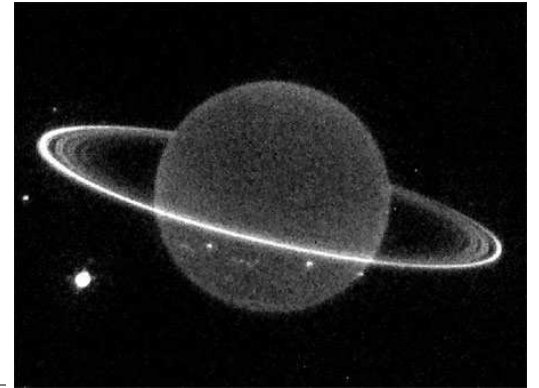# LANL Environmental Chem Modeling:
Today, Marine Organics

LANL –CCS, XCP, T, EES
External – ORNL, IARC, NMT, UW(a), NPS, PNNL
Students –NMT, Columbia, Chicago, UW(i), local high schools
Sponsors –HILAT, RUBISCO, CNLS, CSES, DTRA, ASC for TR, NA-24, Outreach

(What is the Galaxy Made of?

...Seriously)

LANL –SE
External – Help!
Students –Help!
Sponsors –Help!

Breadth of Effort (Complexity 4 SM):

Philosophy

(Redmods for packaging)
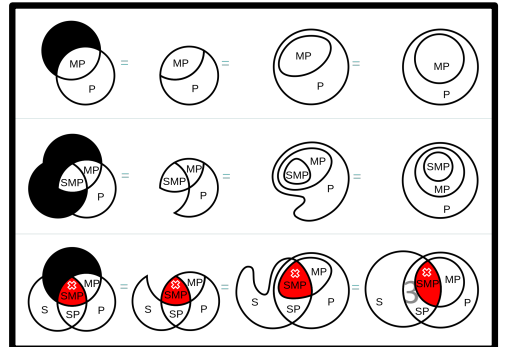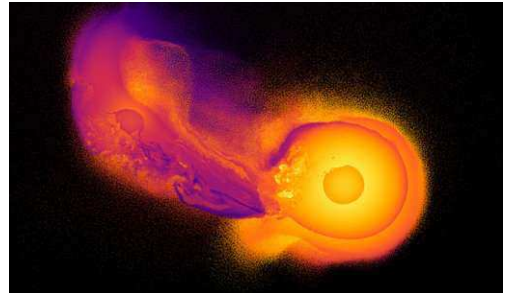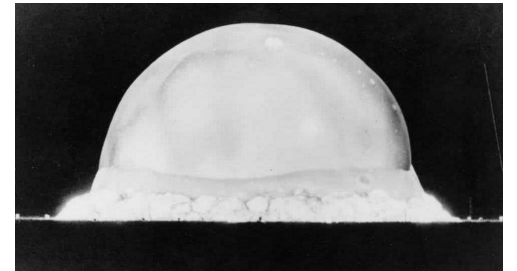
Up the Energy Scale

(Nukes near bottom!)

High Latitude Ocean

(Open, rivers, analysis)

ET Processes

(Giant impact)

Addenda

(Theory)

Weapons Effects: the Low End

Began at Fallout Range
(Reduction on trajectories)
Adapt smog aerosol dynamics
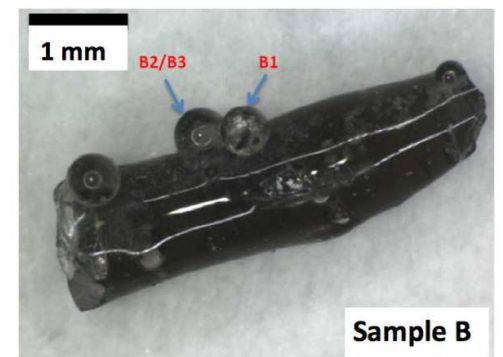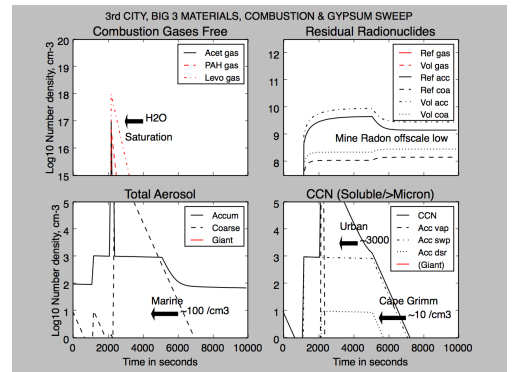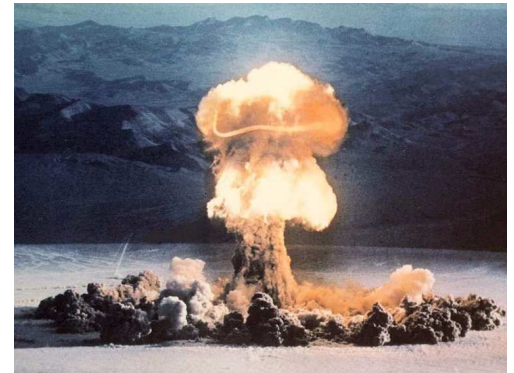*(But from 3000 Kelvin)*
Don't forget sweep
(Global Geology)
Back to Fireball Core
(Plasma, radiation etc.)
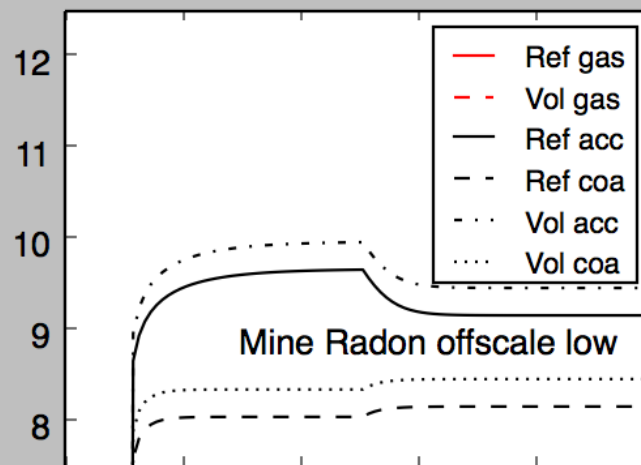Identify huge uncertainties
(Manageable schemes)

