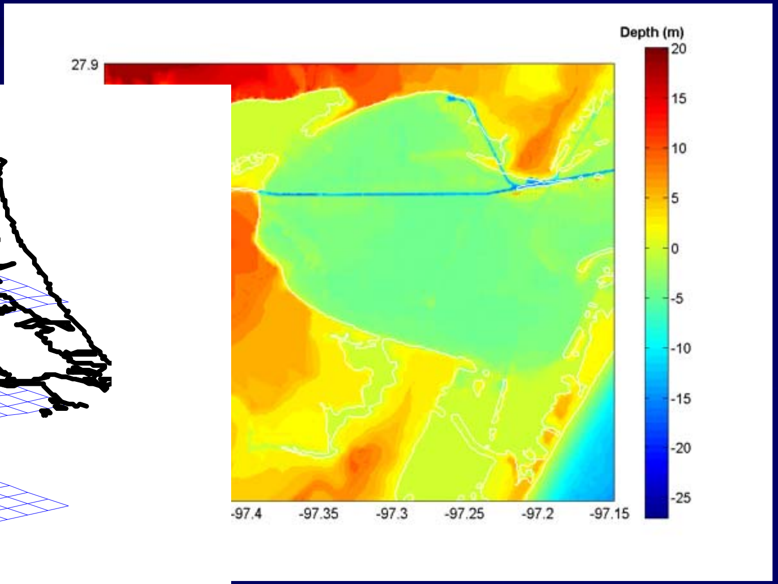
Transport

Kinetics

- **Model coefficients**
  - **Velocity, dispersion, coalescence**
- **Solution provides concentration profile C_k of the k^{th} component**

Computational Grid and Bathymetry





Background Theory - Diffusion

Turbulent Diffusion

$$K_i = \overline{u_i^{'2}} \int_0^t R_i(\tau) d\tau$$

$$K_i = \overline{u_i^{'2}} T_i$$

$$T_i = \int_0^t R_i(\tau) d\tau$$

(Integral time scale of turbulence)

$$R_i(\tau) = \frac{\overline{u_i^{'}(t) u_i^{'}(t+\tau)}}{\overline{u_i^{'}(t)^2}}$$

(Lagrangian autocorrelation Function)

Shear Diffusion

$$K_{xe} = \left(h^2 \overline{u^{'2}} / \overline{K_z} \right) I$$

$$K_{xe} = \overline{u^{'2}} T_c . I$$

$$T_c = h^2 / \overline{K_z}$$

$$I = -\int_0^1 u^{''} \left[\int_0^{z^{'}} \frac{1}{K_z^{'}} \left(\int_0^{z^{'}} u^{''} dz^{'} \right) dz^{'} \right] dz^{'}$$

Depends on time to complete vertical mixing (quasi-steady state) or initialization time, Tn

- **Proportional to characteristic time scale, Tc**
  - **Tn = ϑ.Tc**
- **Typical values of ϑ**
  - **1.0 (Chatwin, 1972)**
  - **0.4 (Fischer, 1968)**
  - **$1/\pi^2$ or 0.1 (Okubo and Carter)**
- **ϑ = 1 equivalent to using full depth for the mixing length**

Background Theory - Coalescence

Advection – Dispersion – Reaction Equation

$$\frac{\partial C_k}{\partial t} = D_z \frac{\partial^2 C_k}{\partial z^2} - w_k \frac{\partial C_k}{\partial z} + r_k$$

Upper Boundary (Partially Absorbtive)

$$D_z = f_{surf} w_i C_k$$

Bottom Boundary (Reflective)

$$\mathrm{D_z} = 0$$

Surfacing Velocity (*Stokes Equation*)

$$v_{s,i} = \frac{(\rho_{oil} - \rho_{water}) d^2 g}{\mu_w}$$

Coalescence Kinetics

$$\frac{\partial C_k}{\partial t} = r_k = \frac{1}{2} \sum_{i+j=k} \alpha\beta(\upsilon_i, \upsilon_j) n_i n_j - \sum_{i=1}^{\infty} \alpha\beta(\upsilon_i, \upsilon_k) n_i n_k$$

Evaluation of Turbulent Diffusivity

- Using computed values of T_L
  - Equation (5) is applied in discretized form to the time-series
  - Current averaging is performed using a sliding window
    - Equivalent to applying a low-pass filter
  - Filter size determined with the aid of spectral analysis on time-series of velocity
- K_i is the product of mean square velocity $\langle u_i^2 \rangle$ and T_L
  - Computed over the same time interval as R_i

Evaluation of Shear Diffusivity

- Determine T_c using K_z from turbulent diffusivity calculations (Eq. 17)
- Obtain vertically averaged square velocity $\langle u_i^2 \rangle$
- Obtain characteristic integral, *I* using discretized form of Eq. 16
  - Values of *I* falls within range recommended (Fischer, 1973); 0.06-0.15
- K_i is product of all three quantities evaluated over time
  - Generates time-series of K_i values

