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Multiphase Transport with Large Deformations Undergoing Rubbery-Glassy Phase Transition: Applications to Drying

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Overview

- Drying of biomaterials involves mass, momentum and energy transport along with large shrinkage of the porous material
- Material exists in different states (Rubbery/Glassy) during drying affecting product quality critically
- Complex Shrinkage pattern is observed leading to Case-Hardening
- Case-Hardening affects key Quality Attributes of the dried product such as Porosity and Bulk Density

What is Case-Hardening?

- Thin and significantly dried layer (crust/shell) on the outside of the material

- A glassy matrix characterized by different Mechanical and Transport properties compared to the core

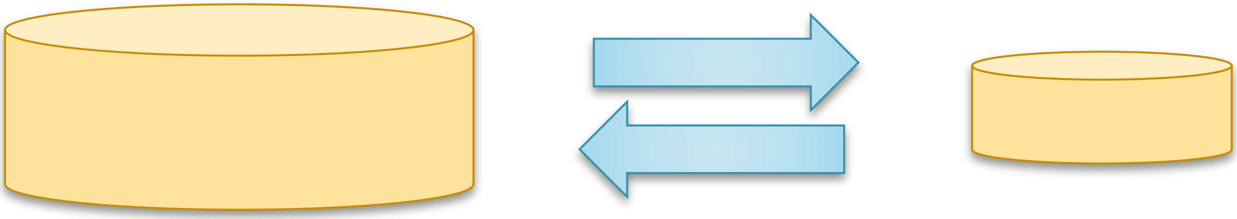
- As a result, the material shrinkage deviates from the amount of water lost

Objectives

- To develop a fundamentals-based multiphase porous media model coupled with large deformations undergoing Rubbery-Glassy phase transition to simulate drying processes
- To predict the complex shrinkage patterns, case hardening effects and deviations in volumetric shrinkage observed during drying
- To predict key Quality Attributes such as degree of crust formation, gas porosity and bulk density

Hot air convective drying

- Convective drying carried out at three different temperatures (40^{0}C, 70^{0}C, 150^{0}C)
- Assumptions:
  - The different phases are in continuum
  - Thermal Equilibrium
  - Pressure shared by all phases

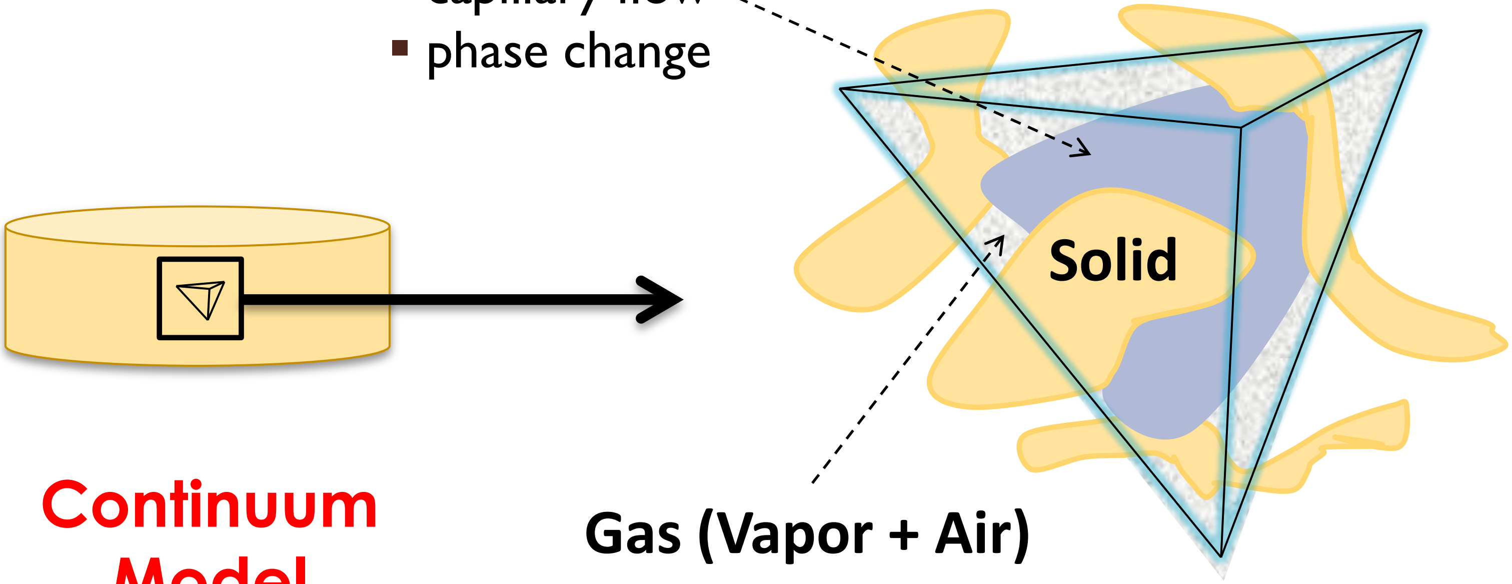


Multiphase transport in porous medium

Large Deformations

Prediction of Key Quality Attributes

Modeling Framework



Water

- bulk flow/convection
- capillary flow
- phase change

Heat transfer

(for the mixture)

Continuum Model

Gas (Vapor + Air)

- bulk flow
- binary diffusion
- phase change

Representative elementary volume

Transport Model

Mass Conservation

Water:

$$\frac{\partial c_w}{\partial t} + \overbrace{\left(\mathbf{v_w} - \underbrace{\mathbf{v_s}}_{\text{Solid Velocity}}\right)\cdot\nabla c_w + c_w\nabla\cdot\mathbf{v_w}}^{\text{Convection}} = \nabla\cdot\underbrace{\left(D_w\nabla c_w\right)}_{\text{Diffusion}} - \overbrace{\dot{I}}^{\text{Phase change}}$$

