

# Modeling Concurrent Damage Due to Environmental and Mechanical Effects

*P. Murru, Z. Grasley, K.R. Rajagopal, P. Alagappan*  
Texas A&M University

Anna Maria XVIII  
Holmes Beach, FL  
Nov 15-17, 2017

# Motivation & objective

- Damage = reductions in either/both **stiffness** and ultimate **capacity**
- Caused by both simultaneous mechanical and chemical loadings!
  - Existing methods tend to use CDM to quantify “damage”; do not fully couple
- Hypothesis: Damage may be defined in terms of microstructural density changes
- Objective: Derive and evaluate *Density Driven Damage Mechanics* (3D-M)

# 3D-M advantageous over competing approaches

	Fracture mechanics	Continuum damage mechanics	3D-M
Simultaneous chemical & mechanical degradation	X	X	✓
Single constitutive equation for all stress states	X	X	✓*
Properly handles kinematics	X	✓	✓
Quantifies strength reductions	✓	✓	✓
Quantifies stiffness reductions	X	✓	✓
Non subjective constitutive model	✓	X	✓

\* Preliminary results indicate this possibility upon mesh refinement

# Why a density based model?

- Damage ought to be a function of an intensive variable
- What intensive properties can be measured on a chunk of material?

Of intensive properties we can measure directly without choice of a reference configuration, **DENSITY** is most likely related to damage

- Mass concentration
- Molar concentration
- Mass density
- Melting point

- Strain energy!
- Invariants of stress/strain?

Calculated from Force & Displacement, but these are **SUBJECTIVE** since they are changes from some reference configuration

# 3D-M framework: mixture theory

- Must consider locally large deformation gradients
- Conventional continuum mechanics does not allow for chemical degradation by its very nature (i.e., the requirement of a continuum)

$$\frac{d\rho}{dt} = -\rho \operatorname{div}(\mathbf{v})$$

- Mixture theory couples density changes due to chemical and mechanical effects

For species  $i$ :  $\frac{d\rho^i}{dt} = \dot{\rho}_{gen}^i - \rho^i \operatorname{div}(\mathbf{v}) - \operatorname{div}(\mathbf{j}_m^{i-mix})$      $\sum_{i=1}^n \mathbf{j}_m^{i-mix} = 0$      $\sum_{i=1}^n \rho^i = \rho$      $\sum_{i=1}^n \dot{\rho}_{gen}^i = 0$

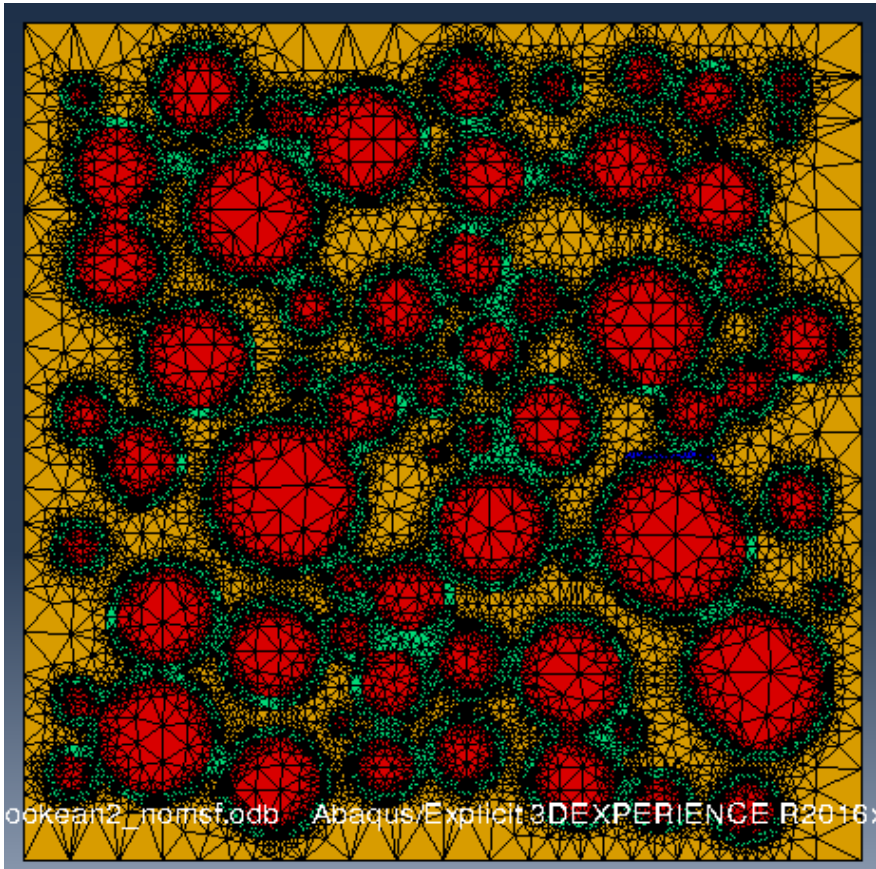
$$\rho^i = \frac{\Delta m_{gen}^i}{1 + \ln[J]} + \frac{\rho_0^i}{1 + \ln[J]}, \text{ where } J = \det(\mathbf{F})$$

