Numerical model for predicting heat and mass transfer phenomena during cake baking

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• Objectives
  • Implementation of a numerical model for predicting:
    • Temperature fields
    • Moisture content fields
    • Gas pressure fields
    • Swelling
  • Use this model and associated experiments for improving material and mechanisms understandings:
    • Water diffusion coefficients (liquid-vapour) in a porous deformable medium
    • Reaction kinetic of C0₂ production (caused by the leavening agents)
    • Evapo-condensation phenomena
    • ...
Composition:
- Flour
- Eggs
- Fatty substance
- Sugar
- Chemical leavening
Coupled physical phenomena

Energy conservation

\[ \frac{\partial \hat{h}}{\partial t} + \nabla \cdot (\hat{v} \hat{h}) = -\nabla \cdot (q + n_T h_t + n_p h_p + n_{co2} h_{co2}) \]

Momentum conservation

\[ \nabla \cdot \sigma = \nabla p_g \]

Viscoelasticity approach based on Kelvin – Voigt model

Water mass conservation

\[ \dot{\rho}_s \left( \frac{\partial W}{\partial t} + \dot{v} \cdot \nabla W \right) = -\nabla \cdot (n_T + n_p) \]

Solid mass conservation

\[ -\rho_s ^{\mathrm{di}} \frac{\partial \varepsilon}{\partial t} + \nabla \cdot (\rho_s \dot{\varepsilon}) = 0 \]

Porosity development

\[ \dot{\varepsilon} = \rho_s \dot{\varepsilon} \]

CO2 mass conservation

\[ \dot{\rho}_s \left( \frac{\partial \rho_{co2}}{\partial t} + \dot{v} \cdot \nabla \rho_{co2} \right) = -\nabla \cdot (n_{co2} + \dot{G}_{co2}) \]
Conservation equations

Assumptions:
- 3 phases: solid (s), liquid (l), gas (g)
- 2 species in gaseous phase: water (v) et CO₂
- Local thermodynamic equilibrium
- Gaseous phase: ideal gas mixture

Masse conservation:

Solid:
\[
\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\nu_s \rho_s) = 0
\]

Liquid (water):
\[
\frac{\partial \rho_l}{\partial t} + \nabla \cdot (\nu_s \rho_l) = -\nabla \cdot n_l - \dot{G}_W
\]

Vapour (water):
\[
\frac{\partial \rho_v}{\partial t} + \nabla \cdot (\nu_s \rho_v) = -\nabla \cdot n_v + \dot{G}_W
\]

CO₂:
\[
\frac{\partial \rho_{co2}}{\partial t} + \nabla \cdot (\nu_s \rho_{co2}) = -\nabla \cdot n_{co2} + \dot{G}_{co2}
\]

\[\dot{\rho}_i\] Mass concentration (kg.m⁻³)
\[\nu^s\] Deformation velocity (m.s⁻¹)
\[\dot{G}\] Species Production / consumption (kg.m⁻³.s⁻¹)
\[n\] Species flow (kg.m⁻².s⁻¹)
\[W\] Moisture content (kg.kg⁻¹)
Assumptions:
- 3 phases: solid (s), liquid (l), gas (g)
- 2 species in gaseous phase: water (v) and CO₂

Masse conservation:

Liquid water transport (Fick’s law):

\[ n_l = -D_{eff,l} \nabla \rho_l = D_T^{l} \nabla T + D_W^{l} \nabla W + D_{P_g}^{l} \nabla P_g \]

Vapour water transport (Darcy and Fick laws):

\[ n_v = -\rho_g^g D_{eff,v} \nabla \omega_v = -\rho_v^g \frac{k_{rg}^g k_g^g}{\mu_g} \nabla P_g^g = D_T^v \nabla T + D_W^v \nabla W + D_{P_g}^v \nabla P_g^g \]

CO₂ transport (Darcy and Fick laws):

\[ n_{CO_2} = -\rho_g^g D_{eff,CO_2} \nabla \omega_{CO_2} = -\rho_{CO_2}^g \frac{k_{rg}^g k_g^g}{\mu_g} \nabla P_g^g = D_T^{CO_2} \nabla T + D_W^{CO_2} \nabla W + D_{P_g}^{CO_2} \nabla P_g^g \]

\[ k_r \kappa \text{ Permeability (m}^2\text{)} \]
\[ \varepsilon \text{ Porosity} \]
\[ P \text{ Pressure (Pa)} \]
\[ D_{eff} \text{ Diffusion coefficient (m}^2\text{s}^{-1}) \]
\[ \omega \text{ Mass fraction} \]
\[ \mu \text{ Dynamic viscosity (Pa.s)} \]
Assumptions:
- 3 phases: solid (s), liquid (l), gas (g)
- 2 species in gaseous phase: water (v) et CO₂
- Local thermodynamic equilibrium
- Gaseous phase: ideal gas mixture

