Biocomplexity In Subsurface Bioremediation Problems

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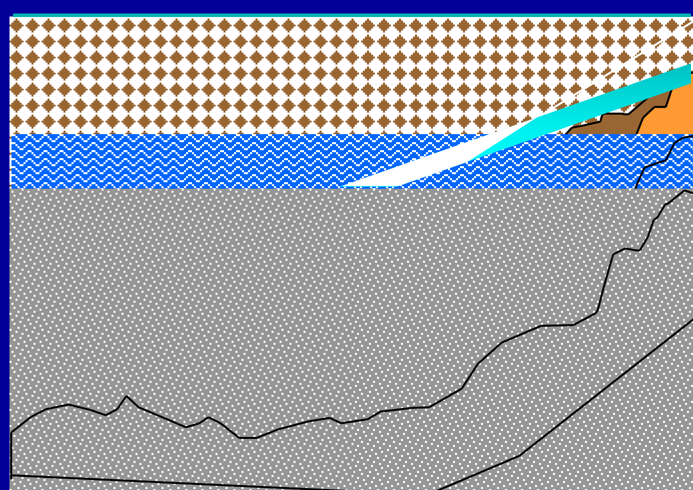
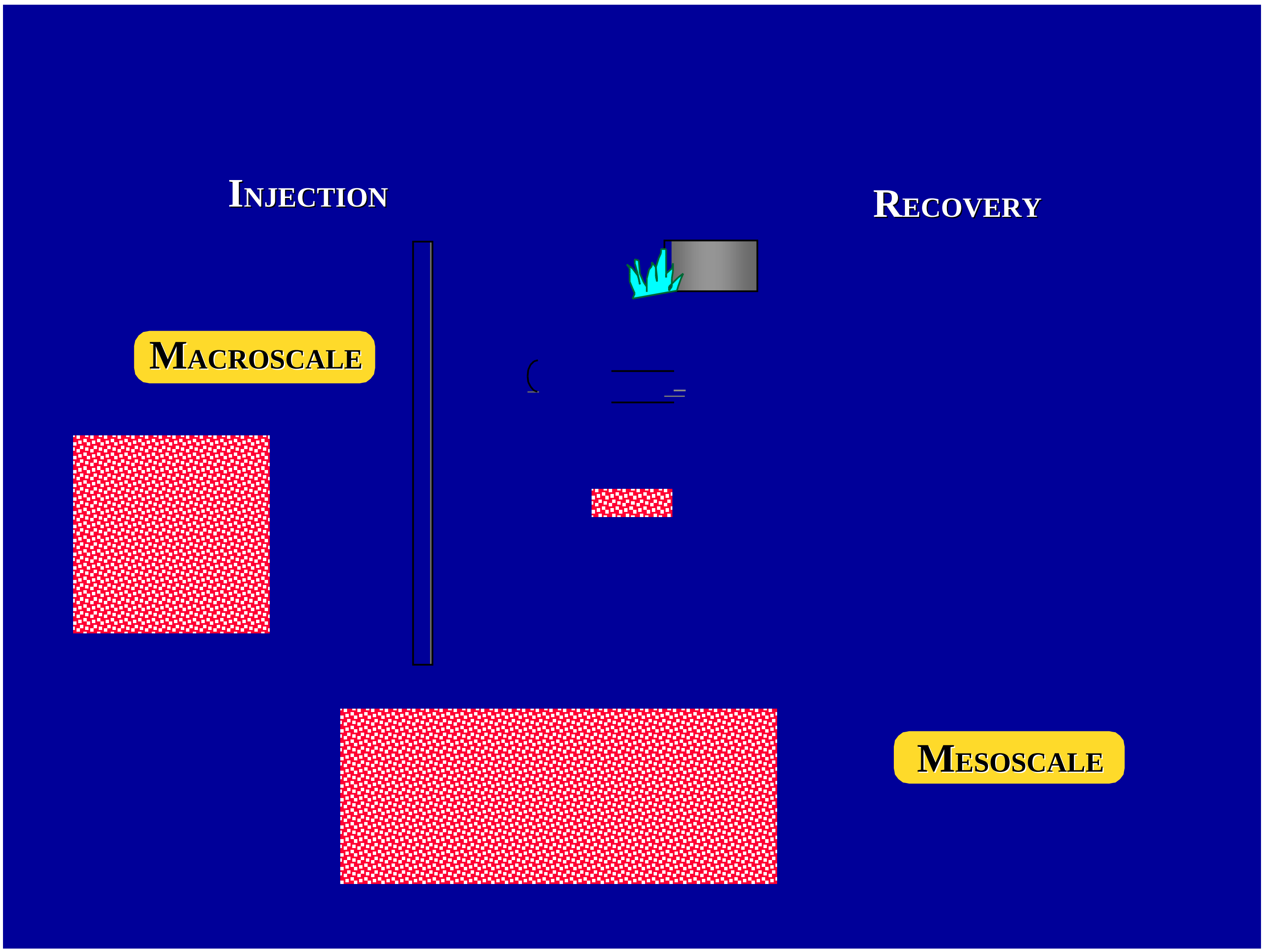
LEAKY UNDERGROUND STORAGE TANKS



