Modeling Flow and Deformation during Salt-Assisted Puffing of Single Rice Kernels

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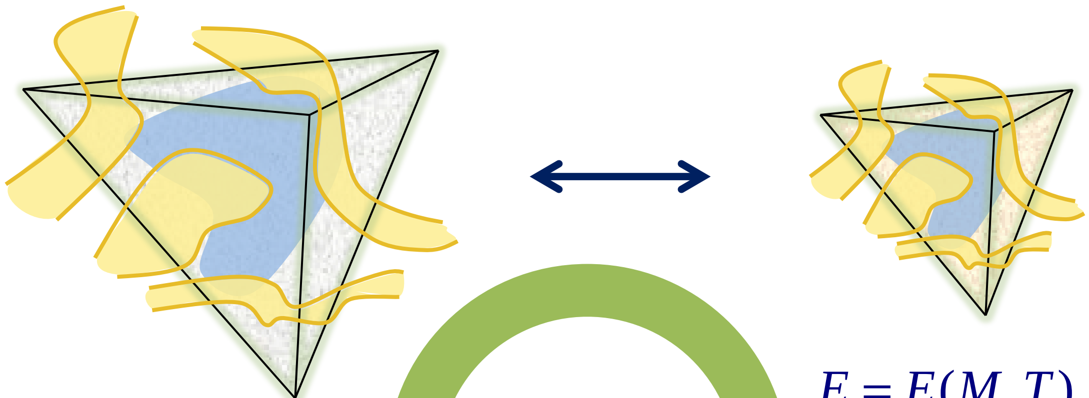
COMSOL CONFERENCE
2014 BOSTON

Puffing

Puffing: Salient Features

- Quick process and a complex interplay of mass, momentum and energy transport with Large Deformations
- Rapid evaporation of water to vapor
- Phase Transition from Glassy (brittle) to Rubbery (ductile) state
- Large volumetric expansion of the kernel due to Gas Pressure generation and Phase Transition
- Large Plastic (inelastic) deformation of the material

Transport Process in Deformable Porous Media



$E = E(M, T) \quad p_f$

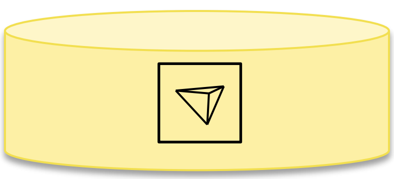
Multiphase, multicomponent transport

Poromechanics, phase dependent properties

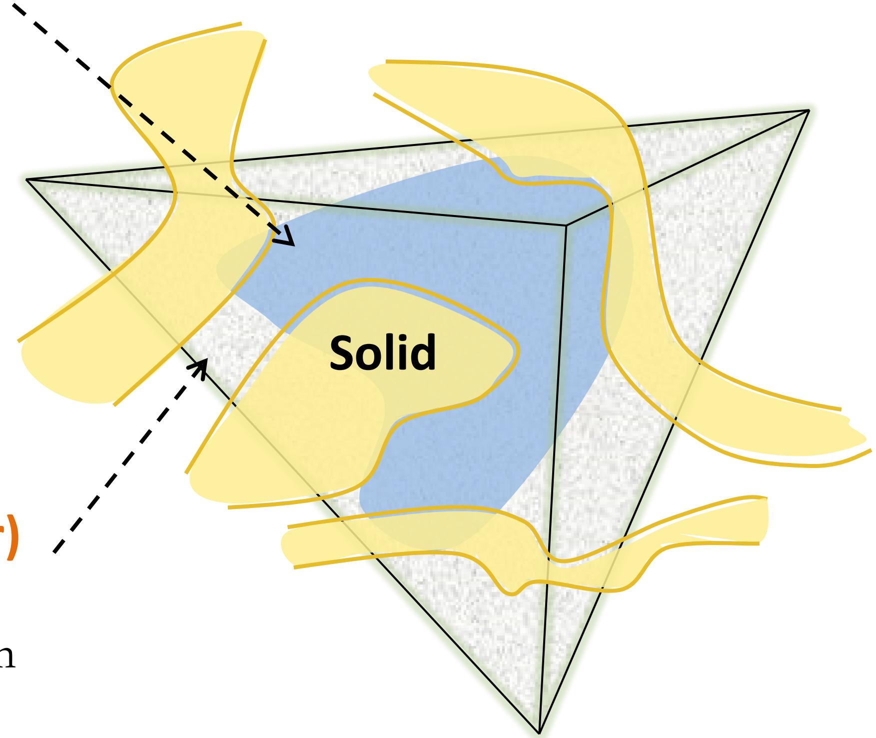
$$\mathbf{n}_{\mathrm{i,G}} = \mathbf{n}_{\mathrm{i,s}} + c_i \mathbf{v}_{\mathrm{s,G}}$$

Transport Process Porous Media[1,2,3]

Water
- bulk flow/convection
- capillary diffusion
- phase change



Porous material



Gas (Vapor + Air)
- bulk flow
- binary diffusion
- phase change

Element

[1]Whitaker (1997)
[2]Ni H et al., (1999)
[3]Halder A et al., (2007)

