Finite Element Modeling of Coupled Heat and Mass Transfer of a Single Maize Kernel Based on Water Potential Using COMSOL Multiphysics Simulation

Authors:

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Main research area of our Institute is grain drying since the 1980’s.

Experimental convective drying tunnel

Testing of grain dryers

Thermographic image of the dryer

Introduction
Besides experimental research drying modeling of a single kernel was initiated.

For example, the mass diffusion relationship was determined for different maize hybrids:

\[ D = e^{a+bX+cT^{-1}} \]

where:
- \( D \) = moisture diffusion coefficient;
- \( X \) = kernel average moisture content (dry basis);
- \( T \) = average temperature of kernels;
- \( a, b, c \) = constants.

(These constants for the Pioneer 3780 hybrid were found: \( a = -3.1411 \); \( b = 3.2159 \); \( c = -6696.6 \))
Based on the measurements mathematical modeling studies of drying were carried out using Finite Element method:

\[ \rho \cdot c \frac{\partial T}{\partial t} = k \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + L \cdot \rho \frac{\partial X}{\partial t} \]

for heat transfer

\[ \frac{\partial X}{\partial t} = D \left( \frac{\partial^2 X}{\partial x^2} + \frac{\partial^2 X}{\partial y^2} \right) \]

for mass transfer

where: \( X \) is moisture content d.b. [kg/kg];
\( \rho \) is density [kg/m³];
\( T \) is temperature [K];
\( K \) is thermal conductivity [W/mK];
\( L \) is latent heat of vaporisation of water [J/kg].

\( D \) is diffusion coefficient [m²/s];
\( c \) is specific heat [J/kgK];
\( t \) is time [s];
\( x,y \) are directions;
FE modelling with **COSMOS 1.71**

**Mass transfer**

5 min

35 min

50 min

85 min of drying

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COMSOL MULTIPHYSICS simulation
(FEMLAB 2.2 package)
Heat Transfer: \( \rho \cdot c \frac{\partial T}{\partial t} = k \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + L \cdot \rho \frac{\partial X}{\partial t} \)

Mass Transfer: \( \frac{\partial X}{\partial t} = D \left( \frac{\partial^2 X}{\partial x^2} + \frac{\partial^2 X}{\partial y^2} \right) \)

FE modelling with FEMLAB 2.2

Before

10 min

20 min

30 min of drying
Magnetic resonance imaging (MRI) studies were carried out to evaluate the accuracy of the FE models.
**FEMLAB model:** the moisture content changes inside a single kernel during drying.

- the model is based on the **m.c. gradients**
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- the model is based on the **m.c. gradients**
Moisture content of the particles vs. whole maize kernels (Florencia)

Average moisture content of the whole kernel, $X$ [kg/kg]

Moisture content of the constituents, $X$ [kg/kg]

- endosperm
- scutellum

40 °C
Considering capillary (water) potential

The modified Luikov’s model of mass transport,

\[ \frac{\partial X}{\partial \tau} = \text{div}D \cdot \text{grad}X \]

can be rewritten:

\[ \frac{\partial X}{\partial \Psi} \frac{\partial \Psi}{\partial \tau} = \frac{\partial}{\partial x} \left[ D \frac{\partial X}{\partial \Psi} \frac{\partial \Psi}{\partial x} \right] + \frac{\partial}{\partial y} \left[ D \frac{\partial X}{\partial \Psi} \frac{\partial \Psi}{\partial y} \right] + \frac{\partial}{\partial z} \left[ D \frac{\partial X}{\partial \Psi} \frac{\partial \Psi}{\partial z} \right] \]

and thus the equation gives:

\[ \frac{\partial X}{\partial \Psi} \frac{\partial \Psi}{\partial \tau} = \text{div}K \cdot \text{grad} \psi \]

where:
- \( X \) is moisture content;
- \( \tau \) is time;
- \( D \) is mass diffusion coefficient.

where:
- \( \Psi \) is capillary (water) potential;
- \( K \) is hydraulic conductivity \((K = D \cdot \partial X/\partial Y)\).
Desorption curves of maize kernel’s particles

Equilibrium moisture content, d.b., X [kg/kg]

Relative humidity, ϕ

Endosperm
Scutellum

ROTRONIC water activity meter

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\[ [\Psi]_X = \frac{R_U \cdot T}{m_v} \ln \varphi \]

where:
\( \varphi \) is the relative humidity of the air (decimal);
\( R_U \) is the universal gas constant;
\( m_v \) is the molecular weight of vapour;
\( T \) is the absolute temperature;
\( X \) is moisture content, d.b.
Boundary conditions

Neumann type:

\[ n \cdot (c \nabla u) + qu = qu_\infty \]

where:

- \( u \) is stands for the water potential (\( \Psi \));
- \( n \) is the normal vector.

\[ d_a = \frac{\partial X}{\partial \psi} \]
Modelled $\Psi$ changes based on grad $\Psi$

$X$ changes based on grad $\Psi$

Water potential, \( [\text{kJ/kg}] \)

Endosperm
Scutellum

Moisture content, \( [\text{kg/kg}] \)

40 °C

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Modelled $\Psi$ changes

$X$ changes based on grad $\Psi$

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Modelled $\Psi$ changes $X$ changes based on $\text{grad} \, \Psi$

Water potential, [kJ/kg]

Endosperm
Scutellum

0 0.1 0.2 0.3 0.4 0.5 0.6
0 50 100 150 200

40 °C

Moisture content, d.b., $X$ [kg/kg]

Water potential, [kJ/kg]

Moisture cotent, [kg/kg]

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Modelled \( \Psi \) changes

\( X \) changes based on \( \text{grad } \Psi \)

Water potential, \([\text{kJ/kg}]\)

Endosperm
Scutellum

Moisture content, \([\text{kg/kg}]\)

40 °C

0 0.1 0.2 0.3 0.4 0.5 0.6

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Modelled $\Psi$ changes

$X$ changes based on grad $\Psi$

Water potential, $\Psi$ [kJ/kg]

Endosperm
Scutellum

Moisture content, $X$ [kg/kg]

40 °C

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Modelled $\Psi$ changes

$X$ changes based on $\text{grad } \Psi$

Water potential, [kJ/kg]

Moisture content, [kg/kg]

Endosperm
Scutellum

Water potential, $\Psi$ [kJ/kg]

Moisture content, $X$ [kg/kg]

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Modelled $\Psi$ changes based on grad $\Psi$

Water potential, $\Psi$ [kJ/kg]

Endosperm
Scutellum

40 °C

Moisture content, $X$ [kg/kg]

Water potential, Moisture content

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Modelled $\Psi$ changes

$X$ changes based on grad $\Psi$

Water potential, [kJ/kg] vs. Moisture content, [kg/kg]

Endosperm
Scutellum
Modelled $\Psi$ changes

$X$ changes based on grad $\Psi$

Water potential, $\Psi$ [kJ/kg]

Moisture content, $X$ [kg/kg]

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Modelled $\Psi$ changes

$X$ changes based on grad $\Psi$

Water potential, $\Psi$ [kJ/kg]

Moisture content, $X$ [kg/kg]

40 °C

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CONCLUSIONS

• In the governing equation using water potential as the driving force has exact physical meaning, instead of the moisture gradient drying force.

• One multiphysical equation system gives more accurate solutions instead of iteration solutions.

• Further studies needs to be done to determine water potential above hygroscopic moisture content.
THANK YOU FOR YOUR ATTENTION!

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