Accounts for chemical degradation

Accounts for mechanical degradation

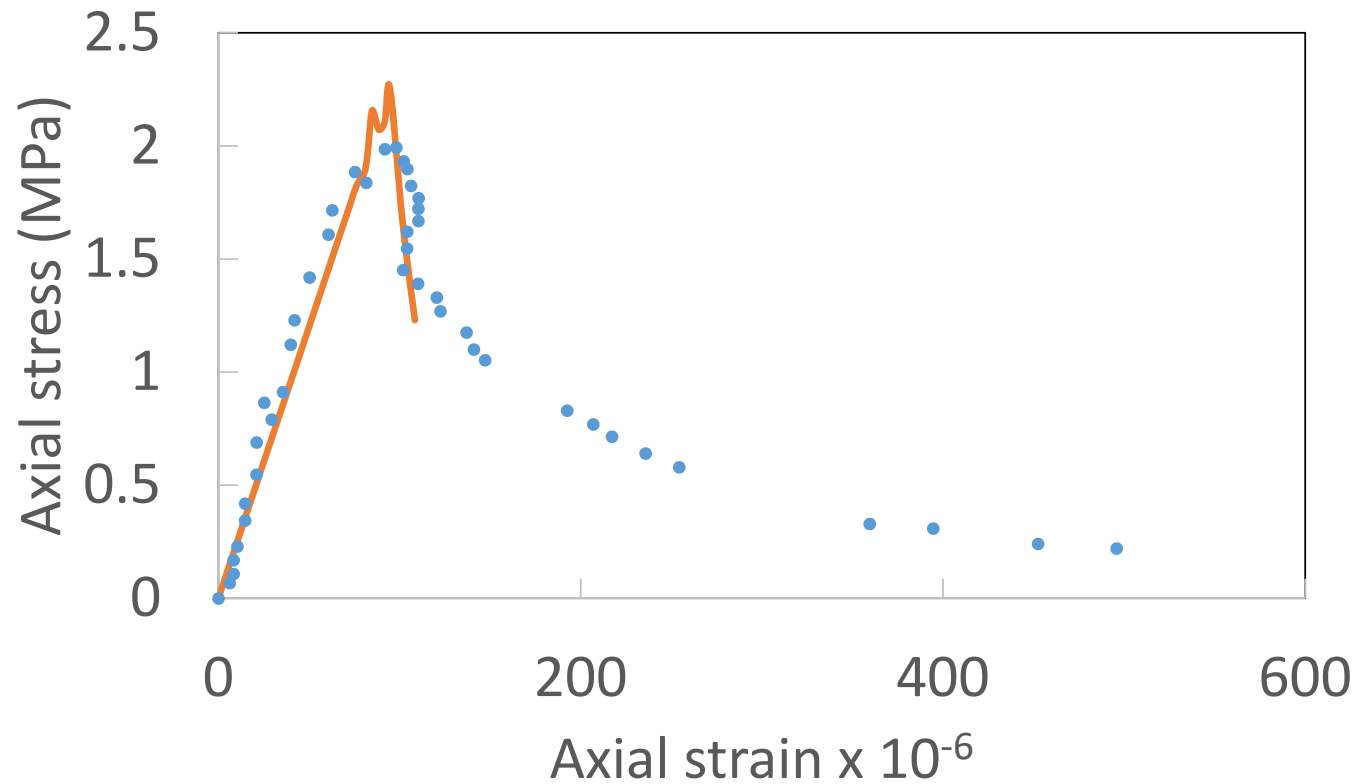
$$G^i, K^i = f(\rho^i)$$

# Test 2D microstructure



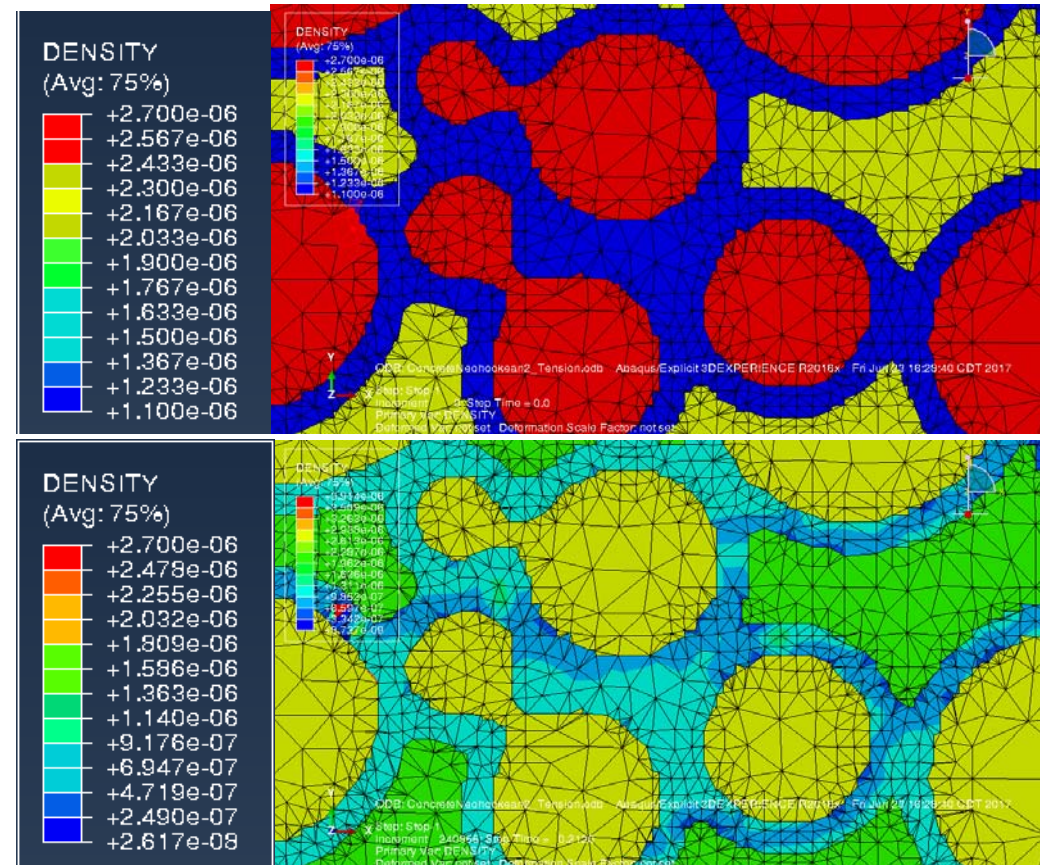
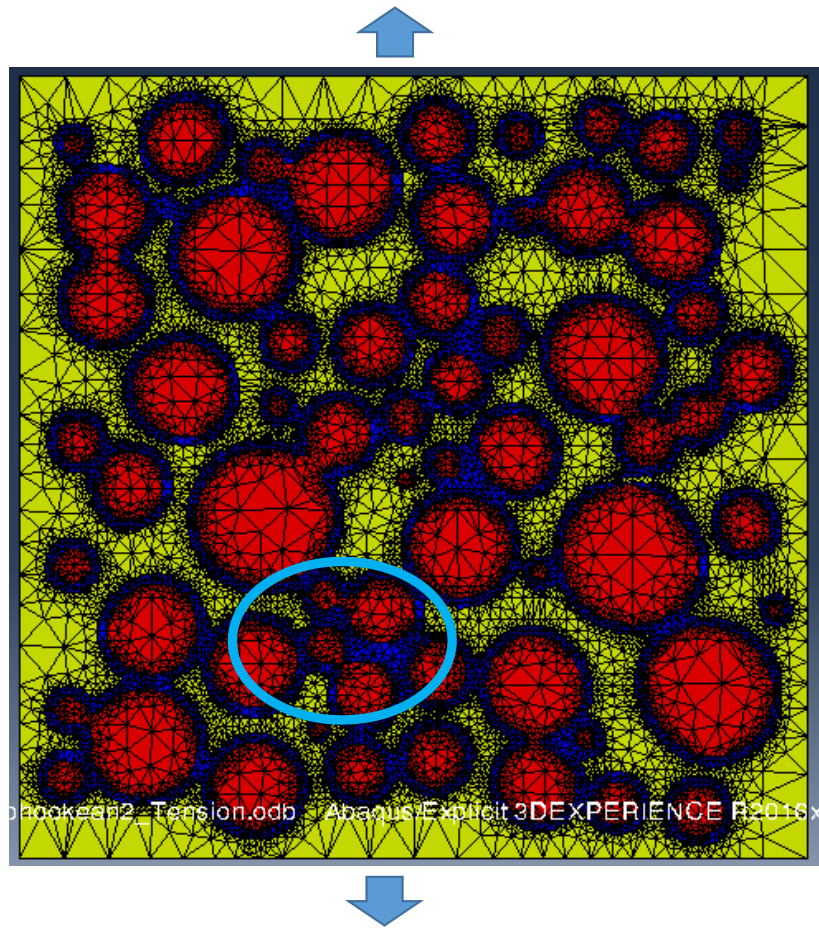
- 3 phase elastic composite
  - Mortar matrix
  - Coarse aggregate
  - ITZ
- Coarse aggregate volume fraction = 0.38
- ITZ thickness = 1/12 aggregate dia.
- Initial densities:
  - $\rho_{agg} = 2700 \text{ kg/m}^3$
  - $\rho_{itz} = 1100 \text{ kg/m}^3$
  - $\rho_{mortar} = 2200 \text{ kg/m}^3$