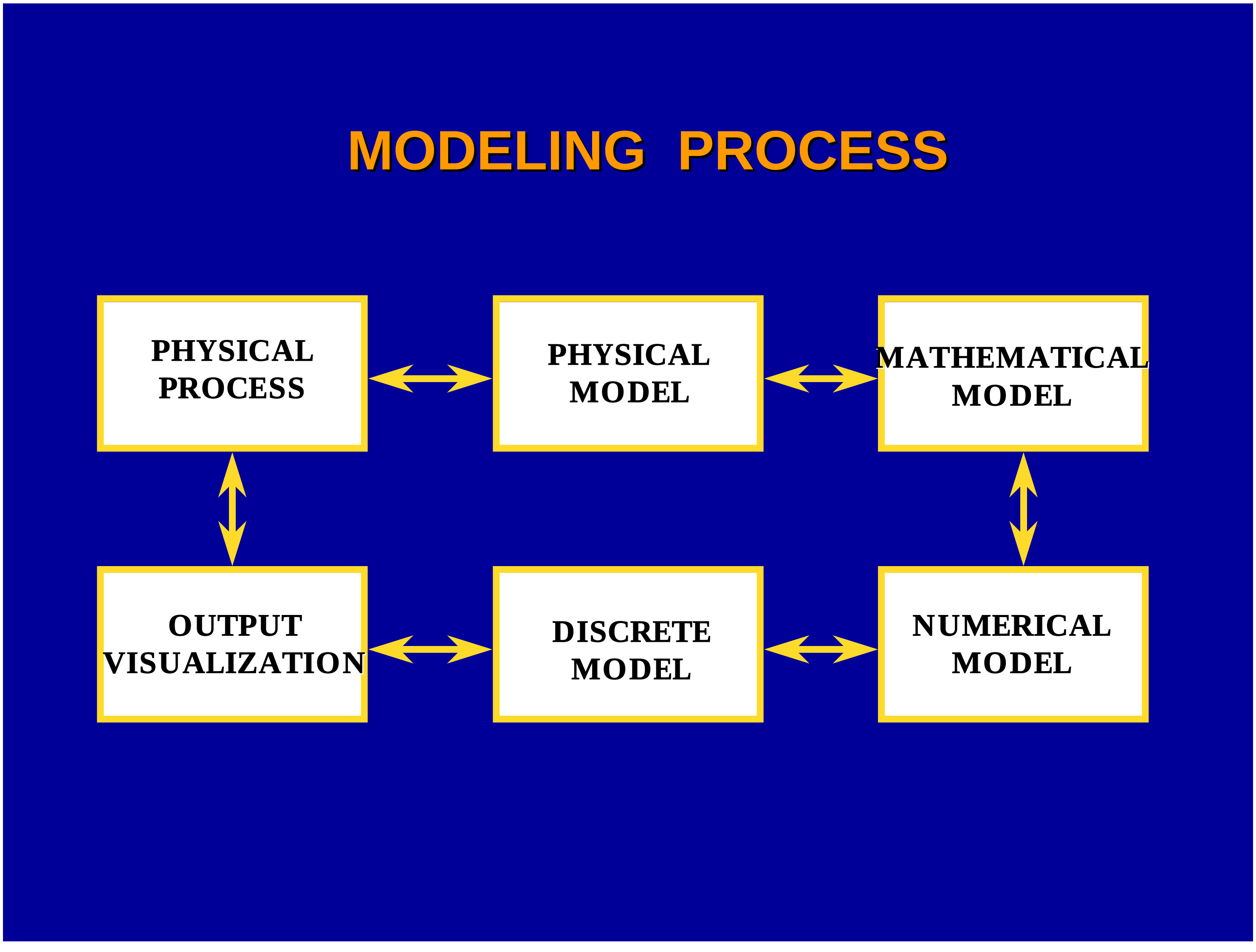

INJECTION
RECOVERY
MACROSCALE
MESOSCALE

NEED FOR SIMULATION

- Develop Better Understanding Of Nonlinear Behavior
  - Computational Laboratory ⟷ Experiments
  - Understand Sensitivities Of Parameters
  - Isolate Phenomena then Combine
- Scale - Up Information And Understanding
  - Pore ⟶ Laboratory ⟶ Field
- Obtain Bounding Calculations
- Develop Predictive Capabilities
  - Optimization And Control

REQUIREMENTS (SCALE - RELATED)

- Effective Physics And Equations
- Effective Parameters And Functions
- Measurable Input Data
- Efficient Implementation Procedures
- Accurate Numerical Methods


MODELING PROCESS
PHYSICAL PROCESS
PHYSICAL MODEL
MATHEMATICAL MODEL
