Developments in Numerical Modeling of Oil Spills Before & After Deepwater Horizon Spill

MOSSFA Synthesis Workshop I

Texas A&M University at Galveston

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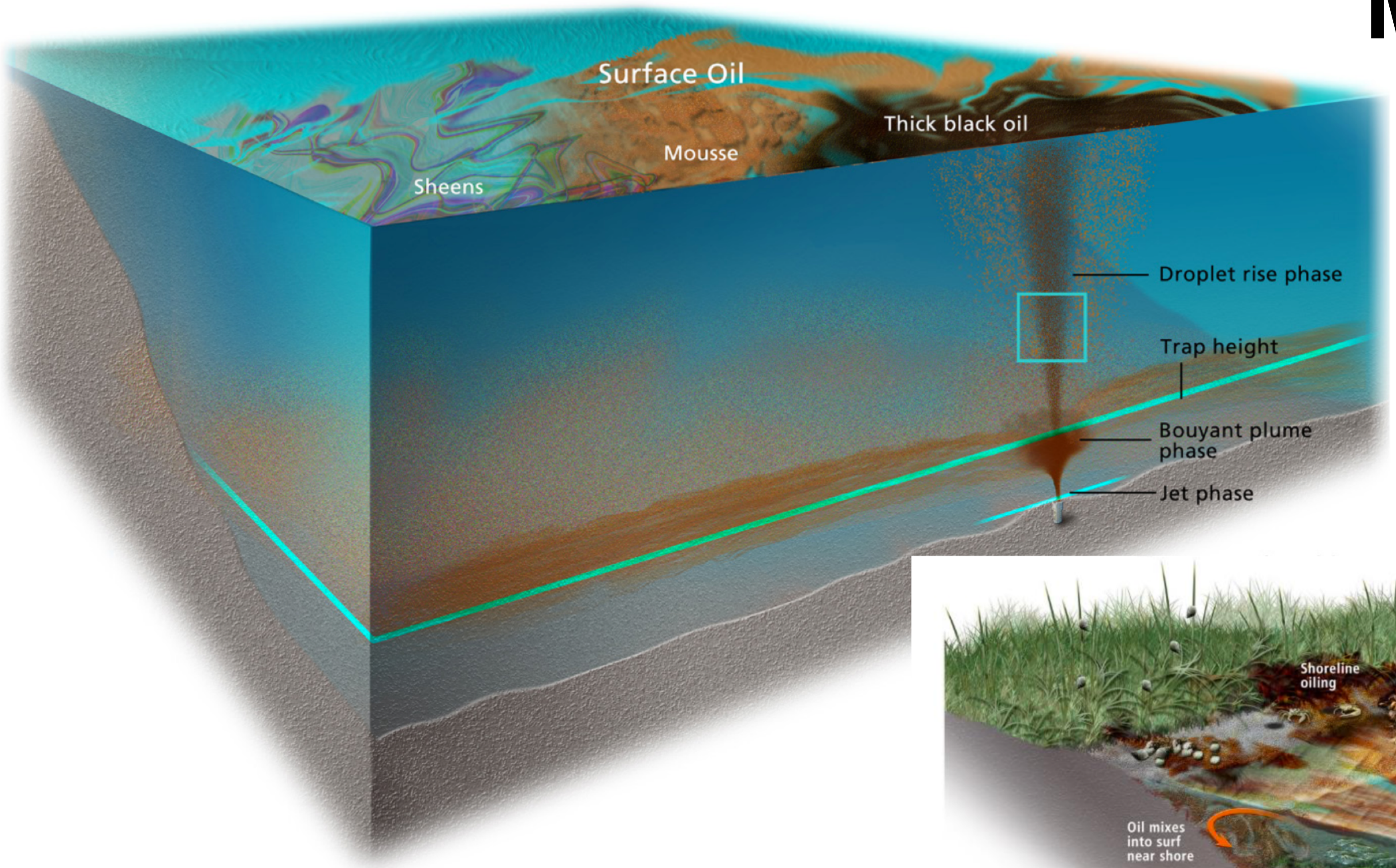
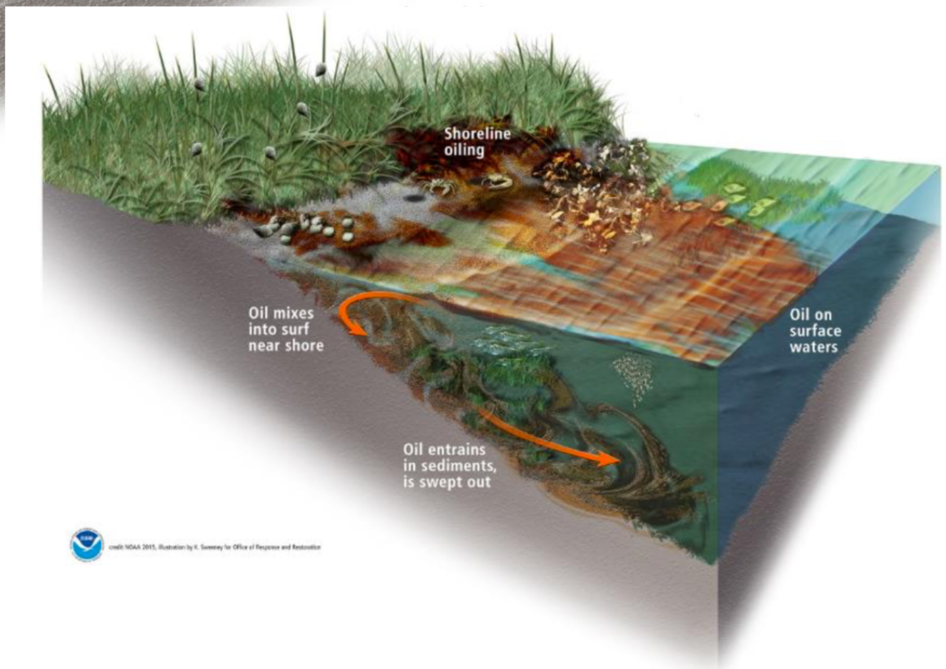
Oil Spill Models