Gas:

$$\frac{\partial c_g}{\partial t} + \left(\mathbf{v_g} - \mathbf{v_s}\right)\cdot\nabla c_g + c_g\nabla\cdot\mathbf{v_g} = \dot{I}$$

Vapor:

$$\frac{\partial c_v}{\partial t} + \left(\mathbf{v_g} - \mathbf{v_s}\right)\cdot\nabla c_g + c_g\nabla\cdot\mathbf{v_g} = \nabla\cdot\underbrace{\left(\varphi S_g\frac{C^2}{\rho_g}M_a M_v D_{eff,g}\nabla x_v\right)}_{\text{Binary Diffusion (vapor and air)}} + \dot{I}$$

Transport Model

Energy Conservation

$$\frac{\partial}{\partial t}\left[\sum_{i=s,w,v,a}\left(c_i c_{p,i} T\right)\right]+\sum_{i=w,v,a}\overbrace{\left(\mathbf{v_i}-\mathbf{v_s}\right)\cdot\nabla\left(c_i c_{p,i} T\right)+\sum_{i=w,v,a}\left(c_i c_{p,i} T\nabla\cdot\mathbf{v_i}\right)}^{\text{Convection}}-c_{p,w}T\nabla\cdot\left(D_c\nabla c_w\right)$$

$$=\underbrace{\nabla\left(k_{eff}\nabla T\right)}_{\text{Conduction}}-\lambda\dot{I}$$

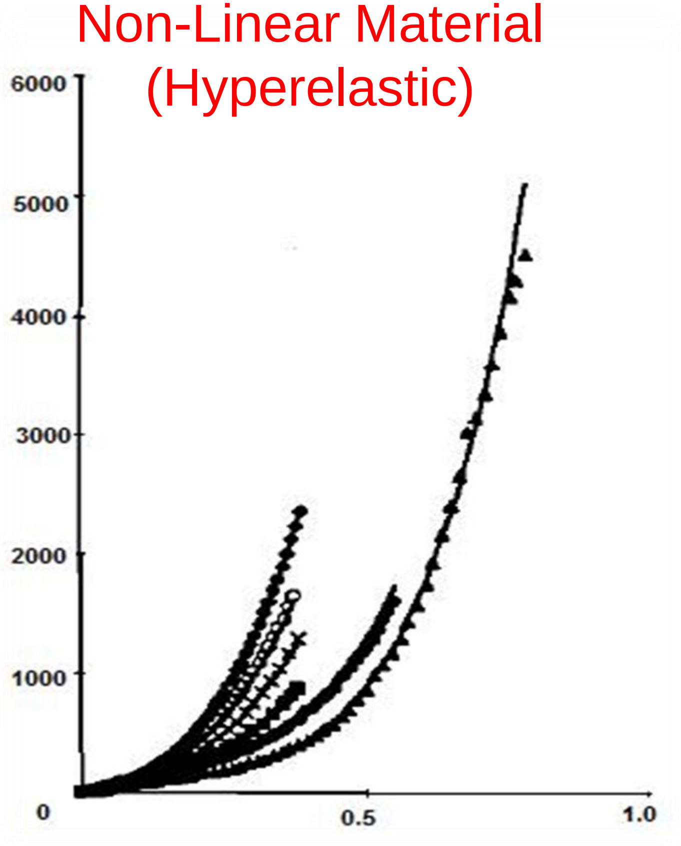
Momentum Conservation

Darcy's Law:
(water and gas)

$$\mathbf{v}_i-\mathbf{v}_s=-\frac{k_i k_{r,i}}{S_i\phi_i\mu_i}\nabla P$$

Solid Mechanical Model

Non-Linear Material
(Hyperelastic)



Stress-Strain curves for potatoes at different moisture contents (Krokida et al., 2000)

Linear Momentum Balance

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

$$-\nabla.\sigma = 0$$

Non-Hookean Material

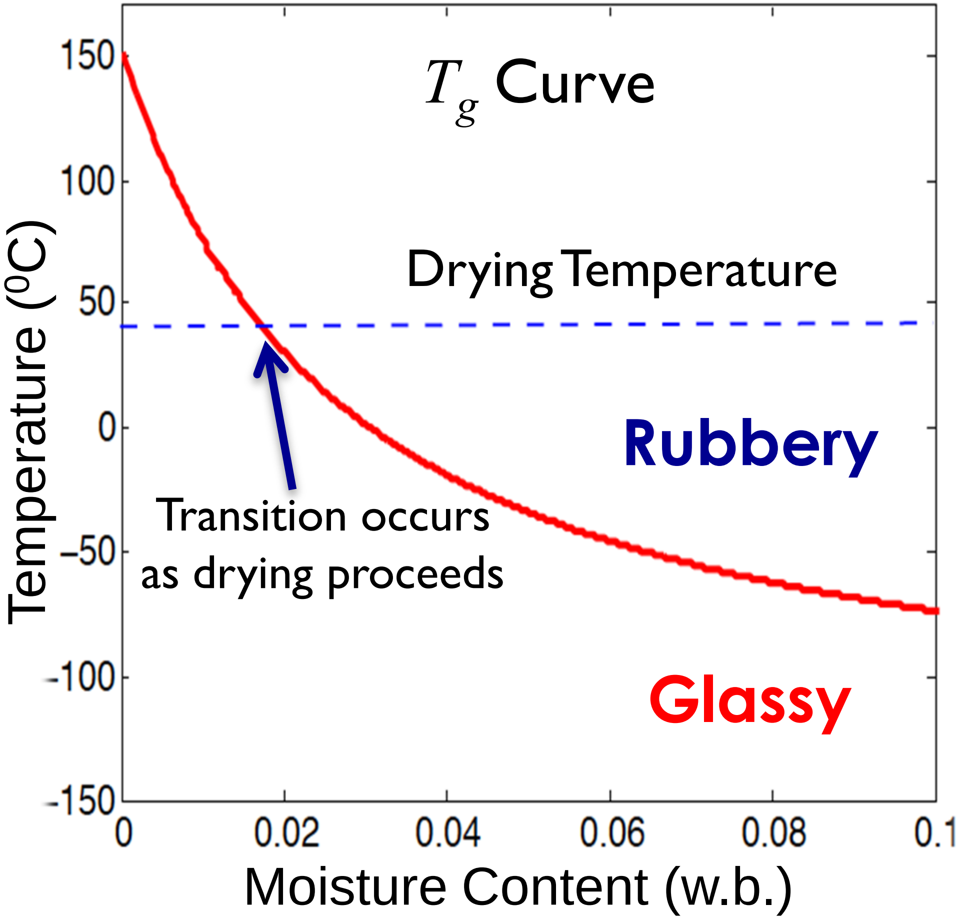
$$W_S = \frac{1}{2}\mu\left(I_1 - 3\right) - \mu \ln\left(J_{el}\right) + \frac{1}{2}\lambda\left[\ln\left(J_{el}\right)\right]^2$$