OUTPUT VISUALIZATION
DISCRETE MODEL
NUMERICAL MODEL

MICROSCOPIC BIOFILM MODEL

- NAVIER - STOKES FLOW:

$$\frac{\partial u}{\partial t} + u \quad u \quad p = \frac{1}{Re} \quad {}^{2}u$$

$$u = 0$$

- CONSTITUENT TRANSPORT:

$$\frac{\partial c_i}{\partial t} + \quad c_i u - D_i \quad c_i = R_i \qquad i = 1, \ldots, NC$$

MICROSCOPIC BIOFILM MODEL
(CONTINUED)

- KINETICS OF BIOTRANSFORMATION:

$$\frac{\partial X}{\partial t} = \mu_{max} \frac{X c}{K + c} - bX$$

$$\frac{\partial c}{\partial t} = \frac{\mu_{max}}{Y_{X/c}} \frac{X c}{K + c}$$

- ATTACHMENT / DETACHMENT:

$$r_A = k_A c$$

$$r_D = k_D L_1^2$$

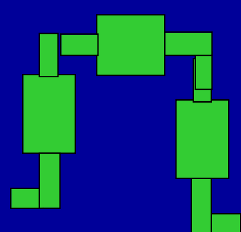
MICROSCOPIC BIOFILM MODEL
(CONTINUED)

