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

Tushar Gulati
Cornell University
Today I Feel Like.com
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 Porous Media\textsuperscript{1,2,3}

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

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

\textsuperscript{1}Whitaker (1997)
\textsuperscript{2}Ni H et al., (1999)
\textsuperscript{3}Halder A et al., (2007)
Transport Process Porous Media

Momentum Conservation

**Darcy Law**

\[
\frac{\partial c_g}{\partial t} + \nabla \cdot \left( n_{g,G} \right) = I
\]

\[
n_{g,s} = -\rho_g \frac{k_g k_{r,g}}{\mu_g} \nabla P
\]

\[
v_i = -\frac{k_i k_{r,i}}{\mu_i} \nabla P
\]

**Darcy Velocity**

\[i = \text{water, gas}\]

Mass Conservation

**Liquid Water**

\[
\frac{\partial c_w}{\partial t} + \nabla \cdot \left( \rho_w \mathbf{v}_w \right) = \nabla \cdot \left( D_w \nabla c_w \right) - \dot{I}
\]

**Water Vapor**

\[
\frac{\partial c_v}{\partial t} + \nabla \cdot \left( \rho_v \omega_v \mathbf{v}_g \right) = \nabla \cdot \left( \varphi S_g \frac{C^2}{\rho_g} M_a M_v D_{eff,g} \nabla \mathbf{x}_v \right) + \dot{I}
\]

Energy Conservation

**Thermal Balance for Mixture**

\[
\frac{\partial}{\partial t} \left[ \sum_{i=s,w,v,a} \left( c_{i,p} \right) \right] + \nabla \cdot \left[ \sum_{i=s,w,v,a} \left( c_{i,p} n_i T \right) \right] = \nabla \left( k_{eff} \nabla T \right) - \lambda \dot{I} + Q_{mic}
\]

Phase Change

**Evaporation-Condensation**

\[
\dot{I} = K \frac{M_v}{RT} \left( p_{v,eq} - p_v \right)
\]

**Non-Equilibrium Formulation**
Deformation in Porous Media: Poromechanics

\[
\bar{\sigma} = \bar{\sigma}' - p_f I
\]

- **Balance of Linear Momentum:** \( \nabla \cdot \bar{\sigma}' = \nabla p_f \)
- **Constitutive Model** for the Solid Skeleton:
  \( \nabla \cdot (D \cdot \varepsilon) = \nabla p_f \)
  
  \( p_f = S_g p_g + S_w p_w \)

1. Perre & May (2001)
Phase Transition

Glassy

Rubbery

Textural Attributes

Porosity & Bulk Density

Volume Shrinkage/Expansion

Stress Cracking

1Roos, Y.H. (2010)
Multiphase transport (Gas Pressure Driven)

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

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

- Hard & rigid
- Glass Transition
- Young’s Modulus
- Soft & compliant
- Poisson’s ratio

Mechanical Property vs. Temperature (K)
Model implementation

Geometry & Boundary Conditions

- Rice kernel as prolate spheroid

2D Axisymmetric

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

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

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

Convective losses

Moisture lost primarily by evaporation

Expansion due to Glass Transition and Evaporation

Material is Glassy

Expansion is more along the tip

Moisture Content

Volume Ratio

Dimension Changes

Major Axis

Minor Axis
Puffing: Actual and Simulated Expansion

Actual volume expansion

Simulated volume expansion
Puffing: Porosity and Microstructure Development

Experiment 0.74

Model 0.751
Puffing: Simulated Process

Temperature    Bulk Modulus    Pressure    Plastic Deformation
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)

![Graph showing volume expansion over puffing time with and without salt](image-url)

- **With salt:**
  - 20% more predicted expansion

- **Without salt:**
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
Any questions?