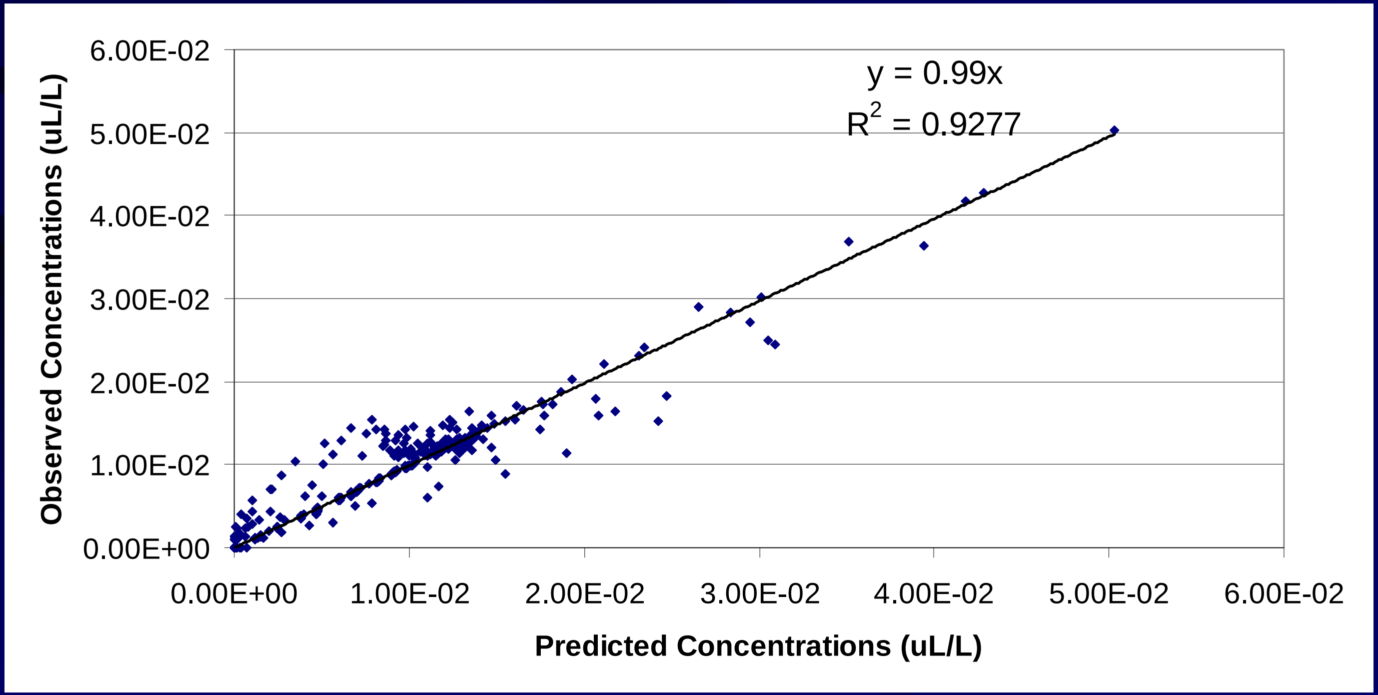
Evaluation of Droplet Coalescence Kinetics

- **Collision Frequency (β)**
  - Depends on Hydrodynamic *Energy*
  - *Energy* characterized using scaling parameter, G_m (mean velocity gradient)
  - Modeled as the sum of collision frequencies due to the Brownian (β_{Br}), shear (β_{Sh}), and differential sedimentation (β_{ds}) mechanisms (Ernest *et al.*, 1995)
  - $\beta(\nu_i,\nu_j)$ and $\beta(\nu_i,\nu_k)$ are the collision frequencies between droplets with volumes of ν_i and ν_j and ν_i and ν_k
- **Collision Efficiency (α)**
  - Depends on droplet interaction forces
  - Repulsion force influenced by *Salinity*
  - fraction of collisions that result in droplet coalescence
  - Based on chemistry; empirically determined
  - $n_{i,j,k}$: particle number concentration in a size interval
  - *i,j* are subscripts designating droplet size class

$$r_k = \frac{1}{2}\sum_{i+j=k} \alpha\beta(\upsilon_i,\upsilon_j) n_i n_j - \sum_{i=1}^{\infty} \alpha\beta(\upsilon_i,\upsilon_k) n_i n_k$$

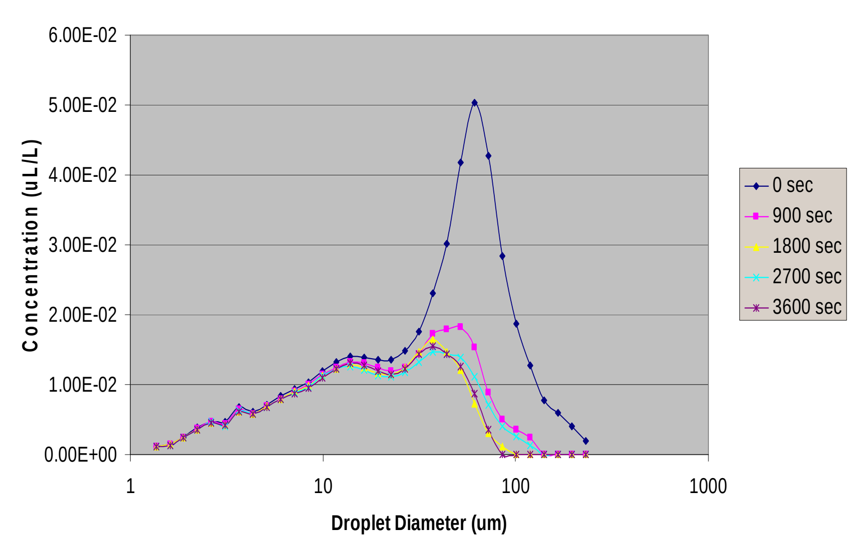
30 0/00, 40 s-1

- Dispersed oil in batch reactor
- All data slides
  - @ $30^{0}/_{00}$, $40 s^{-1}$
  - Predicted $\alpha = 0.89$
  - Time (0-3600 sec)