# Example simulation: uniaxial tension



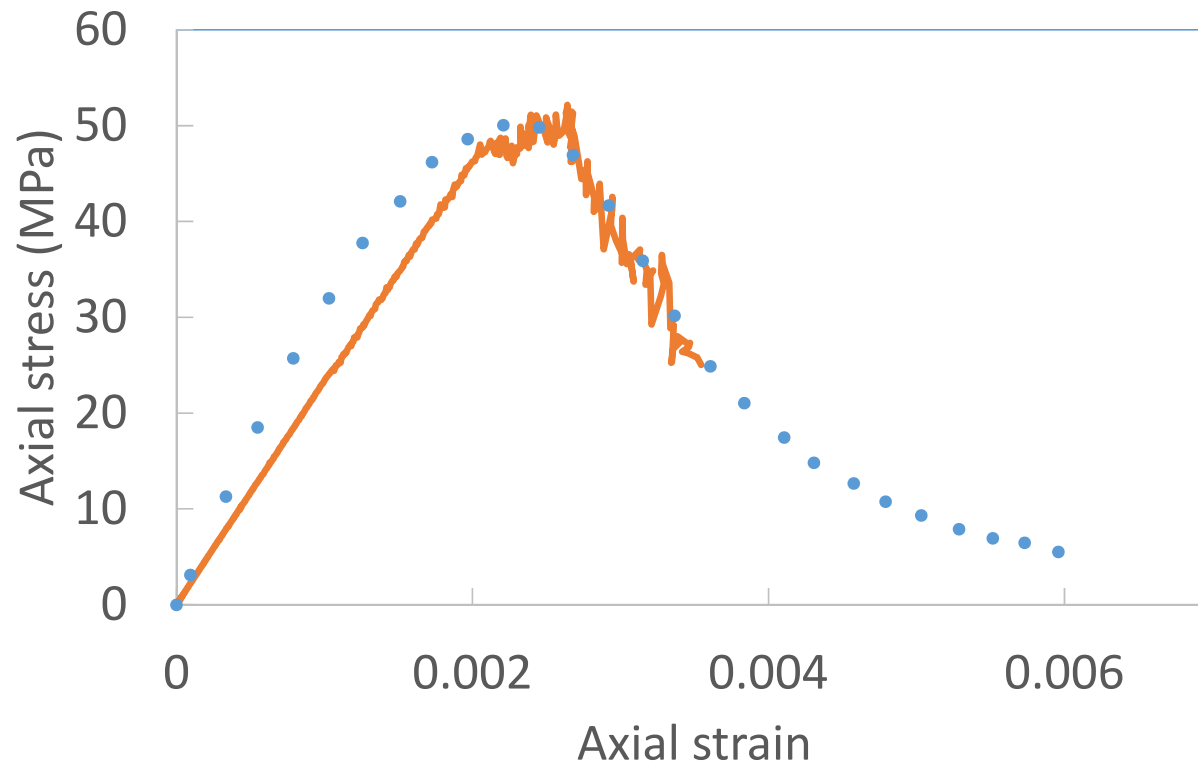
Data from: Zhao, Z. F., et al. (2009). "Fracture Behaviors of Dam and Wet-Screening Concrete by Direct Tensile Test." Key Engineering Materials 400-402: 233-238

