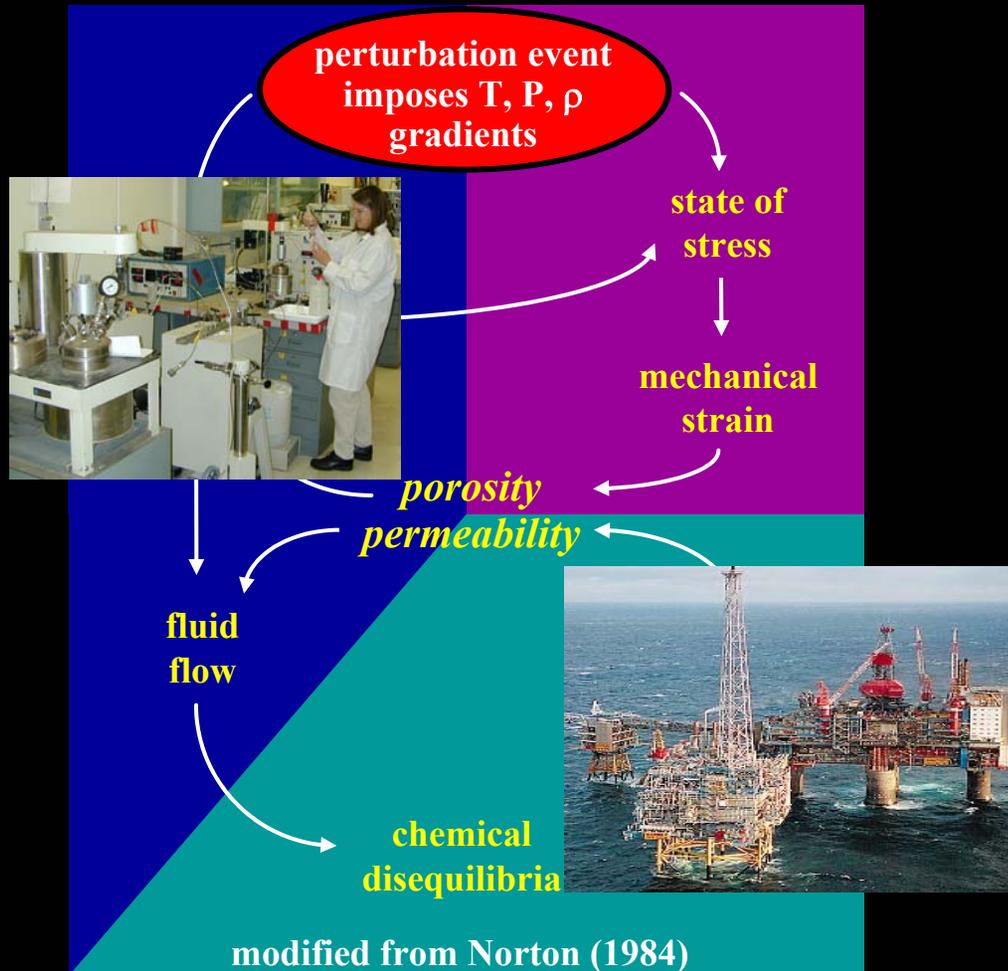


# Requirements & challenges for modeling the isolation performance of geologic CO<sub>2</sub> storage



**James W. Johnson**

*Lawrence Livermore  
National Laboratory  
Livermore, CA*

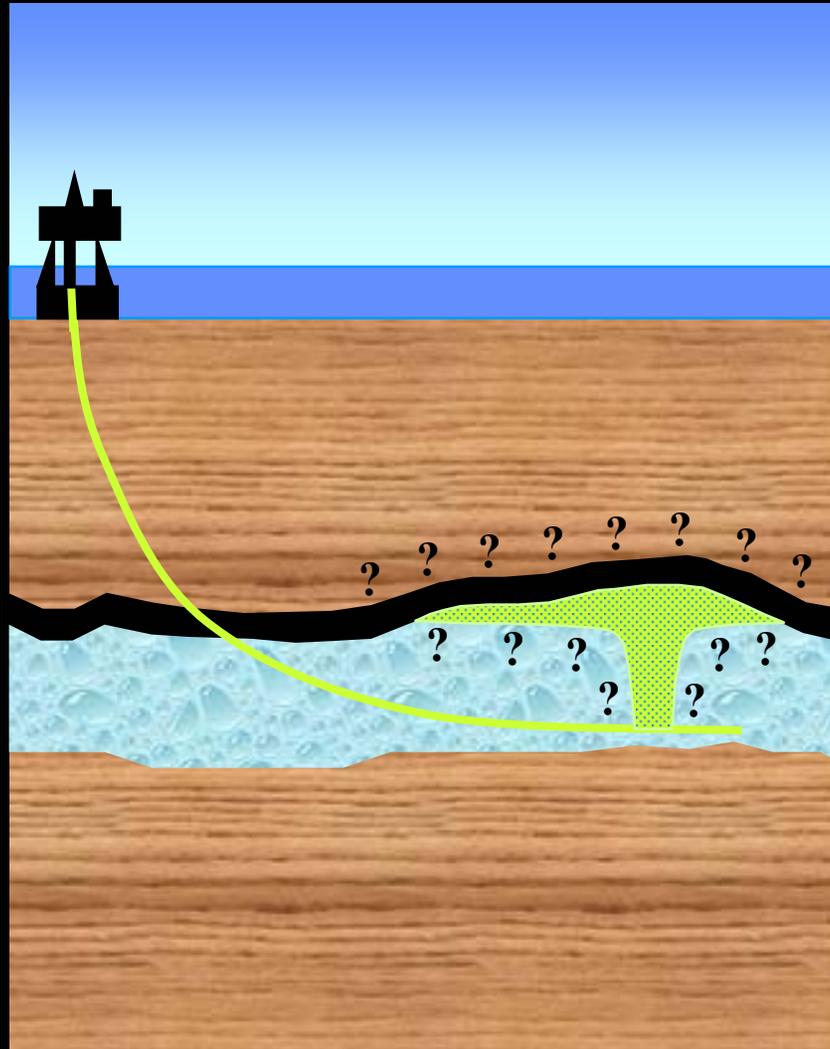
**5<sup>th</sup> Annual Conf. Carbon  
Capture & Sequestration  
May 8-11, 2006  
Alexandria, VA**

