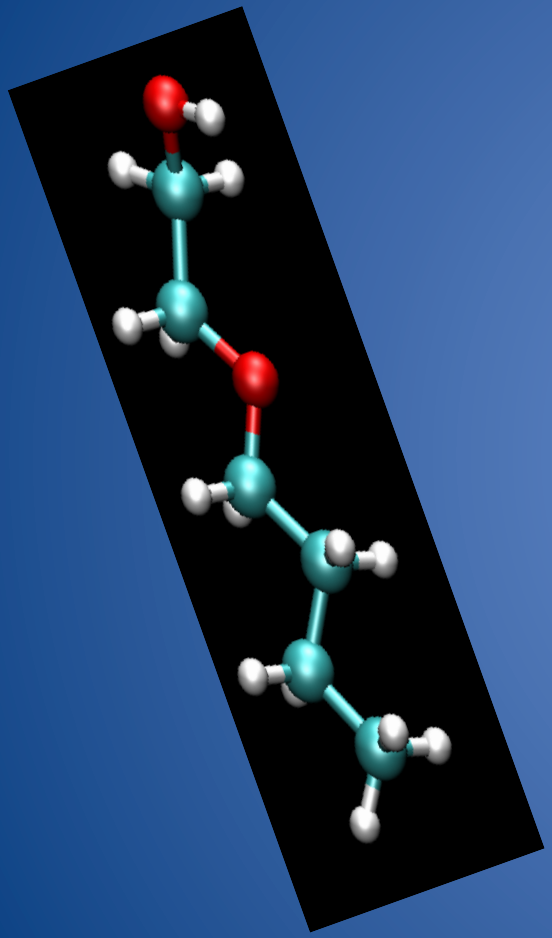
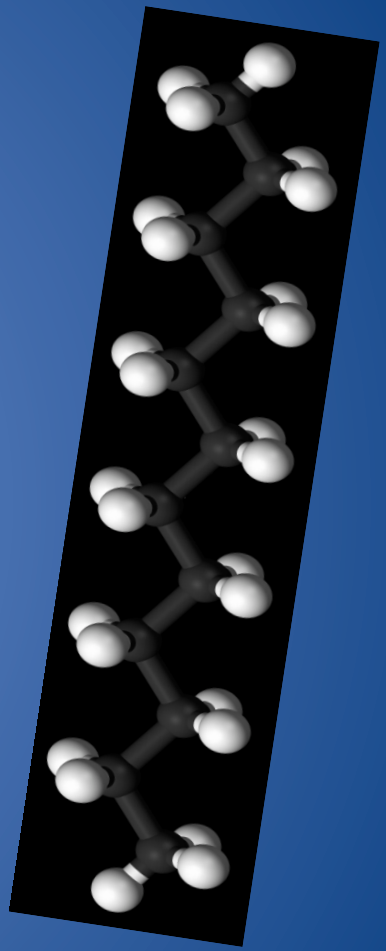
How do Oil Dispersants actually Disperse?





Chris Campbell

Dr. Collin Wick

LA TECH

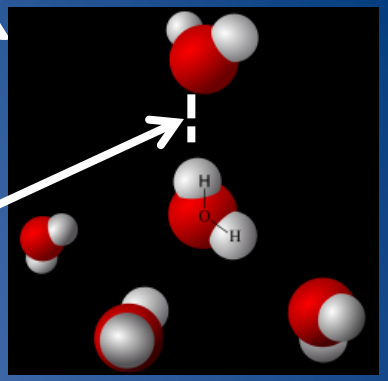
LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

Now what?