# Density contour plot during tensile loading



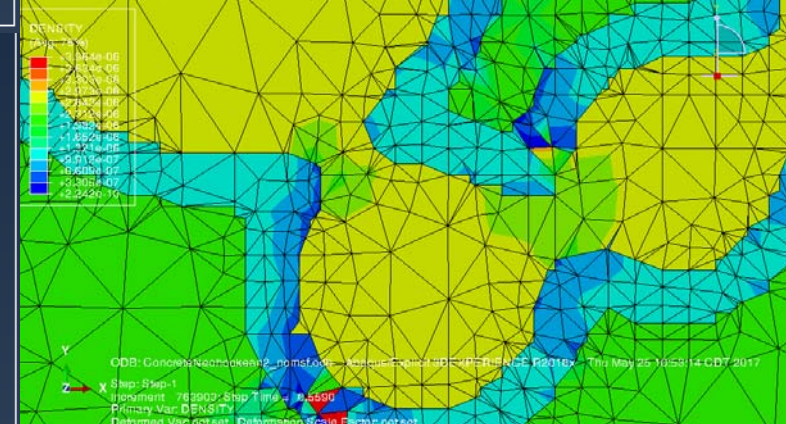
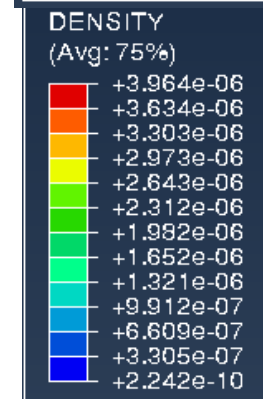
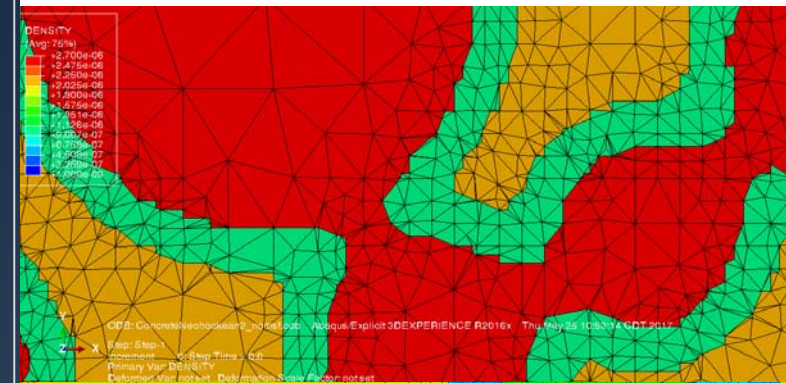
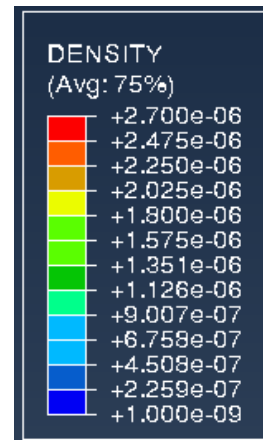
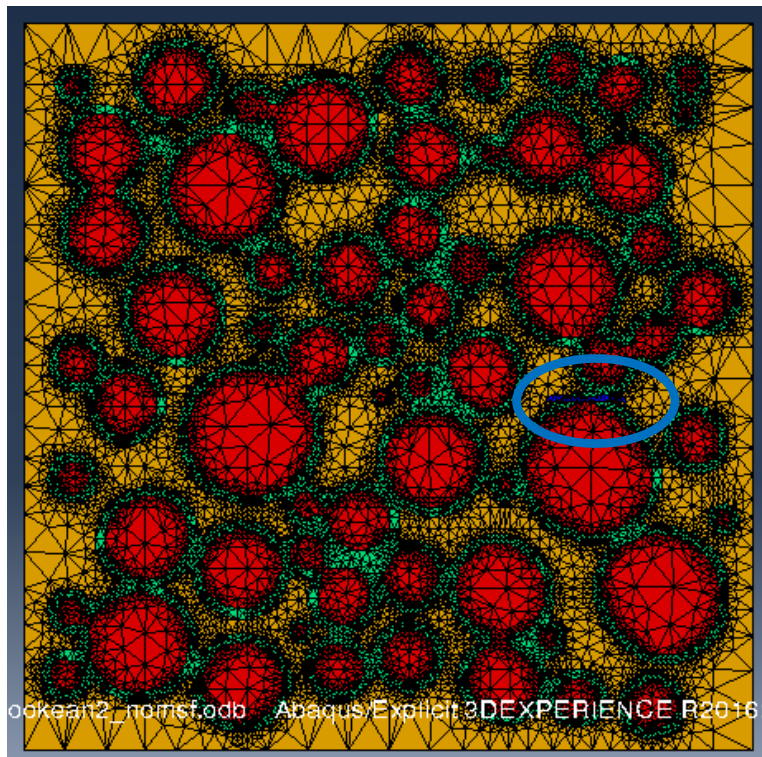


