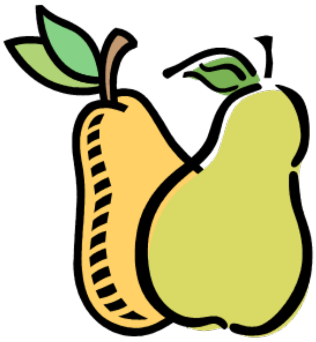
The Pear Project

Solving a macroscale respiration–diffusion model

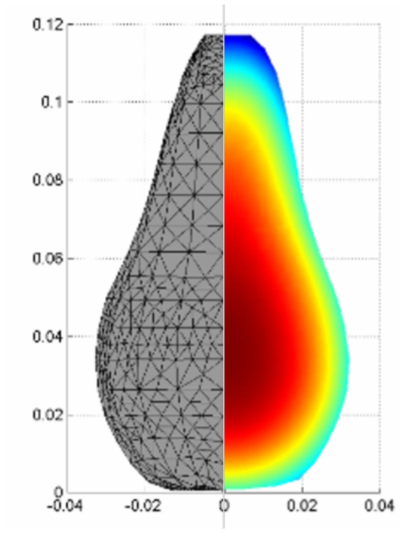
2016 – 2017



After harvest, the respiration metabolism of pome fruit, apple and pear, still remains active. In order to maintain fruit quality for a long period of time, consumption of oxygen and production of carbon dioxide need to be controlled. In practice, this is done by cold and controlled atmosphere storage: low temperature in combination with a reduced oxygen concentration and a slightly increased carbon dioxide concentration slow down the respiration metabolism. However, suboptimal or extreme storage conditions can cause physiological disorders in fruit. For example, if the oxygen concentration is too low and the carbon dioxide concentration is too high, this can lead to core breakdown in *Conference* pears (tissue browning around the core, development of cavities). It is believed that this phenomenon is due to altered respiration (a switch from aerobic to anaerobic respiration or fermentation) and gas exchange properties of the tissue (diffusivity of metabolic gasses).

As the exchange of metabolic gasses, such as oxygen and carbon dioxide, is crucial for maintaining normal *metabolic/physiological* functioning, it is important to study/understand how these gasses are transported and distributed within the fruit structure.

At present, no good methods are available to measure internal gas concentrations in fruit. Therefore, in recent years, a scientific computing approach has been adopted to simulate and predict internal gas concentrations/distributions. Furthermore, this approach allows to study the effect of fruit geometry (shape and size) or controlled storage conditions on local oxygen and carbon dioxide concentrations, while reducing experimental costs.



Goals: Students develop and implement numerical solutions of a macroscale respiration–diffusion system for metabolic gas exchange in pears using the Finite Element Method. Programming and simulation. Code verification/testing against analytical solutions of simplified models.

Contact: nico.scheerlinck@cs.kuleuven.be ; karl.meerbergen@cs.kuleuven.be

General Respiration–diffusion model

As diffusion is considered to be the main mechanism of gas exchange in pear fruit, Fick's laws of diffusion are used to describe an effective diffusion process driven by concentration gradients. Gas exchange is coupled with respiration kinetics. Oxygen consumption and carbon dioxide production are described using Michaelis-Menten reaction kinetics, including a non-competitive inhibition of carbon dioxide on oxygen consumption and inhibition of high oxygen concentrations on the fermentative part of carbon dioxide production.

The model under study consists of a set of two coupled non–linear reaction–diffusion equations, defined on a one-, two- or three-$d$imensional bounded spatial domain $\Omega \subset \mathbb{R}^d$, with a mixed type of conditions at the boundary Γ:

$$\left\{\begin{array}{rcl} \dfrac{\partial C_u}{\partial t} & = & D_u \nabla^2 C_u - R_u(C_u, C_v) \\ & & \\ \dfrac{\partial C_v}{\partial t} & = & D_v \nabla^2 C_v + R_v(C_u, C_v) \end{array}\right. \quad \text{in } \Omega \ , \ t > 0.$$