Large Deformations

$$\mathbf{E}_{\mathbf{el}} = \frac{1}{2}\left[(\nabla.\mathbf{u})^T + \underbrace{\nabla.\mathbf{u}}_{\text{Solid displacement}} + (\nabla.\mathbf{u})^T \nabla.\mathbf{u}\right]$$

Quality Attributes

- Mechanistic approach to predicting Quality Attributes



Bulk Density

$$\rho_b = \rho_s\left(1-\phi_g\right)\left[\left(\frac{1+X}{1+\left(\rho_s/\rho_w\right)X}\right)\right]$$

Crust Formation

$$\Delta T_g = T - T_g$$

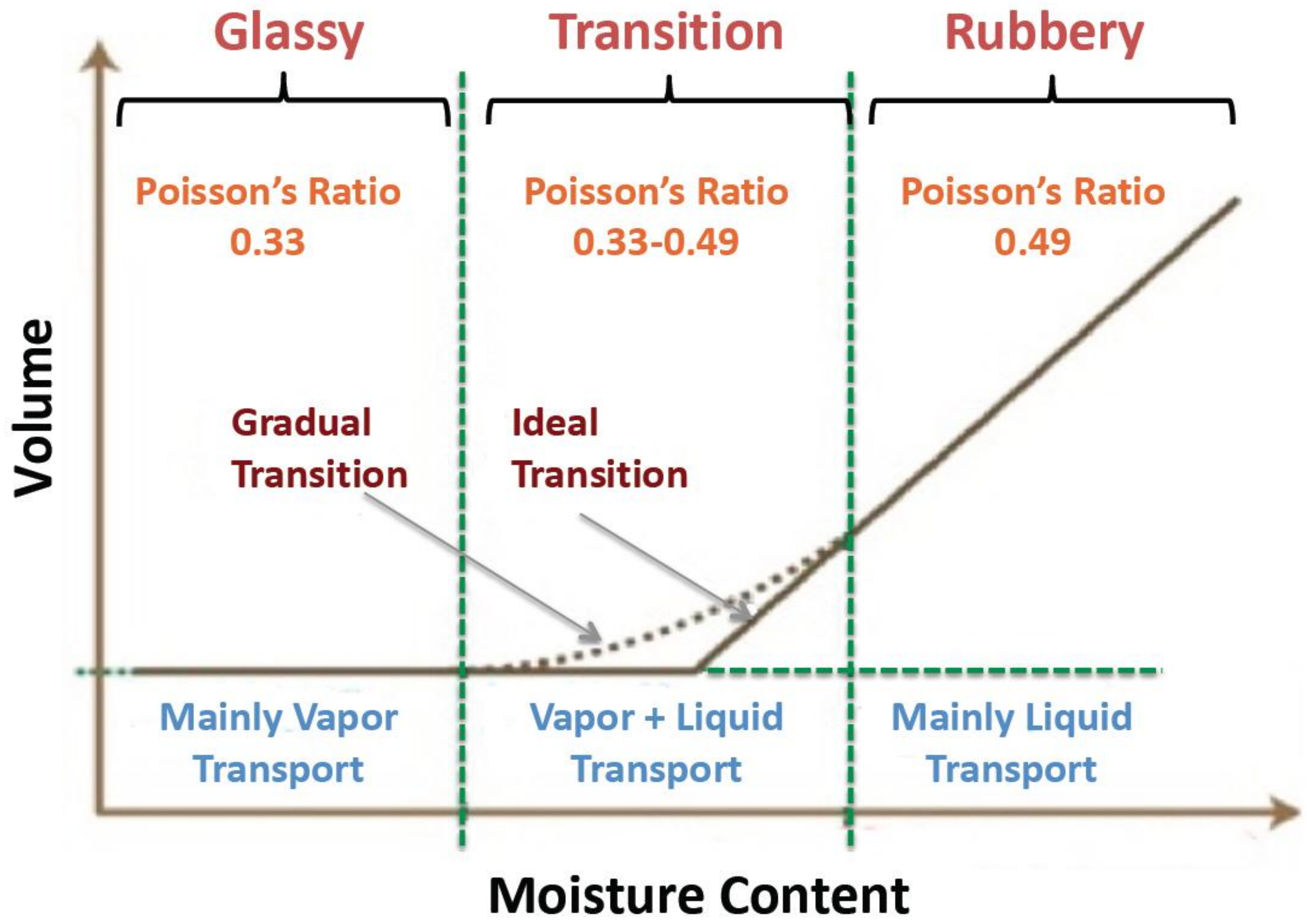
Gas Porosity

$$\phi_g = S_g\left(1-\frac{1-\phi_0}{J}\right)$$

Shrinkage

$$J = \frac{V}{V_0}$$

Transport and Mechanical Properties



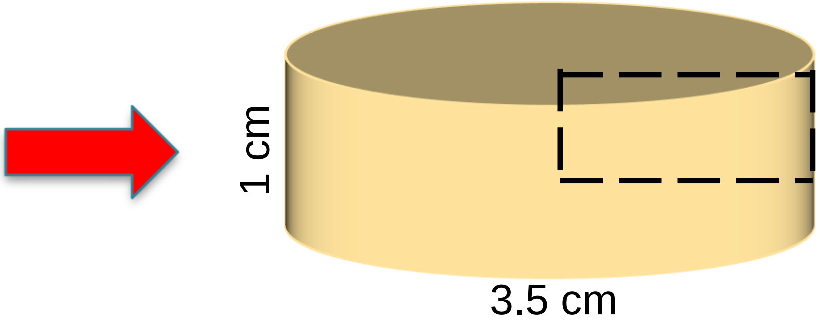
Transport and Mechanical Properties

- Transport and Mechanical Properties are functions of Moisture Content