# Ultimate technical goal



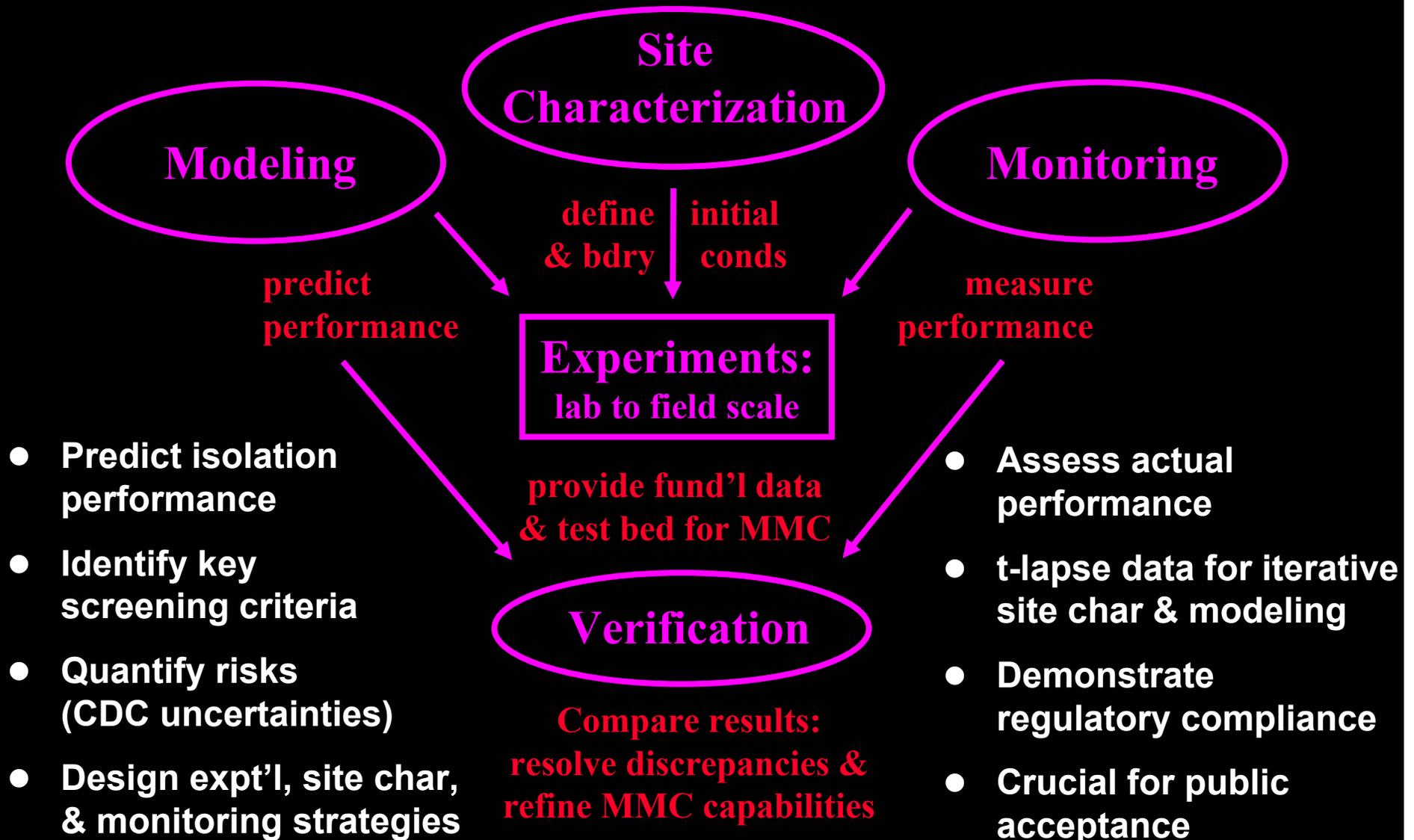
- **Develop two fundamental abilities**
  - ✓ Match injection-stream & disposal-site chars such that requisite isolation performance is *predicted* by advanced modeling capabilities
  - ✓ Match site chars, modeling results, and monitoring techniques such that predicted isolation performance can be *verified*
- **Injection-stream characteristics**
  - ✓ Projected incremental/total flux, impurity comps/concs, #/spacing of injection wells
- **Site components & characteristics**
  - ✓ Target reservoir(s), cap rock(s), localized wellbore environment, & overburden
  - ✓ Myriad hydrological, compositional, geo-mechanical, dimensional, & structural props
- **“Requisite” isolation performance**
  - ✓ That which provides regulatory compliance