3rd CITY, BIG 3 MATERIALS, COMBUSTION & GYPSUM SWEEP

1 mm

B2/B3   B1

Sample B

Modernize the Urban Firestorm

Zoom on Effectiveness/Effects
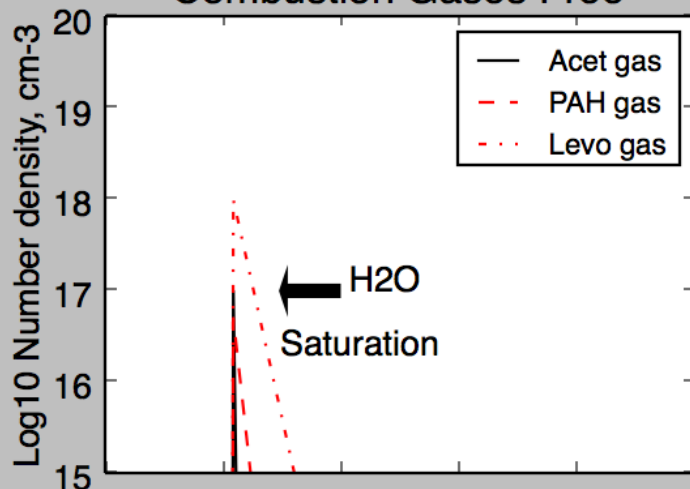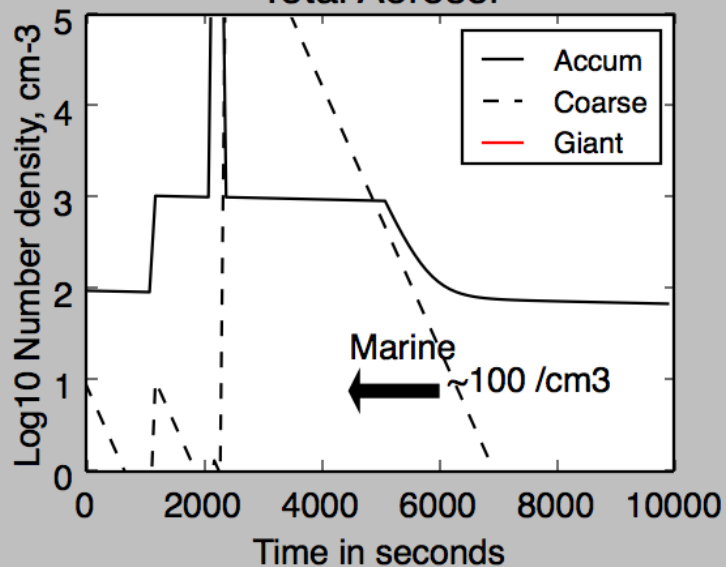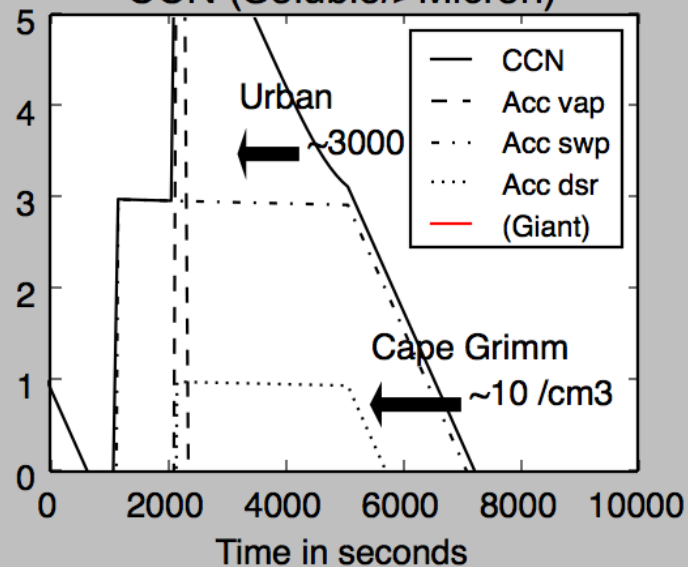
Marine Chem of: Reduced Carbon

SKIP

DMS, methane clathrates
(Small molecules)

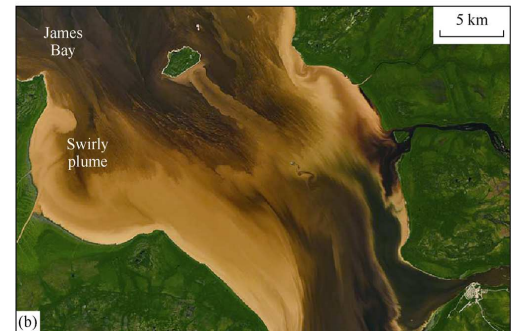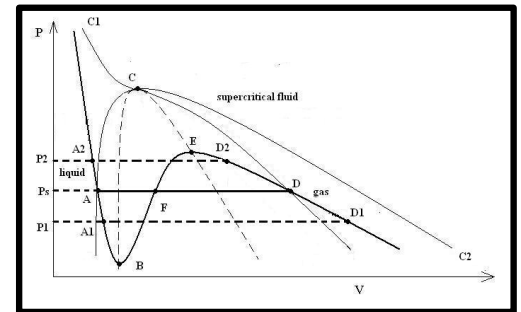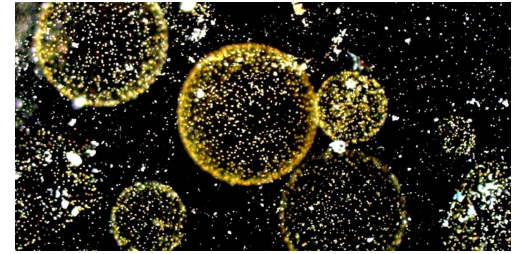Primary Organic Aerosol
(Surfactants)

Biogeochemical EOS
(Gaia in a huge way)

Arctic Rivers
(Jump start IOMB)
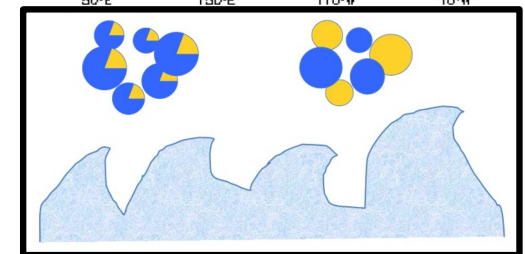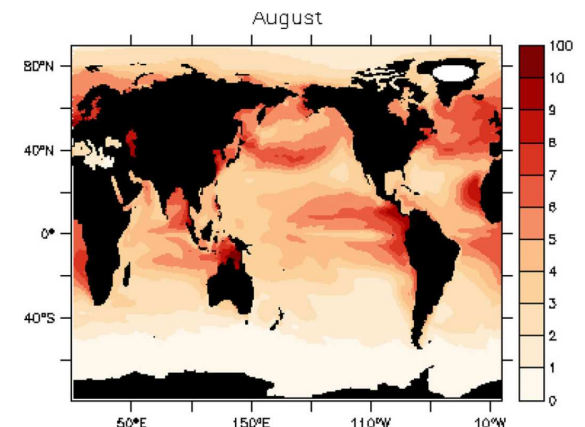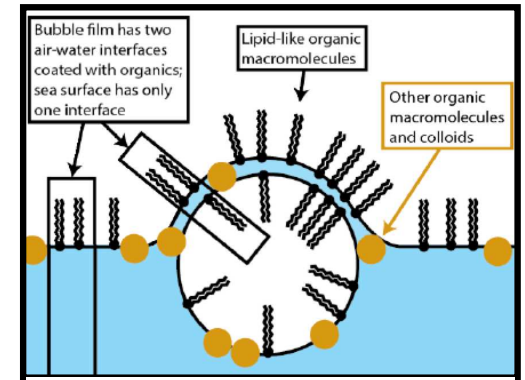
Energetics?
(Blooms, melts, fluxes)

Start from Surfactants and POA:

Standard Story Line
 (Bubble burst)
Macromolecular Adsorption
 (Prots, lipids, hetpc)
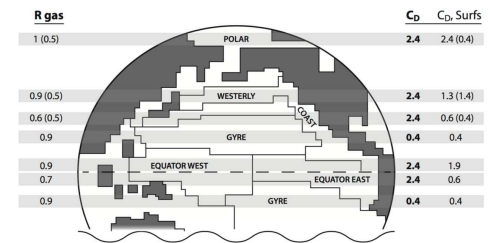Ogunro Maps Accordingly
 (Global patterns)
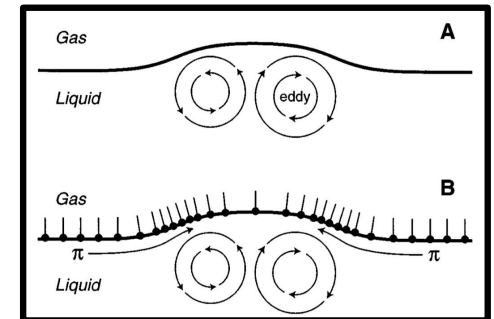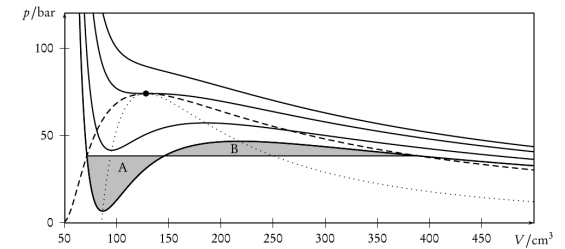Burrows OCEANFILMS
 (-4 W/m2)

Effect Interface Energetics Too!
A Biogeochemical Equation of State:

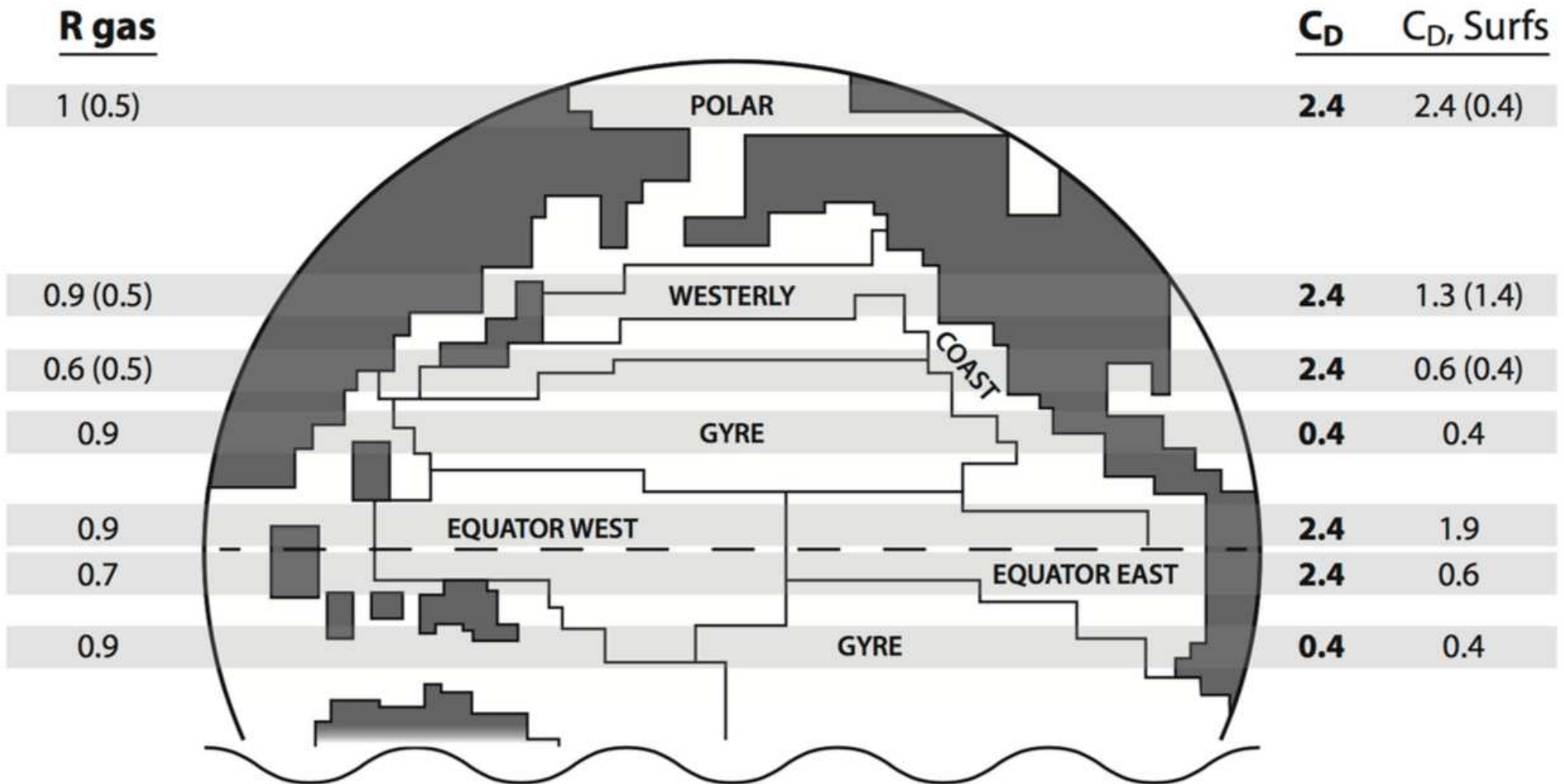### Think Van der Waals but 2d
(Planar g, l, s)
Surface Tension & Eddy Control
(Prots, lips most effective)
Elliott Maps Accordingly
(Under referee duress)
If Correct, Super-Gaian
(Phyto steer currents...)
(Momentum transfer and also)
(heat, water vapor, trace gases)