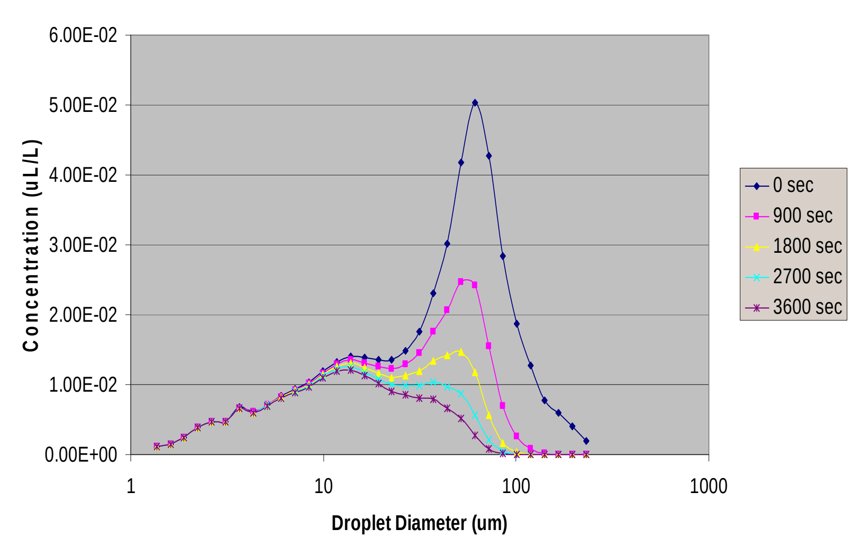


Droplet Distribution

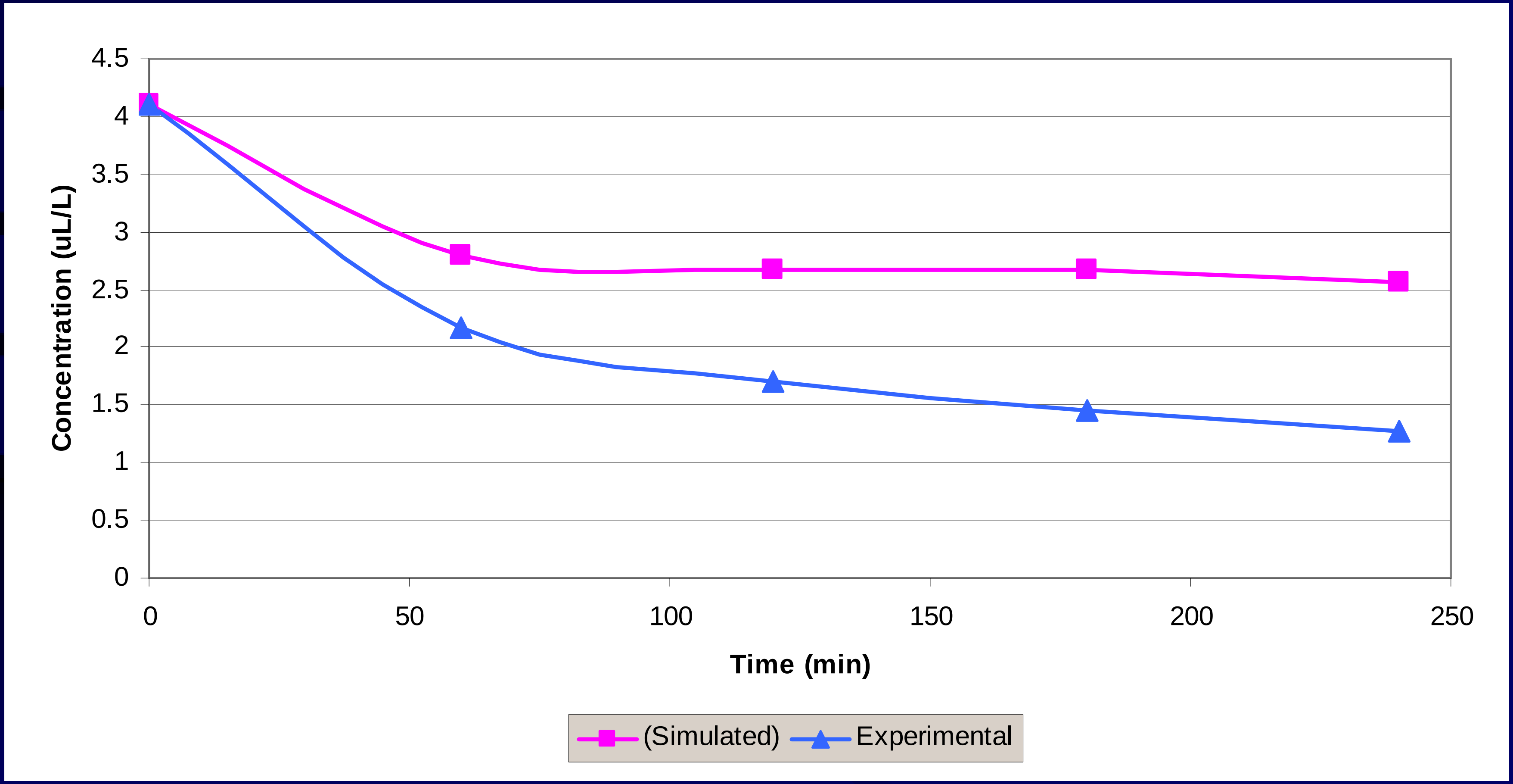
Observed