Transport Process Porous Media

Momentum Conservation

Darcy Law

$$\frac{\partial c_g}{\partial t} + \nabla \cdot \left(\mathbf{n}_{\mathbf{g,G}} \right) = \dot{I}$$

$$\mathbf{n}_{\mathbf{g,s}} = -\rho_g \frac{k_g k_{r,g}}{\mu_g} \nabla P$$

$$\underbrace{\mathbf{v}_{\mathbf{i}} = -\frac{k_i k_{r,i}}{\mu_i} \nabla P}_{\text{Darcy Velocity}}$$

i = water, gas

Mass Conservation

Liquid Water

$$\frac{\partial c_w}{\partial t} + \nabla \cdot \underbrace{\left(\rho_w \mathbf{v}_{\mathbf{w}} \right)}_{\text{bulk flow}} = \nabla \cdot \underbrace{\left(D_w \nabla c_w \right)}_{\text{capillary flow}} - \overbrace{\dot{I}}^{\text{phase change}}$$

Water Vapor

$$\frac{\partial c_v}{\partial t} + \nabla \cdot \underbrace{\left(\rho_g \omega_v \mathbf{v}_{\mathbf{g}} \right)}_{\text{bulk flow}} = \nabla \cdot \underbrace{\left(\varphi S_g \frac{C^2}{\rho_g} M_a M_v D_{eff,g} \nabla x_v \right)}_{\text{binary diffusion}} + \overbrace{\dot{I}}^{\text{phase change}}$$

Energy Conservation

Thermal Balance for Mixture

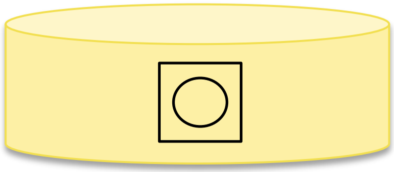
$$\frac{\partial}{\partial t}\left[\sum_{i=s,w,v,a} \left(c_i c_{p,i} T \right) \right] + \nabla \cdot \underbrace{\left[\sum_{i=w,v,a} \left(c_{p,i} \mathbf{n}_{\mathbf{i}} T \right) \right]}_{\text{convection}} = \underbrace{\nabla \left(k_{eff} \nabla T \right)}_{\text{conduction}} - \overbrace{\lambda \dot{I}}^{\text{phase change}} + \underbrace{Q_{mic}}_{\text{microwave source}}$$

Phase Change

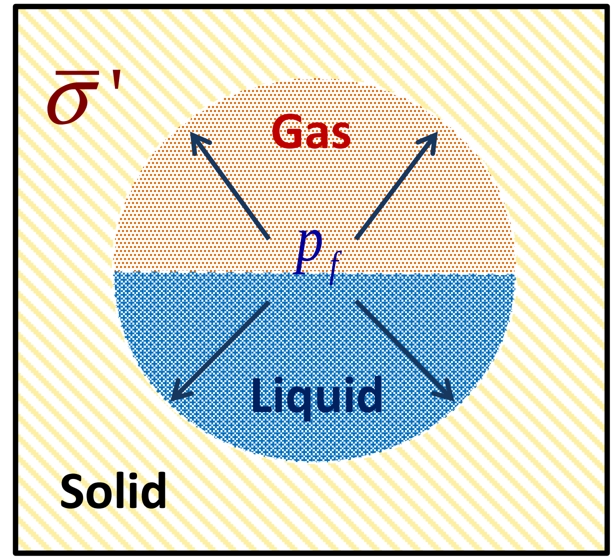
Evaporation-Condensation

$$\dot{I} = K \frac{M_v}{RT} \underbrace{\left(p_{v,eq} - p_v \right)}_{\text{Non-Equilibrium Formulation}}$$

Deformation in Porous Media: Poromechanics[1,2,3]



Porous material



$$p_f = S_g p_g + S_w p_w$$

Average Stress in REV	=	Stress due to solid skeleton	+	Stress due to fluids inside pore

$$\bar{\boldsymbol{\sigma}} = \bar{\boldsymbol{\sigma}}' - p_f \mathbf{I}$$

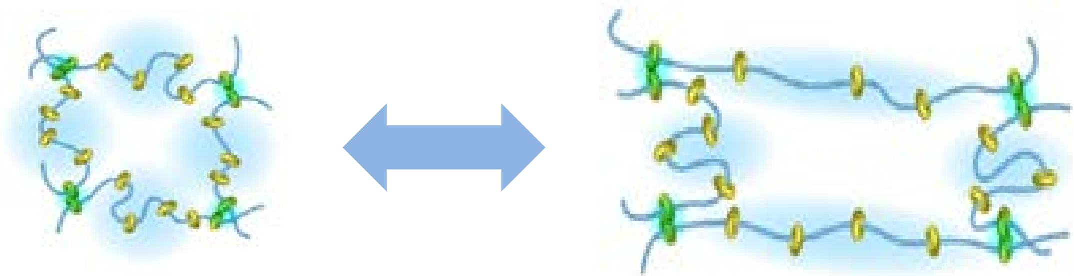
- **Balance of Linear Momentum:** $\nabla \cdot \bar{\boldsymbol{\sigma}}' = \nabla p_f$
- **Constitutive Model** for the Solid Skeleton: $\nabla \cdot \underbrace{(\mathbf{D} \cdot \boldsymbol{\varepsilon})}_{\text{Elasto-Plastic}} = \nabla p_f$