# Fundamental components of long-term isolation performance

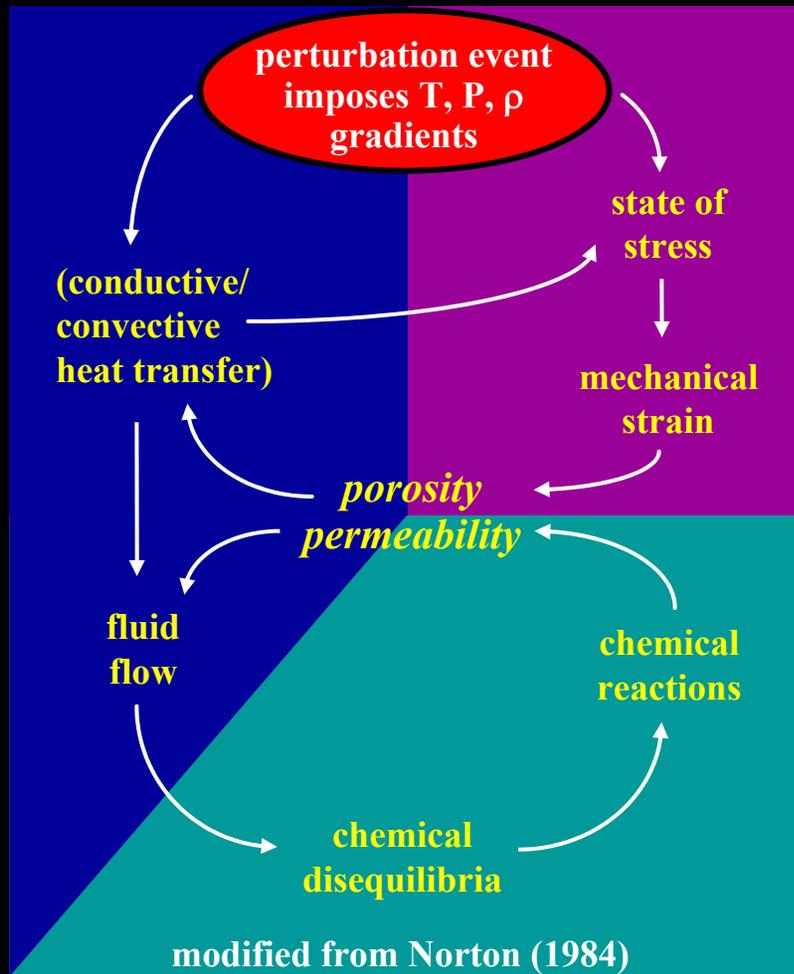


- **Capacity (incremental & cumulative mass)**
  - ✓ Res dims/depth, por/perm mag/het, resid satn, ambient flow field
  - ✓ Must demonstrate for ER credits
- **Density (areal & volumetric footprint)**
  - ✓ Depth, struct, seqn partitioning among geochem & residual trapping mechs
  - ✓ Spatial extent of monitoring programs
- **Containment (hydrodynamic seal capacity)**
  - ✓ Cap-rock/wellbore integrity as f(geochem/geomech processes)
  - ✓ Must demo for regulatory compliance
- **Risk (uncertainty limits on CDC estimates)**
  - ✓ Economic: +/- ER credits & spatial extent of monitoring responsibility
  - ✓ Environmental: +/- resume & impact of potential leakage mechanisms

# Requisite integrated technology portfolio for geologic CO<sub>2</sub> storage



# Modeling the integrated processes & isolation performance of geologic CO<sub>2</sub> storage



- **Process quantification requires theoretical geoscience expertise**
  - ✓ Mathematical reps, numerical methods
- **Practical implementation requires computational expertise & facilities**
  - ✓ Software, solvers, hardware, visualizn
- **Applications require diverse system-specific field & experimental data to represent:**
  - ✓ Initial & boundary conditions: Site characterization data that define the physical domain
  - ✓ Dynamic system evolution: Site-independent data that underpin the process models