	Rubbery	Glassy
Mechanical		
• Elastic Modulus	10^5 Pa	10^7 Pa
• Poisson's Ratio	0.5	0.33
Transport		
• Liquid Diffusivity	10^{-9} m^2/s	-
• Vapor Diffusivity	-	10^{-11} m^2/s

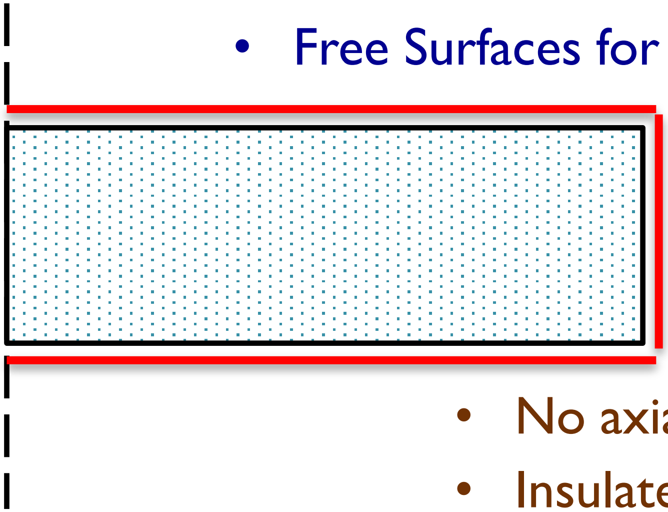
COMSOL Implementation

Cylindrical
Shaped Potato
Samples



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

2D Axisymmetric



- No axial displacement
- Insulated for Energy and Moisture transfer

COMSOL Implementation

Heat and Mass Transport

COMSOL Multiphysics:

- Transport of Dilute Species
- Transport of Concentrated Species (Maxwell-Stefan)
- Heat Transfer in Fluids
- Darcy Flow

ALE frame for Mesh Movement

Primary Variables: temperature, concentration, pressure, velocity

Solid Mechanics

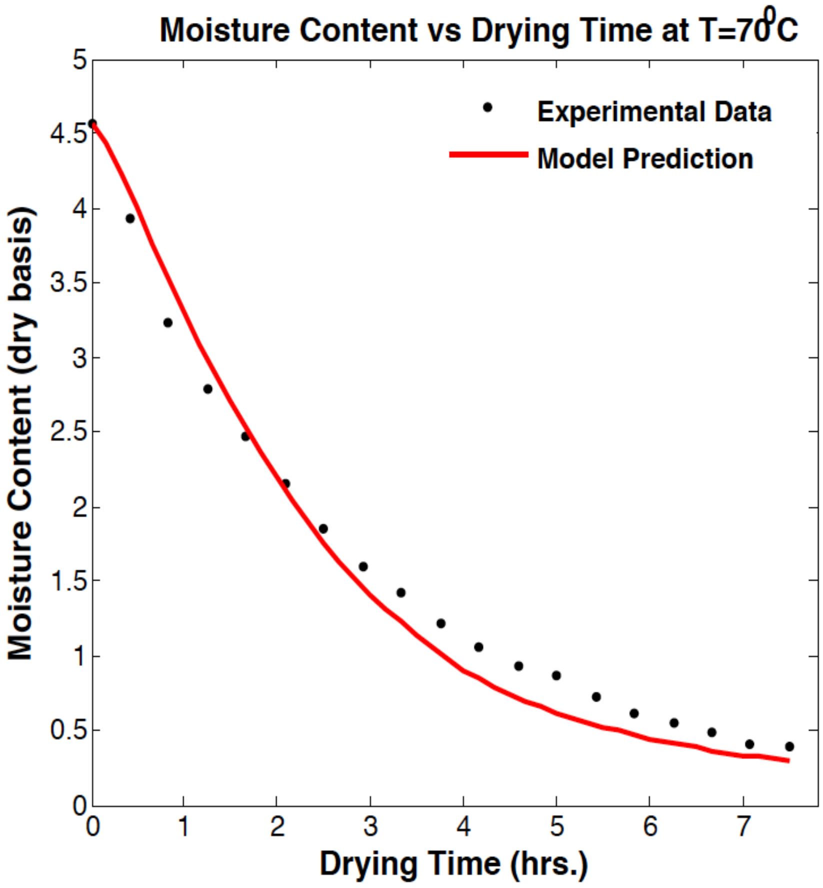
Large deformations:

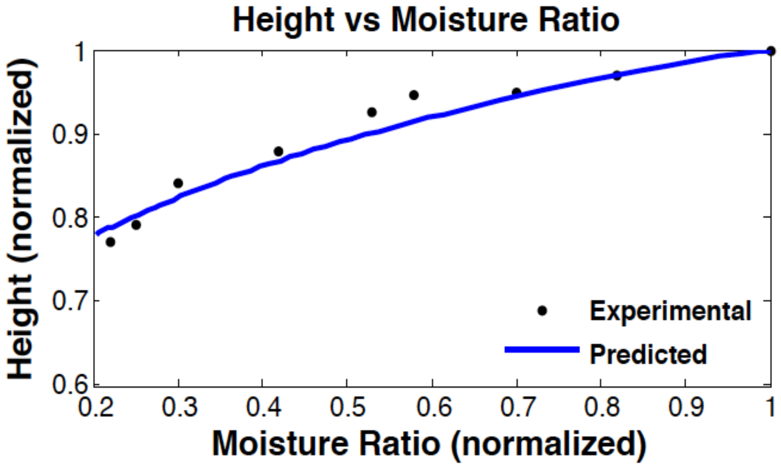
- Hyperelastic material (Neo-Hookean Model)
- Geometric non-linearity

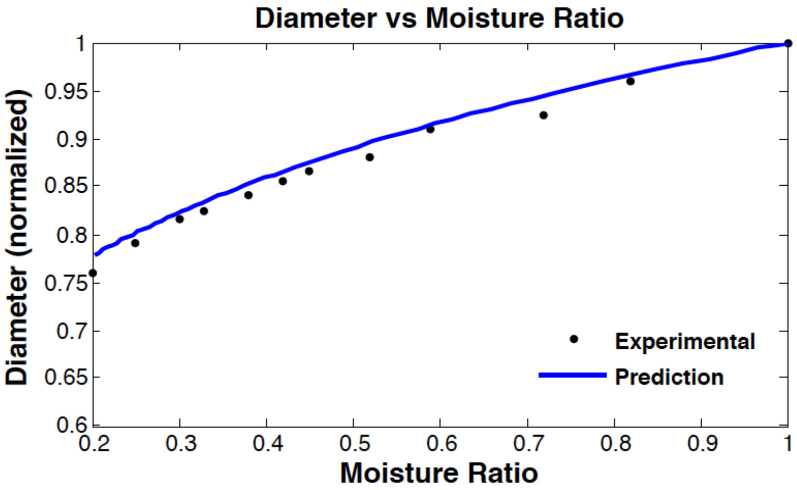
Primary Variables: Stresses (2nd PK), Strains (Cauchy-Green)

Results: Model Validation

- The drying model was validated for moisture, height and diameter histories *(Yang & Sakai, 2001)*

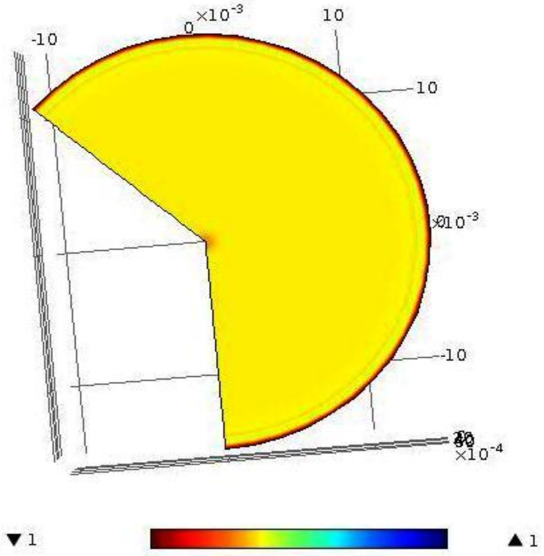




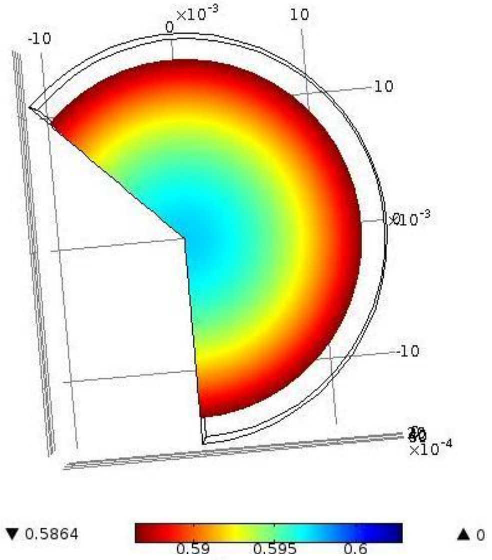


Simulated shrinkage vs. time (T=70^{0}C)

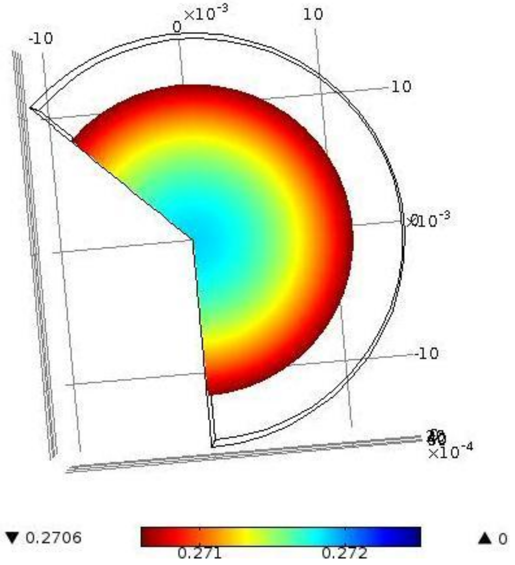
0 Hrs.