Zoom for ORNL Benefit

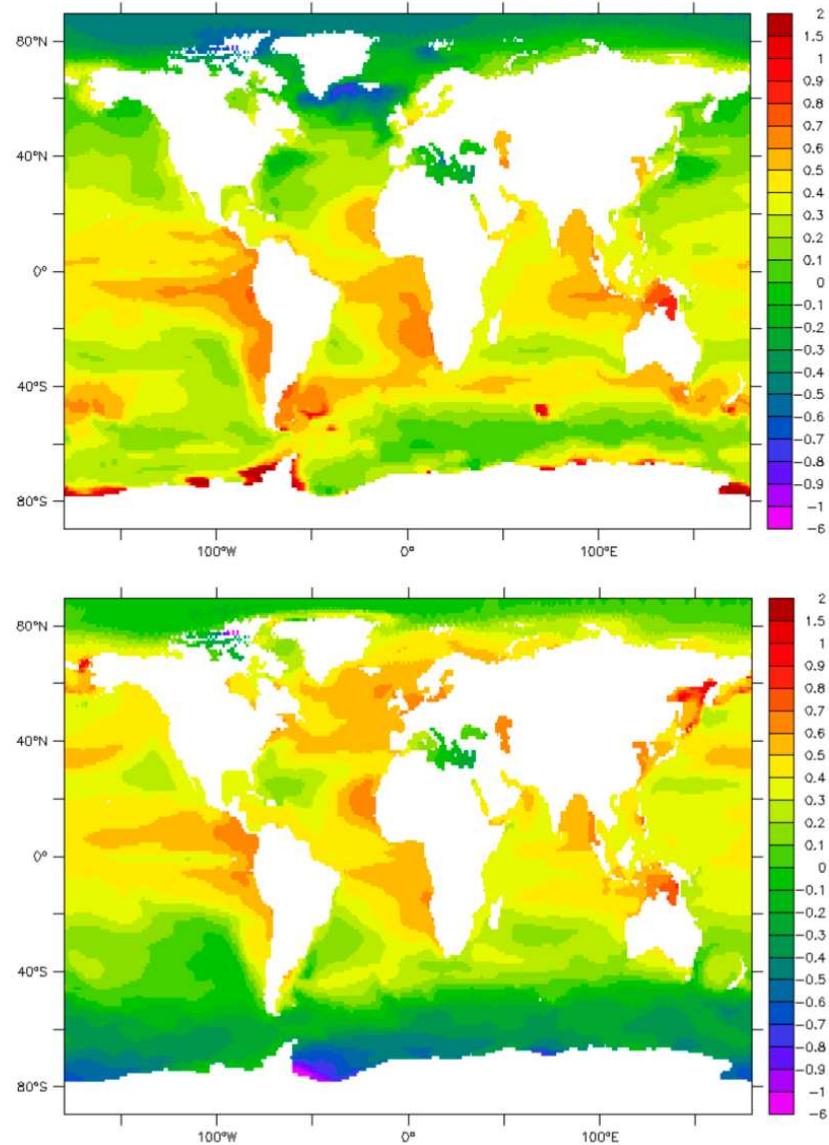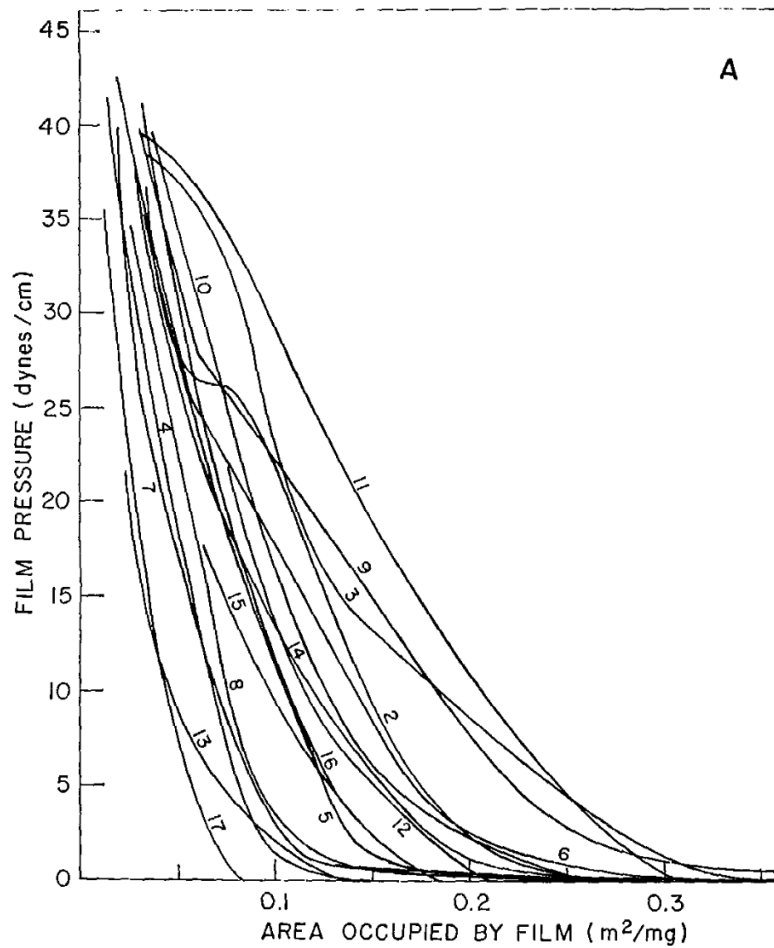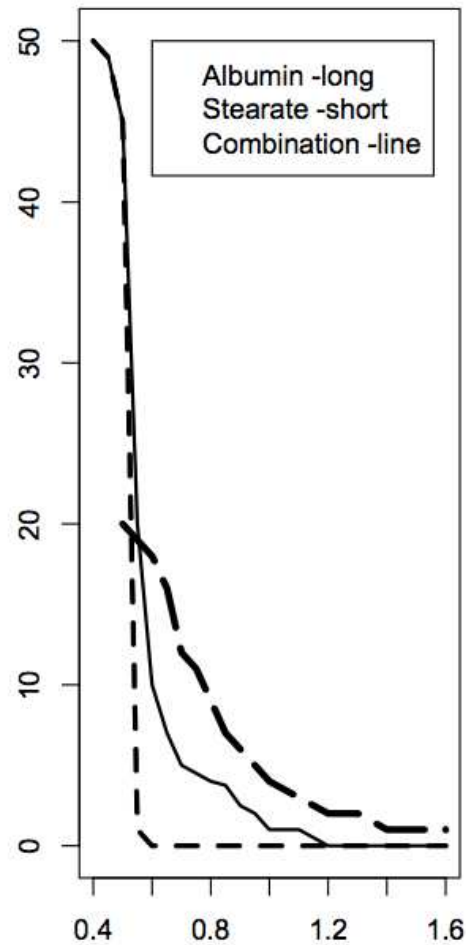| R gas		C_D	C_D, Surfs
1 (0.5)	POLAR	2.4	2.4 (0.4)
0.9 (0.5)	WESTERLY	2.4	1.3 (1.4)
0.6 (0.5)	COAST	2.4	0.6 (0.4)
0.9	GYRE	0.4	0.4
0.9	EQUATOR WEST	2.4	1.9
0.7	EQUATOR EAST	2.4	0.6
0.9	GYRE	0.4	0.4

