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Combustion-generated nanoparticles and their health effects

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theVioligroup

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Risk Assessment of Environmental Nanoparticles

- **RISK = HAZARD + EXPOSURE**
- Too often, the 'exposure' part of this equation is omitted and hazard is equated with risk.
- Recent toxicity studies have demonstrated that high-dose, intratracheally-instilled, SWNT in the lungs of rats may produce unusual foreign-body tissue reactions.

- *But what is the exposure levels of carbon nanotubes?*

Negligible

In summary

- Nanoparticles from diesel source
- Epidemiological studies
- Factors" Solubility, chemical composition, surface area, number, shape, singlet or agglomerates, etc...

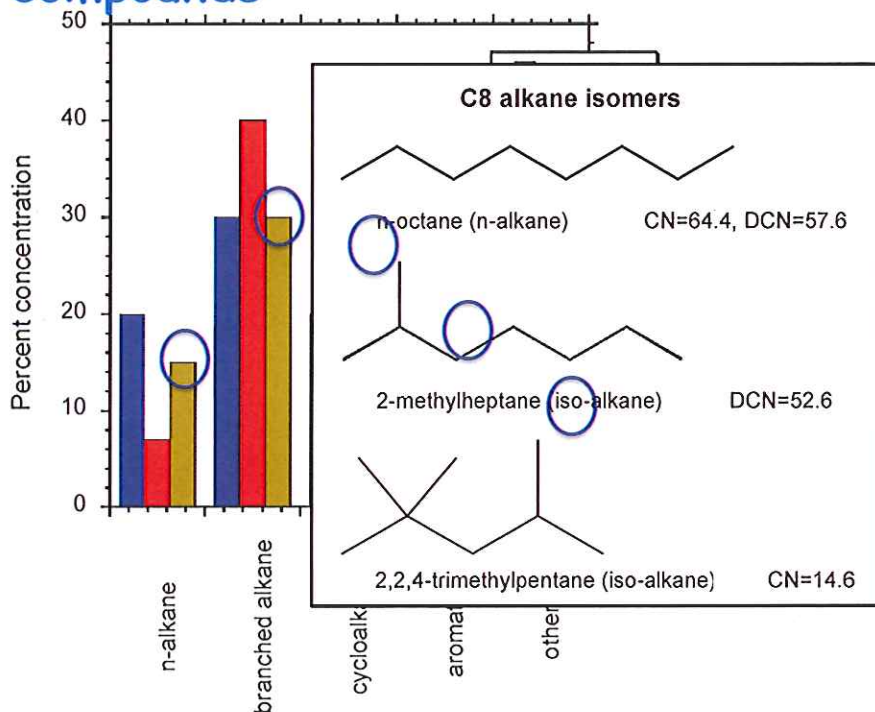
Main questions

- How combustion-generated nanoparticles look like?
- What is the mode of **entry** into cells?

The flow...

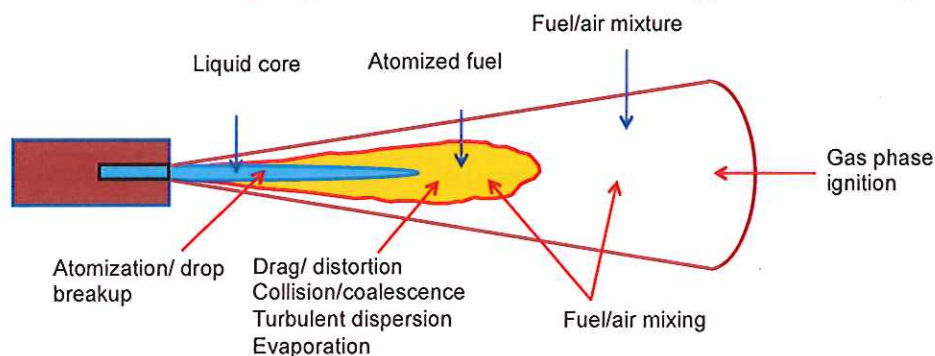
- Model diesel engines:
 - What fuel? Is heptane a good model for diesel fuels?
- Nanoparticle formation in diesel conditions
- Interactions with biological cells