Deepwater Horizon – April 2010

Oil and Water Don't Mix



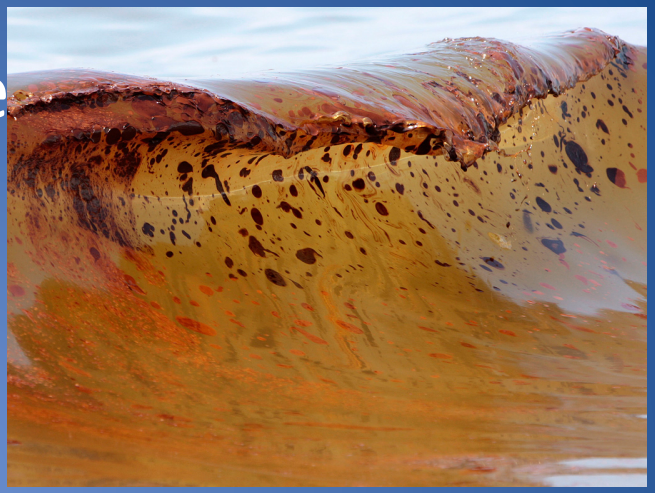
- Hopefully we know this, but why?
- Water-water interactions have strong hydrogen bonding interactions
- Oil interacts via weaker nonpolar (London forces) interactions
- Water likes itself better than oil, so it expels oil

LA TECH

LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

Oil looks ugly, and it can harm wildlife

- Tar balls and asphalt at the beach
- Oily pelicans ☹



LA TECH

LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

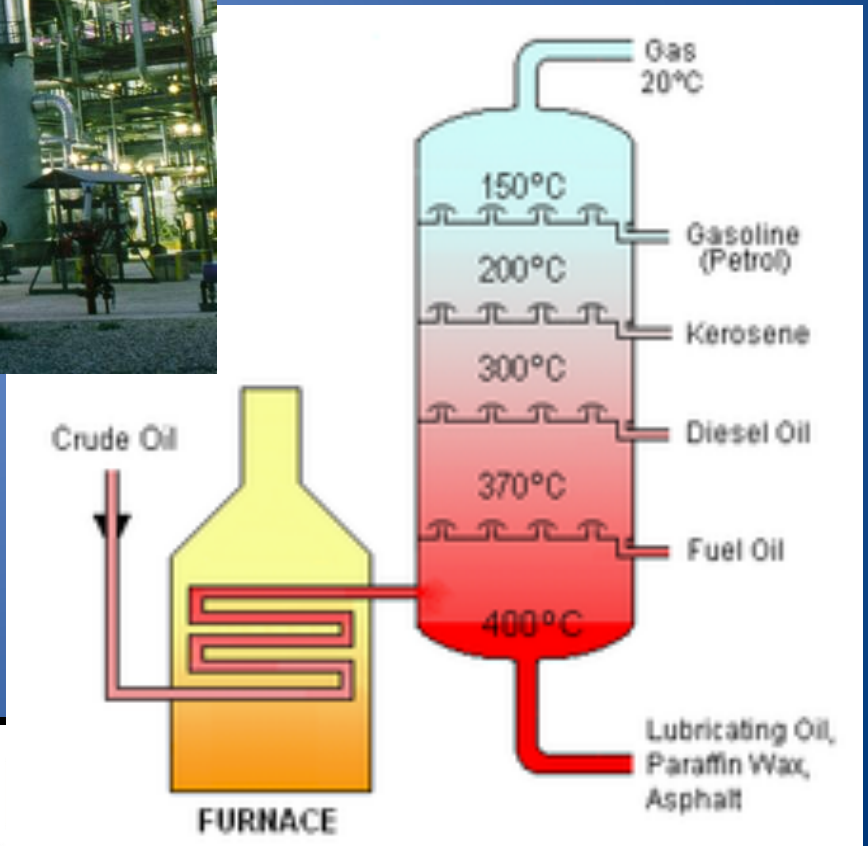
Crude Oil is a "GUMBO" of Hydrocarbons, benzenes, asphaltenes, paraffins (waxes), etc.