Elasto-Plastic

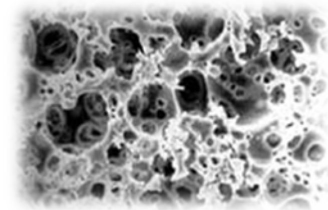
[1]Perre & May (2001)
[2]Kowalski (2000)
[3]Coussy (2004)

Phase Transition

Glassy **Rubbery**



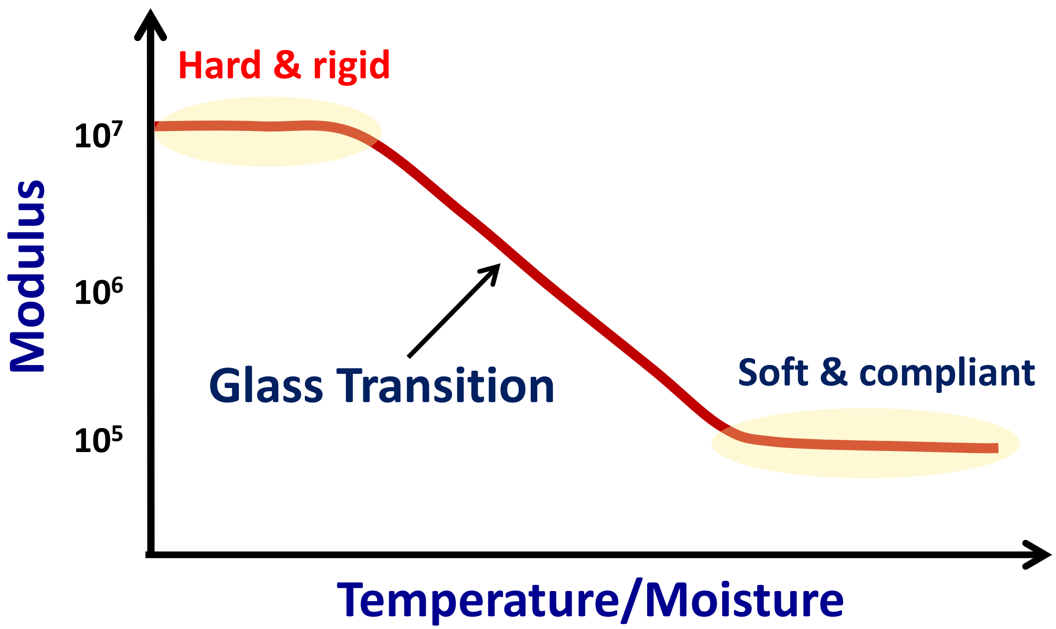
Textural Attributes



Porosity & Bulk Density

Volume Shrinkage/Expansion

Stress Cracking



[1]Roos, Y.H. (2010)

Puffing: Modeling Framework

- Salt-Assisted Puffing carried out at 200^0C for 15s

Multiphase transport
(Gas Pressure Driven)

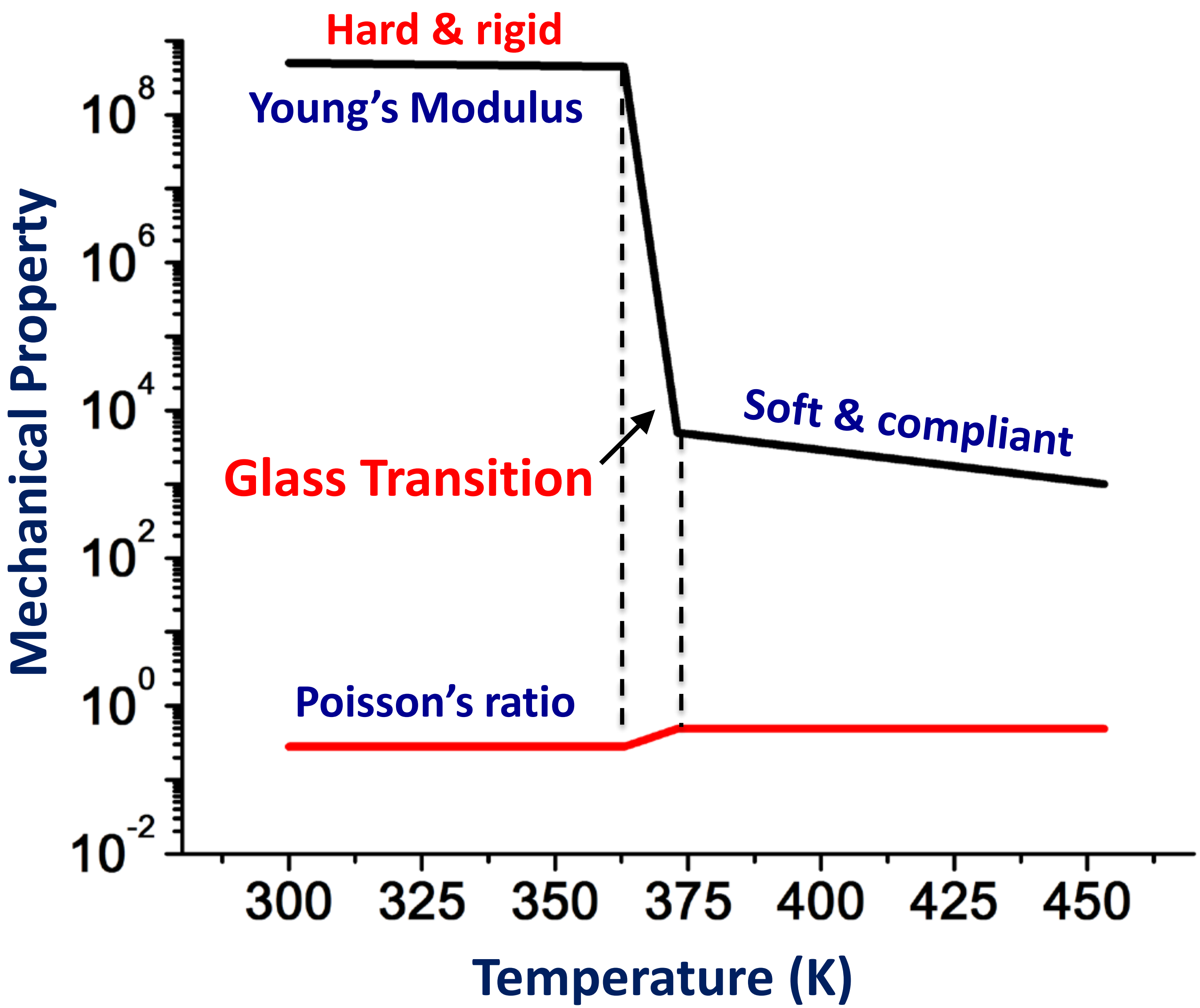
Large Deformations
(Elastic, Perfectly-Plastic Material)