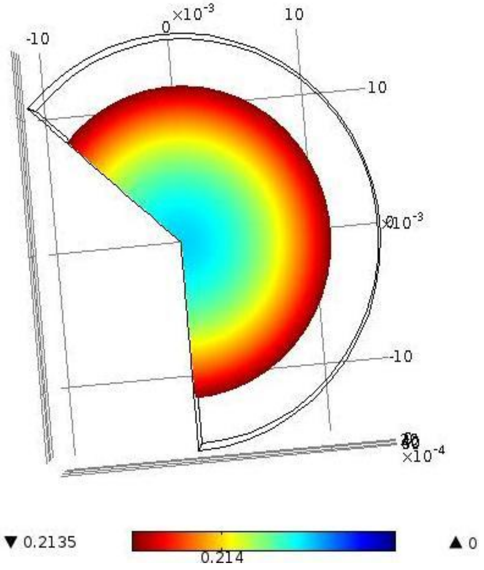
2 Hrs.



4 Hrs.



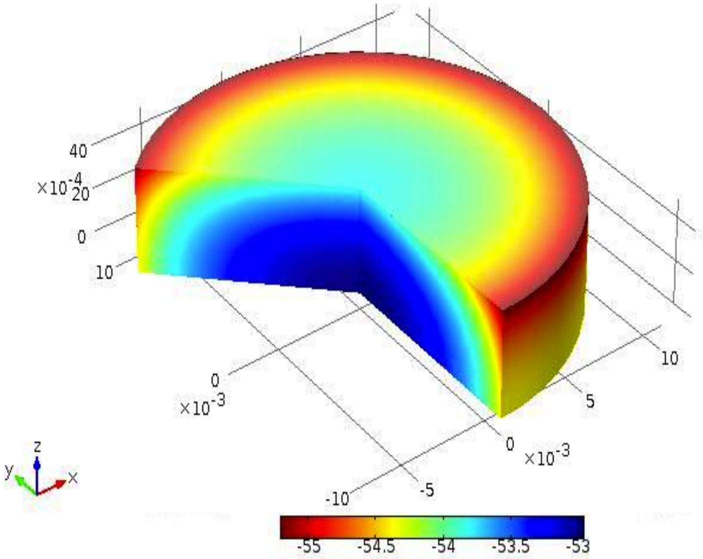
8 Hrs.



Degree of Crust Formation (ΔT_g)

- $\Delta T_g > 0$ indicates material is in Rubbery State
- $\Delta T_g < 0$ indicates material is in Glassy State

Completely Glassy

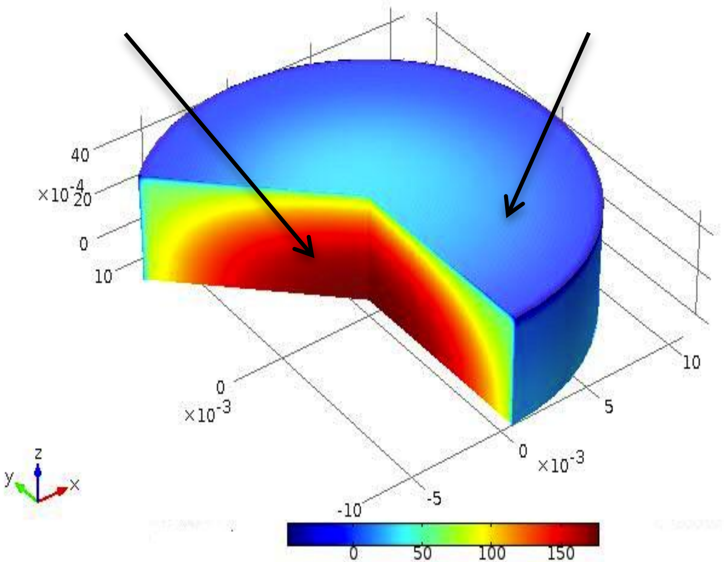


-55.2^0C -52.95^0C

Low Temperature (70^0C)