# Fundamental Challenges for modeling

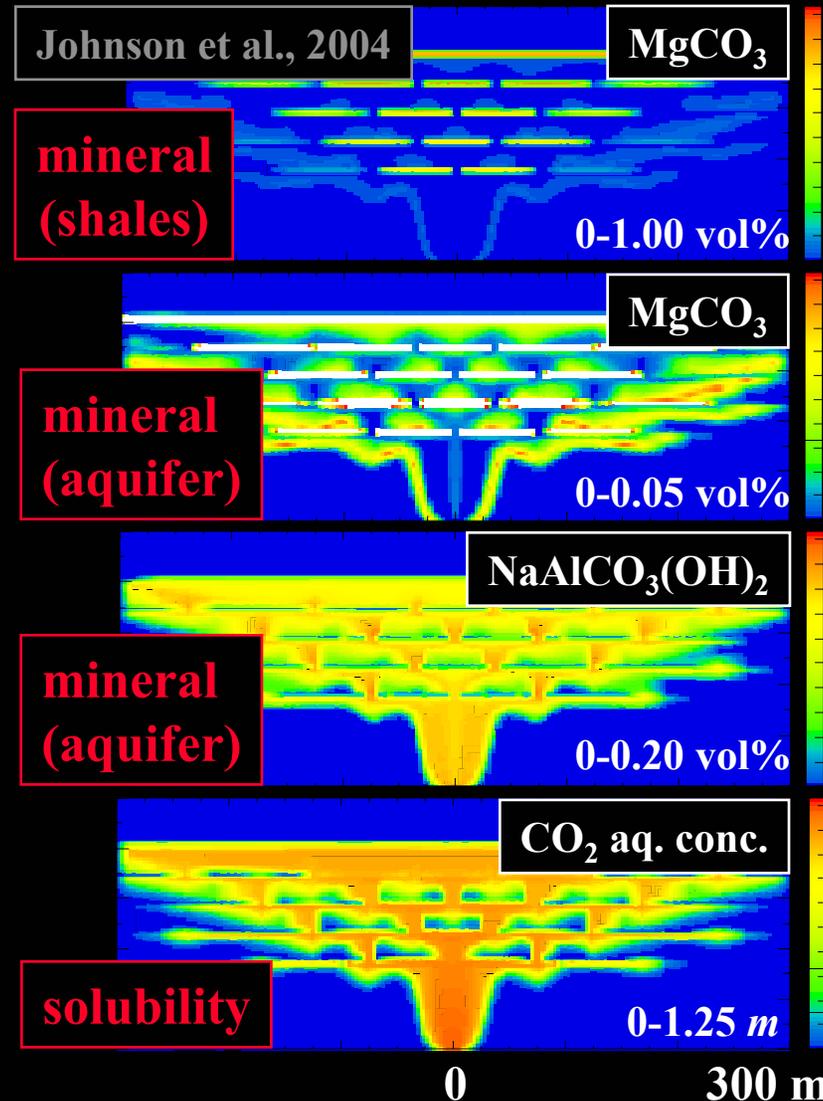


- **Ultimate goal**
  - ✓ Develop ability to match injection-stream & disposal-site chrs such that requisite isolation performance is *predicted*
- **Challenges**
  - ✓ Identify key screening criteria that facilitate such correlations (CDC components)
  - ✓ Quantify & reduce the uncertainties that surround such predictions (R component)
- **Potential screening criteria**
  - ✓ Myriad hydrological, compositional, structural, & dimensional properties
- **Sources of uncertainty**
  - ✓ Process & process coupling: rep'n & accur.
  - ✓ Site-independent data: accuracy
  - ✓ Site characterization: accuracy -- spatial distribution of heterogeneous properties

# Identification of screening criteria for optimized source/sink matching

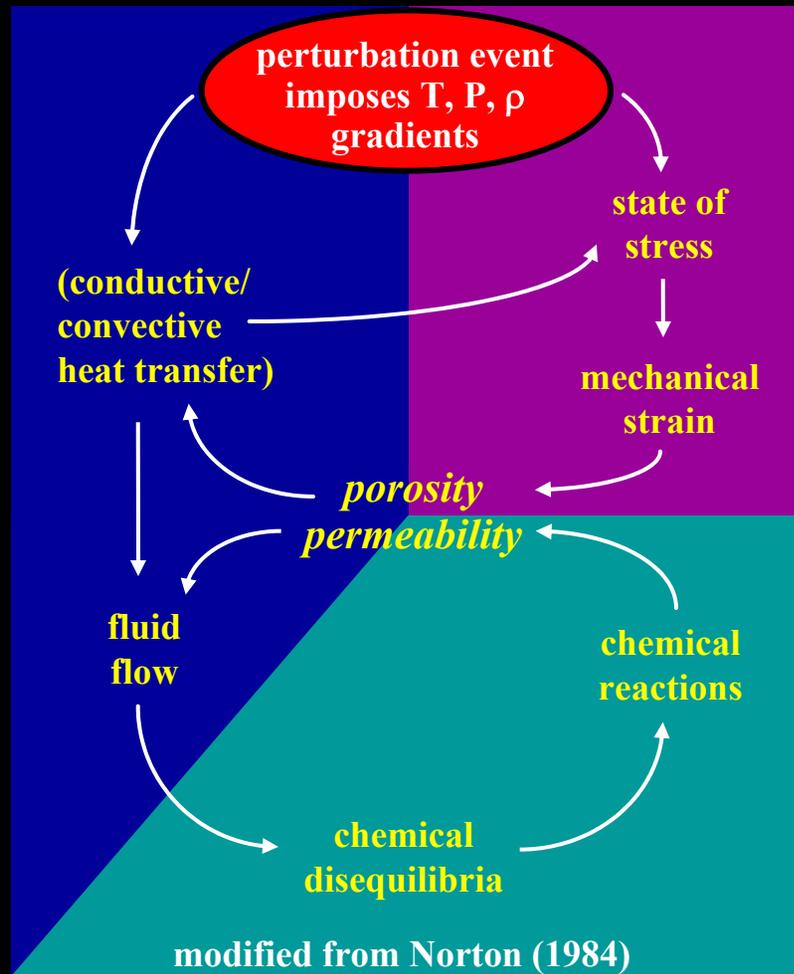


## trapping mechanisms (DSH: 20 yrs)



- Approach: quantify CDC sensitivity to the range of key property variations
- Compositional
  - ✓ CO<sub>2</sub> impurities: e.g., SO<sub>x</sub>, NO<sub>x</sub>, CH<sub>4</sub>, H<sub>2</sub>S
  - ✓ Res/cap-rock min: carb-forming cations
  - ✓ Ambient fluids: aqueous & HC phases
  - ✓ Wellbore environs: mud, cement, casing
- Hydrological
  - ✓ CO<sub>2</sub> & ambient fluid fluxes
  - ✓ Poros/perm of res/cap-rock/wellbore envs
  - ✓ Residual saturations: CO<sub>2</sub>, aqueous, HC
- Structural
  - ✓ Res lateral cont; res/cap interface topog.
- Depth & geothermal gradient (P-T conds)
  - ✓ Eq. ref. frame for chem mass transfer
  - ✓ Fluid-phase density contrasts