Transportation Fuels: mixtures of many compounds

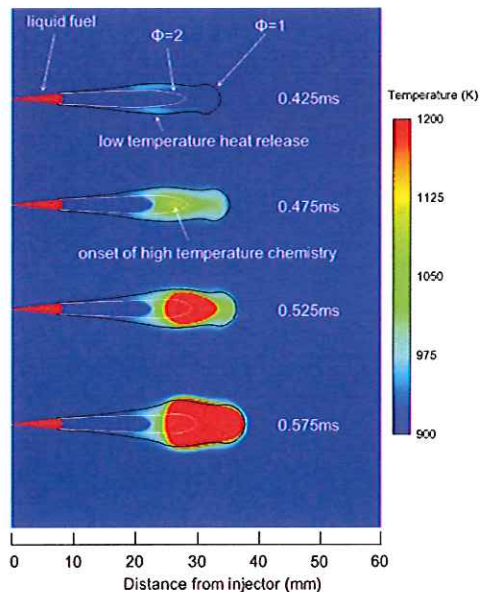


Fuel Surrogate and Engine Simulations

- Model compounds that reproduce real fuels
- We matched some physical and chemical properties (density, vapor pressure, viscosity, specific heat for liquid length and chemical composition)
- We looked at spray characteristics and ignition delay

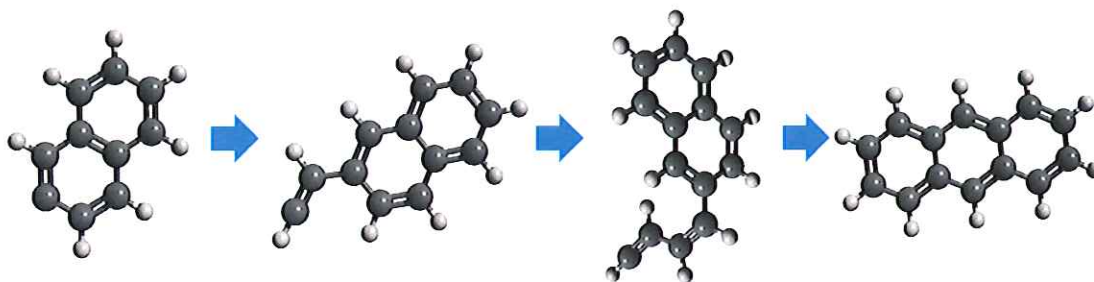


Engine Simulations



- CFD simulations for diesel surrogate
- We used spatial/temporal information from the CFD to look at the formation of nanoparticles
- For example, T, P, hydrocarbon concentrations

SNAPS for nanoparticle formation in combustion



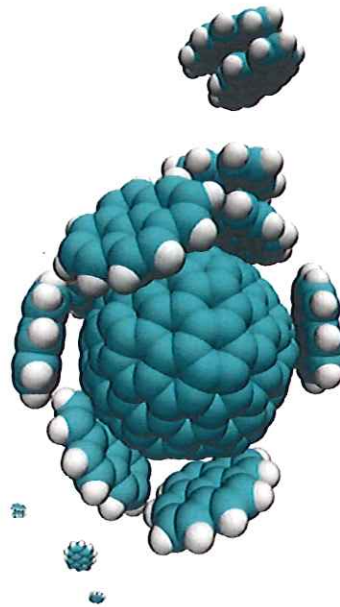
- Stochastic Nanoparticle Simulator – SNAPS code.
- It links chemistry, environment (T, P, Gas Phase Species) to **molecular structure**
- Detailed particle **morphology**
- Both **elementary** and global reactions

In addition

Presence of nanoparticles influence growth mechanisms of other species.

Nanoparticles can act as nuclei

Fullerene and PAHs



Our contribution to the field

- RISK = HAZARD + EXPOSURE (ASSESSMENT)