On average, crude oils are made of the following elements or compounds:

Carbon - 84%
Hydrogen - 14%
Sulfur - 1 to 3% (hydrogen sulfide, sulfides, disulfides, elemental sulfur)
Nitrogen - less than 1% (basic compounds with amine groups)
Oxygen - less than 1% (found in organic compounds such as carbon dioxide, phenols, ketones, carboxylic acids)
Metals - less than 1% (nickel, iron, vanadium, copper, arsenic)
Salts - less than 1% (sodium chloride, magnesium chloride, calcium chloride)

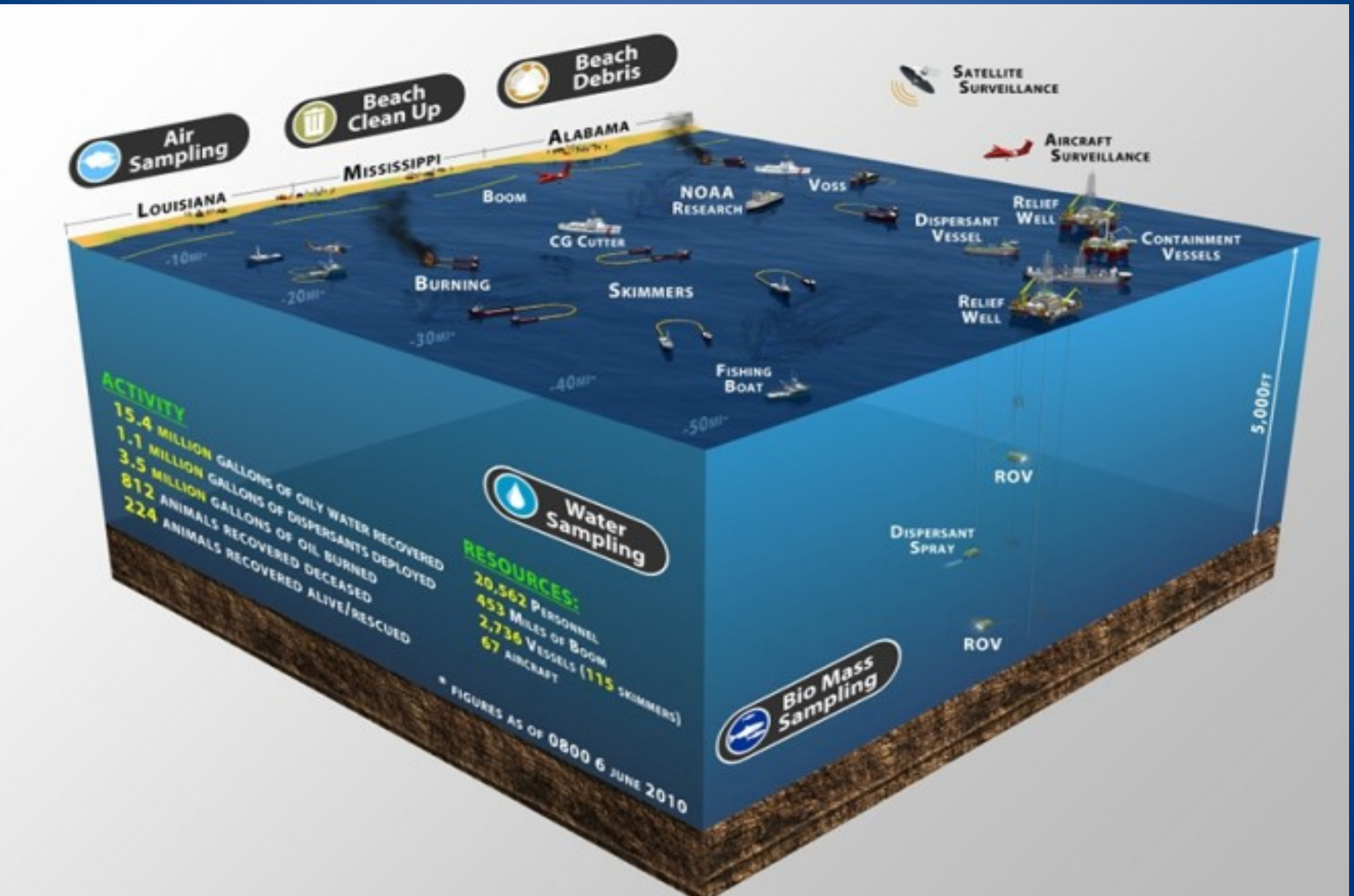
LA TECH

LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications



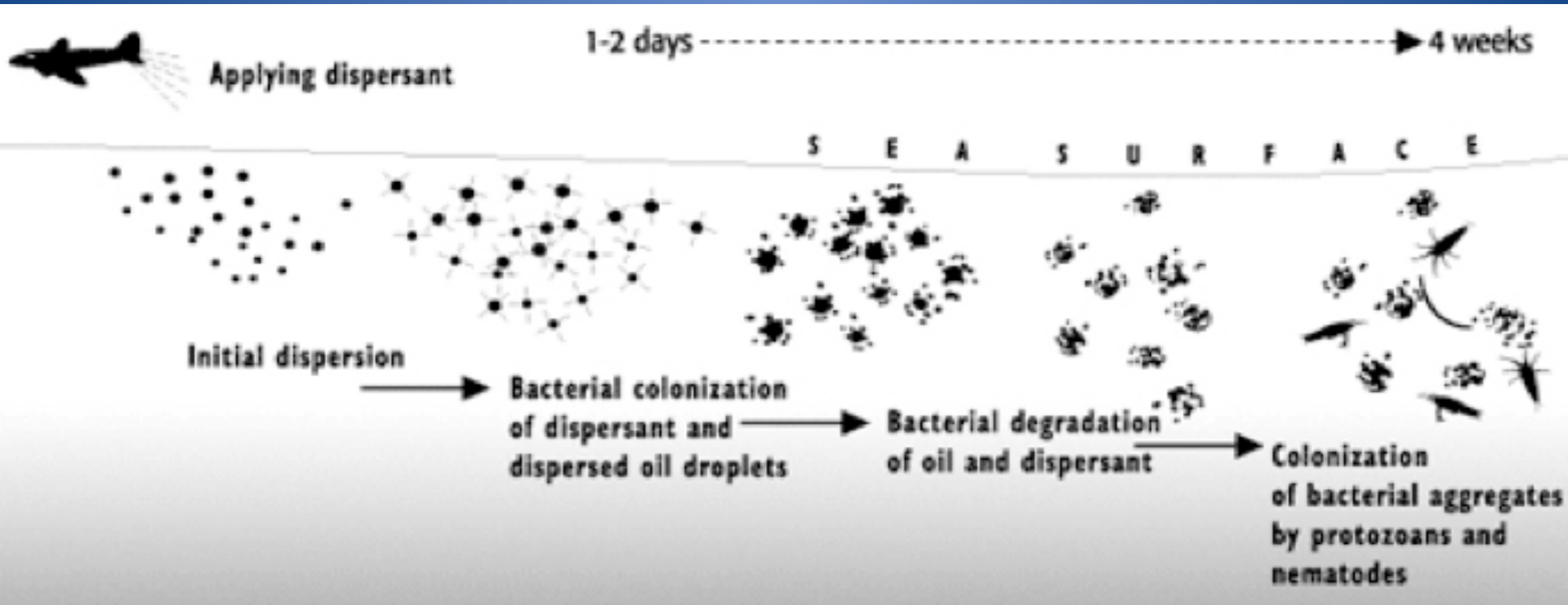
LA-SiG
Louisiana Alliance for Simulation-Guided M