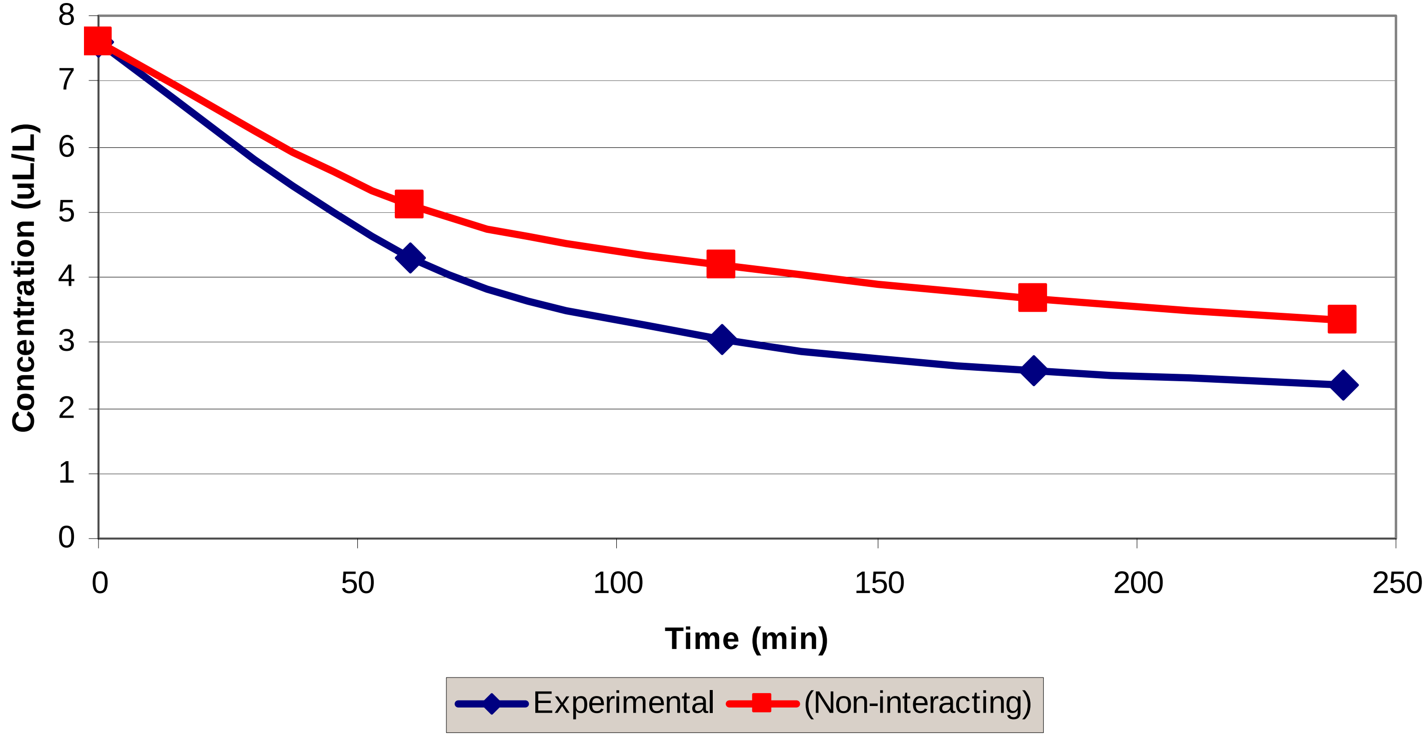
Predicted



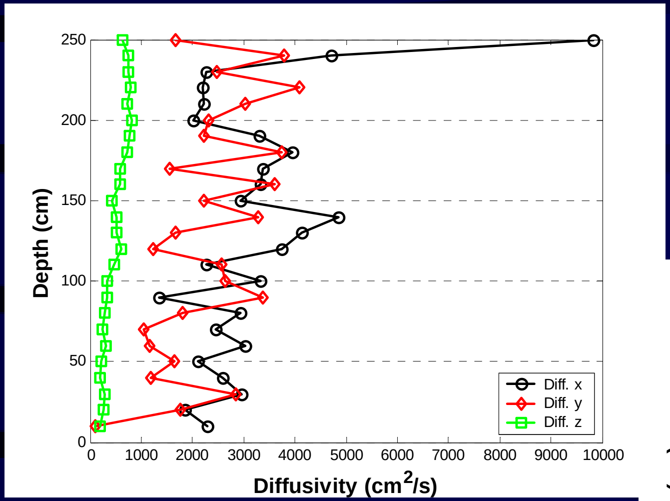
Dispersed Oil Distribution: 30 $^0/_{00}$, 30 s^{-1}