# Example simulation: uniaxial compression

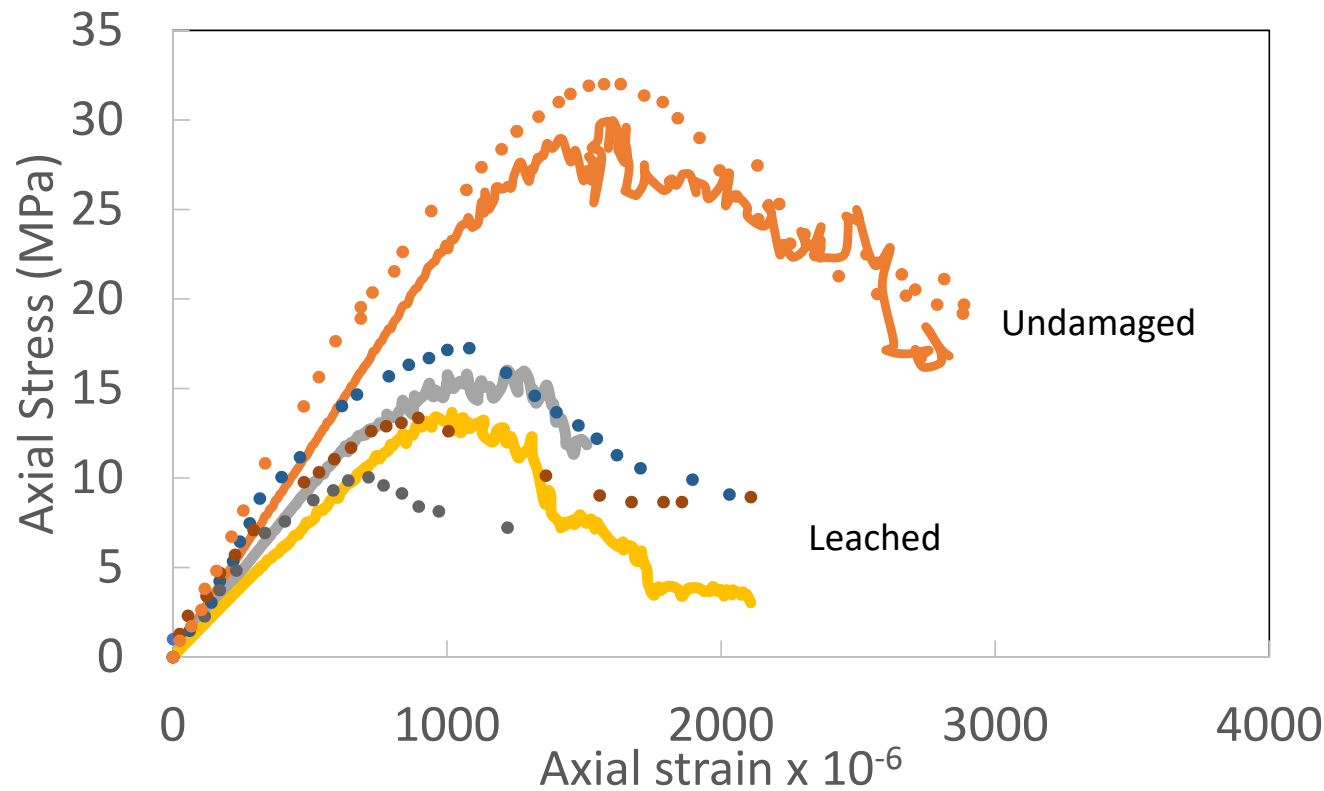


Data from: Lu, Z.-H. and Y.-G. Zhao (2010). "Empirical Stress-Strain Model for Unconfined High-Strength Concrete under Uniaxial Compression." *Journal of Materials in Civil Engineering* 22(11): 1181-1186.