# Current challenges in developing robust process models



## • Multiphase flow processes

- ✓ Fm H<sub>2</sub>O, impure CO<sub>2</sub>, HC (liq, gas)
- ✓ EOS, visc, 2-3 phase relative perm
- ✓ Residual saturation descriptions
- ✓ Hysteretic capillary pressure functions

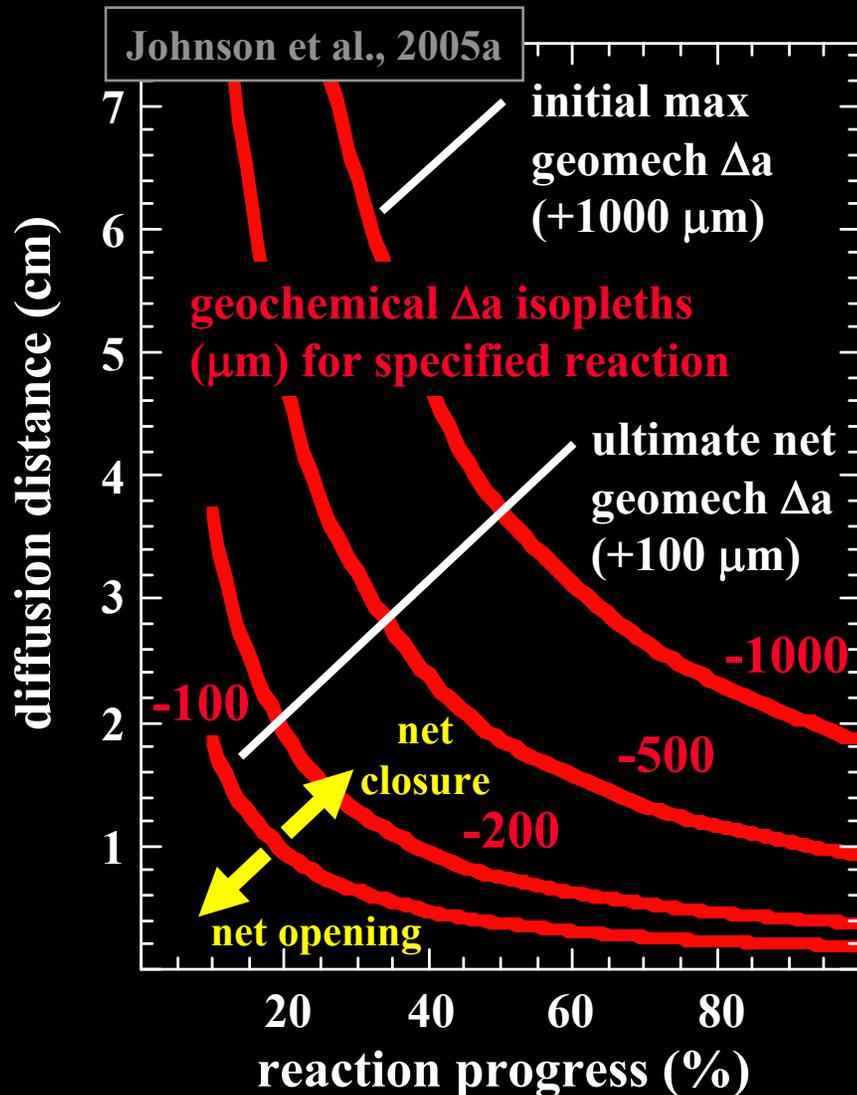
## • Geochemical processes

- ✓ Equilibrium reference frame: well-estb
- ✓ Intra-fl & fl/min mass transfer: less mature
- ✓ Min diss/pptn kinetics (processes & data): nucl & growth, near-equil rates, SSA
- ✓ CO<sub>2</sub> impurities; H<sub>2</sub>O solub in “immisc” CO<sub>2</sub>
- ✓ CO<sub>2</sub> crit phenom; biogeochem processes
- ✓ *Perm(continuum-rep poros(min diss/pptn))*