Zoom on ΔTension... C_d Needed

Figure 1. Log surface pressure maps (Δtension) assembled using the baseline Ogunro et al. model output [33] plus marine 2D equations of state described in Appendix A. The color bar has been set so a reference range of 0.3–3 mN/m is central (−0.5 to 0.5 in log units). February and August monthly averages are shown for a typical year near the turn of the millennium.
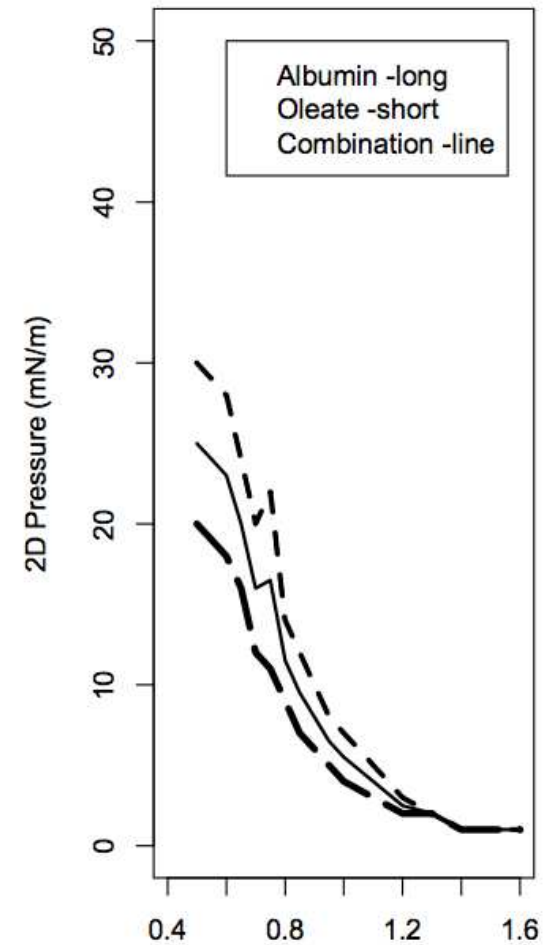
Zoom on Validation... IOMB Needed

Spread with Solid

Albumin -long
Stearate -short
Combination -line

(A)

Spread with Liquid

Albumin -long
Oleate -short
Combination -line

(B)

(OGUNRO DID DOC TABLES, BUT...)

Arctic Riverine Chemistry:

Total organic mechanisms
  (From headwaters)
All dissolved classes, functions
  (Open sea plus aromatics)
Floodplain is dilution driven
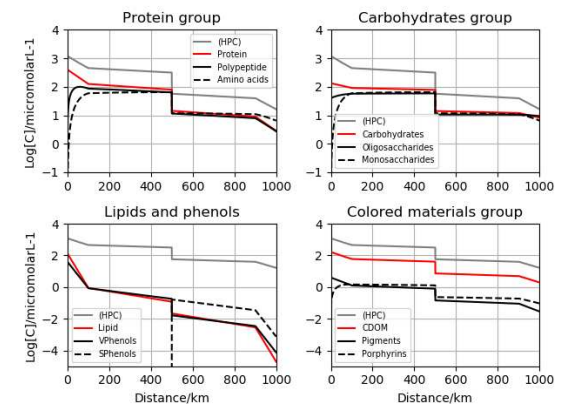 *(Initialize for RVIC, MOS)*
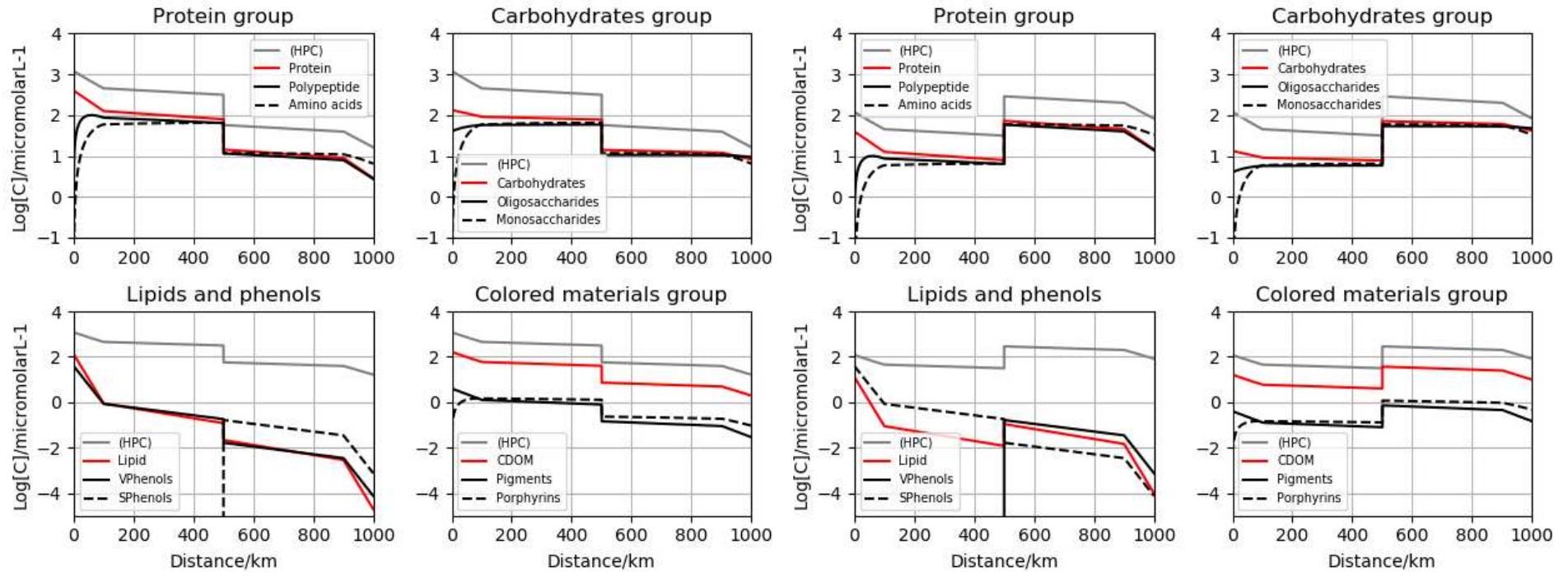Mixed particulates soon
  (POC plus minerals)
Multiple effects
  (Turbidity, surfactants,)
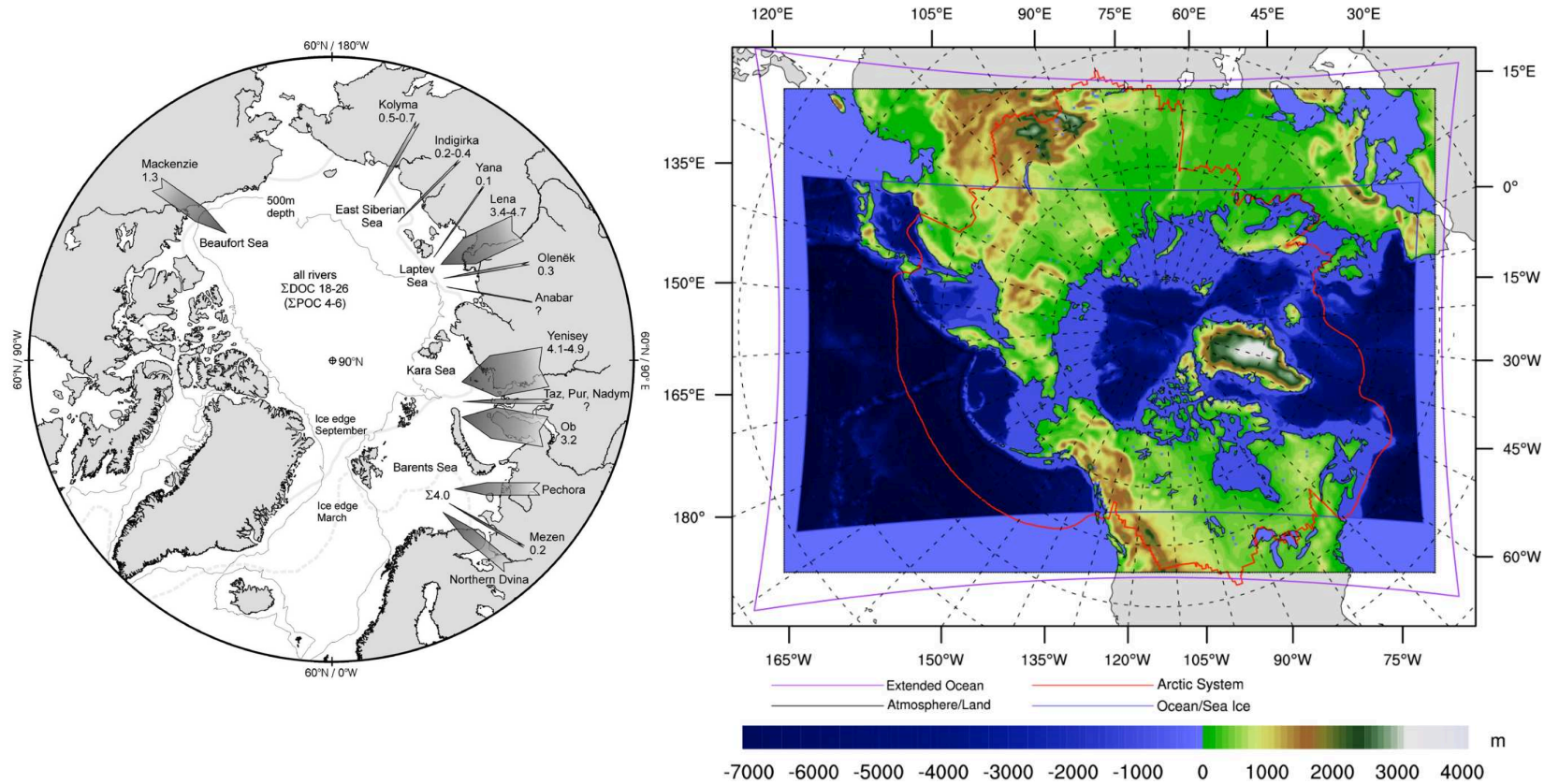 *(Antifreeze...)*
  (And of course N)