- KINETICS OF BIOTRANSFORMATION:
- FILTRATION
- DEATH / SLUFFING

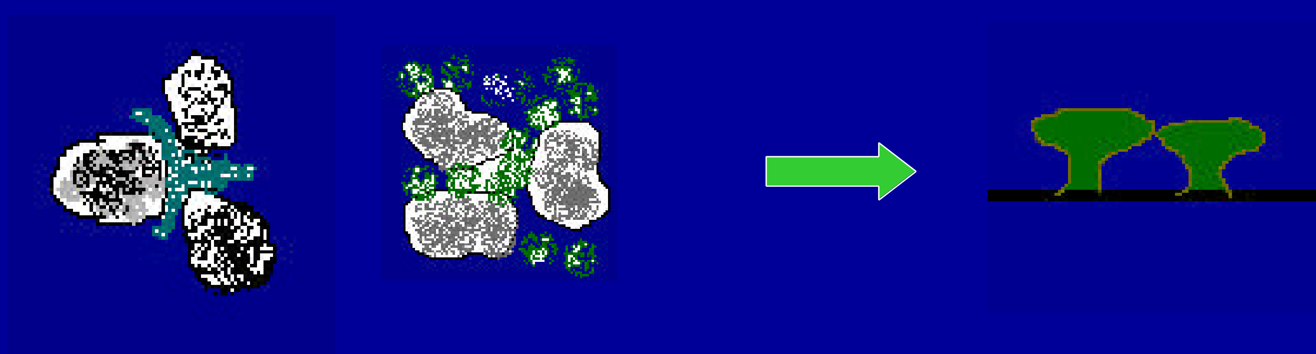
- CHEN, CUNNINGHAM, EWING, PERALTA, VISSER - NMPDE

LABORATORY EXPERIMENTS

CENTER FOR BIOFILM ENGINEERING
(Montana State University)

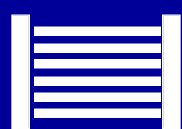


ETCHED MICROMODELS
COMPLEX STRUCTURE



LABORATORY EXPERIMENTS
(CONT'D)

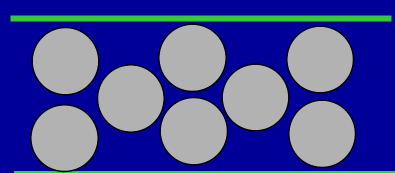
PLANNED



MEASURE:

- CHANGES IN PORE SIZES
- CHANGES IN WETTABILITY

2-D:



3-D:

USE NAVIER STOKES CODE: UNIV. STUTTGART

COUPLE WITH 2-D & 3-D BIOFILM MODEL

--MONTANA STATE UNIVERSITY

INVERSE PROBLEMS FOR PARAMETERS/KINETICS

UPSCALING

$$\tilde{u} = -\frac{\tilde{K}}{\mu} \quad \Phi, \qquad \tilde{K} = \text{effective permeability}$$

$$\frac{f}{ft}(\varphi c) + \quad (\tilde{u}c) - \quad \tilde{D}(\tilde{u}) \quad c = \hat{q}c, \quad \tilde{D} = \text{macrodispersity}$$

- **Gelmar, Axness – Water Res. Res., 1983**
- **Dagan – Flow & Trans. Porous Media, 1989**
- **Ewing, Russell, Young – 10 Spe Res. Sim., 1989**
- **Espedal, Langlo, Saevareid, Gislefoss,**
- **Hansen – 11 Spe Res. Sim., 1991**
- **Durlofsky – Water Res. Res., 1991**
- **Glimm, Lindquist – Comp. Meth. Water Res., 1992**
- **Glimm, Lindquist, Pereira, Zhang – Trans. Porous Media, Ta**
- **Amaziane, Bourgeat, Koebbe – Trans. Porous Media, Ta**
- **Langlo, Espedal – Adv. Water Res., Sub.**
- **Proc. 2nd Kovacs Symposium – Uncertainty – Unesco**

SINGLE-PHASE FLOW EQUATIONS

D'ARCY'S LAW: $$u = -\frac{K}{\mu}\left(\; p - \rho g \; z \right)$$

MASS BALANCE: $$\frac{\partial}{\partial t}(\varphi\rho) + \quad (u\rho) = q$$

TRANSPORT:

$$\frac{\partial}{\partial t}(\varphi c) + \quad uc - \quad D(u) \; c = \lambda(c) + qc$$

WHERE

$$D_{ij} = \varphi(x)\; d_m I + \frac{d_\ell}{|u|}\begin{pmatrix} u_1^2 & u_1 u_2 \\ u_1 u_2 & u_2^2 \end{pmatrix} + \frac{d_t}{|u|}\begin{pmatrix} u_2^2 & -u_1 u_2 \\ -u_1 u_2 & u_2^2 \end{pmatrix}$$