- **CDOG** - Comprehensive Deepwater Oil and Gas Blowout Model at Clarkson University, Potsdam NY by Yapa et al.
- **SIMAP/OILMAP** - Integrated Oil Spill Impact Model System/Oil Spill Model and Response System - Models at RPS Ocean Science (ASA) in Rhode Island by French McCay et al. and Spaulding et al.
- **OSCAR** - Oil Spill Contingency And Response Model at SINTEF Norway by Reed et al. and Johansen et al.
- **GNOME** - General NOAA Operational Modeling Environment - Model at NOAA by Bill Lehr, Chris Barker and CJ Beegle Krause
- **TAMOC** - Texas A&M Oil Spill (Outfalls) Calculator by Socolofsky et al.
- **CMS** - Connectivity Modeling System by Paris et al.
- **LTRANS** - Lagrangian TRANSport model by North et al.
- **BLOSOM** – The National Energy Technology Laboratory (NETL) Blowout and Spill Occurrence Model
- **MOHID** – Water Modeling System - Portugal

Model Description

- Near-Field model
- Far-Field model
- Bubble and droplet break-up model
- Physical, chemical and biological processes of bubbles and droplets
- Interaction with land (coast, sea bottom)



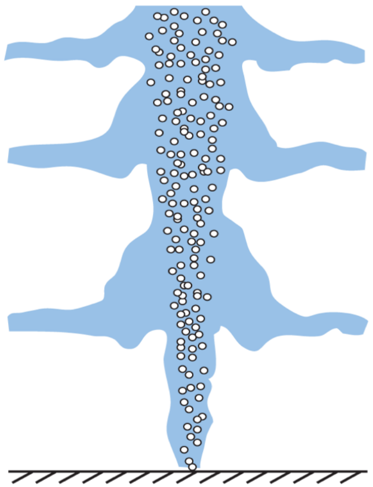


Picture Credits: Kate Sweeny/NOAA

Integral Plume Models

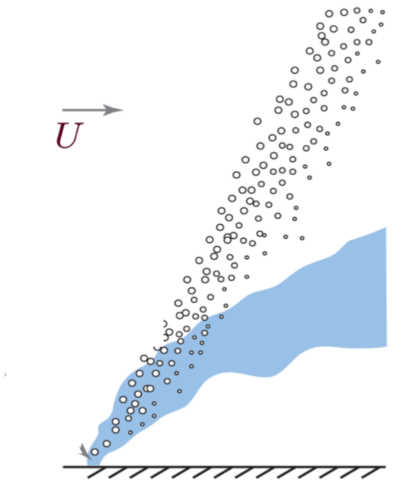
- ➢Implemented in Texas A&M Oil Spill (Outfalls) Calculator.
- ➢Use to simulate single and multiphase plume.
- ➢Use an entrainment hypothesis and top hat velocity profiles.

Stratified Plume Model



Eularian integral model, based on **double plume** model approach for **stratification dominant** environments

Bent Plume Model



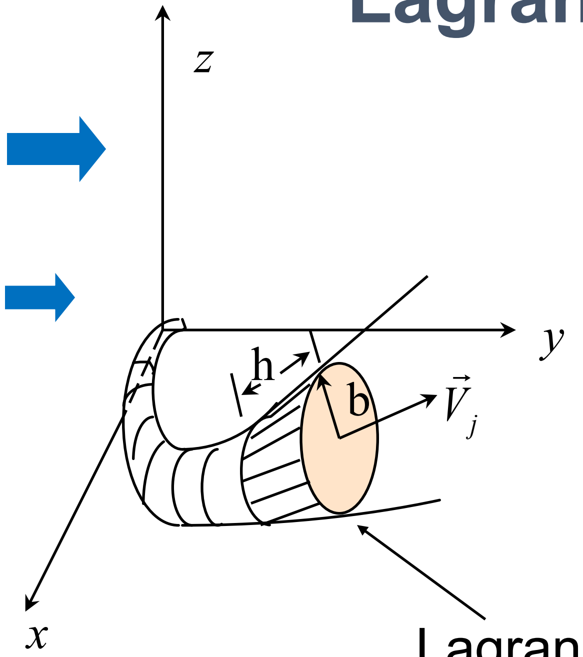
Lagrangian integral model simulates plumes in **cross flow dominant** environments

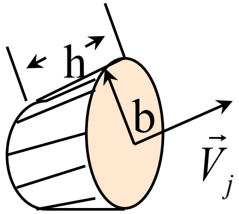
Socolofsky et al. (2008) JHE, Dissanayake et al. (2018) EFM