Inside Wet and Rubbery

Outside Dry and Glassy



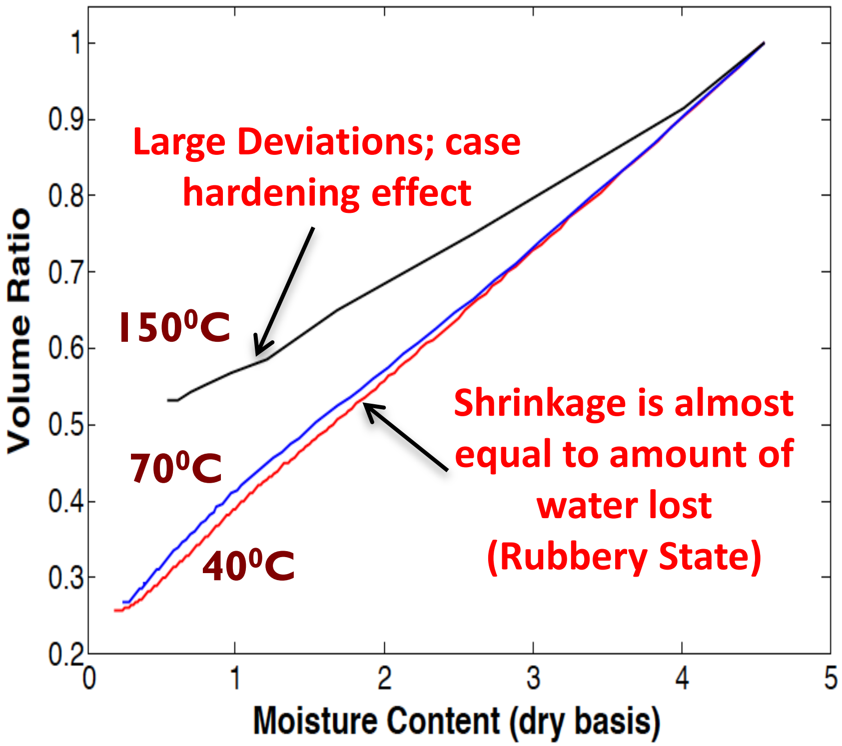
-47.9^0C 177.1^0C

High Temperature (150^0C)

Deviations in Volumetric Shrinkage

- High drying rates results in Case-Hardening leading to large deviations in volumetric shrinkage

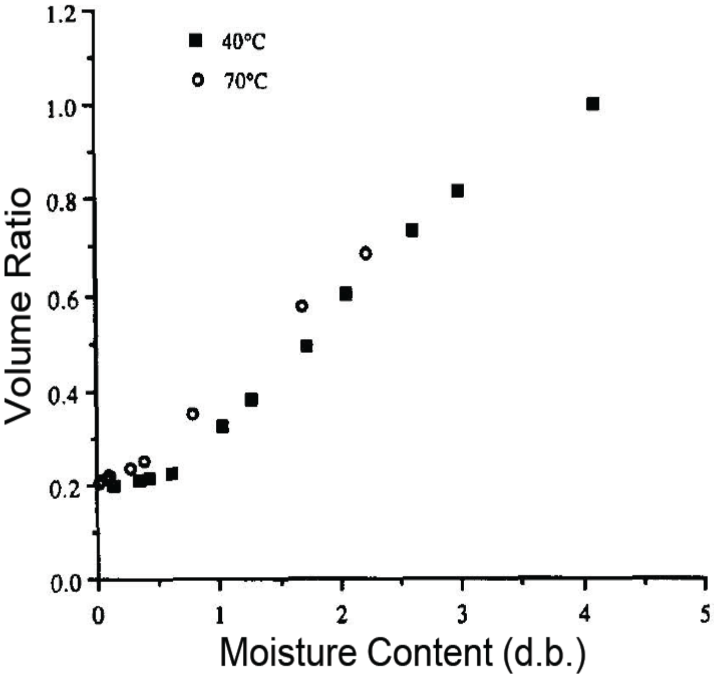
Predicted Volume Ratio at different temperatures



Large Deviations; case hardening effect

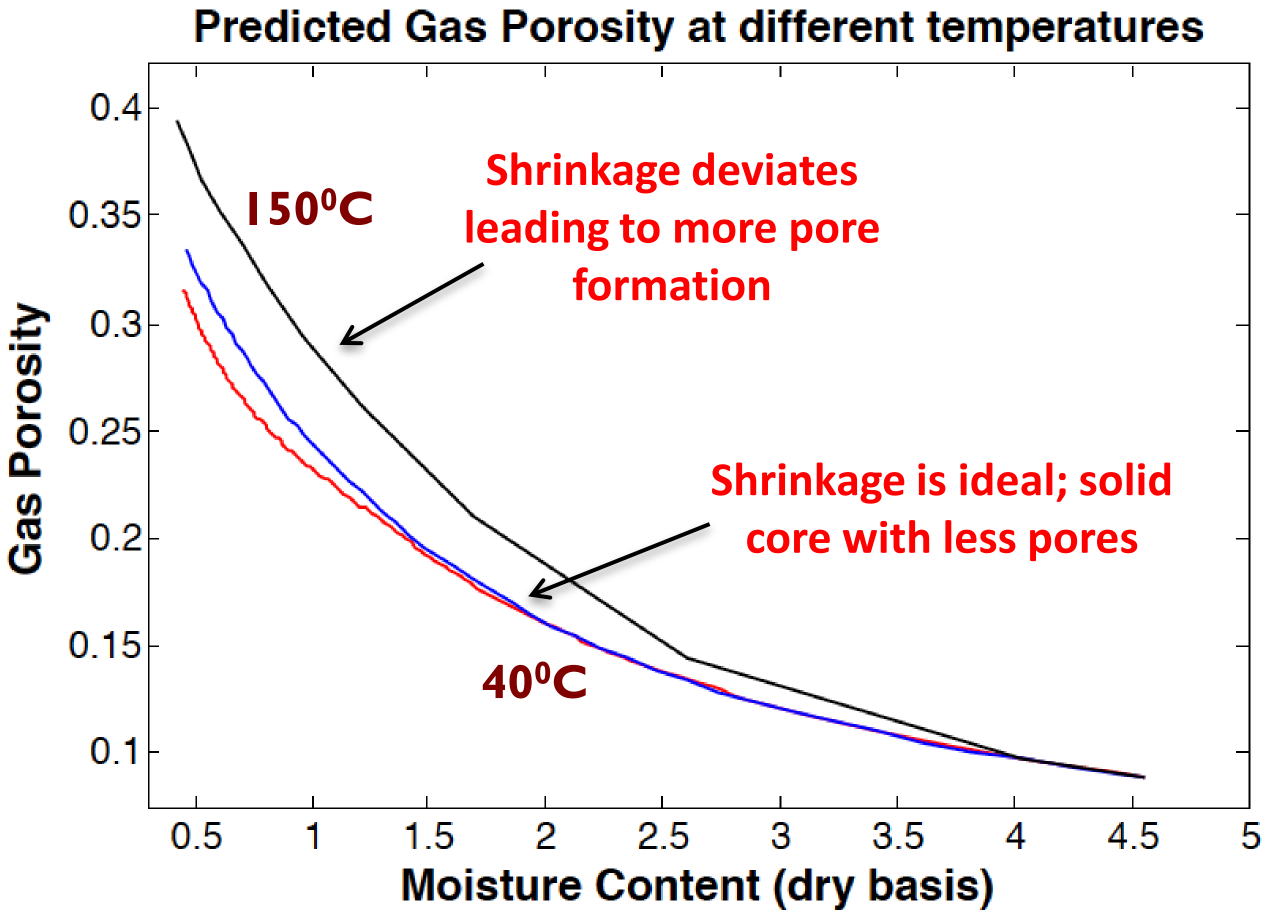
Shrinkage is almost equal to amount of water lost (Rubbery State)