+ Nonlocal Dispersion (t)

SINGLE-PHASE FLOW EQUATIONS
(CONTINUED)

COMMON ASSUMPTION:

$$k = \begin{pmatrix} k_{11} & 0 & 0 \\ 0 & k_{22} & 0 \\ 0 & 0 & k_{33} \end{pmatrix}$$

HOMOGENIZATION:

$$k = \begin{pmatrix} k_{11} & k_{12} & k_{13} \\ k_{12} & k_{22} & k_{23} \\ k_{13} & k_{23} & k_{33} \end{pmatrix} \quad \text{(LOCALLY)}$$

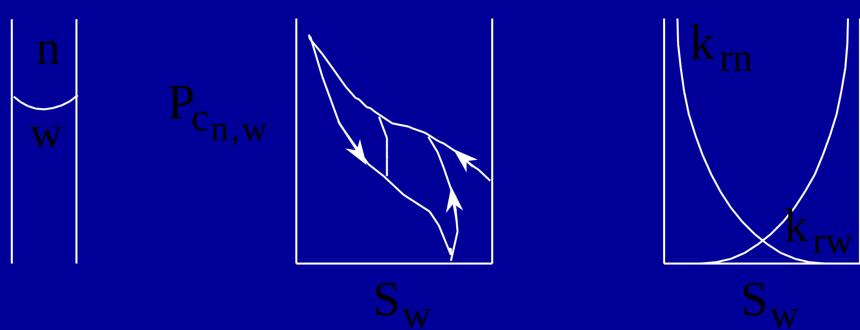
TWO-PHASE FLOW

D'ARCY'S LAW: $u_i = -\frac{Kk_{ri}}{\mu_i}\left(\quad p_i - \rho_i g \quad z\right)\ , \quad i = w, n$

MASS BALANCE: $\frac{f}{ft}\left(\phi\rho_i S_i\right) + \qquad \left(\rho_i u_i\right) = q_i \rho_i \ , \quad i = w, n$

$p_{c_{n,w}} = p_n - p_w \ , \quad S_n + S_w = 1$

w = Wetting Phase
n = Nonwetting Phase



TWO-PHASE FLOW

- **D'ARCY'S LAW:**

$$u_t = -K\lambda \left(p_t - G \right) \quad , \quad u_t = u_a + u_w$$

$$\lambda_i = k_{ri} / \mu_i \;, \; i = a, w \;, \; \lambda = \lambda_a + \lambda_w$$

$$f = \lambda_i / \lambda \quad , \; i = a, w$$

$$u_1 = f_i u_t + \text{CAP. PRES. TERM}_i + \text{GRAV. TERM}_i \;, \; i = a, w$$

$$p_t = S_a p_a + S_w p_w + \text{CAP. PRES. TERM}_i$$

$$\frac{f\varphi}{ft} + \quad u = -\sum_{i=a}^{w} \frac{1}{\rho_i} \varphi S_i \frac{f\rho_i}{ft} + u_i \quad \rho_i - q_i \rho_i = -\sum_{i=a}^{w} R_i$$