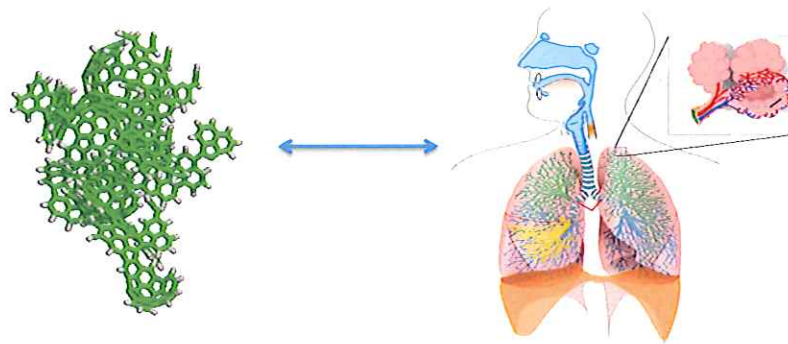
Investigating the behavior of **combustion-generated nanoparticles**

- Go beyond correlations, focusing on “molecular mechanisms of interactions between nano and biological systems”

(what chemical and physical properties of nanoparticles influence mode of entry and fate?)

Nano-Bio Interface

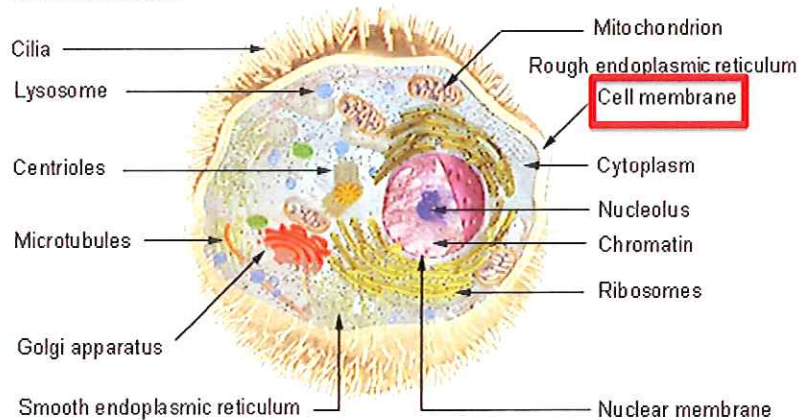
Interactions of Carbonaceous Nanoparticles with Biological Systems



Cell: smallest unit of living organisms

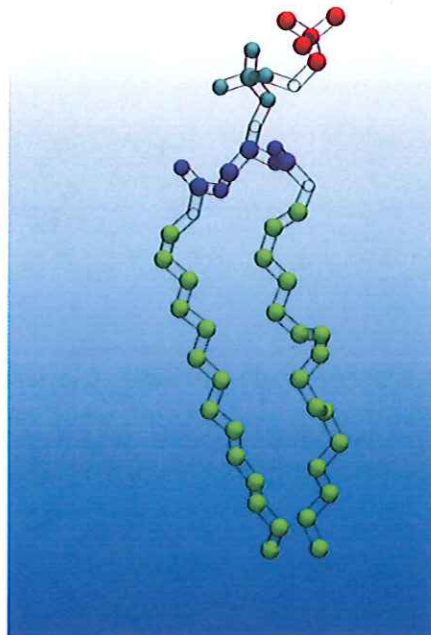
There are many different types of cells in the body. However, they all contain three parts: the cell membrane, the nucleus, and the cytoplasm.

Cell Structure

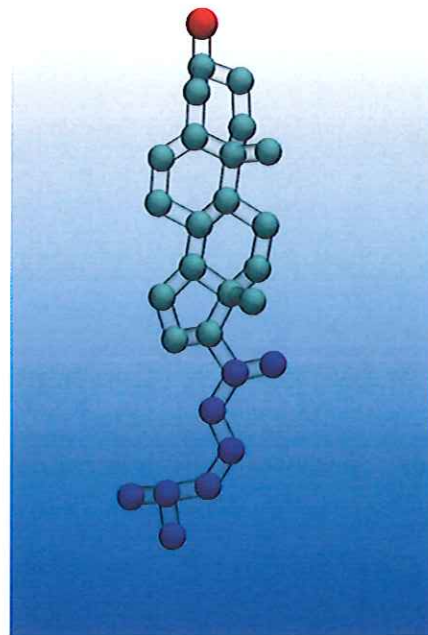


Molecular dynamics simulations

- Systems: lipid bilayers of POPC/CHOL and carbonaceous nanoparticles
- Code: NAMD 2.7b4; PLUMED 1.2.0
- *Force fields CHARMM27 + CGenFF*
- *Thermostat 310 K; Barostat 1 atm*
- Compute: Dynamics and Free energy profiles



POPC



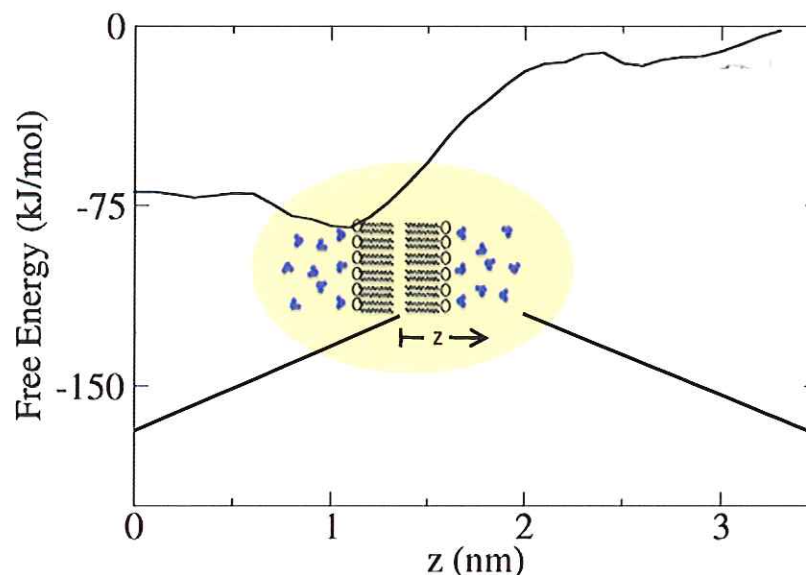
CHOL

Properties of interest

Size, solubility, chemical composition, surface area, number, shape, singlet or agglomerates, etc...

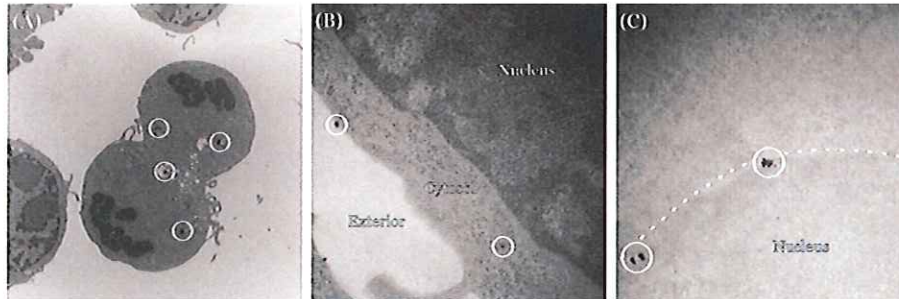
- Upon exposure, NPs may enter cells by **different mechanisms** dependent on their size, material, and surface characteristics.
- The pathways of **entry** and the subsequent intracellular particle distribution influence the biological effects caused by particles.

Free Energy Profile from MD simulations



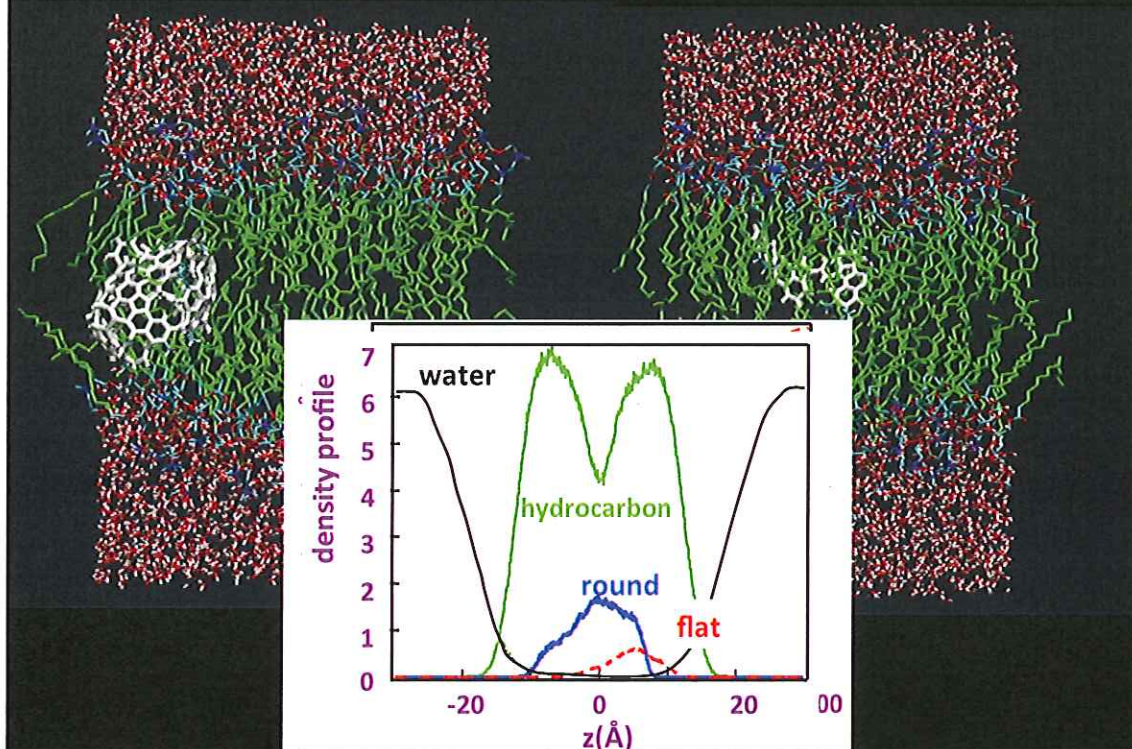
Biological experiments

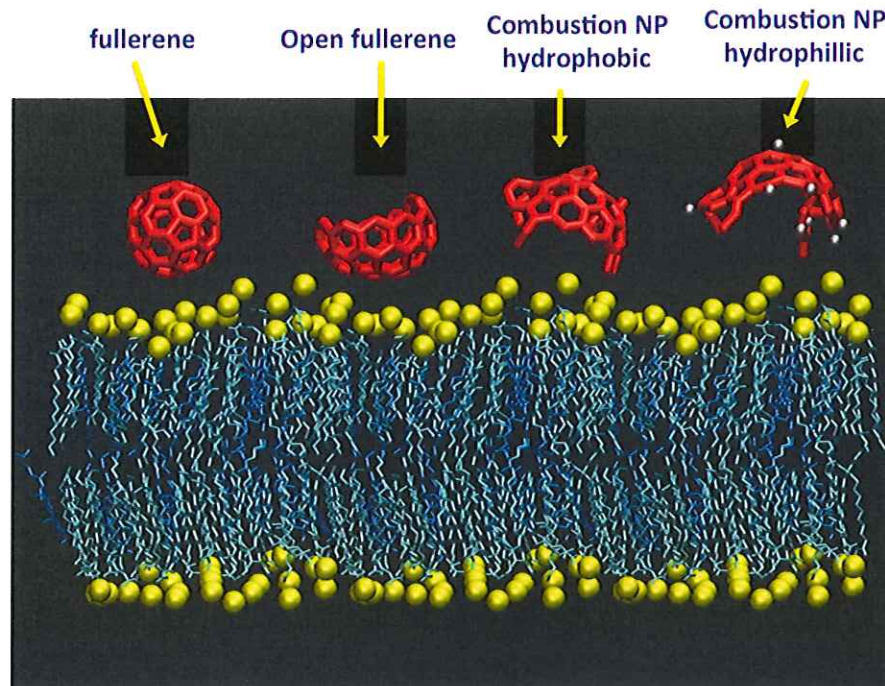
- We exposed RAW 264.7 immortalized macrophages to different concentrations of fullerenes.



- TEM micrograph of RAW 264.7 with C_{60} .
 (A) in cytoplasm; (B) adjacent to cell membrane.
 (C) Clusters that are not contained in classical phagocytotic structures

Combustion-generated Nanoparticles in lipid bilayer





Fiedler and Violi, Biophysical Journal 99: 144-152 (2010)



Need for extended set of parameters for particle penetration in biological systems

- **C60 is limited** in its ability to generically represent the toxicity of similarly sized nanoparticles.
- **Surface area and chemical composition** appear to be the parameters that influence the permeation process.
- To adequately assess the health effects of anthropogenic carbonaceous nanomaterials, an **expanded and inclusive set** of representative systems should be considered.