Experimental Volume Ratio at different Temperatures (Wang and Brennan, 1993)



Gas Porosity

- High drying rates results lead to increased Pore formation and in some cases, tissue rupture

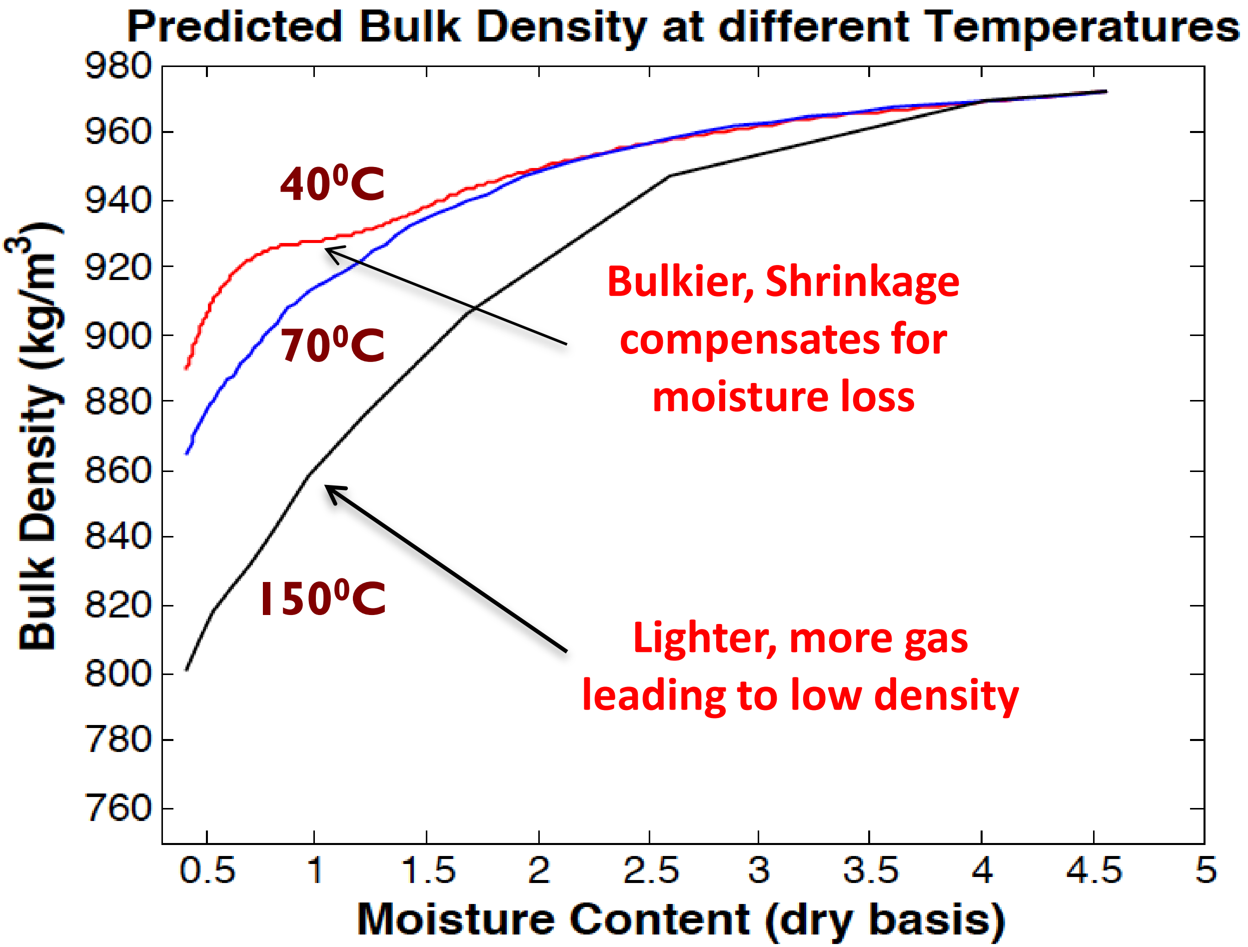


Shrinkage deviates leading to more pore formation

Shrinkage is ideal; solid core with less pores

Bulk Density

- Low drying rates lead to uniform shrinkage, material reduces to a solid core resulting in a denser product



Bulkier, Shrinkage compensates for moisture loss

Lighter, more gas leading to low density

Summary and Conclusions

- A mechanistic approach to understanding drying of biomaterials taking into account the different states of the material is proposed

- The model predicts Case Hardening and key Quality Attributes with very little empirical information

- Such models could serve as frameworks for quality prediction for many products and processes beyond simple drying that involve a complex interplay of heat and mass transport and large deformation (shrinkage/swelling)

Questions?

Thank You