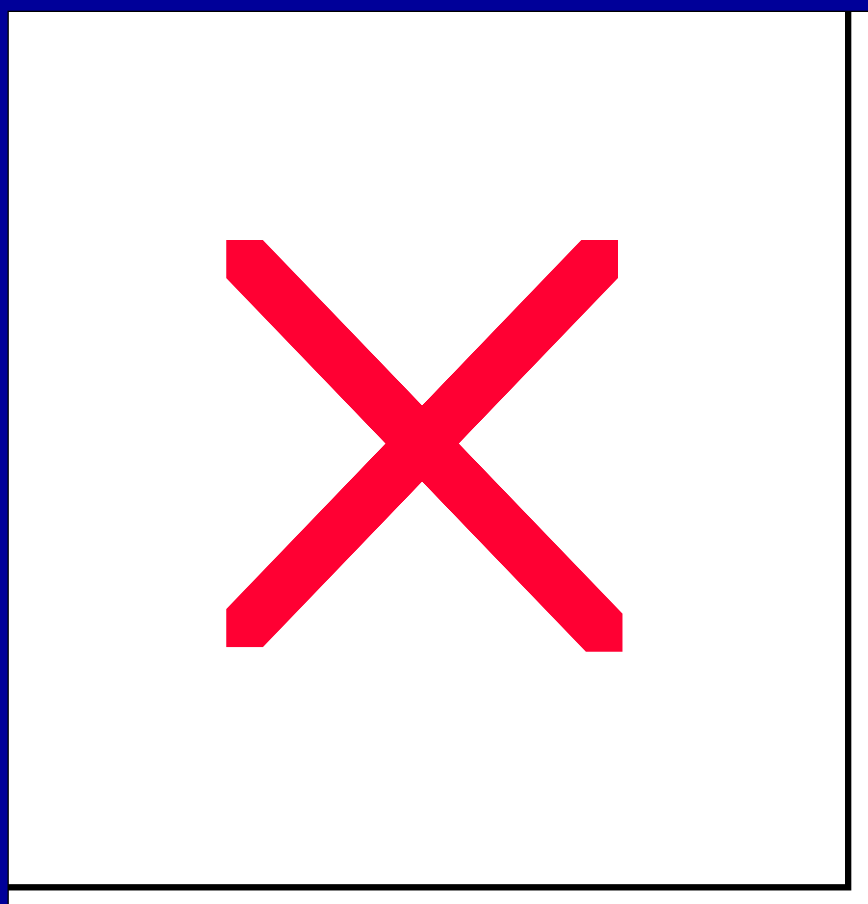
- **MASS BALANCE:**

$$\frac{f}{ft}(\varphi S_w) + \quad f_w(S_w)u_t - \quad D_1 \frac{f p_c}{f S_w} \quad S_w = \text{GRAV. TERM}_w - R_w$$

- **TRANSPORT:**

- **NEED MACROSCOPIC DISPERSION**

Ref: Chavent, Jaffre - 1978
Chen, Ewing, Espedal - CMWR X, 1994



Saevareid, Espedal, *et al.* 1992.

LABORATORY EXPERIMENTS -- CONT'D

PLANNED

- Imaging Laboratory (Texas A&M University)
  - NMR Imaging of Cores:
  - Obtain: Porosity Distribution
Velocity Distributions
Permeability
  - Grow Biomass in Cores
- Repeat and Compare
- Inverse Problems for Models

- Montana State University
  - Bench Scale Experiments
  - Development of Biobarriers
  - Development of Models

- VEGAS (University of Stuttgart)
  - Large Flumes
  - Room-speed Experiments
    - --Biobarriers

DNAPL INFILTRATION

VEGAS
UNIVERSITY OF STUTTGART

CONCLUSIONS

- Biosystems in the Subsurface are Complex, Nonlinear, and Highly Heterogeneous.
- Models are Needed at the Micro Scale to Understand the Competitive Interaction of Diverse Species.
- Scale-Up from Micro-Scale to Continuum Models Can Utilize Discrete Pore/Throat System Simulations.
- Uncertainty in the Subsurface Properties Must Be Incorporated Stochastically to Develop Bounding Calculations.

CONCLUSIONS (CONT'D)

- SCALE-UP OF NONLINEAR PHENOMENA : MANY ORDERS OF MAGNITUDE IN BOTH SPACE AND TIME.
- DEVELOPMENT OF PREDICTIVE MODELS FOR BIOSYSTEMS REQUIRES SIGNIFICANT INTERDISCIPLINARY INTERACTIONS.
- VALIDATION OF MODELS AGAINST LABORATORY AND FIELD EXPERIMENTS AT ALL SCALES IS ESSENTIAL.
- MULTIPHASE TRAPPING MECHANISMS AND BIOAVAILABILITY REQUIRE A MODELING CAPABILITY FOR INTERFACIAL PROCESSES.