Masse conservation:

\[ \bar{\rho}_s \left( \frac{\partial W}{\partial t} + \nabla \cdot (\nu_s^s W) \right) = -\nabla \cdot \left( (D_l^W + D_v^W)\nabla W + D_v^T \nabla T + D_v^P \nabla P^g \right) \]

\[ K_T \frac{\partial T}{\partial t} + K_W \frac{\partial W}{\partial t} + K_{P_g} \frac{\partial P^g}{\partial t} + K_{\epsilon} \frac{\partial \epsilon}{\partial t} + \nabla \cdot \left( \nu_s^s \rho_{CO₂} \right) = -\nabla \cdot \left( D_{CO₂}^T \nabla T + D_{CO₂}^W \nabla W + D_{CO₂}^P \nabla P^g \right) + \dot{G}_{CO₂} \]

\[ -\rho_s^s \frac{\partial \epsilon}{\partial t} + \nabla \cdot (\nu_s^s (1 - \epsilon) \rho_s^s) = 0 \]

Moisture content \( W \)

Gas Pressure \( P_g \)

Porosity \( \epsilon \)
**Conservation equations**

**Assumptions:**
- 3 phases: solid (s), liquid (l), gas (g)
- 2 species in gaseous phase: water (v) et CO₂
- Local thermodynamic equilibrium
- Gaseous phase: ideal gas mixture

**Energy conservation (product):**

Enthalpy formulation:

\[
\frac{\partial \rho h}{\partial t} + \nabla \cdot (\nu_s \rho h) = -\nabla \cdot (q + n_l h_l + n_v h_v + n_{co2} h_{co2})
\]

**Momentum conservation:**

Solid approach (Viscous behaviour):

\[
\nabla \cdot \sigma = \nabla \cdot P_g^g
\]

Deformation velocity \(\nu_s\)

\[
\sigma = 2 \mu \dot{\varepsilon}
\]

\[
\dot{\varepsilon} = \frac{1}{2} [ (\nabla \nu_s^s)^T + \nabla \nu_s^s ]
\]

With:

- \(h\) Enthalpy (J.kg⁻¹)
- \(c_p\) Specific heat (J.kg⁻¹.K⁻¹)
- \(L_v\) Latent heat (J.kg⁻¹)
- \(T\) Temperature (K)
- \(q\) Heat flux (W.m⁻²)
- \(k_{eff}\) Effective thermal conductivity (W.m⁻¹.K⁻¹)
Conservation equations

Boundary conditions:

Air / product interface:

\[-n(n_l + n_v) = \frac{k_m M}{R} \left( \frac{P_v}{T} - \frac{P_{v,\infty}}{T_{\infty}} \right) = m_w\]

\[-n(q) = h(T_{\infty} - T) + \varepsilon_p \sigma (T_{oven}^4 - T^4) - n_l L_v\]

Mold / product interface:

\[-n(n_l + n_v) = 0\]

\[-n(-k_{eff} \nabla T) = -n(-k_{mold} \nabla T_{mold})\]

\[T = T_{mold}\]

Mold / air interface:

\[-n(q) = h(T_{\infty} - T_{mold}) + \varepsilon_m \sigma (T_{oven}^4 - T_{mold}^4)\]

Symmetry axis: zero fluxes conditions

\[P_g^g = P_{atm}\]

\[\sigma = 0\]

\[-n(v_s^s \bar{\rho}_s) = 0\] Deformation velocity

\[-n(n_{co2}) = 0\]

\[-n(v_s^s) = 0\] Deformation velocity

\[P_v\] Vapour Pressure (Pa)

\[k_m\] Mass transfer coefficient (m.s\(^{-1}\))

\[m_w\] Water evaporation rate (kg.m\(^{-2}\).s\(^{-1}\))

\[h\] Heat transfer coefficient (W.m\(^{-2}\).K\(^{-1}\))

\[\varepsilon_p\] Emissivity
Implementation of governing equations:

- Comsol Multiphysics 5.2®
  - Transient 2D axisymmetric model
  - 4 equations in PDE formulations in general form \((W, T, Pg, \epsilon)\)
  - Structural Mechanics Module for \(\nu_S^x\)
  - ALE formulation (Arbitrary Lagrangian Eulerian) \(\Rightarrow\) mobile meshing
- Meshing
  - 715 mapped and triangular elements
- Compute time
  - 20 min (CPU Intel Xeon 2,66 GHz (6 cores), Ram 24 GO)
Results
Results

height at the center of the product (mm)

![Graph showing height vs. time]

- **Simulated**
- **Experimental**

![Image of a simulated structure]
Conclusion

• A numerical model was implemented for describing heat and mass transfer into a deformable porous medium.
• This model predicts: temperature, moisture content, gas pressure, porosity and swelling.
• A correct agreement with experimental data for temperatures, mass losses and global deformation is noted. Nevertheless, results could be improved.
• Provide better knowledge about product and the mechanisms.

Perspectives

• Improving the model
  • Gas phase with 3 species: water, CO$_2$ and air
  • Colouring (brownness) prediction
  • Adding mechanical laws and reaction kinetics (coagulation, gelatinization, CO$_2$ production) more realistic.