Dispersed Oil Distribution: 10 $^{0}/_{00}$, 30 s^{-1}

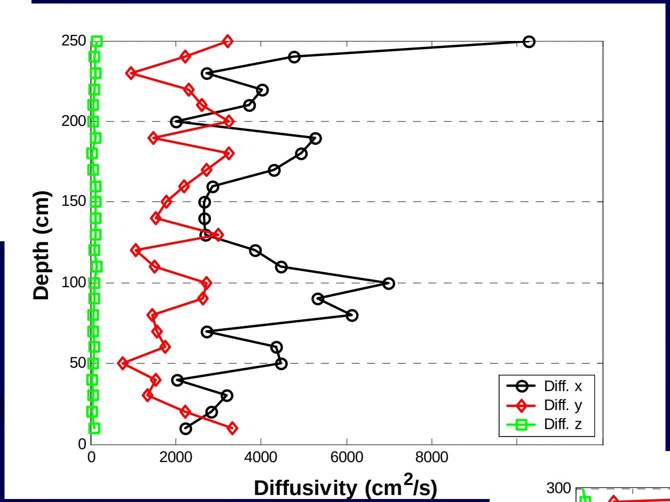


Turbulent Diffusivity vs. Depth

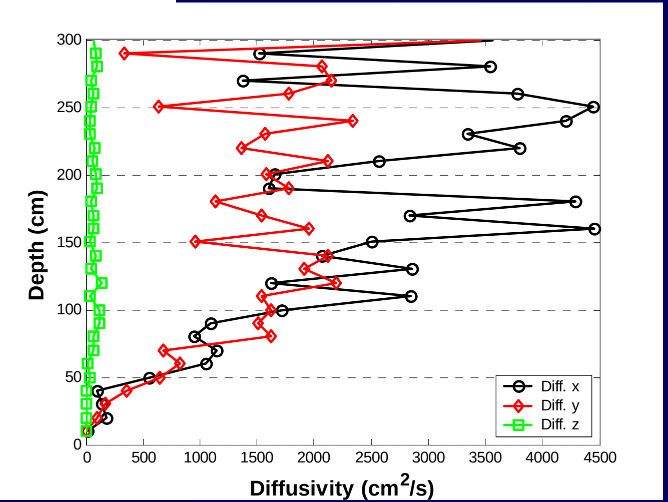


Study 0828_1

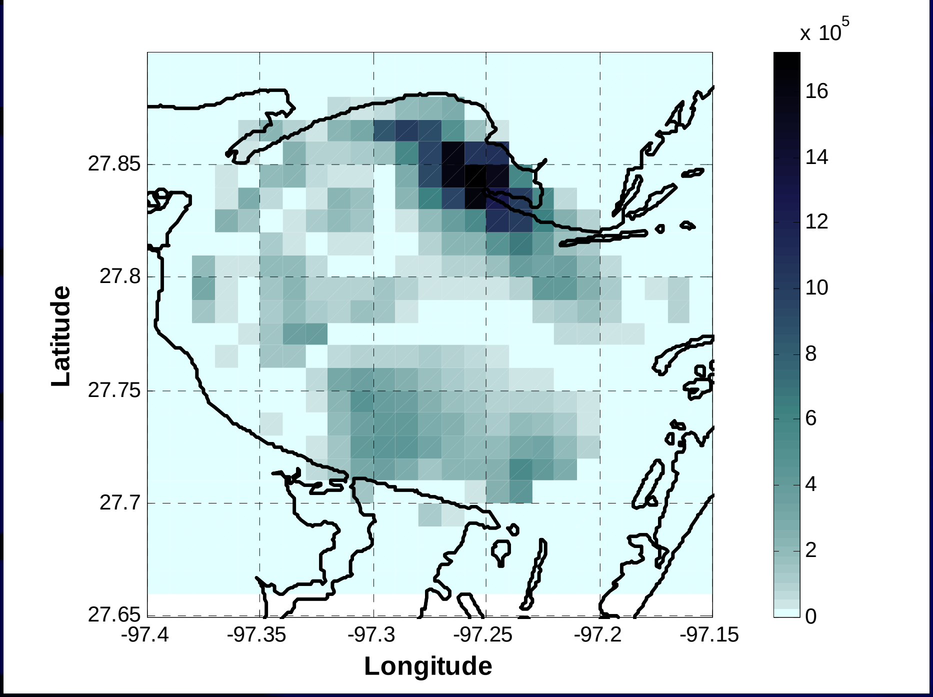
Study 0828_2

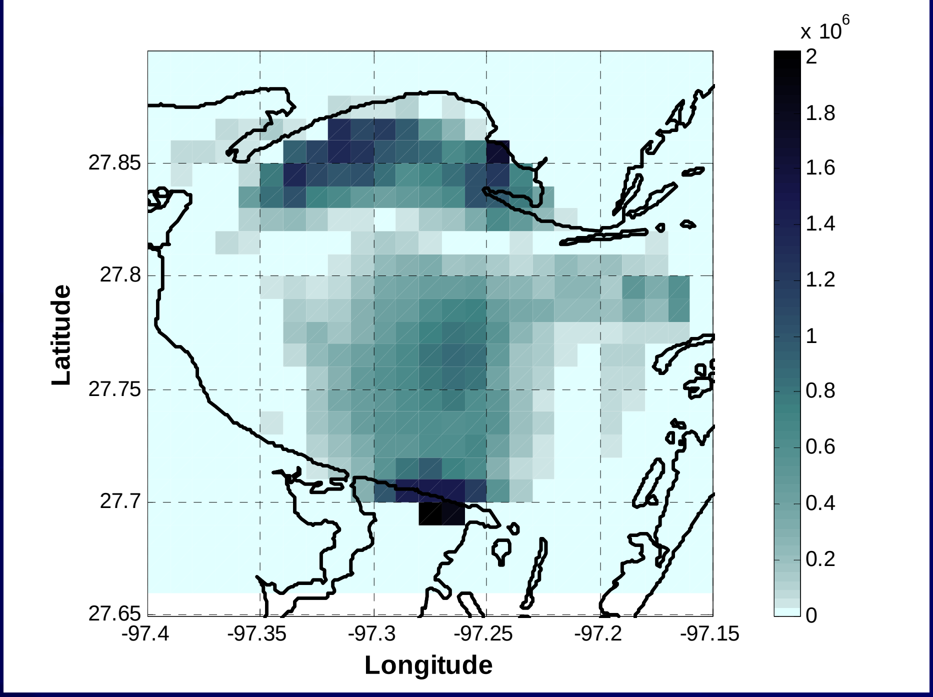