## • Geomechanical processes

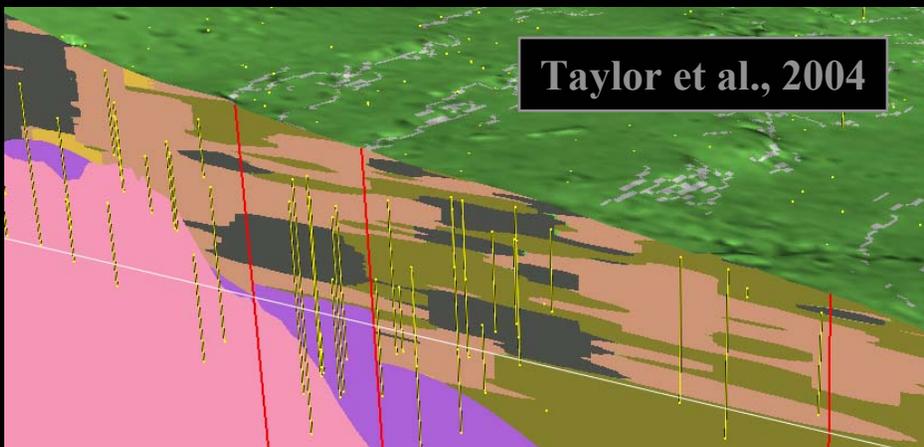
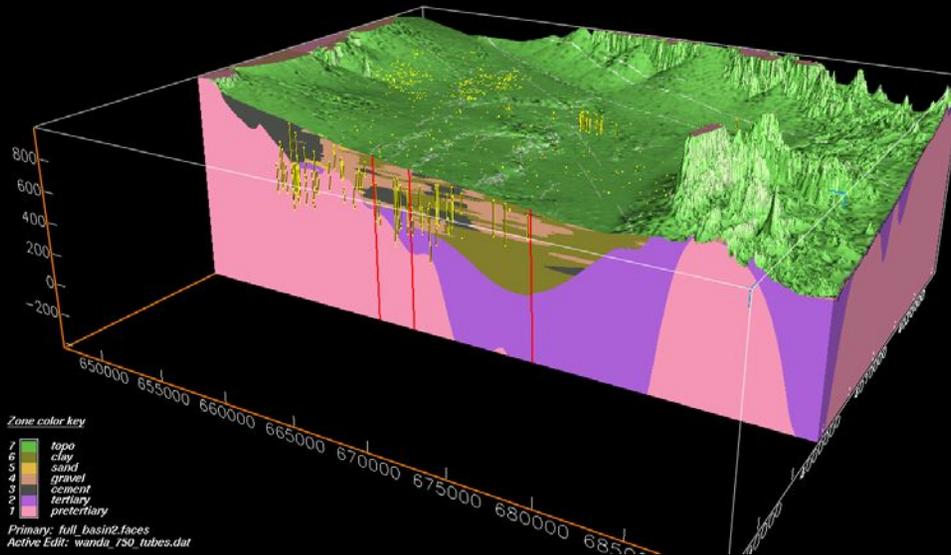
- ✓ Effective stress( $P_f$ , total stress)
- ✓ Stress-strain rels:  $a_{per}(P_f, \text{frac stiff}(a_{per}))$
- ✓ *Perm(DEM-rep poros( $a_{per}$ ))*

# Current challenges in developing seamless process coupling



- **Multiphase flow/geochem interface**
  - ✓ Chemical affinity(aq.,  $\text{CO}_2$ , HC flow)
  - ✓ Min diss/pptn; convective mixing
  - ✓ Fm  $\text{H}_2\text{O}$  dens( $\text{CO}_2$  solub; min diss/ppt)
  - ✓ Rel effect: flow, min diss/ppt, conv mix
  - ✓ Flow(geochem-dep perm)
- **Multiphase flow/geomech interface**
  - ✓ Effective stress( $P_f(\text{CO}_2$  influx))
  - ✓ Flow(geomech-dep perm)
  - ✓ Interfacing continuum & DEM models
- **Geochem/Geomech interface**
  - ✓ Geomech props(composition)
  - ✓ Perm(geochem/geomech components)
  - ✓ Rel rates/mags of indiv components
  - ✓ Interfacing continuum & DEM models

# The up-scale/down-scale challenge of transitioning from lab- to field-scale models



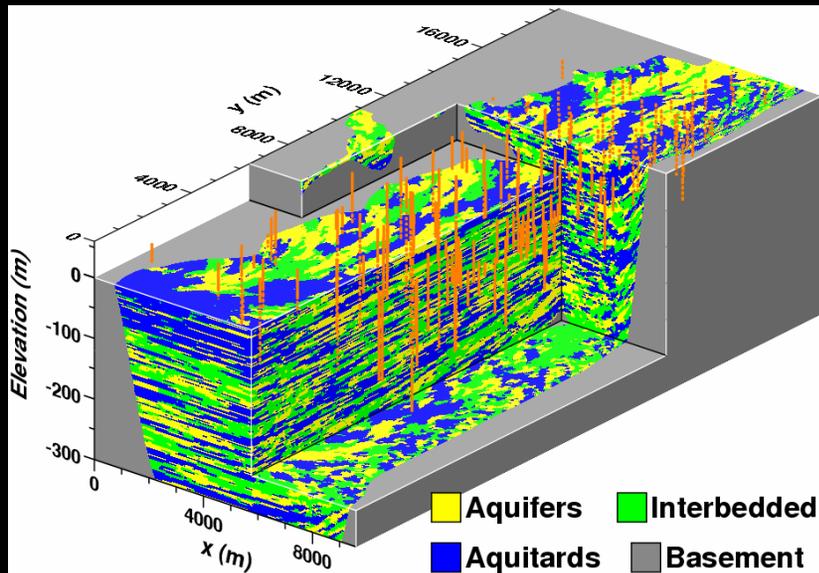
## ● Lab-scale simulations

- ✓ Init/bdry conds are established: por/perm, comp, flow, P-T, stress
- ✓ Perturbation event often observed & sampled directly in situ in its entirety
- ✓ Mass/ener redistribution processes often can be evaluated independently
- ✓ Resolution of prediction/observation discrepancies: model fine-tuning