Prediction of Key Quality Attributes

Porosity   Microstructure   Volumetric Expansion

- Driving force of deformation:
  - Expansion is driven by gas pressure gradients only, shrinkage due to moisture loss is neglected

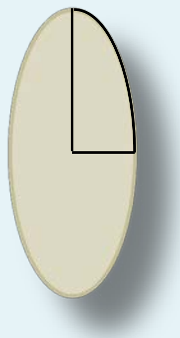
Puffing: Mechanical Properties

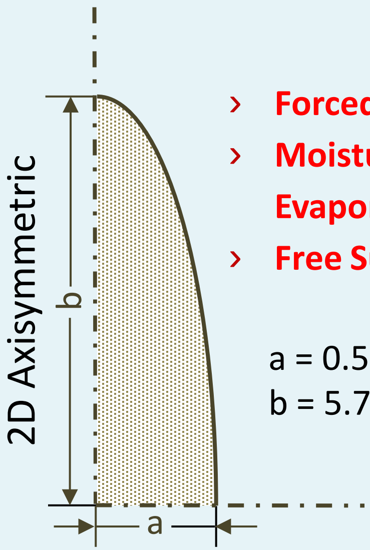


Model implementation

Geometry & Boundary Conditions

Rice kernel as prolate spheroid





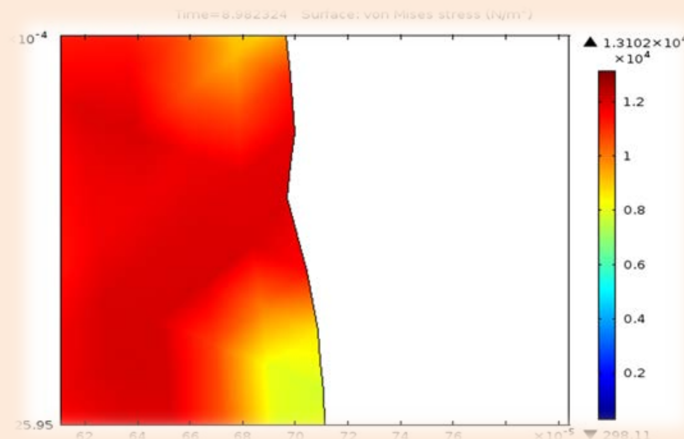
- **Forced Convection Heat Transfer**
- **Moisture Loss through Evaporation**
- **Free Surfaces for Deformation**