Plume Dynamic Stage (PDS) – Cross Flow Dominated Plume

Lagrangian Control Volume

Ambient cross flow





Travels with averaged velocity along the plume centerline

Lagrangian Control Element

Velocity, salinity, and temperature - averaged for the cross section

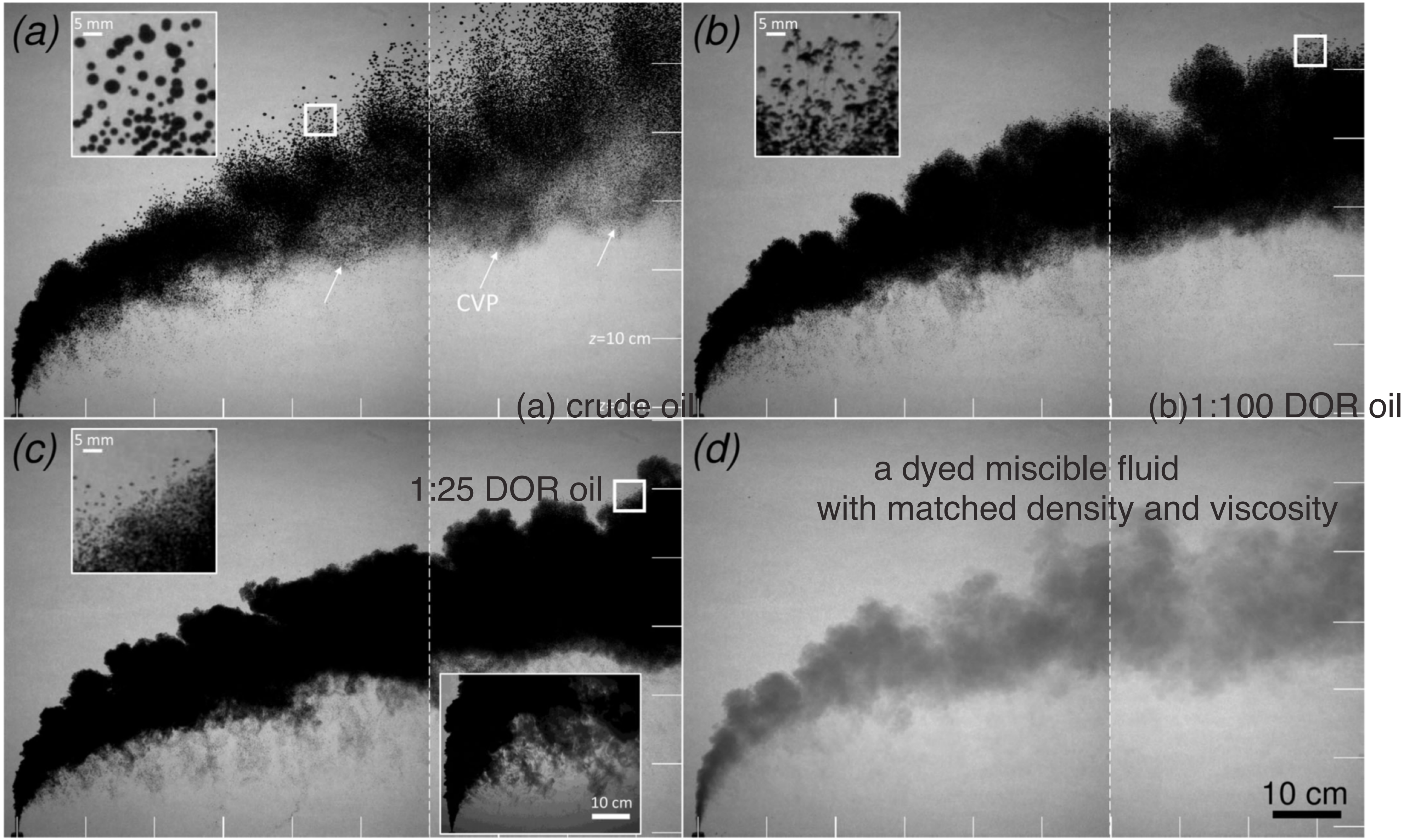
h – Thickness of control volume

b – Radius of control volume

V_j – Plume velocity

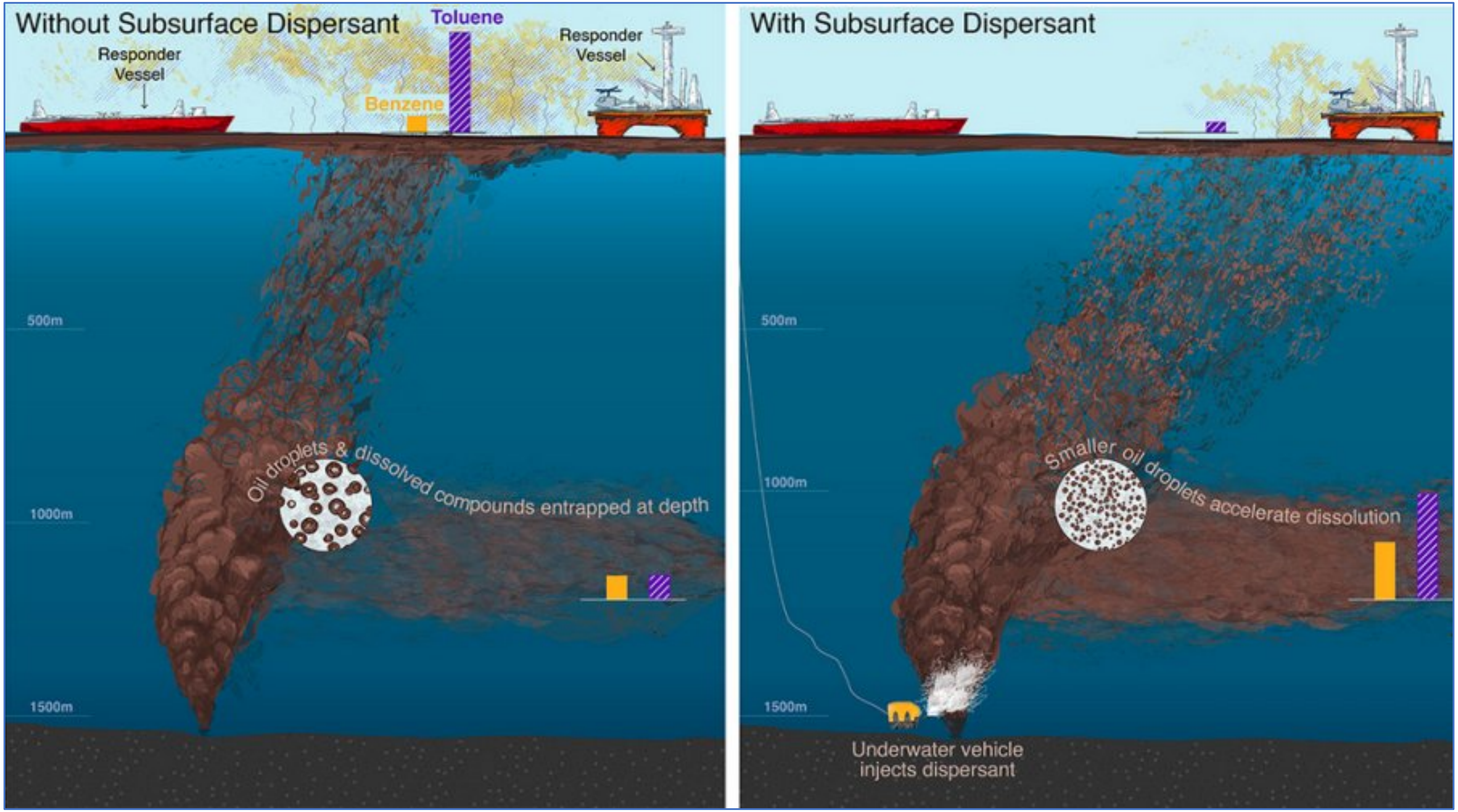
Lee & Cheung (1990) JEE, Yapa & Zheng (1997) JHR

Effects of Dispersants-Laboratory Experiments



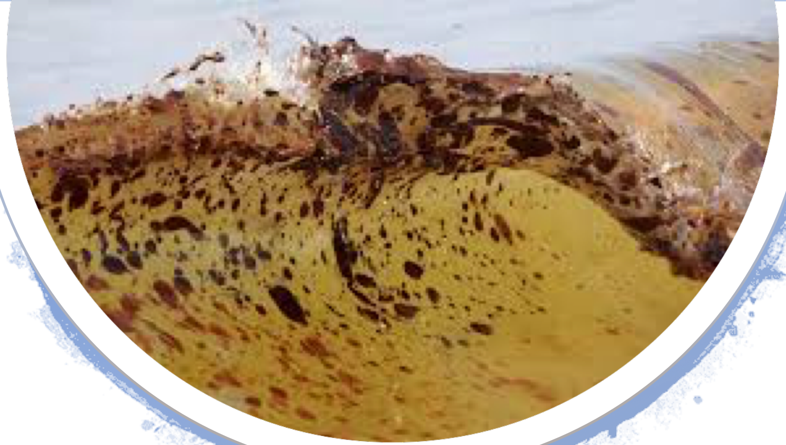
Murphy et al. (2016)