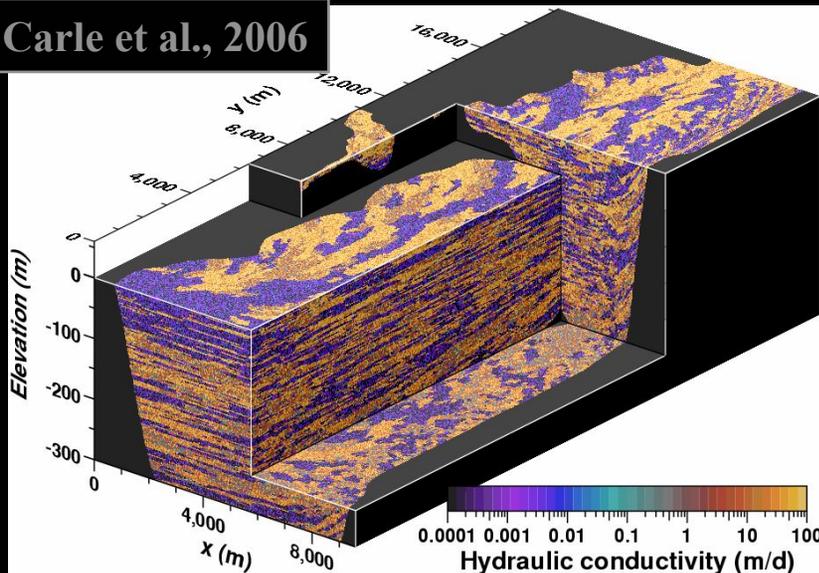
## ● Field-scale simulations

- ✓ Init/bdry conds are poorly known: sparse sampling, extreme heterog.
- ✓ Perturbation event is observed indirectly and sampled at intervals
- ✓ Mass/energy redistribution processes must be evaluated in integrated form
- ✓ Resolution of prediction/observation discrepancies: improved site char & process/computational scaling

# Quantifying & reducing the uncertainty of site characterization

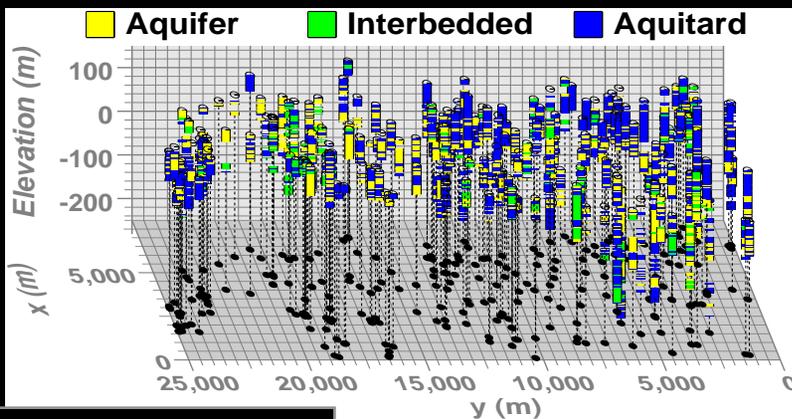


Carle et al., 2006

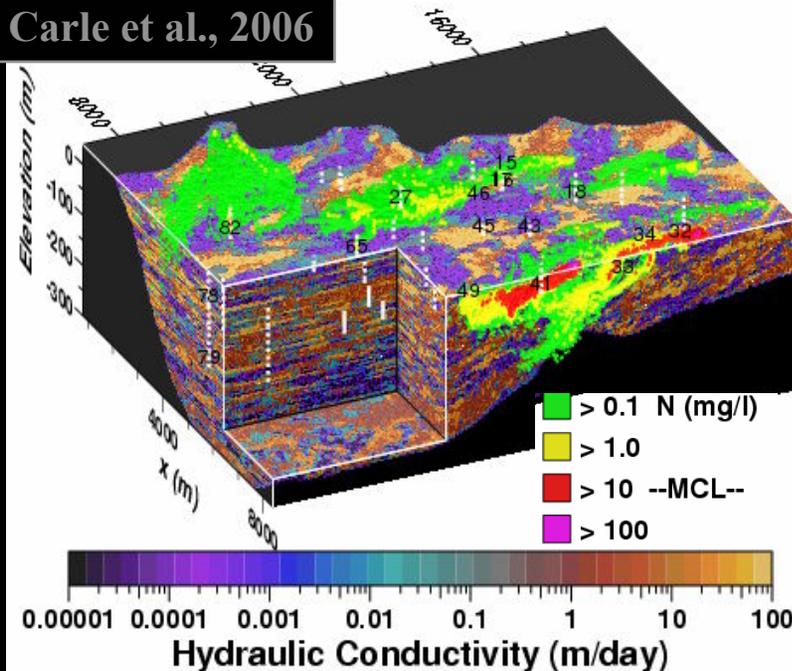


- Fundamental challenge of field-scale performance prediction
- Requires three-pronged approach:
  - ✓ Maximize data density & diversity
  - ✓ Develop improved methods for extracting maximum value from raw data
  - ✓ Repeatedly refine site char efforts by integrating new info from monitoring pgms
- Improved methods
  - ✓ Advanced *in situ* fluid sampling techs
  - ✓ Detailed compositional analyses of core
  - ✓ Facies-based transitional prob. approach for inter-well stratigraphic interpolation
  - ✓ Continuous stochastic random field approach for intra-stratum heterogeneity
- Monitoring data
  - ✓ Often delineates local high/low perm zones that are undetectable *a priori*