Zoom for AJ Benefit

Lena –Swimming Upstream

RASM and Other Sophisticated Grids

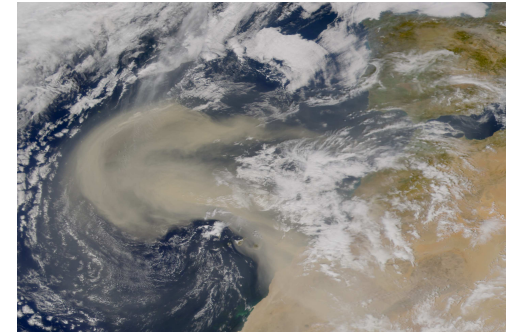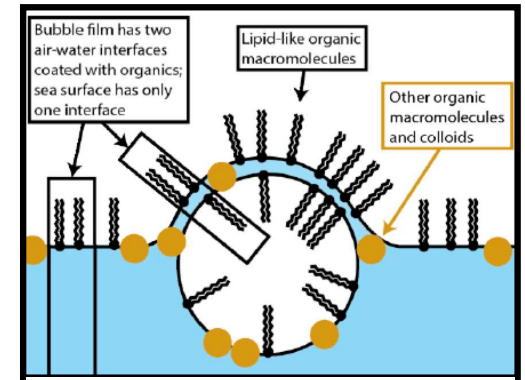# Iron at the Global Interface: UWisc

Use IOMB data, 2D Redmods
   (IT logic)
Are POA polymers ligands?
   (Proteins, polysacchs)
Or adsorbed macromolecules?
   (Proteins, lipids)
Or Meskhidze upper column?
   (alpha hydroxy moeity)
Reduced carbon regulates metal
   (2D bioreactor?)