Simulation of Subsea Dispersants



Gros et al. (2017) PNAS, Picture Credits: WHOI

Models to Predict Size Distributions of Oil & Gas from Underwater Blowouts & Natural Dispersion



- Two main approaches
  - **Equilibrium Correlation Models**

    E.g. Johansen et al. (2013, 2015), Li et al. (2017 a, b)

    - Predict equilibrium droplet size distribution
    - Based on non-dimensional correlations
    - Consider release and ambient fluid properties and flow state
  - **Population Dynamic Models**

    E.g. Bandara and Yapa (2011), Nissanka and Yapa (2016, 2017) – Oildroplets, Zhao et al. (2014), (2017a), (2017b) – VDROP, VDROPJ

    - Predict evolution of size distributions along the plume
    - Based on Break-up and Coalescence
    - Consider release and ambient fluid properties and flow state

Experimental Data for Calibration/Validation of Oil & Gas Break-up Models

- **Data Available in different scales** – Small, Medium, Large (Field scale)
  - **DeepSpill field experiments** - oil and gas release at 844 m depth

    Johansen (2002)
  - **Laboratory Experiment Data** – 6 phases of small and medium scale experiments at SINTEF tower basin, Southwest Research Laboratory and OHMSETT facility, TUHH- Humburg (Brandvik et al., 2013; 2014, 2015, 2016, 2017a, 2017b, Malone et al., 2018, Wang et al., (2018)

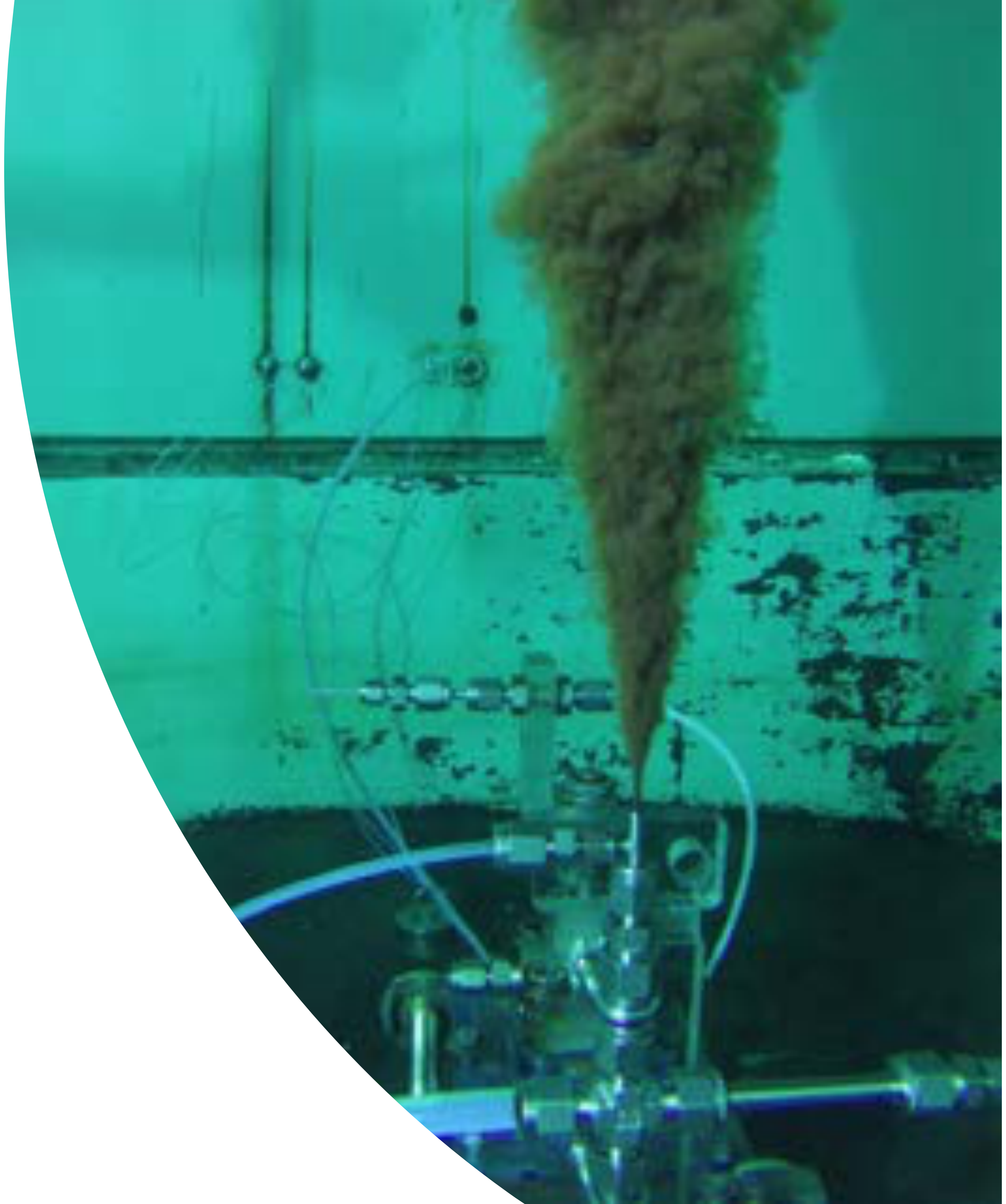


Photo Credit: Brandvik et al. (2015)