There is a multipart strategy to save the coasts

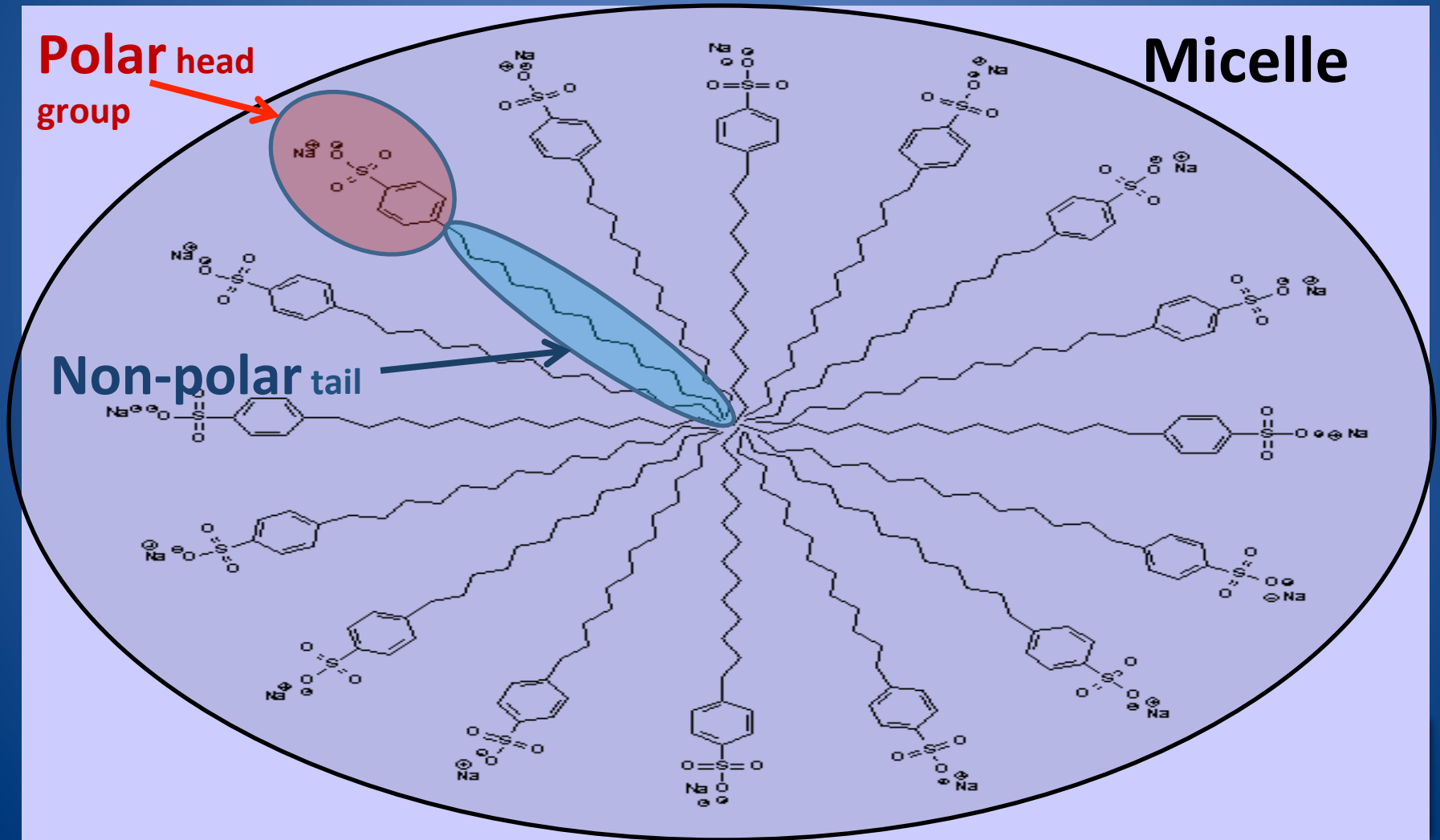


Adding dispersants increases the rate of oil decomposition?

- We can break apart the oil, making minidroplets via the formation of MICELLES
- In small droplets, the oil has much more surface area
- More surface area → more contact with water and bacteria in it → faster decomposition



- Micelles are spherical "blobs" formed by surfactants, which are molecules with two halves
  - A hydrophobic (water fearing) non-polar tail of that interacts with oil (pointing towards the middle)
  - A hydrophilic (water loving) polar head that likes to interact with water
- These allow oil an water to mix!