# Requisite integration of site characterization, modeling, & monitoring activities



Carle et al., 2006

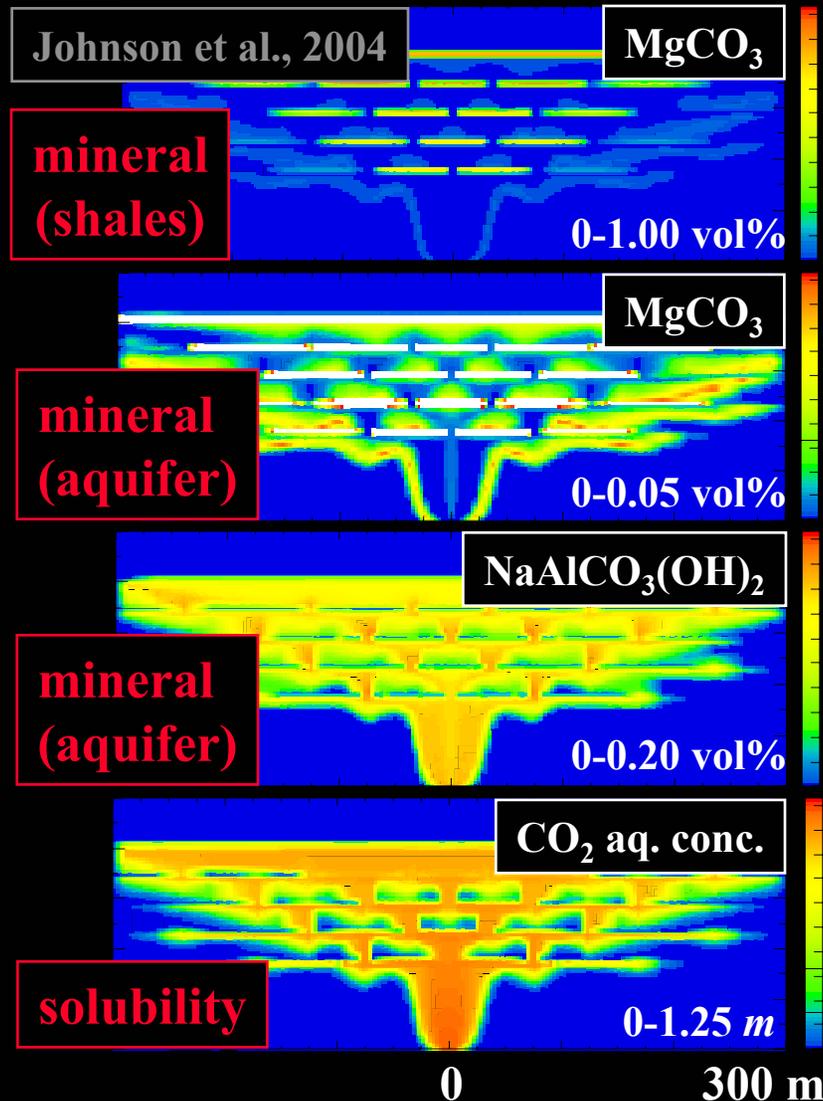


- **Expt-calibrated predictive models**
  - ✓ Screening criteria for isolation performance
  - ✓ Define & prioritize site char activities
- **Site characterization**
  - ✓ Sparse raw data for geostatistical methods
  - ✓ Core (high-res vert), seismic (rel low-res 3D)
- **Geostatistical methods**
  - ✓ 3D heterogeneous property distributions
  - ✓ Perm: spatial framework of CO<sub>2</sub> migration
  - ✓ Comp: efficacy of geochem trapping mechs
- **Site geologic model**
  - ✓ Import to EarthVision & predictive models
- **Model & monitor isolation performance**
- **Minimize prediction/mmt discrepancies**
  - ✓ Iterative staged refinement of het prop dists that honor *all* data (Ramirez et al., 2006)

# Next-generation reactive transport modeling of long-term isolation performance to:



trapping mechanisms (DSH: 20 yrs)



- Quantify impurity constraints (sep reqmts)
  - ✓ Site integrity as  $f(\text{SO}_x, \text{NO}_x, \text{CH}_4, \text{H}_2\text{S})$
  - ✓ Define max non-deleterious limits
- Optimize source/sink matching (perf rank)
  - ✓ Identify key screening criteria
  - ✓ Maximize CDC performance
- Optimize filling strategies (impl. schemes)
  - ✓ #, spacing, geom, influx rates/duration of  $\text{CO}_2$  (+/- associated  $\text{H}_2\text{O}$ ) injection wells
- Quantify & minimize CDC uncertainty (risk)
  - ✓ Expt-calibrated process models & coupling, site-indep data, site characterization
- Design monitoring programs
  - ✓ Identify appropriate technology suite
  - ✓ Determine imaging/sampling locs/freqs
- Interface with atmos & ocean models
  - ✓ Seamless tracking of pot'l release scenarios