$a = 0.5 \times 10^{-4}$ m
$b = 5.75 \times 10^{-4}$ m

- **No axial displacement**
- **Insulated for Energy and Moisture transfer**

Numerical Solution using COMSOL 4.3b

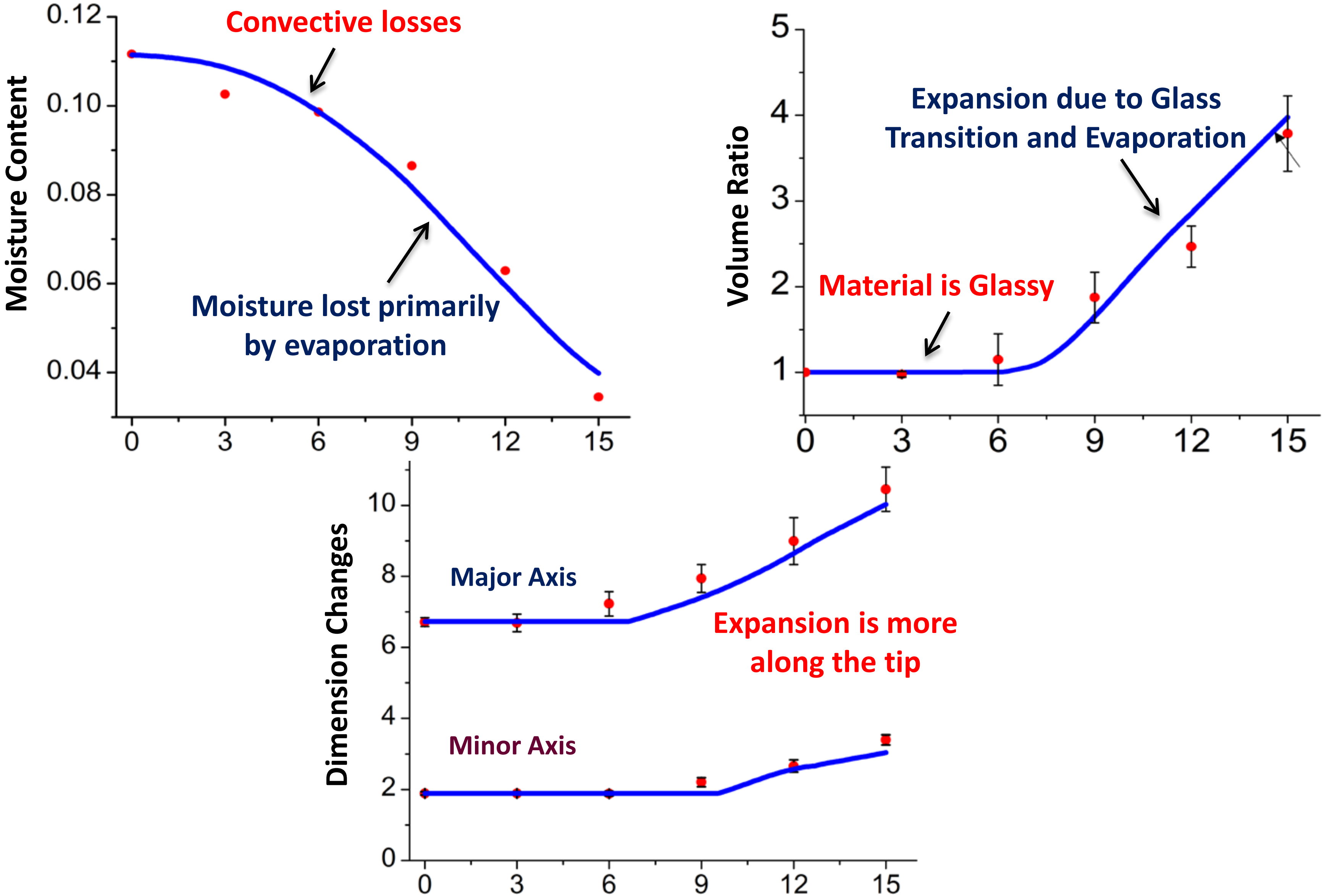
- **A highly-non linear coupled multi-physics problem, convergence issues**



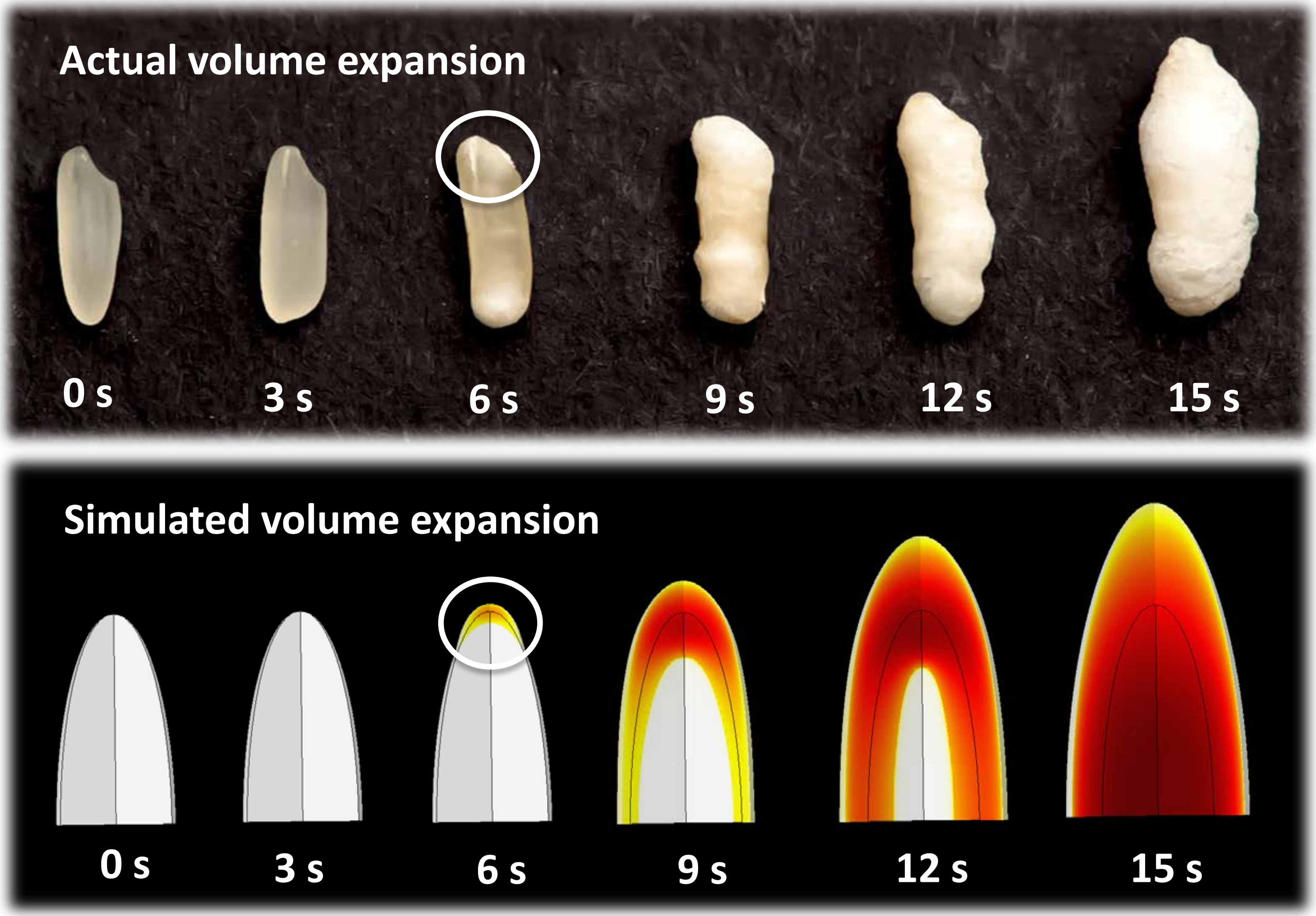
Mesh inverts and leads to convergence problems