Study 1007



Spatial Distribution of Diffusivity

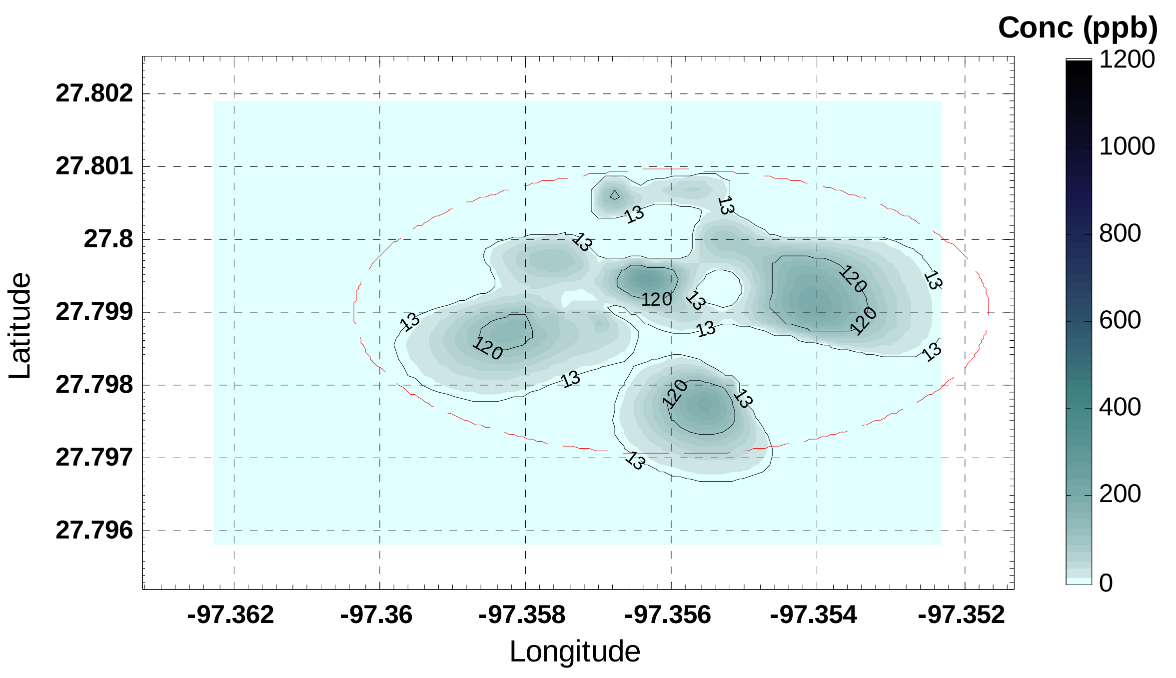




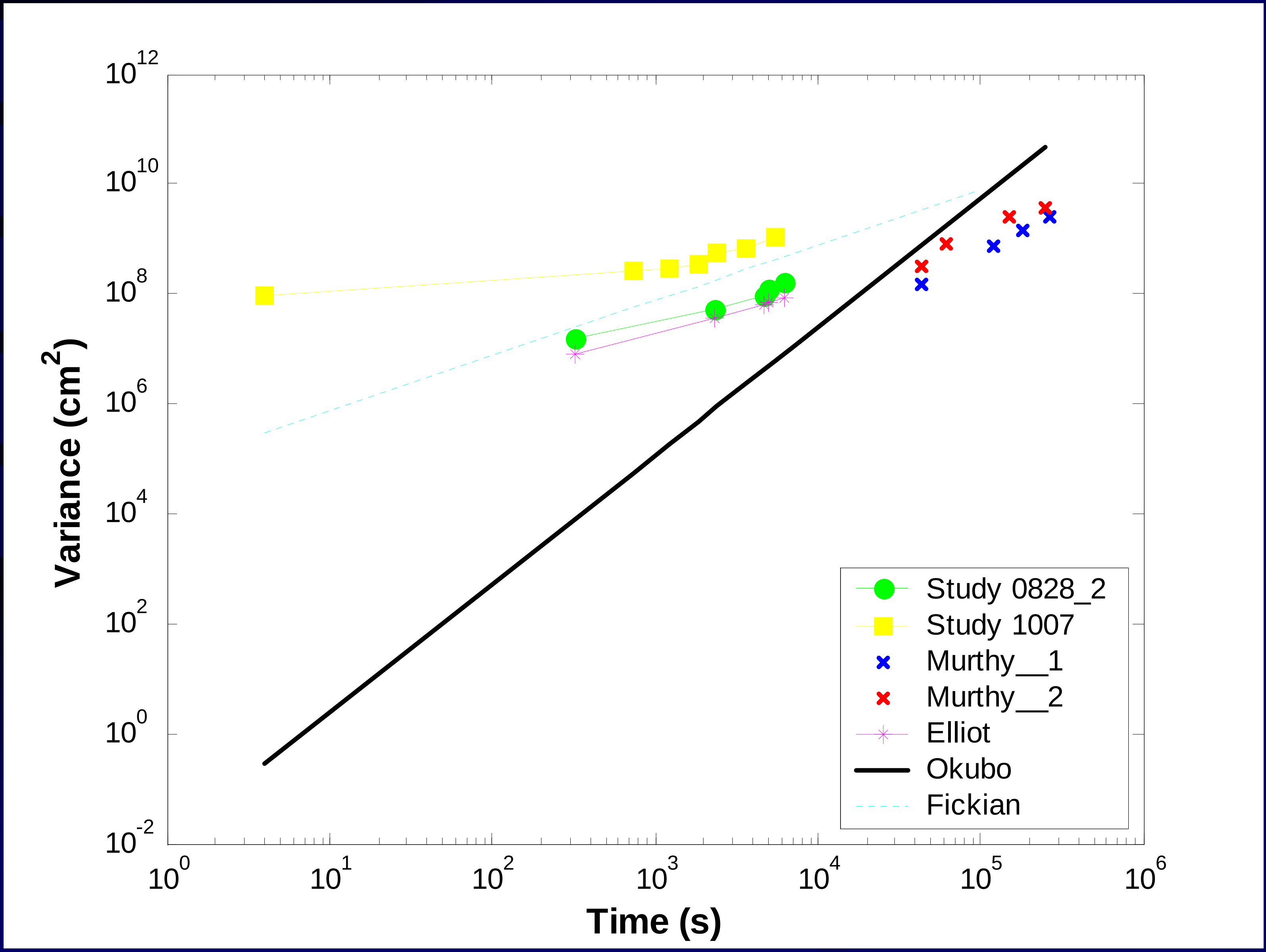
- Diffusivity Values from Hydrodynamic Observations
  - Generates spatially distributed and temporally varying values for ‘dispersion’ when modeling a water body.