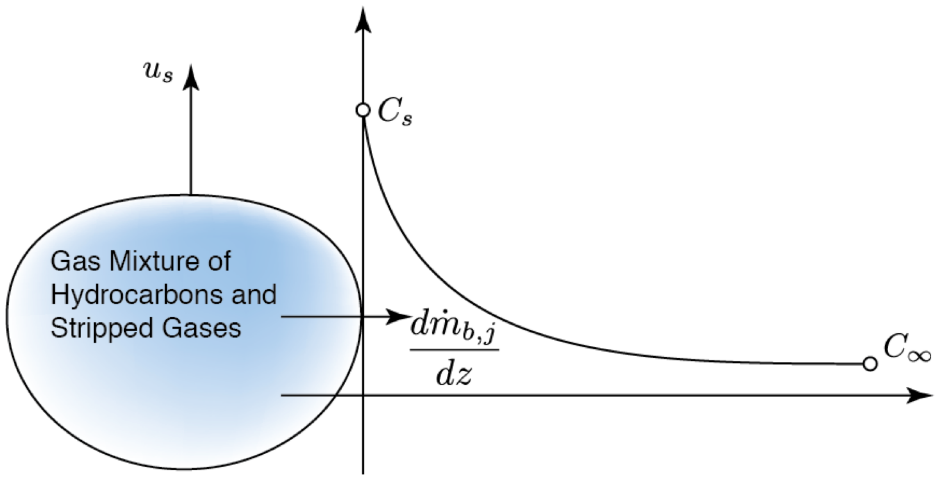
Mass & Heat Transfer of Bubbles & Droplets

Mass Transfer

$$\frac{d\dot{m}_{b,j}}{dz} = -\frac{\pi \dot{n}_b d_e^2}{u + u_s} \beta_j \left(c_{s,j} - c_j\right)$$

Saturation concentration

Mass transfer coefficient



Modified Henry's Law

$$c_{s,j} = H_j f_j$$

Mixture fugacity

$$H_j = H_{0,j} \exp\left(\frac{1}{R}\frac{dH_sol}{dT}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right)\exp(f(S))$$

Henry's law constant

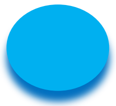
Heat Transfer

$$\frac{d(\dot{m}_p C_p T_p)}{dt} = -\frac{\pi \dot{n}_b d_e^2}{u + u_s} \beta_p (T_p - T_a)$$

Heat transfer coefficient

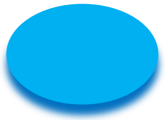
McGinnis et al. (2006) JGR-Oceans

Terminal Velocity of Droplets & Bubbles



$$U_T = (\mathrm{Re}\,\mu / \rho d)$$

Spherical shape
(small size)



$$U_T = \mu M^{-0.149} (J - 0.857) / \rho d_e$$

Ellipsoidal shape
(intermediate size)

$$U_T = 0.711\sqrt{g d_e \Delta\rho / \rho}$$

Spherical-cap
(large size)

ρ - density of ambient fluid

μ - viscosity of ambient fluid

de - equivalent diameter

d - bubble diameter

Re - Reynolds number

ρ - density of ambient fluid

σ - interfacial tension

M – Morton Number

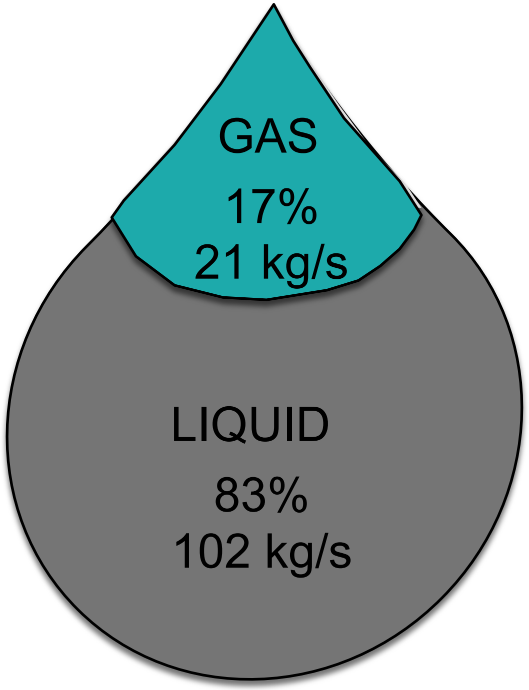
J - f(μ, d,ρ, σ)

Zheng and Yapa (2000) based on Clift et al. (1978)

Release Fluid Equilibrium

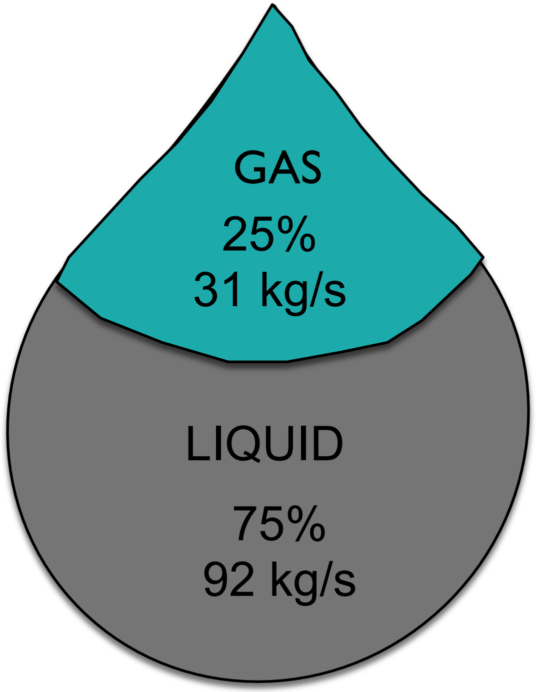
Live Oil under in situ Conditions

Temperature = 105 °C Pressure = 15.2 atm



Dead Oil under STP

Temperature = 15 °C Pressure = 1 atm



Liquid and Gas phase equilibrium and density calculation uses Peng-Robinson Equation of state

Gros et al. (2016)

Far-Field: Advection & Diffusion Stage

For oil and gas

$$\underbrace{\frac{\partial}{\partial t}(C_{vg})}_{\text{Concentration Change}} + \frac{\partial}{\partial x}(uC_{vg}) + \underbrace{\frac{\partial}{\partial y}(vC_{vg}) + \frac{\partial}{\partial z}(wC_{vg})}_{\text{Advection due to Ambient Currents}} = \overbrace{\frac{\partial}{\partial x}\left(D_x \frac{\partial C_{vg}}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial C_{vg}}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C_{vg}}{\partial z}\right)}^{\text{Diffusive Transport}}$$

$$\underbrace{\boxed{+\frac{\partial}{\partial z}(w_b C_{vg})}}_{\text{Advection due to Buoyant Particles}} - \underbrace{S_D}_{\text{Source/ Sink Term}}$$

For dissolved oil and gas

$$\frac{\partial}{\partial t}(C_{vd}) + \frac{\partial}{\partial x}(uC_{vd}) + \frac{\partial}{\partial y}(vC_{vd}) + \frac{\partial}{\partial z}(wC_{vd}) = \frac{\partial}{\partial x}\left(D_x \frac{\partial C_{vd}}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial C_{vd}}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C_{vd}}{\partial z}\right)$$

$$+ S_D$$

Lagrangian Parcel (LP) Method

- A Lagrangian Parcel - A representation of an ensemble of identical multiple particles.
- Each LP has a mass and a set of time-dependent spatial coordinates.
- LPs can be droplets, bubbles, dissolved oil, gas, or solid particles.
- Chemical and physical processes are considered.
- LPs are introduced into water at a rate corresponding to flow rate from the source.
- Use forcing from hydrodynamic models/measured data to model advection.