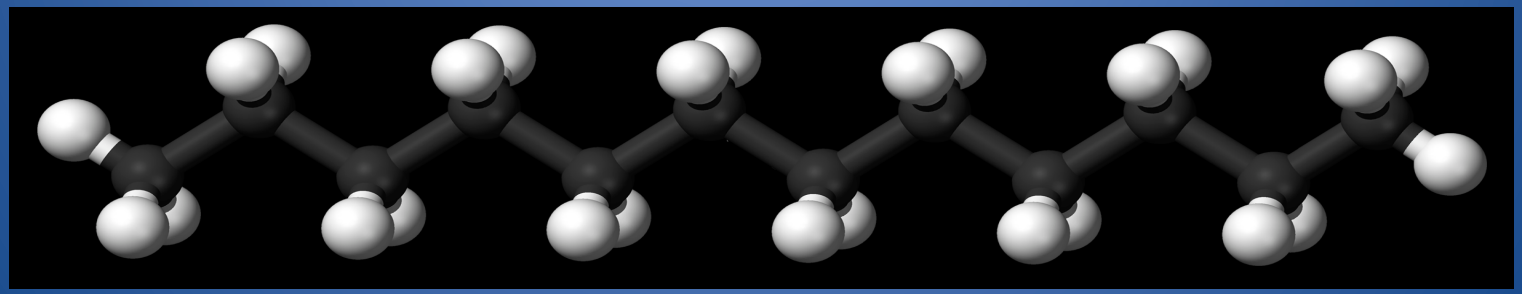


The most commonly used type of surfactant is soap, which disperses dirt/oil

- Soaps disperse dirt and oil in clothing into water so that it can be washed away
- http://www.chemgapedia.de/vsengine/vlu/vsc/en/ch/12/oc/vlu_organik/c_acid/fettsaeuren.vlu/Page/vsc/en/ch/12/oc/c_acid/fatty_acid/fatty_acid.vscml.html for laundering process

Oil is collection of hydrocarbons, so we use models

- We used dodecane (12 carbons) last year as our "model oil", which is a major part of diesel, kerosene, and jet fuel.
- This year we just used spheres to model the oil molecules.