  - Uses data from HF radar and acoustic Doppler current profilers (ADCP).
- This concept replaces the use of single value to represent dispersion when modeling a water body.

Dye Patch Characteristics

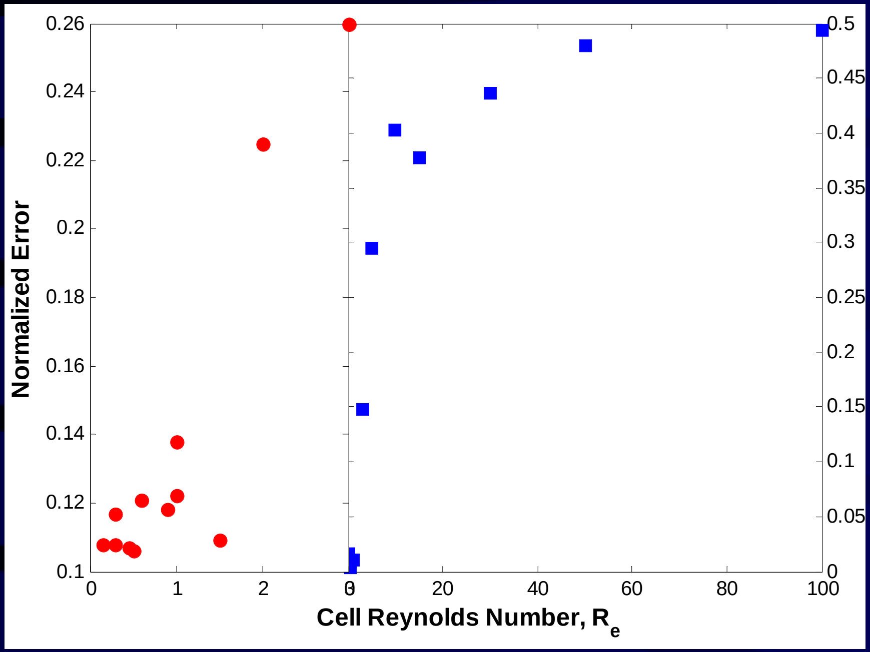
- Computed vs. Observed Spread
- Aspect ratio ??