Physical, Chemical & Biological Processes Associated with Droplets & Bubbles in the Far-filed

- Dissolution
- Biodegradation
- Natural dispersion
- Evaporation
- Photo-oxidation
- Water-in-oil emulsion and tar ball formation
- Interaction with land/ice
- Interaction with sediments/mineral particles in shoreline/coastal environments
- Marine oil snow (MOS) formation – new addition?

MOS Aggregate Formation: Coagulation Theory

$$\frac{dn(m,t)}{dt} = \frac{\alpha}{2}\int_0^m \beta(m_j, m-m_j)n(m-m_j,t)n(m_j,t)dm_j$$
$$-\alpha n(m,t)\int_0^\infty \beta(m,m_j)n(m_j,t)dm_j - n(m,t)\frac{w_s(m)}{Z} + I(m,t)$$

$n(m,t)$ - Particle size spectrum

m, m_j - Particle masses

$w_s(m)$ - Settling velocity of particles of mass m

α - Stickiness (Probability of sticking after a collision)

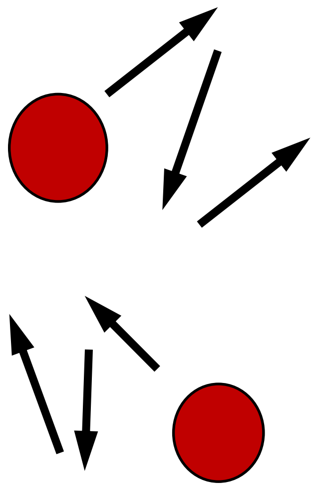
$\beta(m,m_j)$ - Coagulation kernel (Determines rate of collision of m & m_j)

$I(m,t)$ - Rate of formation of particles of mass m

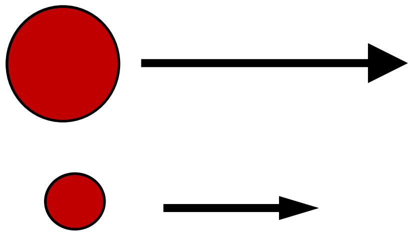
Photo Credits: David Liittschwager

Collision Mechanisms

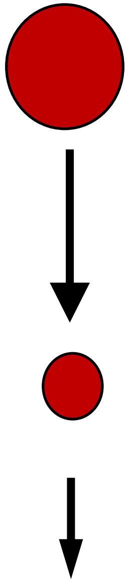
<u>**Brownian Motion**</u>



<u>**Fluid Shear**</u>



<u>**Differential Settling**</u>



Numerical Model of Marine Oil Snow (MOS)

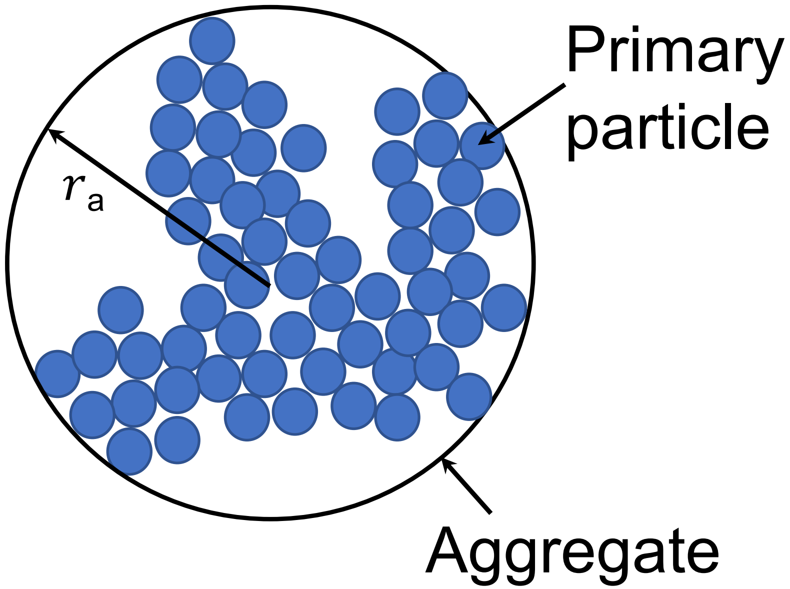
Aggregation Model

- Based on a Stochastic, Lagrangian Aggregate Model of Sinking particles (SLAMS-Jokulsdottir & Archer, 2016).
- Model uses super-droplet method to simulate large number of real particles with one representative particle to increase the calculation efficiency (Zsom & Dullemond, 2008).
- We introduced oil and river sediments to the SLAMS model to simulate MOS formation.