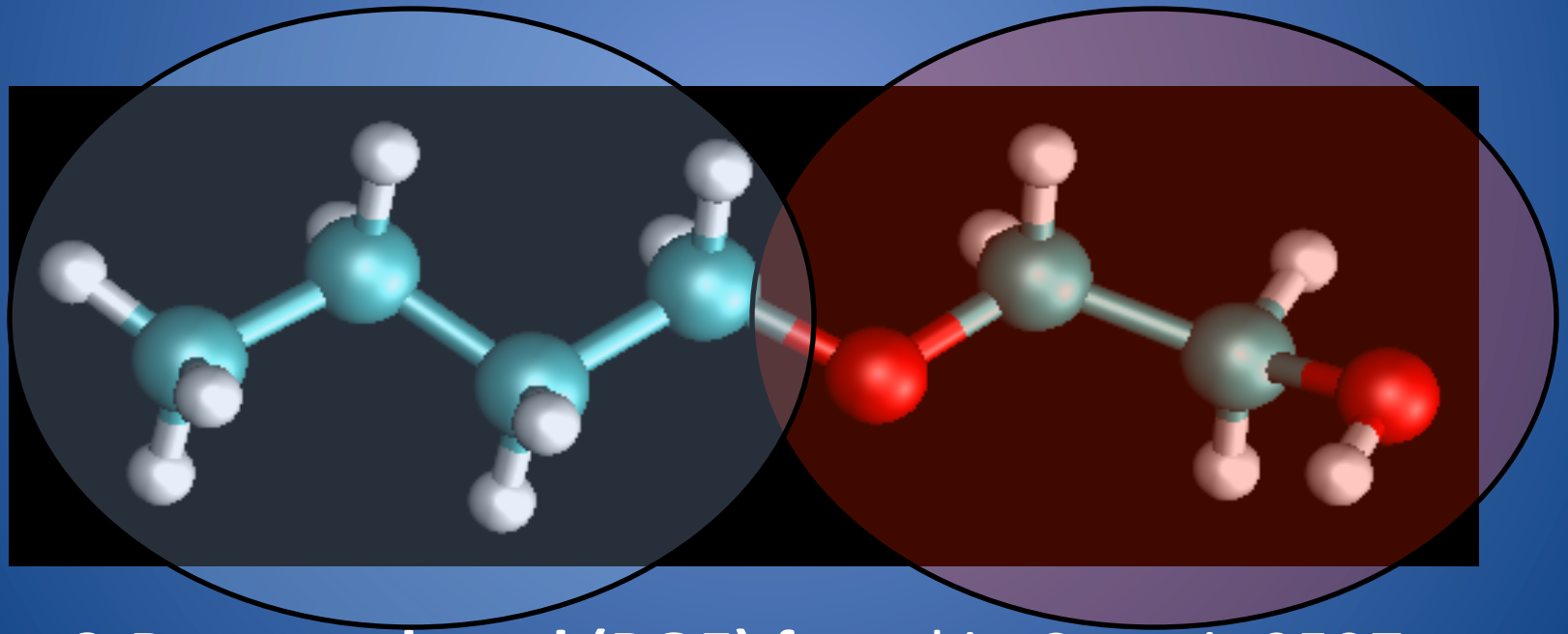
LA TECH

LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

We modeled the most prevalent compound in a commonly used dispersant, Corexit

Non-polar tail

Polar head group

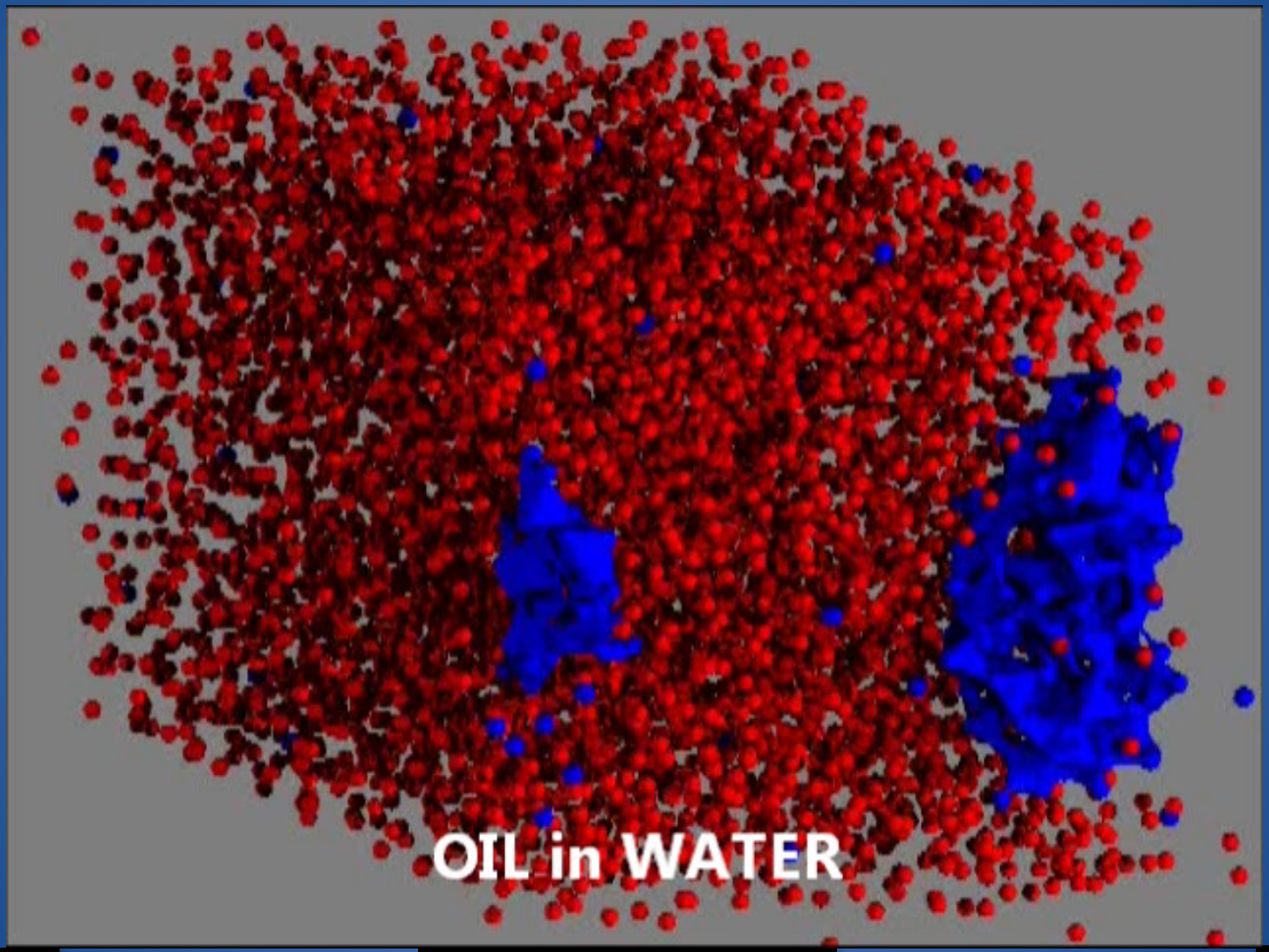


2-Butoxyethanol (BOE) found in Corexit 9527

LA TECH

LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

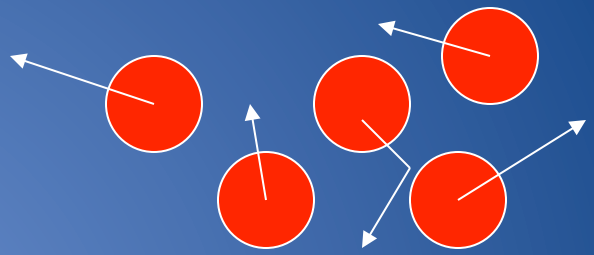
This year's model was much "simpler"



LA TECH

LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

We use the Amber molecular dynamics program which works by following Newton's 2nd Law



- Everything is based off of F=ma.
- Each molecule interactions with all other molecules by bond stretching, bond bending, polar and nonpolar interactions
- These cause a force between atoms
- This forces causes velocities and the system moves following these velocities.
- We move the system in small steps, and calculate the force each step.
- Tweek temperature, bond strengths, locations, etc.

LA TECH

LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

We need input atomic coordinates and velocities to tell the program how the atoms interact, their size, etc.

- We have to generate initial coordinates (see sample code on right)
- We then have to tell the program which molecules are bonded, and how they interact in general (do they bond, have nonpolar interactions, charge (polar) interactions?
- We finally have to tell the program what temperature run at, the timestep (1 femto second 10^{-12} s), how many total steps, etc.

```
implicit none

integer i,j,iunit,ia,ib,ii,m

parameter(iunit=22)

double precision xi(3,iunit),xin(3,iunit,9),vin(3,iunit,9),dx(3)