- **Large strain plasticity adds additional level of numerical challenge,**
- **Need to play extensively with default solver features of the software**

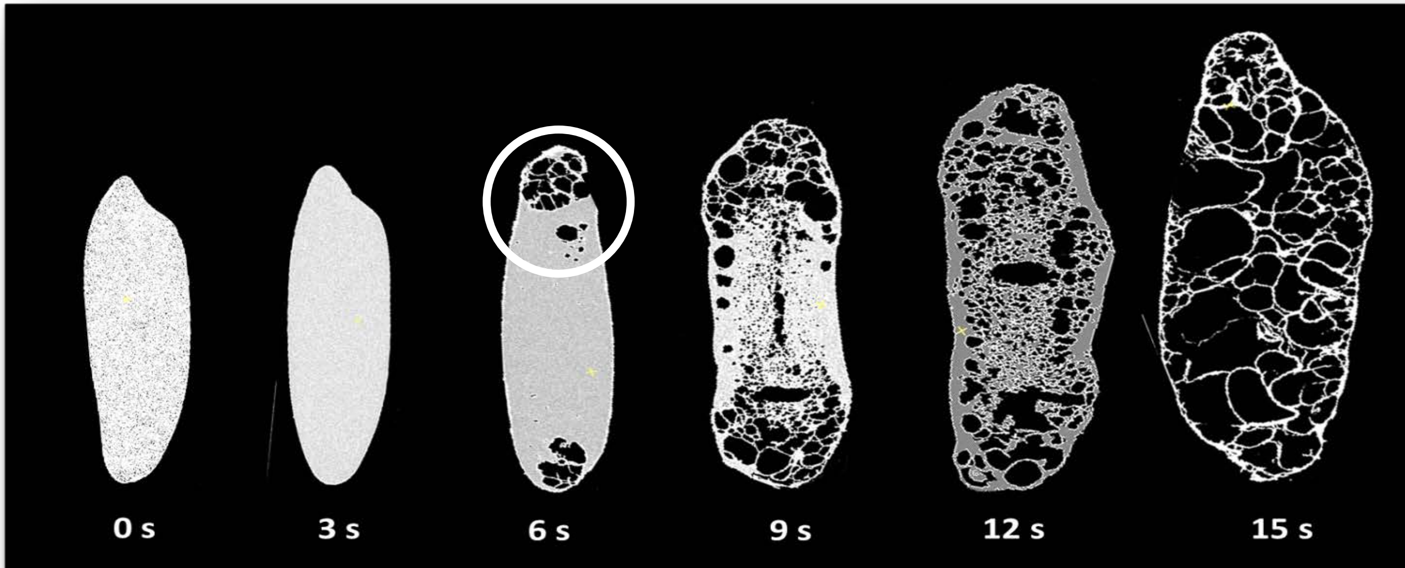
Puffing: Model validation



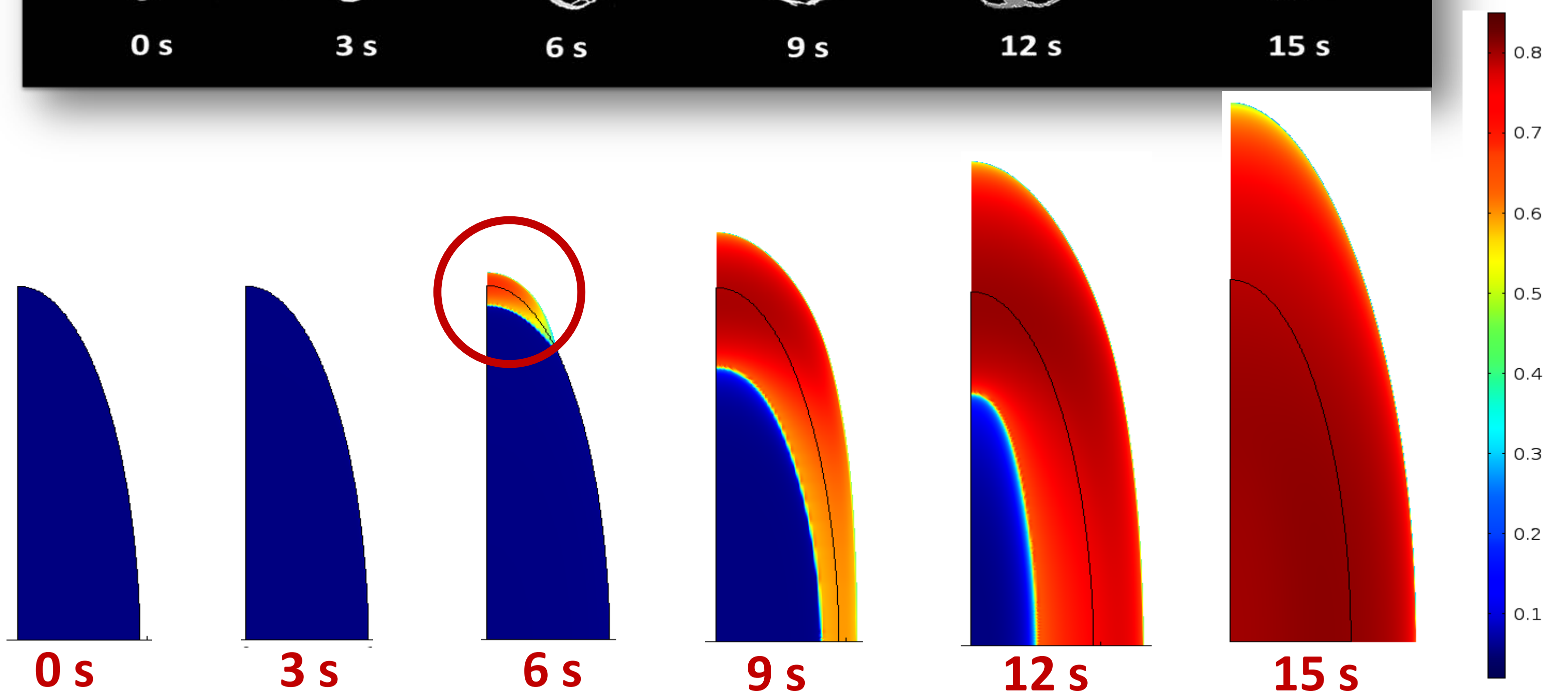
Puffing: Actual and Simulated Expansion



Puffing: Porosity and Microstructure Development



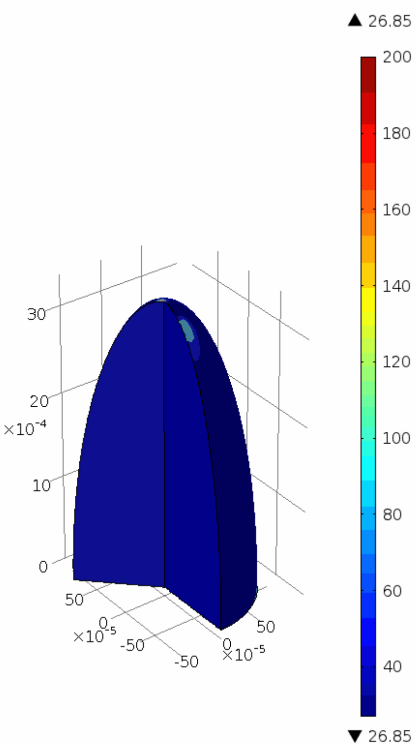
Experiment
0.74



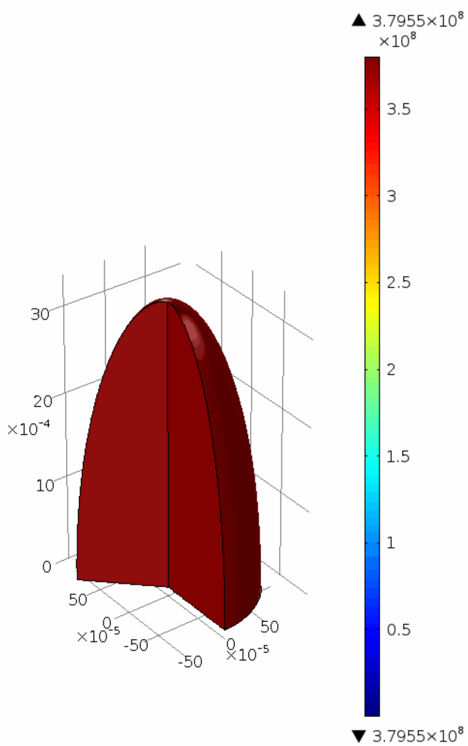
Model
0.751

Puffing: Simulated Process

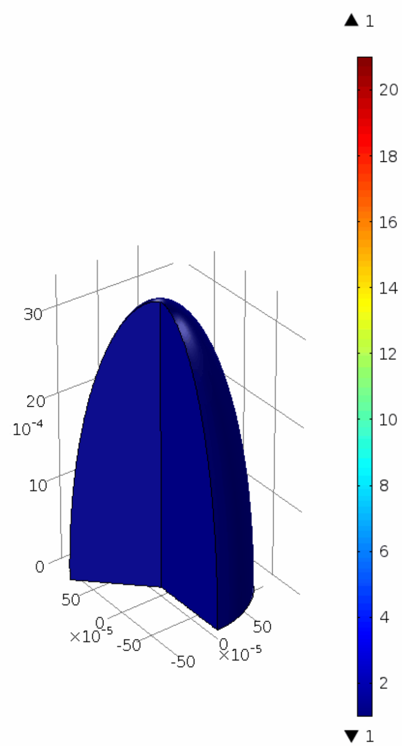
Temperature



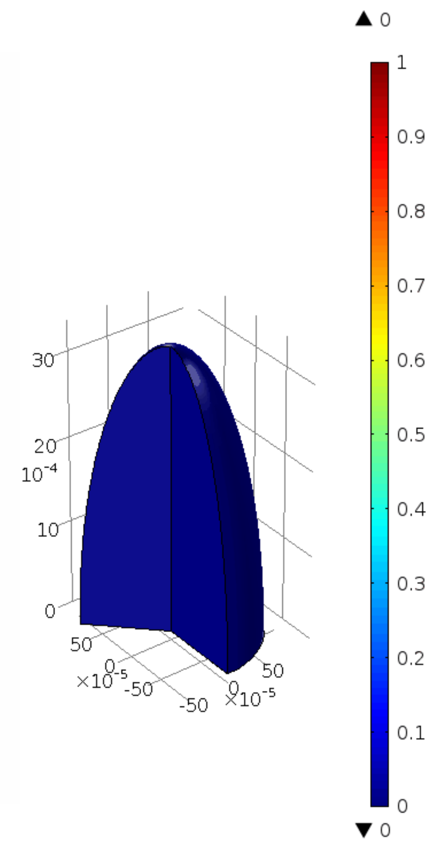
Bulk Modulus



Pressure