# Density contour plot for compression



# Example simulation: leaching



- Measured porosity increase used to calculate density degradation
- 30 d and 60 d of leaching

Data from: B. Huang, C. Qian, Construction and Building Materials 25 (2011) 2649–2654

# Conclusions

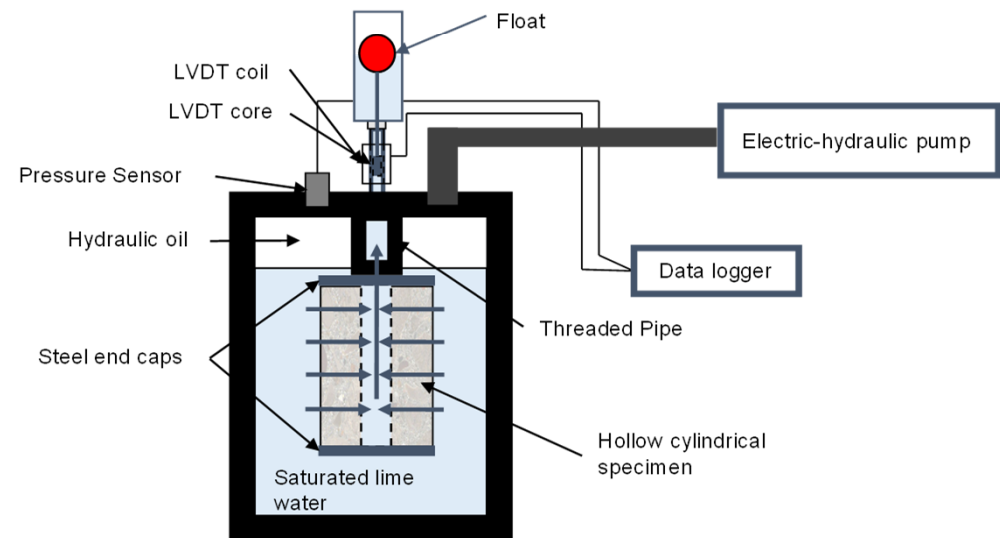
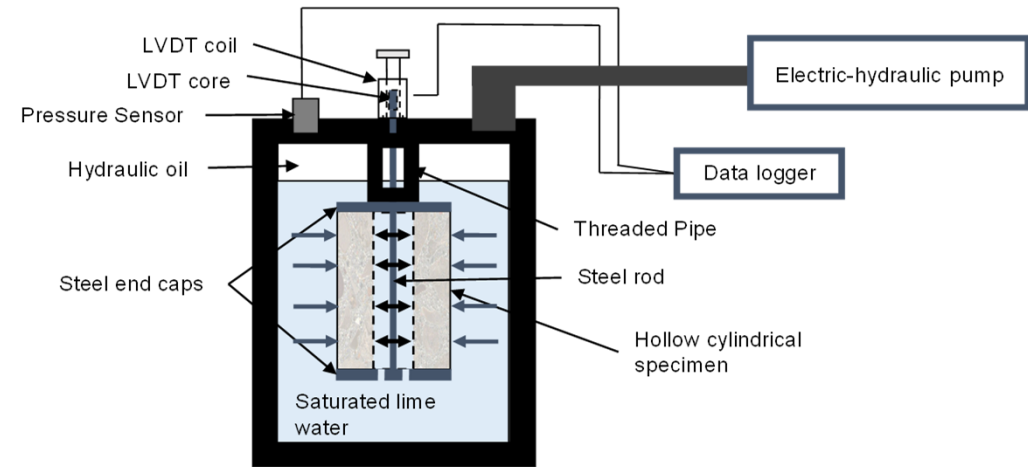
- New damage model introduced
  - Based on microscopic density changes
  - Overcomes many limitation of existing models for damage/fracture/failure
  - Unifies chemical and mechanical degradation via single modeling approach
- Preliminary results encouraging for mechanical and chemical degradation simulations
  - Opens door to much more robust failure predictions/analysis
- Need more research on mesh size dependency in relation to microstructural sizes
  - Verify that a single constitutive function for all stress states might be developed
  - Tie constitutive functions to microstructure evolution in fundamental way... may be truly predictive!
- Model limitations
  - Requires non-linear kinematics (finite deformations)
  - Computationally intensive

# Future work

- Extend model to 3D
- Refine mesh/ improve numerics
- Use real aggregate shapes
  - Spherical harmonics or X-ray CT
- Do leaching tests, compression tests, tension tests all on same concrete
  - See if we can predict tensile failure and effects of leaching from results of compressive loading

# Other Grasley research

- Advanced material development
  - Dispersing high volume fractions of micro/nano particles
- Durability measurements
  - Poromechanics-based permeability measurements
- Modeling
  - Creep & shrinkage
  - Coupled mechanics, thermodynamics, durability
    - F/T, etc.
  - Dispersion
  - Computational materials science