Giant Impact: the High End

The Molecular Cloud
(Scale beyond imagining)
Sub-nebulae
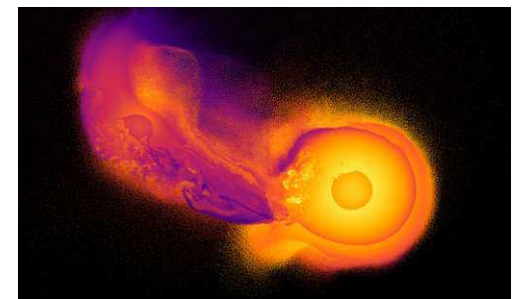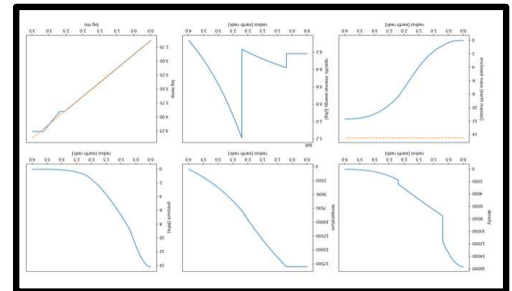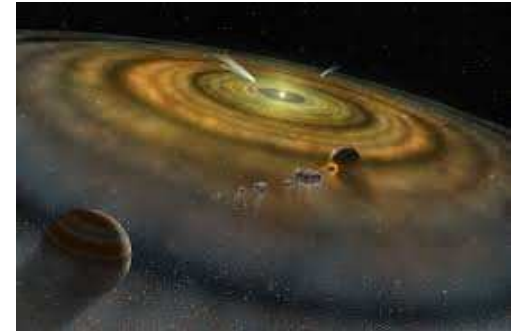*(Planets and rings)*
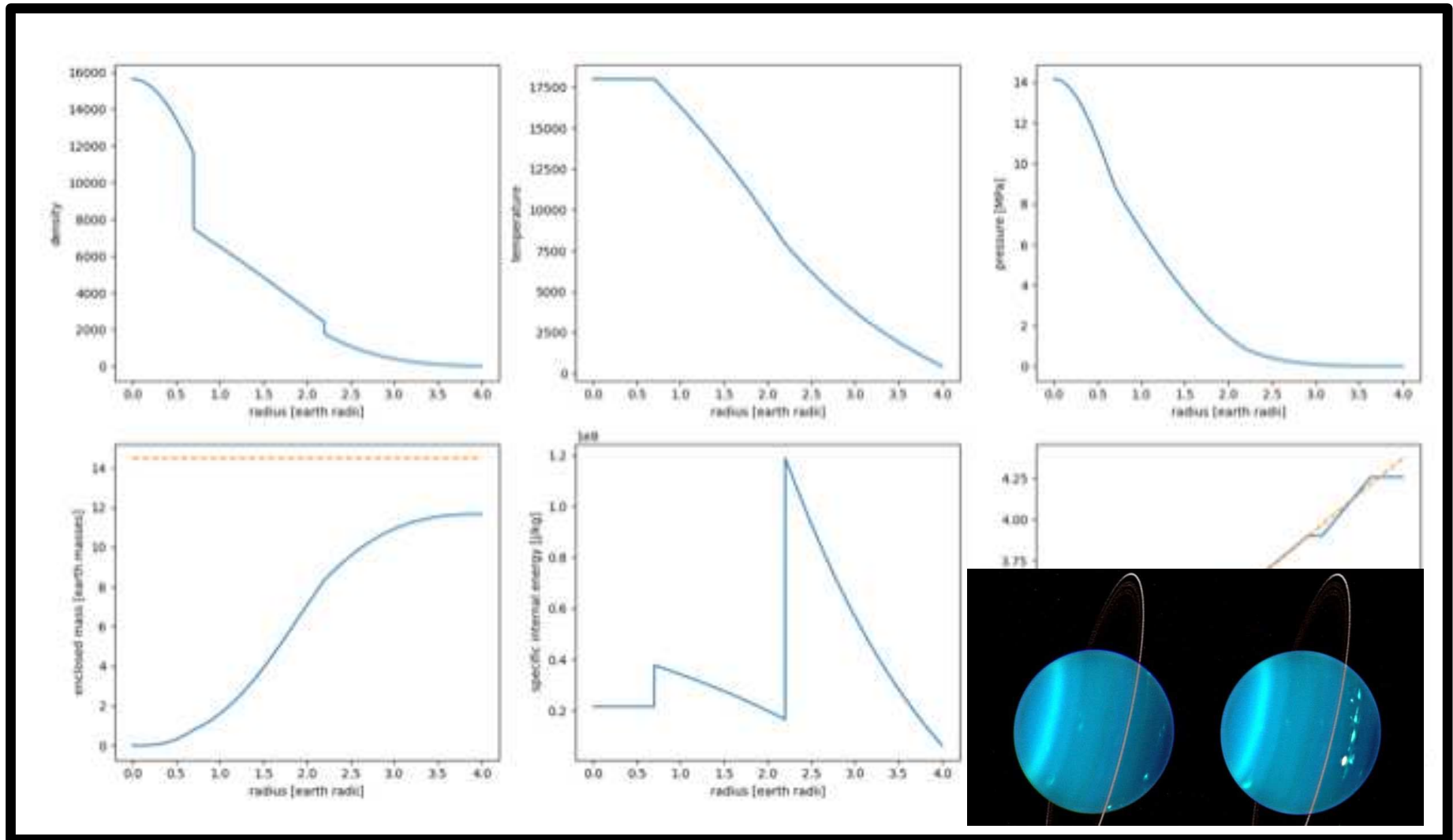Equations of State
(In outer solar system)
CHON Equilibria
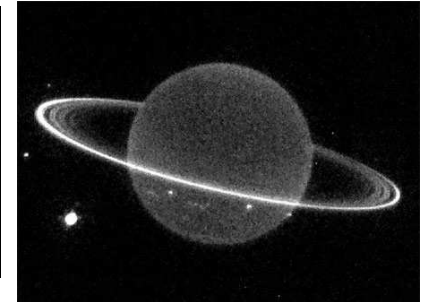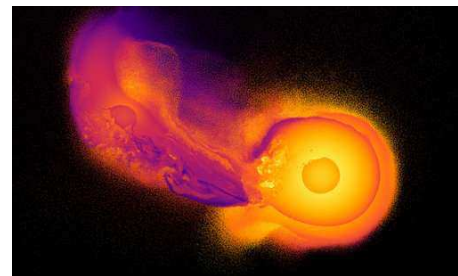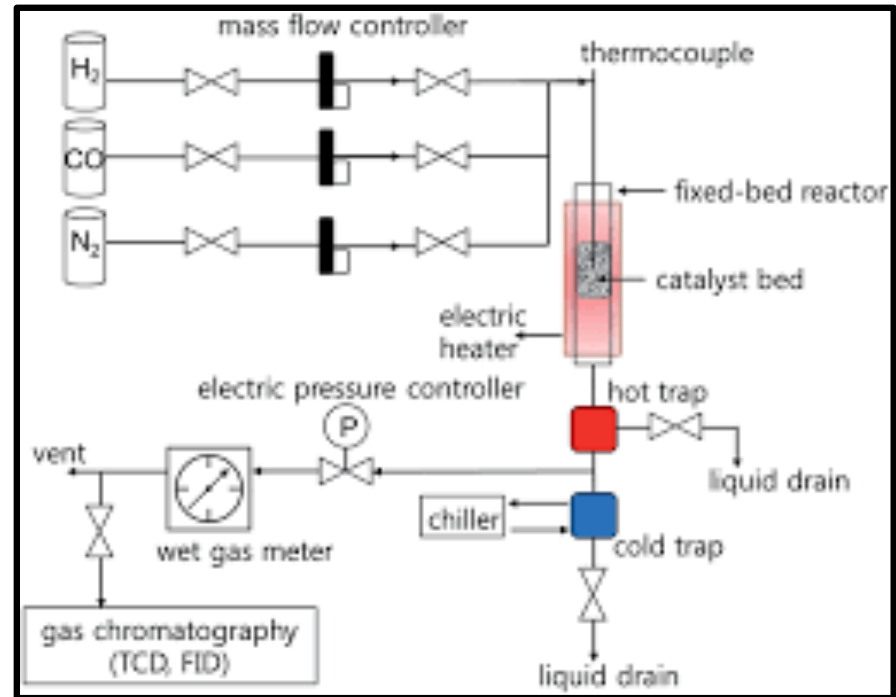*(The molecular "ices")*
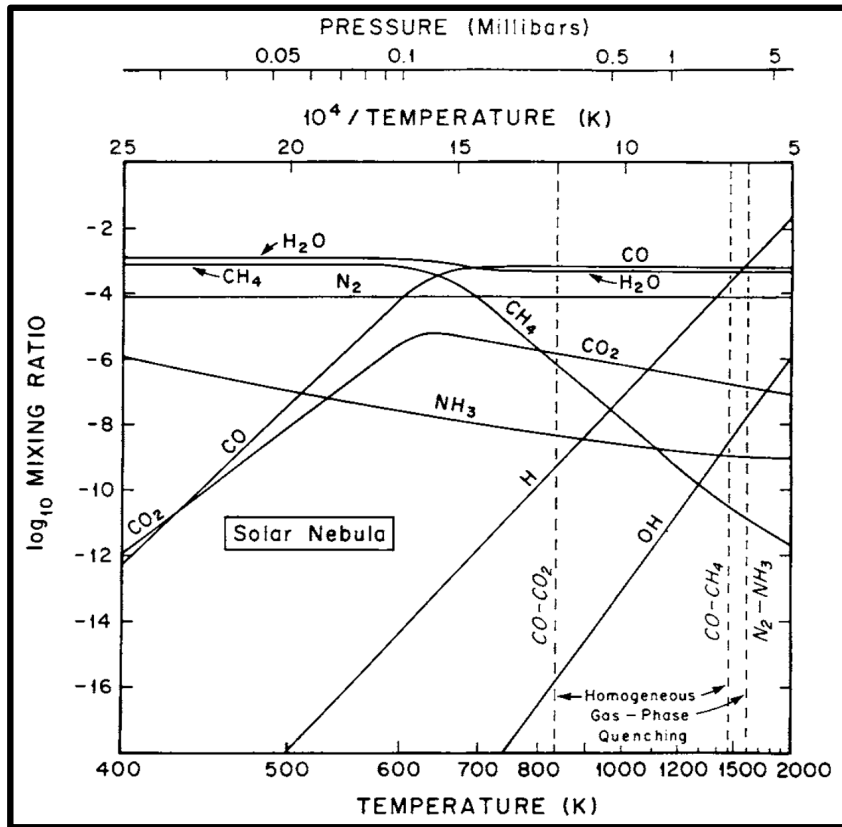Organic synthesis
(E.g. Fischer Tropsch)

