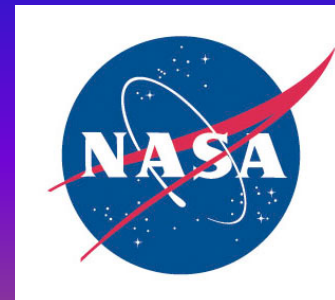


Challenges Associated with Representing DOM and CDOM in Models

Raleigh Hood

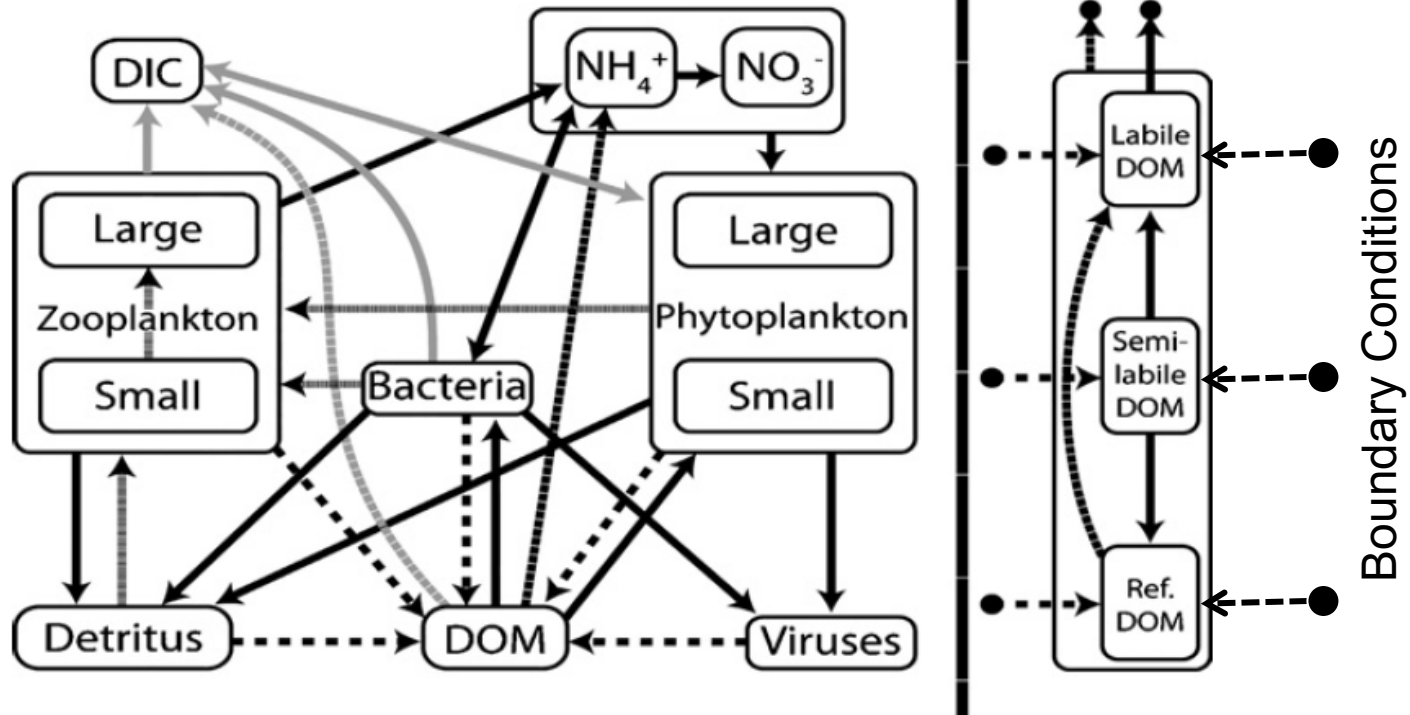
OCB Annual Meeting

Woods Hole, MA, June 26, 2017



Representing DOM and CDOM in models:

From Keller and Hood (2011)



State-of-the-art in 2011: DOM is modeled as labile, semi-labile and refractory pools. Problems:

- Each of these DOM pools represents a very complex mixture of compounds.
- Transformations among pools are poorly constrained.
- Photo-lability and microbial lability are not synonymous with one another.
- CDOM is not represented.
- Terrestrial DOM supply is specified as a poorly constrained boundary condition.
- Planktonic food web DOM sources are poorly constrained.

Representing DOM and CDOM in models:

Constituents of DOM

See Chapter 22 in Libes for structures of organic compounds

Semi-Bio-Labile

High molecular weight >5000 Da (includes colloids)

- proteins
- **polysaccharides** (mucus, structural polymers)
- nucleic acids
- some humic substances

Mixed-Bio-Lability
Some Refractory

Medium Molecular weight 500-5000 Da

- humic substances (**refractory**)
- oligopeptides, oligonucleotides
- lipids
- pigments

Bio-Labile

Low molecular weight < 500 Da

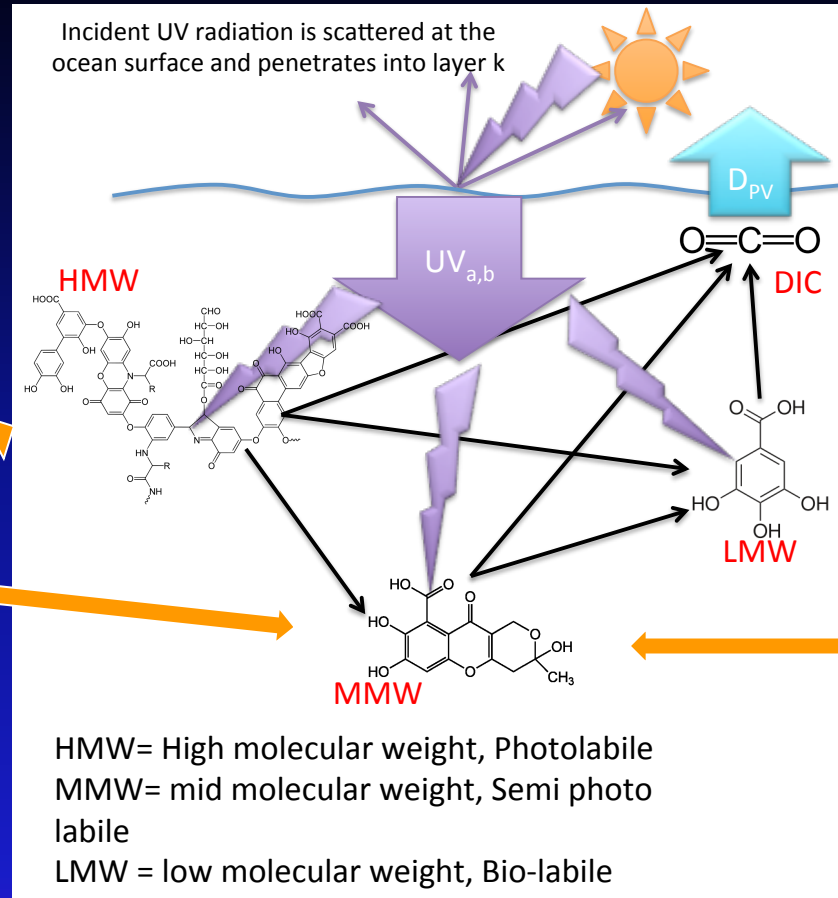
- monomers (sugars, amino acids, fatty acids)
- osmolytes (DMSP, betaines, polyols)
- toxins, pheromones and other specialty chemicals

- Each of these DOM pools represents a very complex mixture of compounds.
- Photo-lability and microbial lability are not synonymous with one another.

Representing DOM and CDOM in models:

- Representing DOM as a set of labile, semi-labile and refractory pools is a gross oversimplification of reality.
- Moreover, where transport is dominated by diffusion (e.g., between the water column and the sediments and in the sediments) this approach violates physicochemical laws of diffusion because diffusion acts on the basis of individual chemicals, i.e., the concentration gradient of individual chemicals – not the bulk pool.
- Technically, this approach is only correct if each pool represents one chemical constituent of DOM. It follows that in order to correctly model DOM and CDOM you must represent every single chemical constituent as a separate state variable and every single transformation as a specific photochemical reaction or microbial enzymatic reaction.
- But there are 1000s of chemical constituents and transformations in DOM and CDOM and many (most?) are not well understood.
- It is not feasible to represent 1000s of chemical constituents and transformations of DOM and CDOM in our models.

Representing DOM and CDOM in models:



- We are pursuing a different approach.
- Construct pools that are informed by state-of-the-art understanding.
- DOM is modeled as high molecular weight (more colored/photolabile), mid-molecular weight (mid-colored/semi-photolabile) and low molecular weight (less colored/bio-labile) pools.
- Terrestrial sources provide mostly HMW, and MMW more colored, photolabile DOM.
- Planktonic foodweb sources provide mostly MMW and LMW, less colored and bio-labile DOM.

Thank You