Aggregate properties

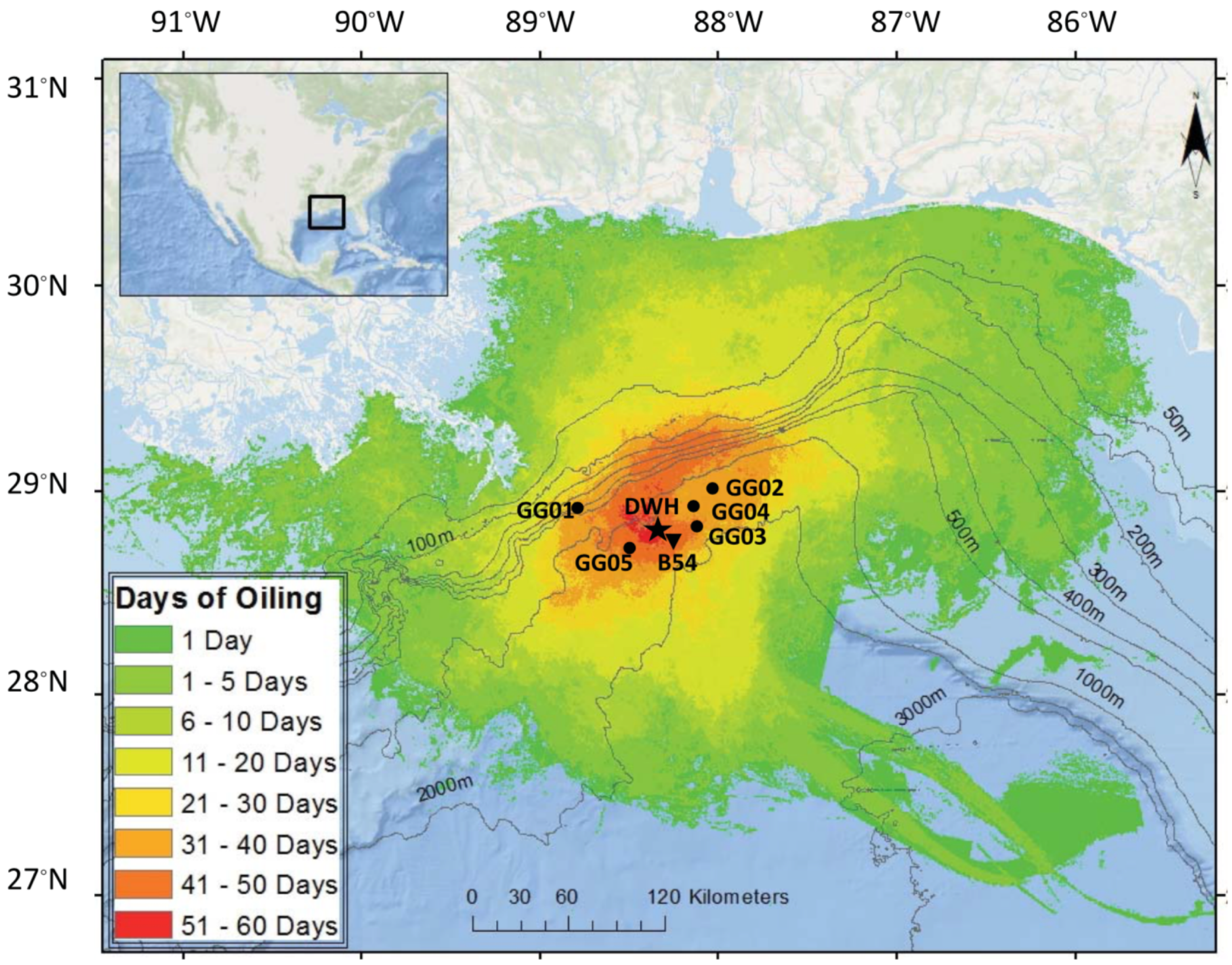
- Fractal scaling
- Porosity

} Aggregate size & density } Terminal velocity



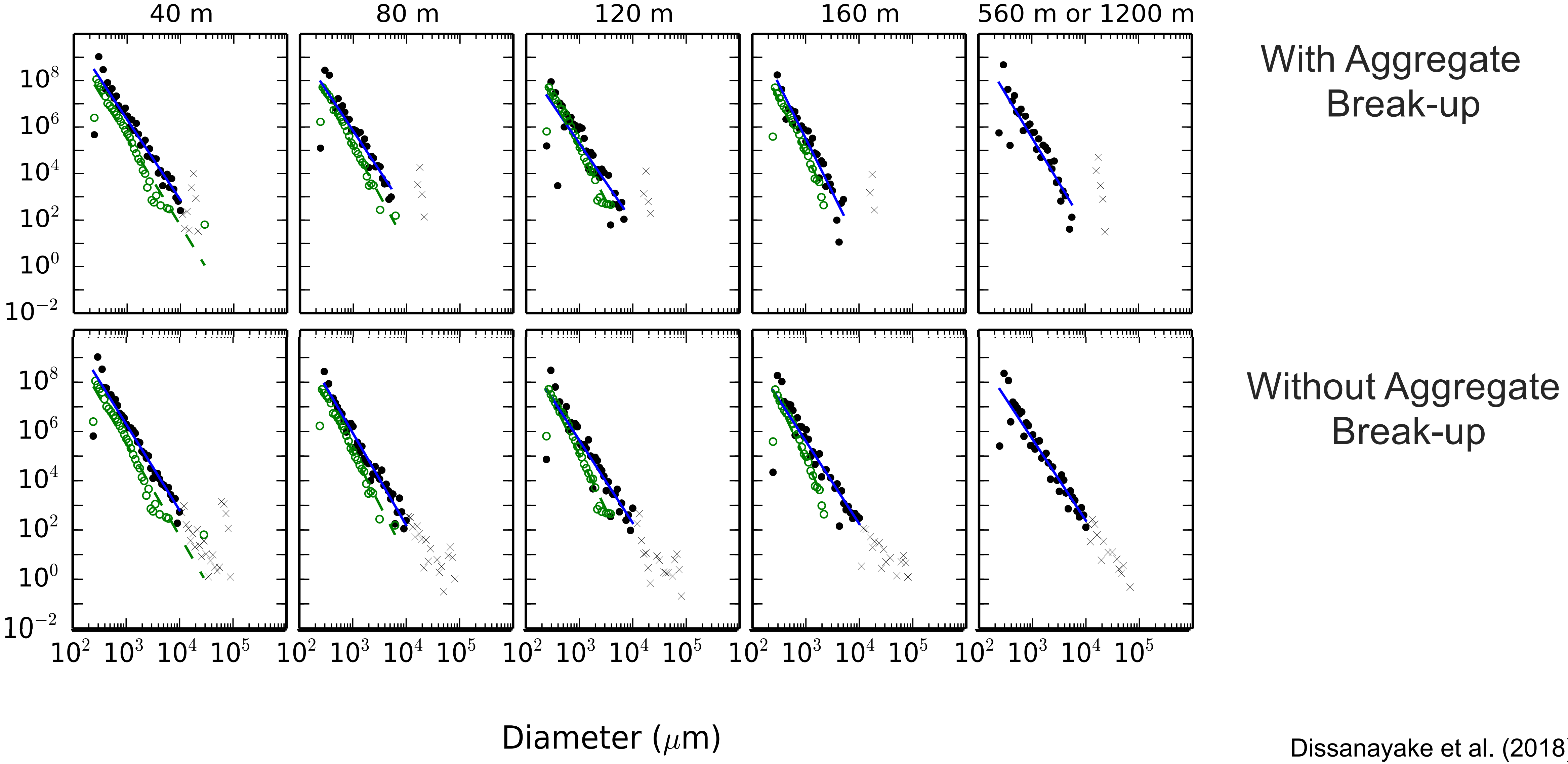
Dissanayake et al. (2018) JGR-Oceans

Field Data Collected



Dissanayake et al. (2018) JGR-Oceans

Simulation Results: Aggregate Size Spectrum



Dissanayake et al. (2018) JGR

Settling Fluxes at the seafloor

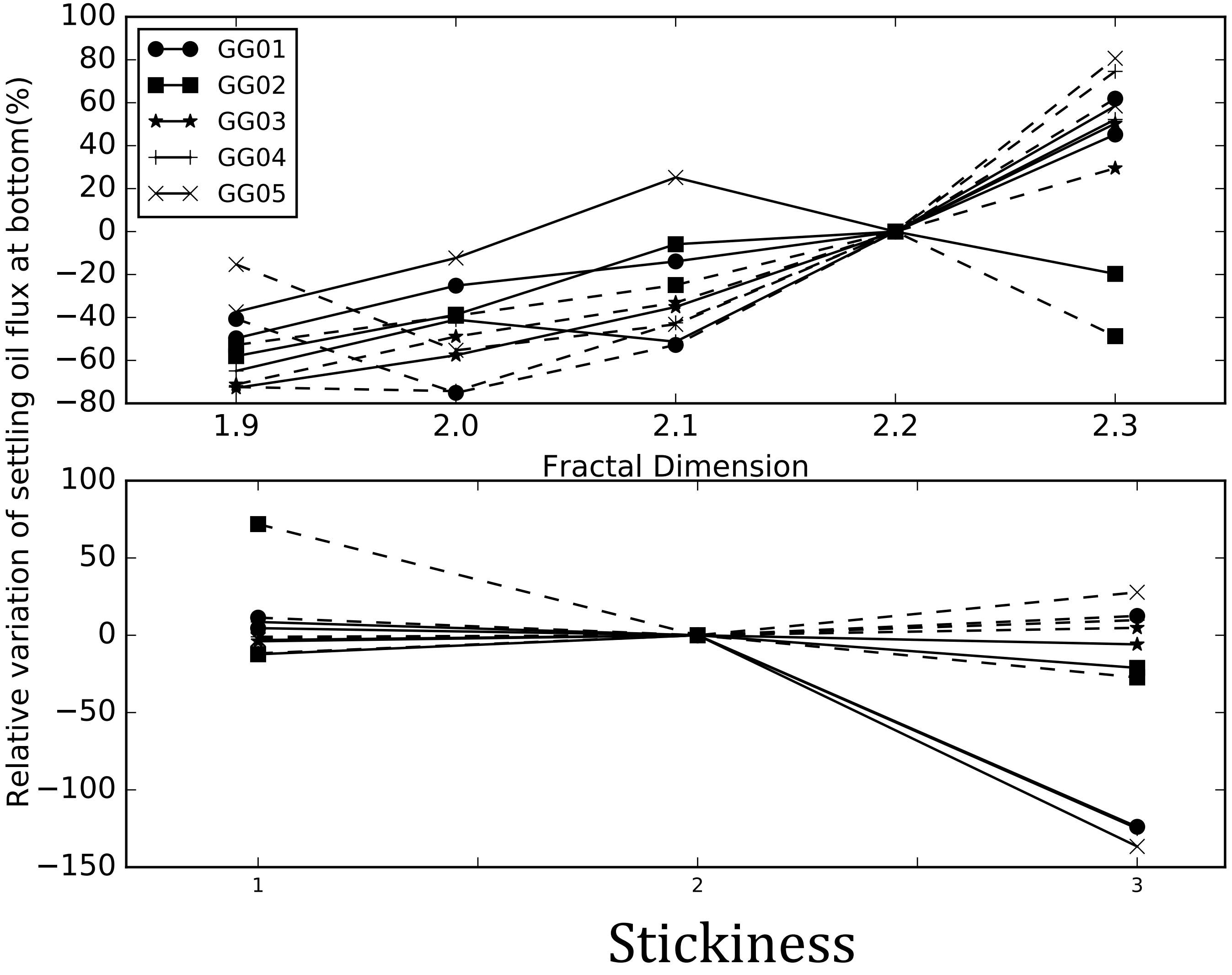
Model Estimation

Station	Seafloor oil Concentration ($g\ m^{-2}$)
GG01	4.03
GG02	14.82
GG03	134.7
GG04	3.38
GG05	5.46

Estimations from field observations

Authors	Seafloor Study Area (km^2)	Seafloor Oil Concentration ($g\ m^{-2}$)
Stout & German [2017]	1030	**20**
Romero et al. [2017]	32648	**0.039–0.098**
	219	**2.39–8.74**

Model Sensitivity



Stickiness Estimation Method

Method 1

$$S_{agg} = (S_{OrgC}\,V_{OrgC} + S_{TEP}\,V_{TEP} + S_{Oil}V_{Oil} + S_{Sed}V_{Sed})/V_{agg}$$

Method 2

$$S_{agg} = (0.1\,V_{OrgC} + V_{TEP})/V_{agg}$$

Method 3

$$S_{agg} = (V_{OrgC} + V_{TEP} + V_{Oil} + V_{Sed})/V_{agg}$$

Conclusions

- There has been new developments/improvements in oil spill models after DWH in near-field, far-field, bubble and droplet break-up models.
- The formation of MOS can be added as an extension to the oil and suspended particle aggregation or oil mineral aggregation in the coastal environments.
- Determining how to define input variables for these models are important.
- Experimental and modeling groups should communicate with each other.
- Future modifications for marine oil snow formation models
  - Model the time evolution of oil and MOS in the water column.
  - Coupling the model with a hydrodynamic model that will allow us to simulate oil and MOS advected within a system.
  - Additional research on the factors controlling aggregate fractal structure, stickiness, and disaggregation rates to improve the model predictions and comparison with data.
  - Biodegradation of oil in MOS aggregates.
  - Define oil in detail. e.g. pseudo components

Acknowledgement

Marine Oil Snow modeling work was made possible by a grant from The Gulf of Mexico Research Initiative to support the Project: Oil-Marine Snow-Mineral Aggregate Interactions and Sedimentation during the 2010 Deepwater Horizon Oil Spill.

Thank you!