$ ,boxl

boxl = 51.2295426

dx(1) = 80.0d0

read(10,*)
read(10,*)
read(10,*) ((xi(m,j),m=1,3),j=1,iunit)

ii = 0
dx(2) = 0.0d0
do ia = 1, 3
dx(2) = dx(2) + boxl/3.0d0dx(3) = 0.0d0
do ib = 1, 3
dx(3) = dx(3) + boxl/3.0d0
ii = ii + 1
do j = 1, iunit
do m = 1, 3
xin(m,j,ii) = xi(m,j) + dx(m)
if (m.eq.1) then
vin(m,j,ii) = -0.2
else
vin(m,j,ii) = 0.0
endif
enddo
enddo
enddo
enddo

write(20,9028) (((xin(m,j,ii),m=1,3),j=1,iunit),ii=1,9)
write(21,9028) (((vin(m,j,ii),m=1,3),j=1,iunit),ii=1,9)

9028 format(6f12.7)

stop
end
```

Other types of code?

- http://www.institute.loni.org/lasigma/ to look at HTML

Is Corexit safe?

EPA Test Results

- "The (acute toxicity test) results indicate that the eight dispersants tested are similar to one another based on standard toxicity tests on sensitive aquatic organisms... These results confirm that the dispersant used in response to the oil spill in the Gulf, Corexit 9500A, is no more or less toxic than the other available alternatives."
- "While the dispersant products alone – not mixed with oil – have roughly the same effects, JD-2000 and Corexit 9500 proved to be the least toxic to small fish..."
- www.epa.gov/bpspill/dispersants-qanda.html#effects2

LA TECH

LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

What about our students

- Oil Spill Sphere Impact Study
  - Hydro- Atmo- Litho- Bio-
- Science Fair/Research Opportunities and FUNDING!
- Toshiba's ExploraVision competition
  - Technology development, use, and future use
- Earth Day activities
- Competitions – LEGO, Olympiad, etc.

LA TECH

LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications