Agent-Based Modeling of Hyporheic Zone Carbon Biogeochemistry

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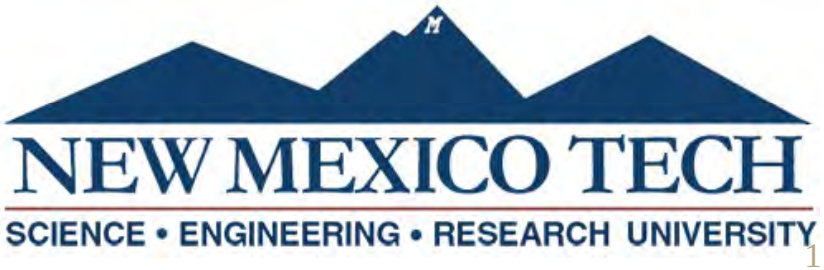
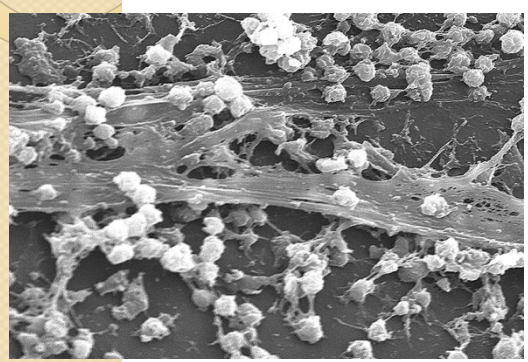
7 April 2011

New Mexico EPSCoR



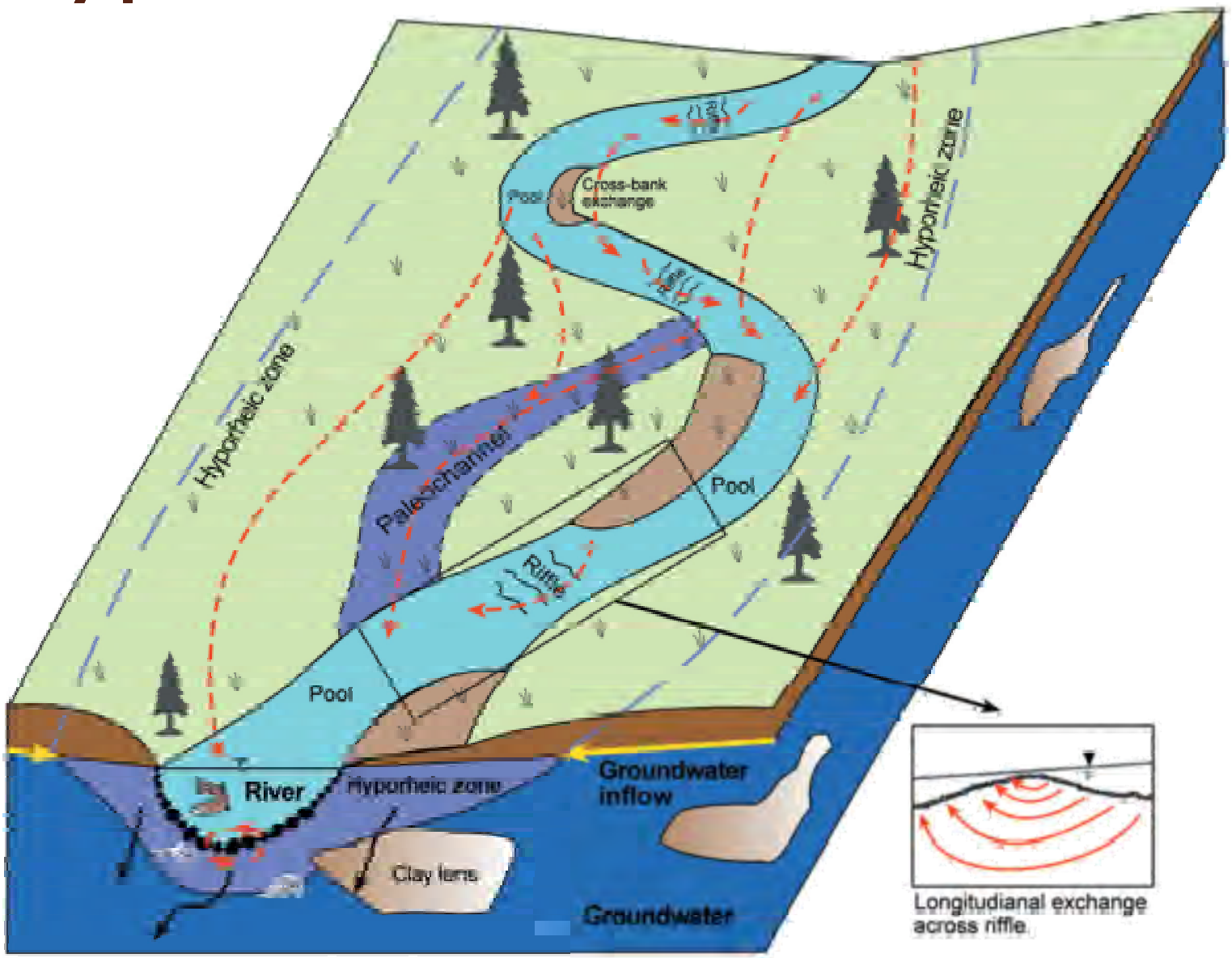
Dissolved Organic Carbon



http://en.wikipedia.org/wiki/File:Staphylococcus_aureus_biofilm_01.jpg

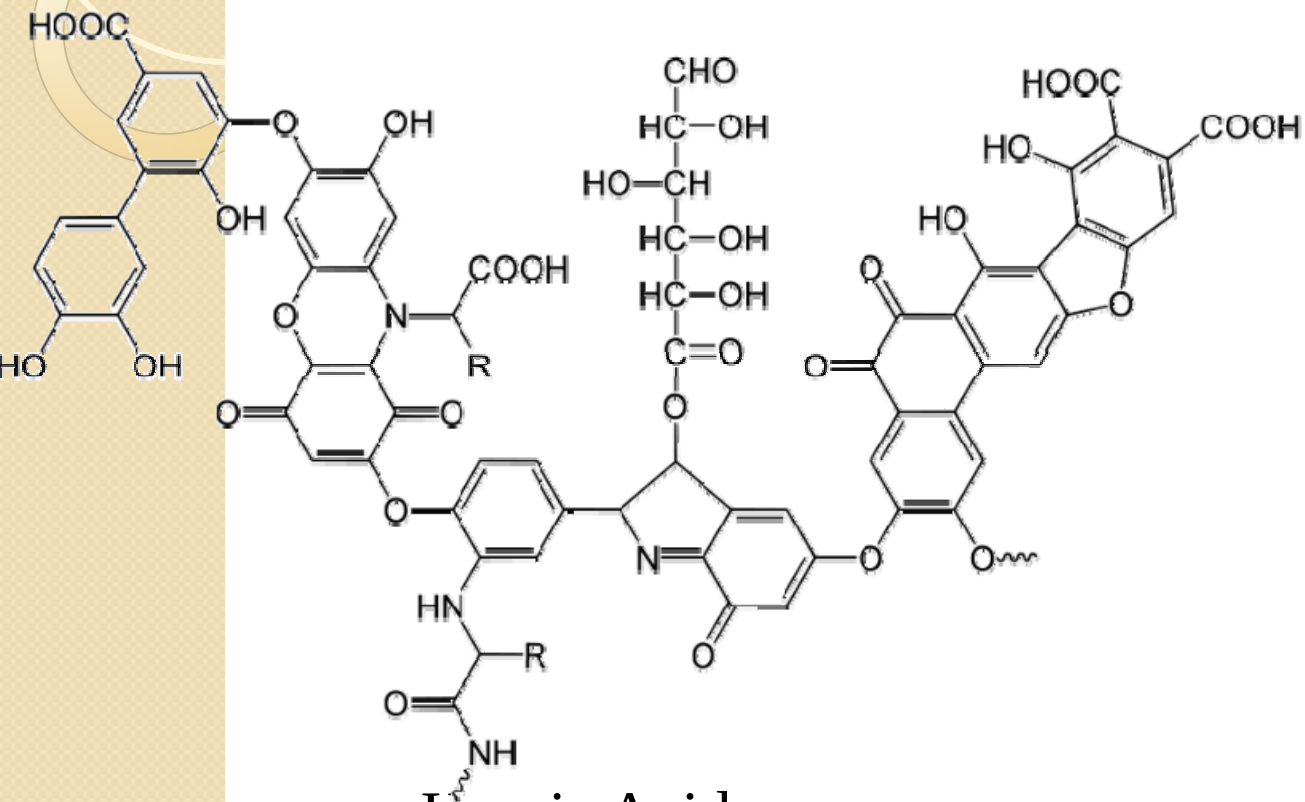
http://www.abcwua.org/content/view/32/25/

Hyporheic Flow

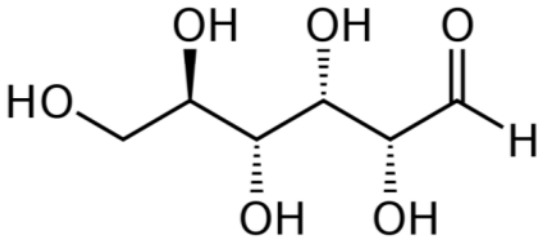


Tonina & Buffington, 2009

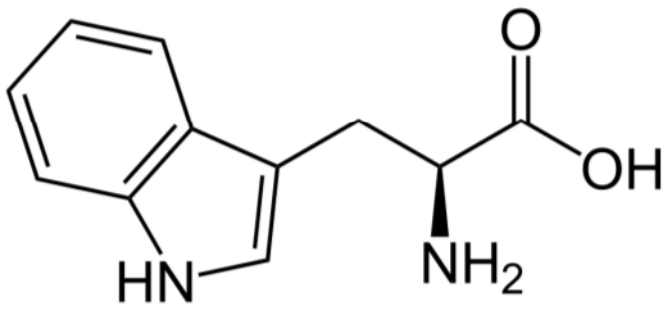
Agent-Based Modeling



Humic Acid
MW = variable



Glucose
MW = 180.16 g/mol



Tryptophan
MW = 204.23 g/mol

AlphaStep: Batch Model

Displaying molecule number 38 | << Back | Go to Molecule 38 | Forward >> | Exit Inspector

Elemental Composition

Carbon	400
Hydrogen	416
Oxygen	101
Nitrogen	0
Sulfur	0
Phosphorus	0

Functional Groups

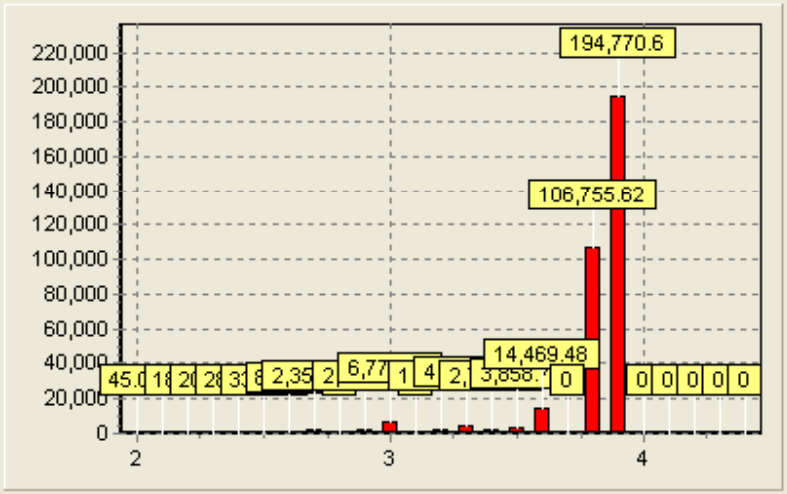
C=C	150	Aldehydes	4
Rings	38	Acids	0
Phenyl	33	Aro. Acids	0
Alcohols	17	Amines	0
Phenols	1	Ring N	0
Ethers	79	Amides	0
Esters	0	Thiols	0
Ketones	1	P-esters	0

Molecular Properties

Molecular Wt.	6840.16
Net Charge	0
Charge Density	0
Aromaticity %	0.75
Bioavailability	0
Kow	0
Kcu	0
Kads	0

Reaction Probabilities

Ester Cond.	0.000E+0
Ester Hydr.	0.000E+0
Amide Hydr.	0.000E+0
Microb. Uptk.	0.000E+0
Dehydration	8.445E-11
Hydration	5.384E-9
Strong Oxid.	8.086E-5
Mild Oxid.	4.043E-4
Alcohol Oxid.	4.312E-5
Aldehyde Oxid.	1.078E-5
Decarboxylation	0.000E+0
Aldol Condens.	6.819E-7



Selected Plot: Mass by log MW

AlphaStep Algorithms

Elemental Composition	Starting materials (precursor compounds)					
	Protein	Cellulose	Lignin	Tannin	Terpenoid	Flavonoid
Carbon	240	360	400			
Hydrogen	382	602	402			
Nitrogen	60	0	0			
Oxygen	76	301	81			
Sulfur	0	0	0			
Phosphorus	0	0	0			
Functional groups						
C=C bonds	15	0	160			
Rings	5	60	40			
Phenyl rings	5	0	40			
Alcohols	10	182	2			
Phenols	0	0	1			
Ethers	0	119	79			
Esters	0	0	0			
Ketones	0	0	0			
Aldehydes	0	0	0			
Acids	6	0	0			
Aromatic Acids	0	0	0			
Amines	6	0	0			
Amides	54	0	0			
Thioethers	0	0	0			
Thiols	0	0	0			
Phosphates	0	0	0			

(1) Ester hydrolysis

$k' = (\#\ \text{Esters})\,[H_2O]\,A\,e^{-\Sigma_a/RT}\,(1 + b\,[H^+] + c\,[OH^-])$

$A = 6 \times 10^5\ h^{-1} \quad E_a = 60\ kJ\ mol^{-1}$ $b = 10^8$ $c = 5 \times 10^8$

(2) Amide hydrolysis

$k' = (\#\ \text{Amide})\,[H_2O]\,A\,e^{-\Sigma_a/RT}\,([H^+] + 10^{-6.54} + b\,[OH^-])$

$A = 6 \times 10^6\ h^{-1} \quad E_a = 50\ kJ\ mol^{-1}$ $b = 10$

(3) Alkene hydration

$k' = (\#\ C{=}C)\,[H_2O]A\,e^{-\Sigma_a/RT}\,[H^+]$

$A = 2 \times 10^{13}\ h^{-1} \quad E_a = 80\ kJ\ mol^{-1}$

(4) Alcohol dehydration

$k' = (\#\ OH)A\,e^{-\Sigma_a/RT}\,[H^+]$

$A = 10^{12}\ h^{-1} \quad E_a = 80\ kJ\ mol^{-1}$

(5) Weak C=C oxidation

$k' = (\#\ C{=}C)\,(A_{enz}[O_2]E_O\,e^{-\Sigma_a/RT} + A_{photo}[O_2]I)$

$A_{enz} = 5 \times 10^9\ h^{-1}\ M^{-1}\ E_a = 50\ kJ\ mol^{-1}$

$A_{photo} = 5 \times 10^7\ h^{-1}\ M^{-1}$

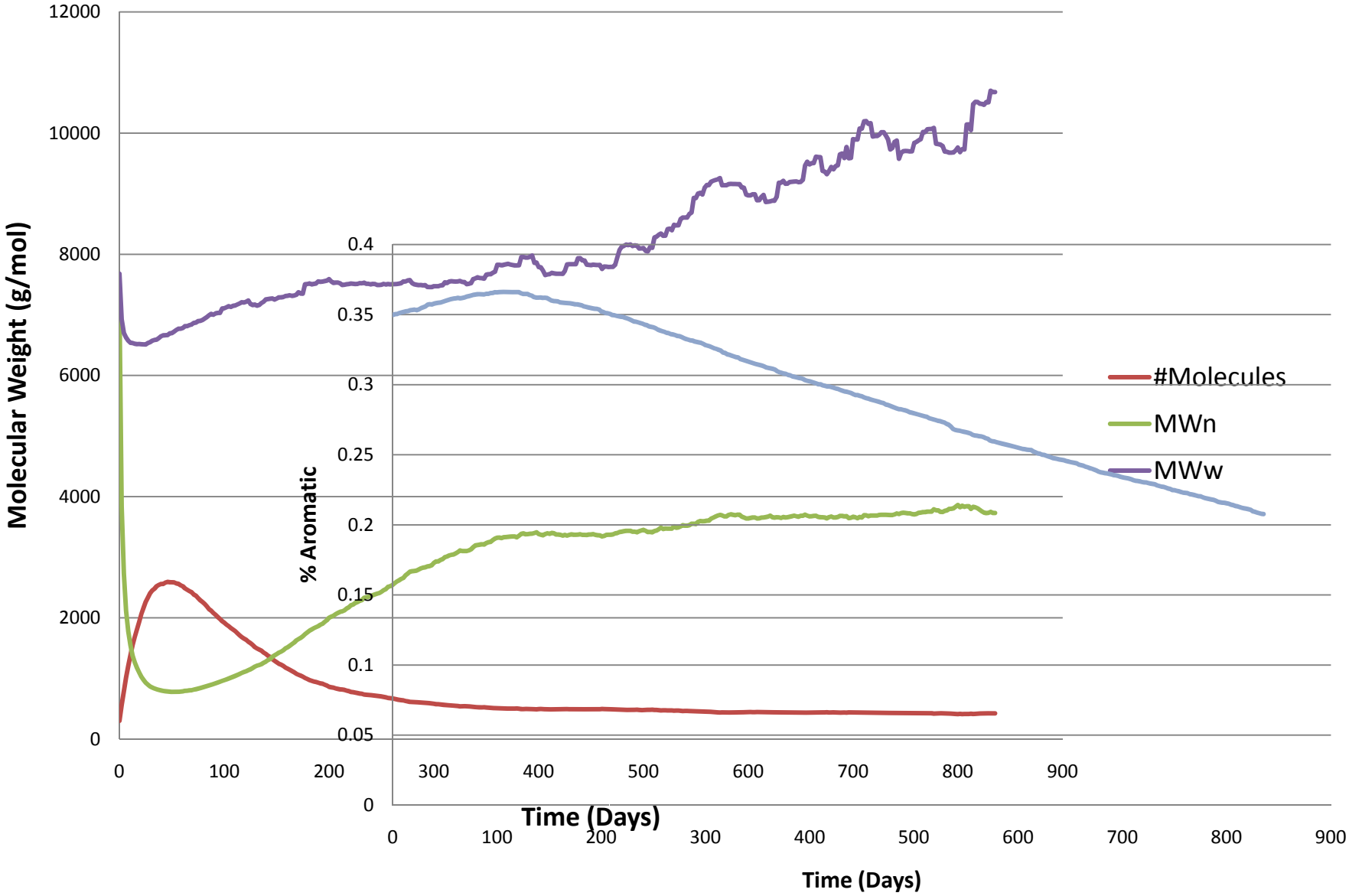
(6) Strong C=C oxidation

$k' = (\#\ C{=}C)\,(A_{enz}[O_2]E_O\,e^{-\Sigma_a/RT} + A_{photo}[O_2]I)$

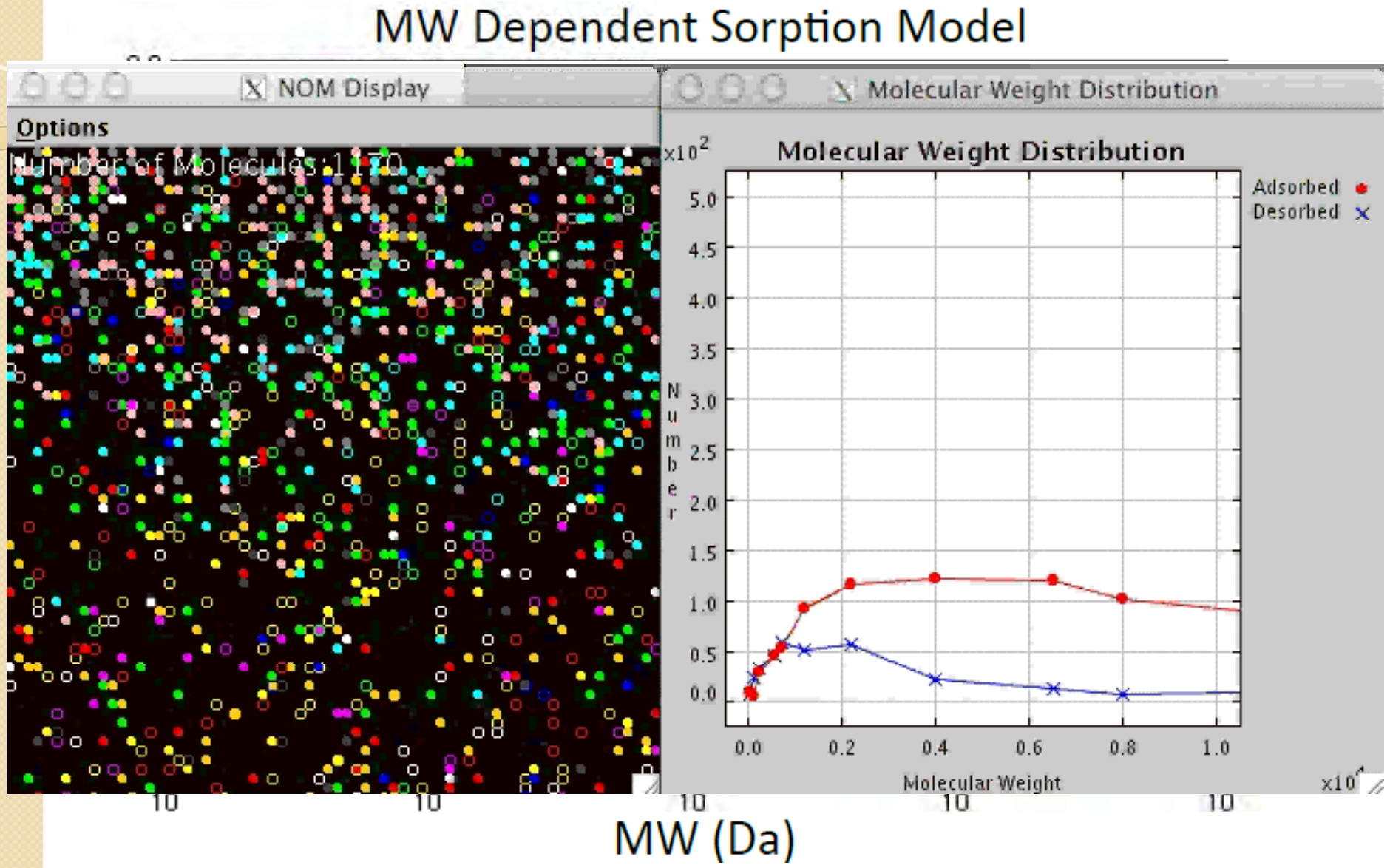
$A_{enz} = 10^9\ h^{-1}\ M^{-1} \quad E_a = 50\ kJ\ mol^{-1} \quad A_{photo} = 10^7\ h^{-1}\ M^{-1}$

22 Jul 2010
T = 8.6 deg C
DO = 0.87 ppm = 0.027 mM
pH = 6.42
100 of each input molecule
Biological conditions

AlphaStep Simulations

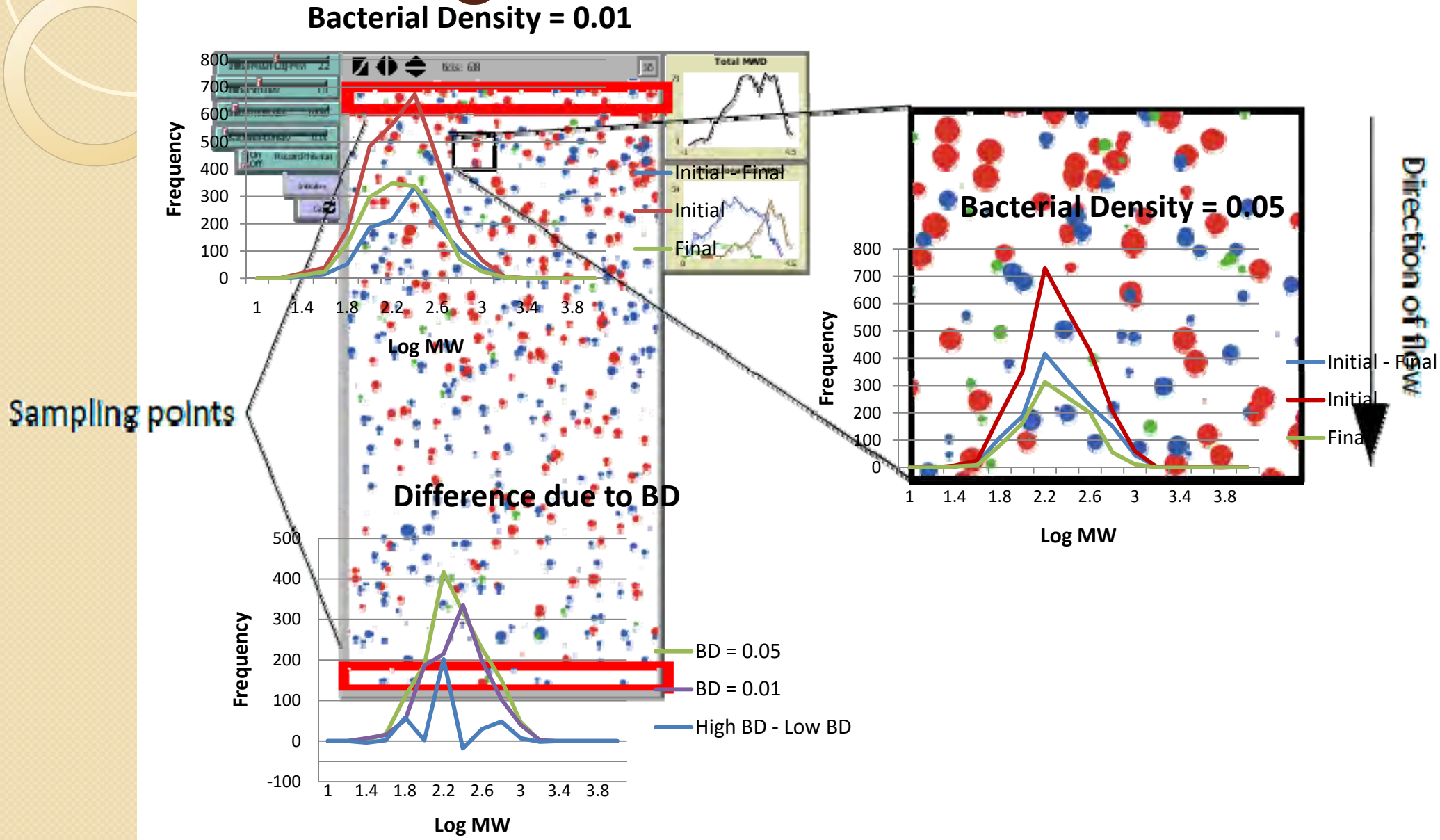


Sorption Model: NOMSim

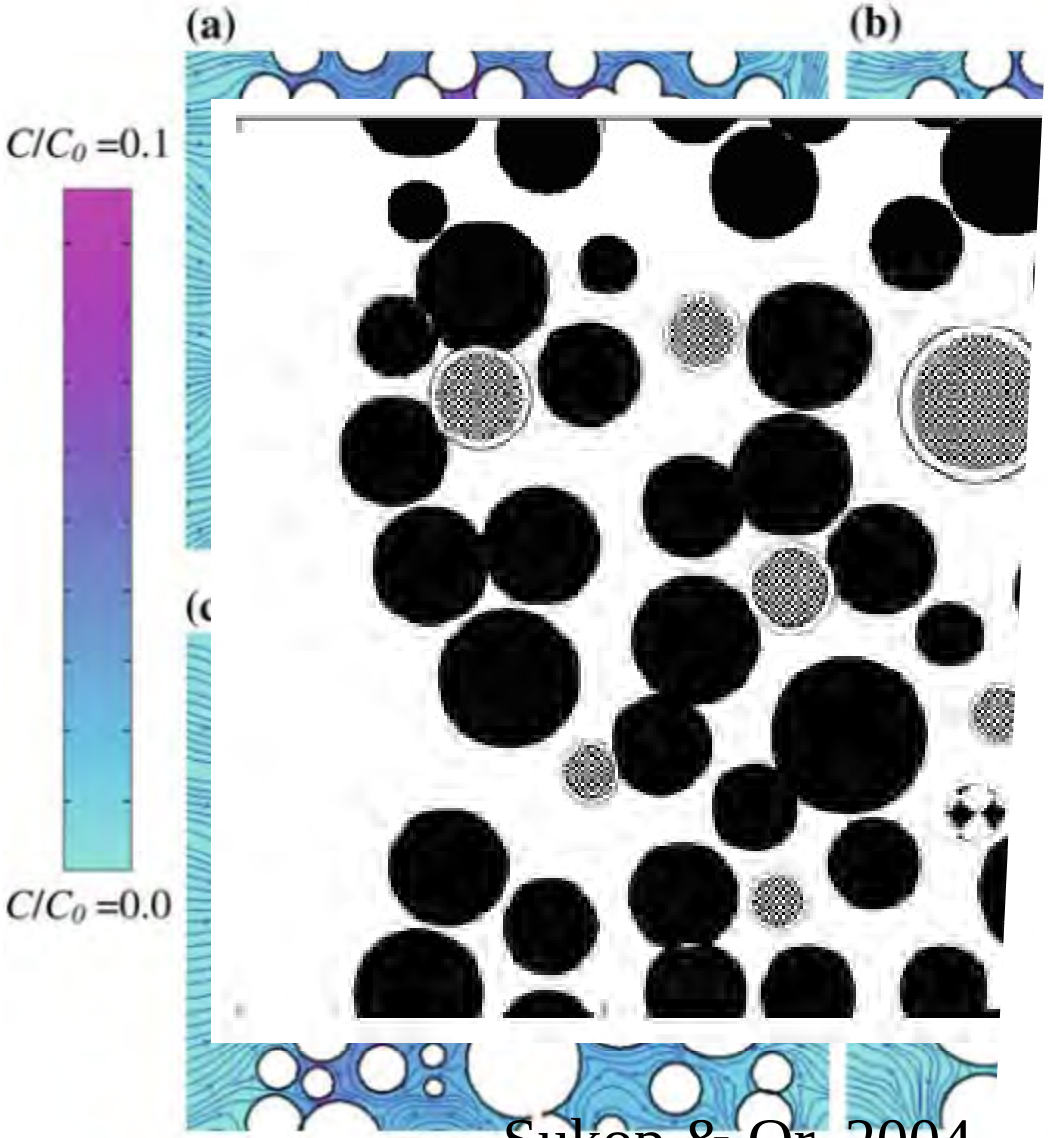


http://www.nd.edu/~nom/Movies/NOM2.mov

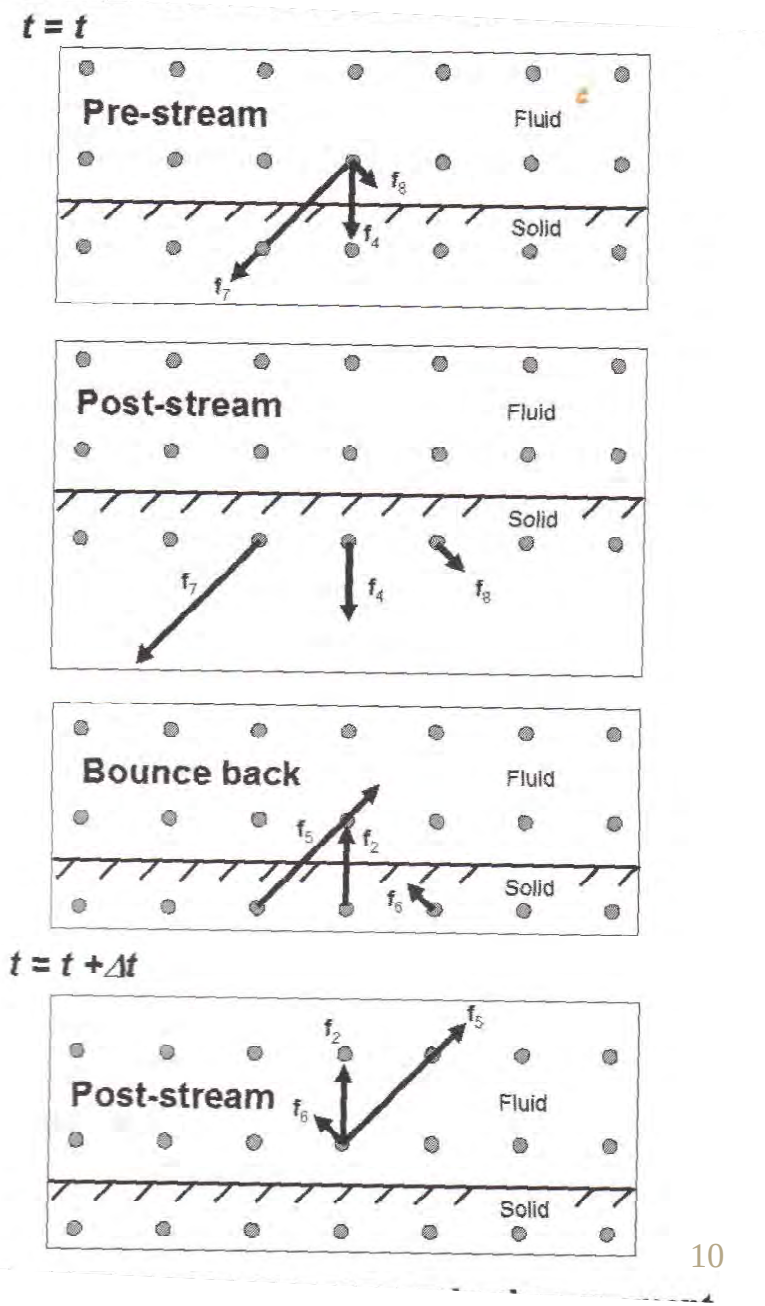
NetLogo Model



Lattice Boltzmann Modeling

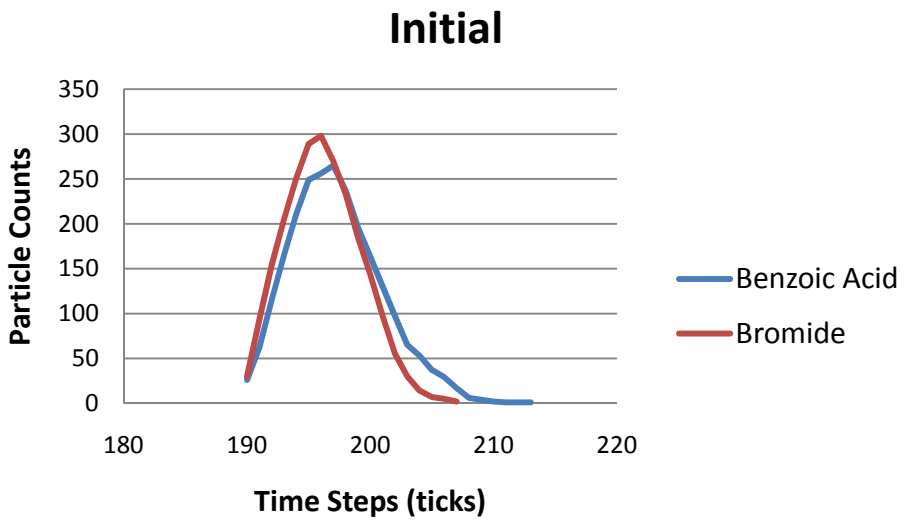


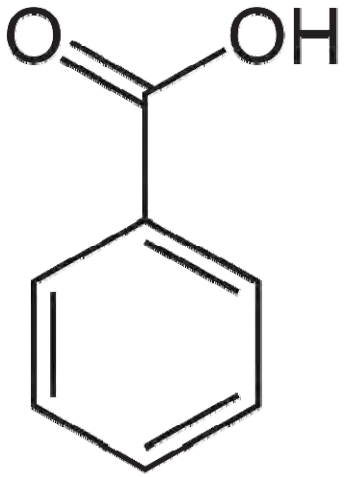
Li & LeBoeuf, 2010



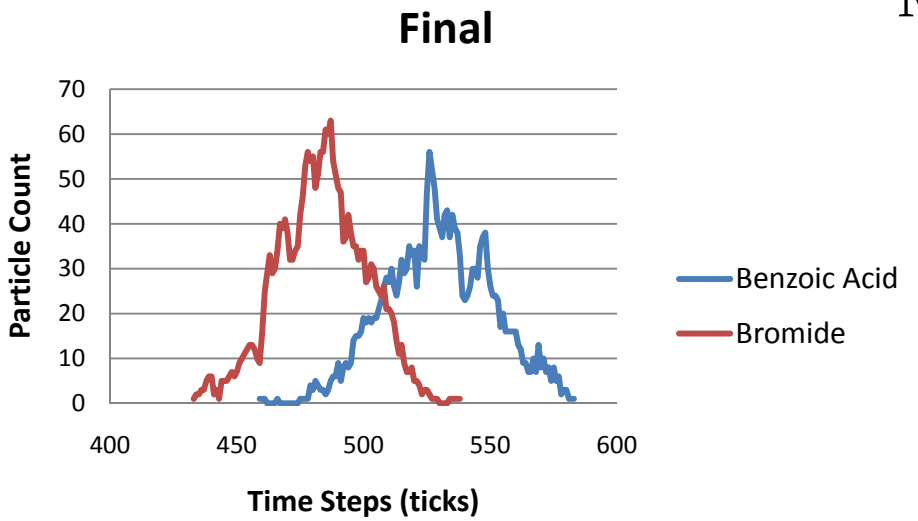
Sukop & Or, 2004

Reactive Tracer Test





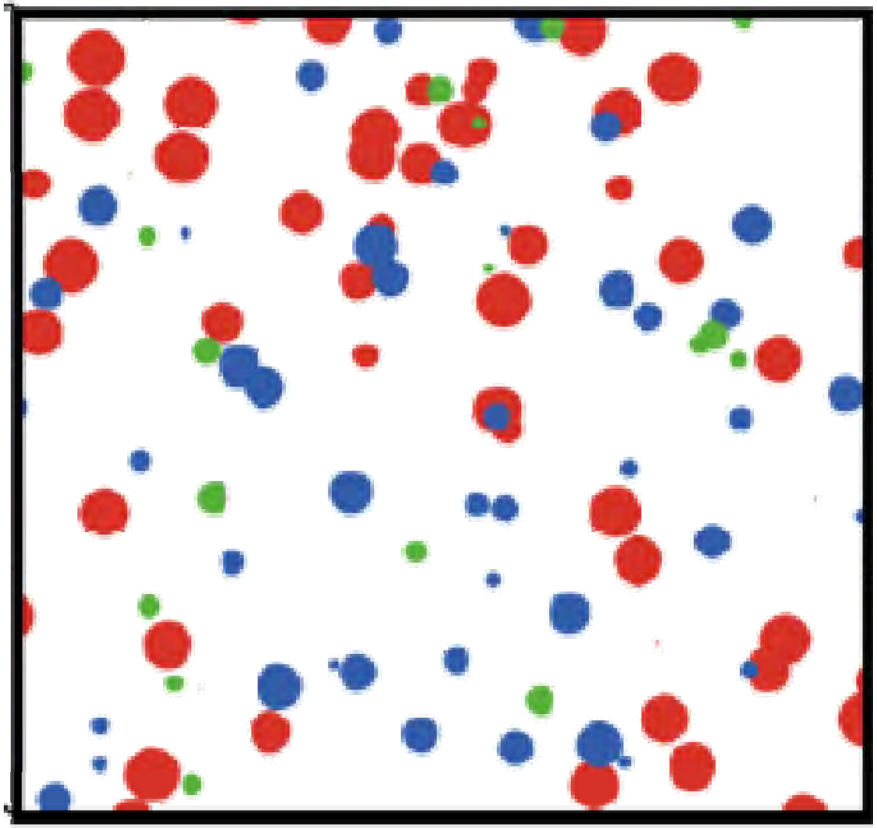
MW = 122 g/mol



Climate Change Scenarios

- Temperature
- Microbial Activity
- Hydrologic Conditions
- DOC Source

Benefits and Limitations



Questions?