# Efforts at Texas A&M

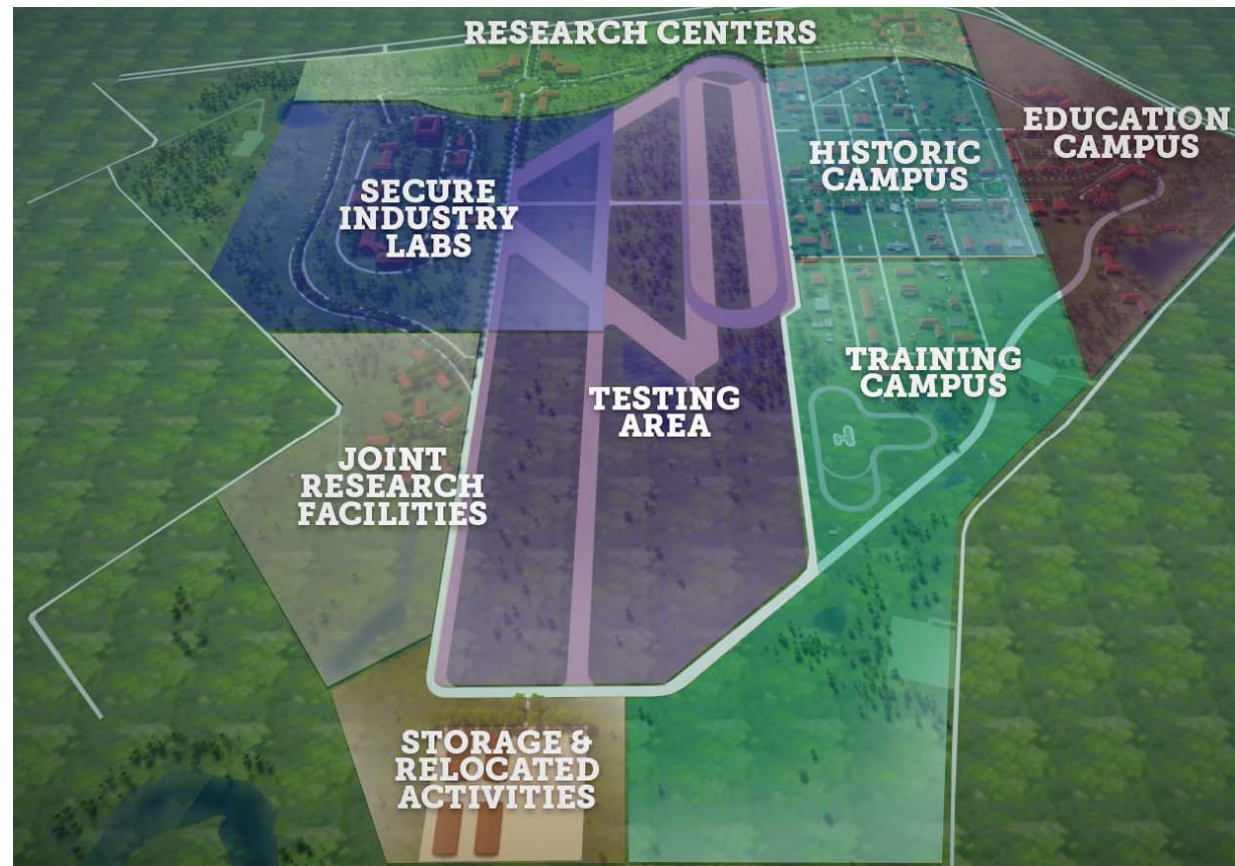
- Looking for forward-thinking industry, university, government, & lab partners
- World-class, unique facility
- You are all invited to schedule a visit!

- New ~\$100M Center for Infrastructure Renewal (CIR) coming online spring 2018
- TTI / TEES Collaboration
- Significant focus on concrete materials, pavements, and structures



# New RELLIS campus

- New 2000+ acre campus
- Multi billion dollar investment
- 10 miles from main campus
- Home of the new CIR
- Extensive outdoor testing areas
- Opportunities for partnership





Thank you!

Zach Grasley PhD | PE | M.ASCE | FACI

Director of the CIR

Presidential Impact Fellow

Professor

Zachry Department of Civil Engineering

Department of Materials Science &

Engineering

Texas A&M University

[zgrasley@tamu.edu](mailto:zgrasley@tamu.edu)



**TEXAS A&M**  
UNIVERSITY.