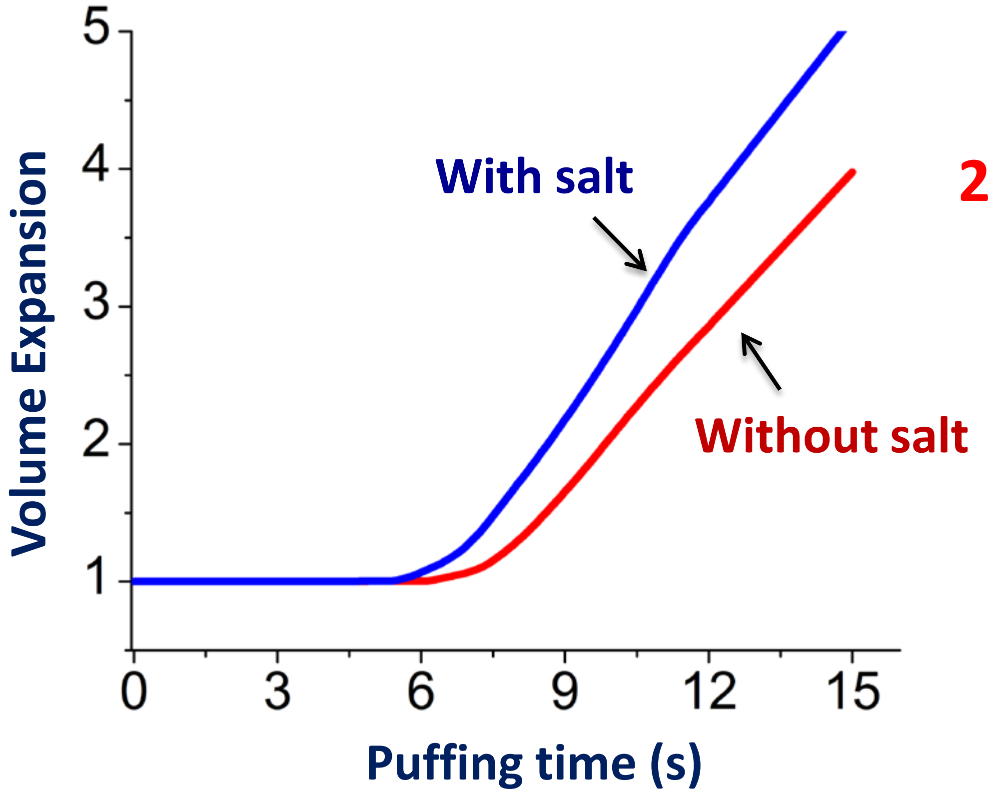
Plastic Deformation



Puffing: Expansion Ratio as a Quality Parameter

Salt preconditioning is done to increase volumetric expansion

- Addition of salt:
  - Decreases the Glass Transition Temperature of the material
  - Increases expansion ratio by at least 15% (found experimentally)



20% more predicted expansion

Puffing: Summary & Potential Applications

- **Physics:** **High temperatures** cause **rapid evaporation** of water generating **large gas pressures** within and, Rubbery-Glassy Phase Transition of the material.

- **Key Observations:** Rice **puffs from the tip** where it Glass Transitions. The expansion front moves inwards eventually causing the entire kernel to puff. **Pore formation** follows a similar trend

- **Process Optimization:** **Salt preconditioning** increases the **expansion ratio** of the kernel

- **Model Extension:** Other **puffing type processes** using **hot oil, gun puffing, extrusion** and **microwave puffing. Starch based-foamed plastics** in the chemical process industry

Acknowledgements

- USDA Grants
- Prof. Ashim Datta
- Prof. Alan Zehnder
- Prof. Shefford Baker
- Alex Warning
- Huacheng Zhu
- Peyman Taherkhani
- Porawon Nitjarunkul
- Dr. Swati Kadam

Thank You