Zoom for XCP Students

Uranian Futures
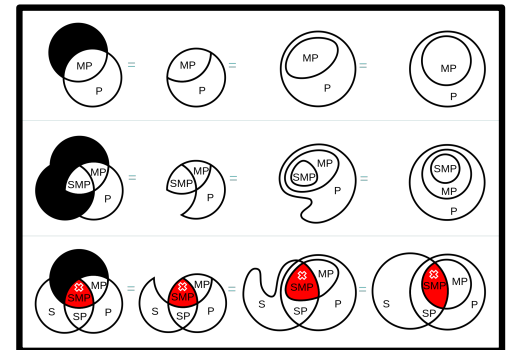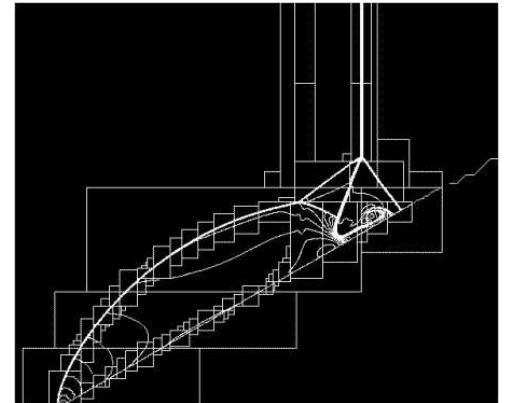
Philosophy and Theory:

Systems a Huge Opportunity
    (Plenty of room 4 procs)
Scan in Reduced Mode, Package
    (Chemistry distilled)
Officially…
    (Minus-First Law,
    (Set theory, Shannon information,
    (Mark-recapture,
    (Reverse selection…
It's UQ Backwards… Impacts NC Stats
IOMB extension to Rivers, Proteins, more

A dash of Info-Theory for IOMB:

Scores require tuning
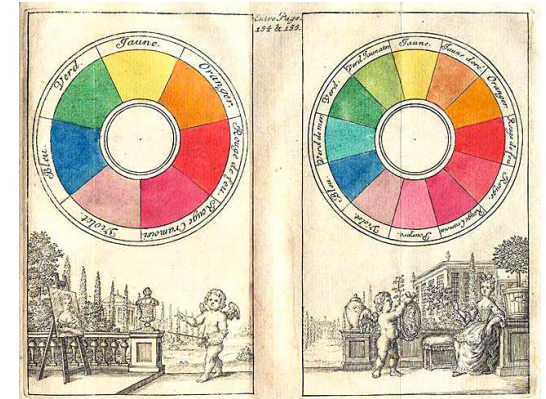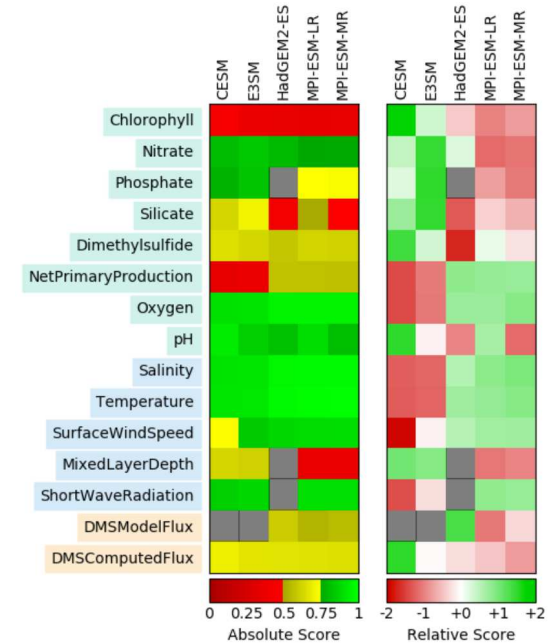*(See Collier et al. 18)*
Shannon Opportunity?
(Between primary colors)
Attend to sparse data
(Identify new processes)
Develop Theory
(AJ digs Stat Mech)

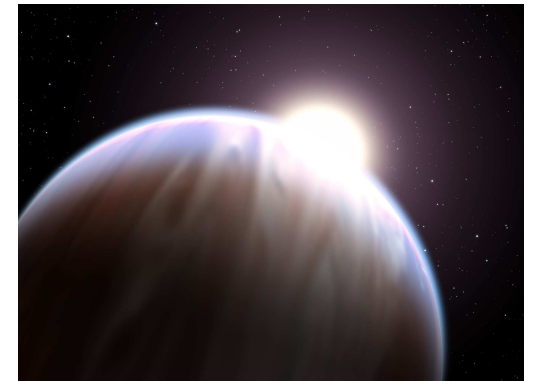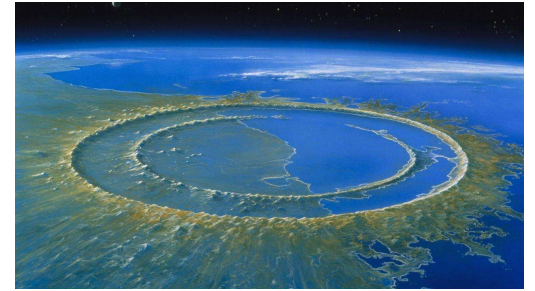# Importance of This Stuff: Cosmic

Pulse Outcomes f(Chemistry)
(Bursts to asteroids)
High Latitude Ocean
(ESM accuracy, GAIA)
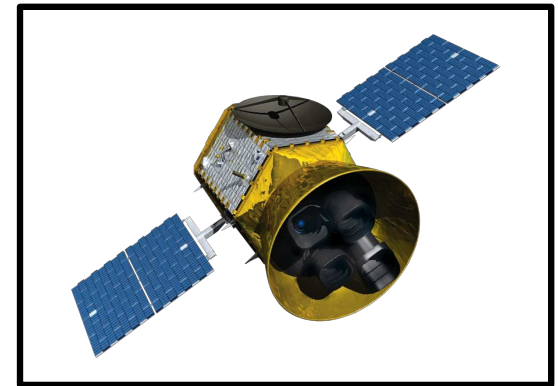Extra-Terrestrial
(Exoplanets coming)

Validation:

Weapons Effects
(Test site etc.)
High Latitudes
(Ongoing, community)
Extra-Terrestrial
(Exoplanets coming!)
Analsys and IOMB
(Sparse data are good data... Orgs!)

Breadth of Effort (Complexity 4 SM):

Philosophy
(Redmods for packaging)

Up the Energy Scale
(Nukes near bottom!)

High Latitude Ocean
(Open, rivers, analysis)

ET Processes
(Giant impact)

Addenda
(Theory)