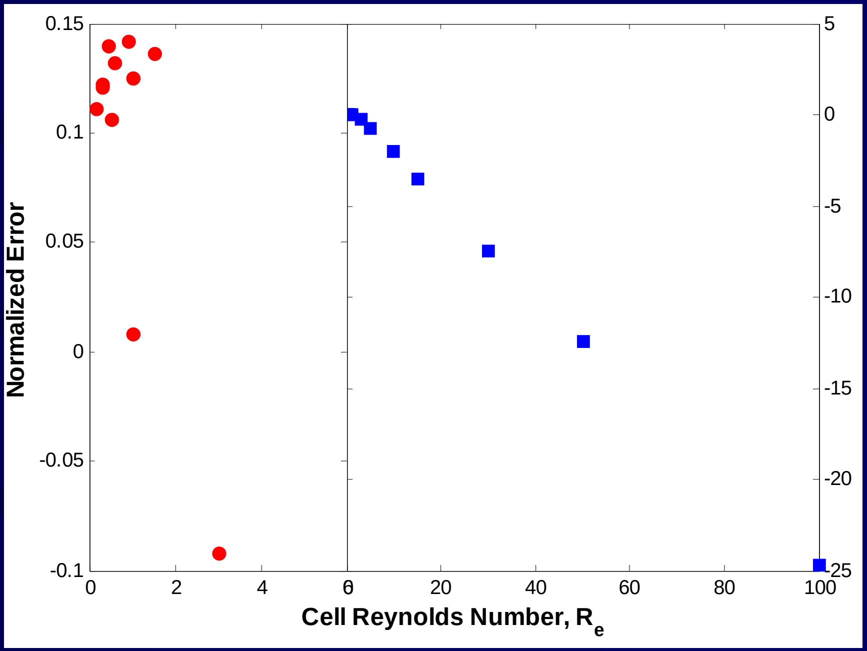


Comparison of Variance Estimates



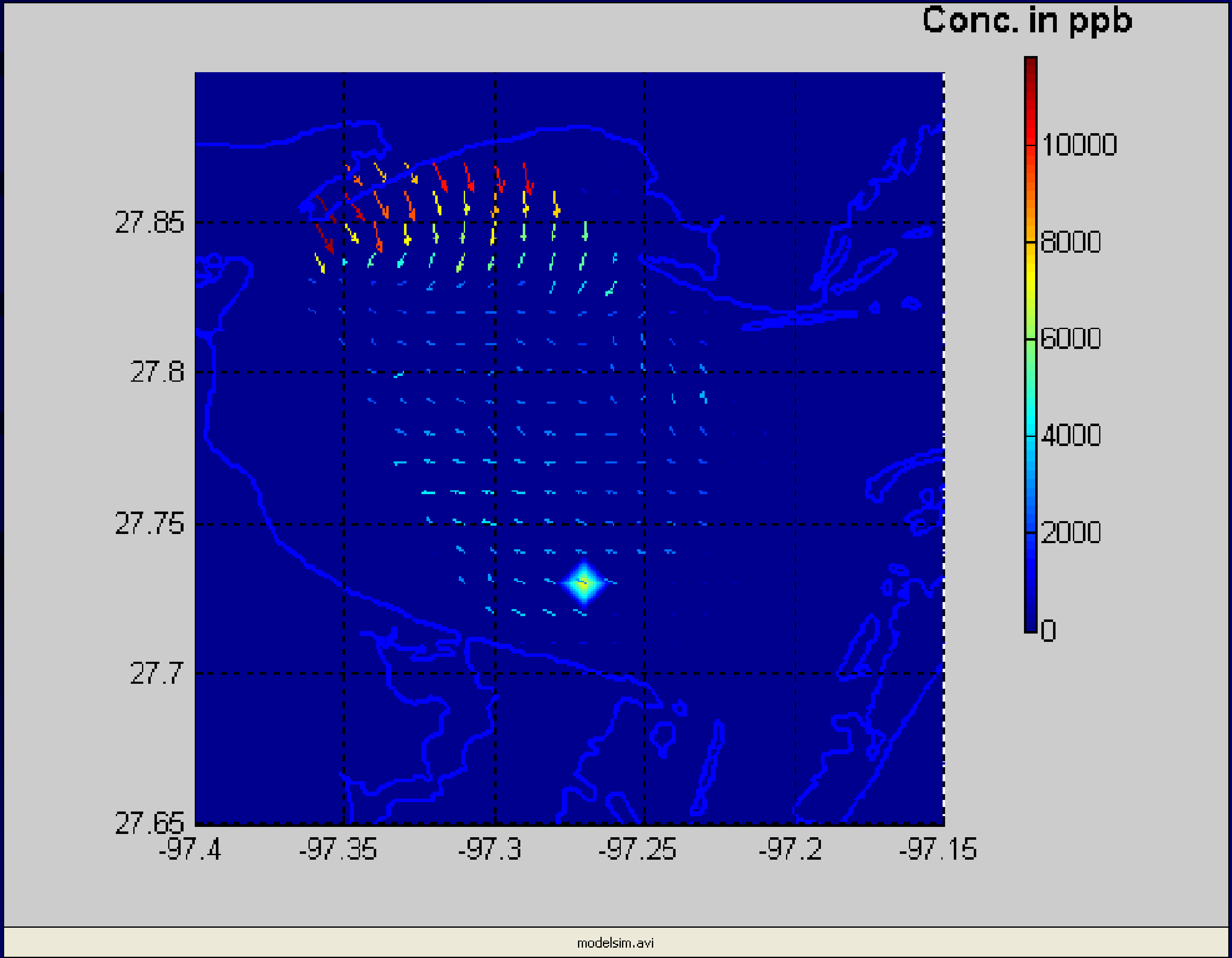
Model Error Analysis





Evolution of Contaminant Plume

From Model Simulation



On-going

Modeling

- Studies conducted
  - Hydrodynamic scaling
    - Transport
      - 2-D
      - 3-D
    - Estimation of dispersion coefficients
    - Shear studies
    - Dye experiments
  - Constituent transport
    - Water quality parameters
    - Dispersed oil
  - Model development

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