$$\left\{\begin{array}{rcl} -\vec{n} \cdot (D_u \nabla C_u) & = & h_u(C_u - C_{uamb}) \\ & & \\ -\vec{n} \cdot (D_v \nabla C_v) & = & h_v(C_v - C_{vamb}) \end{array}\right. \quad \text{on } \ \Gamma \ , \ t > 0.$$

where $C_u \equiv C_u(x, y, z, t)$ and $C_v \equiv C_v(x, y, z, t)$ represent the oxygen and carbon dioxide concentration, respectively. The spatial coordinates are denoted by $x, y, z \in \Omega$, and $t \in \mathbb{R}$ is the time. Gas diffusion is assumed to be isotropic, with D_u and D_v apparent diffusivities of oxygen and carbon dioxide in pear tissue, respectively.
Gas exchange between cells at the boundary of the pear and the environment is modelled by convective mass transfer, with C_{uamb} and C_{vamb} ambient oxygen and carbon dioxide concentrations; $\vec{n}$ is the outward normal to the surface Γ; and h_u and h_v are the convective mass transfer coefficients of oxygen and carbon dioxide, which take into account the pear skin resistance to diffusion.
At $t = 0$, appropriate initial conditions are specified: $C_u(x, y, z, 0) = C_{u0}(x, y, z)$ and $C_v(x, y, z, 0) = C_{v0}(x, y, z)$.

The following equations are used to describe the respiration kinetics $R_u(C_u, C_v)$ and $R_v(C_u, C_v)$, respectively:

$$\left\{\begin{array}{rcl} R_u(C_u, C_v) & = & \dfrac{V_{mu} C_u}{(K_{mu} + C_u)\left(1 + \dfrac{C_v}{K_{mv}}\right)} \\ & & \\ R_v(C_u, C_v) & = & r_q \ R_u(C_u, C_v) + \dfrac{V_{mfv}}{1 + \dfrac{C_u}{K_{mfu}}} \end{array}\right. \quad \text{in } \Omega \ , \ t > 0.$$

with V_{mu} the maximum oxygen consumption rate, K_{mu} the Michaelis-Menten constant for oxygen consumption, K_{mv} the Michaelis-Menten constant for non-competitive carbon dioxide inhibition, r_q the respiration quotient, V_{mfv} the maximum fermentative carbon dioxide production rate, and K_{mfu} the Michaelis-Menten constant of oxygen inhibition on fermentative carbon dioxide production.

Axisymmetric respiration–diffusion model

We are particularly interested in how steady state concentration profiles change as a function of (controlled) atmospheric conditions, such as ambient temperature and oxygen and carbon dioxide concentration. For this purpose we consider the following **steady-state** axisymmetric respiration–diffusion model.

$$\left\{\begin{array}{rcl} \dfrac{1}{r}\dfrac{\partial}{\partial r}\left(D_{u_r} r \dfrac{\partial C_u}{\partial r}\right) + \dfrac{\partial}{\partial z}\left(D_{u_z}\dfrac{\partial C_u}{\partial z}\right) - R_u(C_u, C_v) & = & 0 \\ \dfrac{1}{r}\dfrac{\partial}{\partial r}\left(D_{v_r} r \dfrac{\partial C_v}{\partial r}\right) + \dfrac{\partial}{\partial z}\left(D_{v_z}\dfrac{\partial C_v}{\partial z}\right) + R_v(C_u, C_v) & = & 0 \end{array}\right. \quad \text{in } \Omega \ , \ t > 0.$$

$$\left\{\begin{array}{rcl} -D_{u_r} r \dfrac{\partial C_u}{\partial r} n_r - D_{u_z} r \dfrac{\partial C_u}{\partial z} n_z & = & r h_u (C_u - C_{uamb}) \\ -D_{v_r} r \dfrac{\partial C_v}{\partial r} n_r - D_{v_z} r \dfrac{\partial C_v}{\partial z} n_z & = & r h_v (C_v - C_{vamb}) \end{array}\right. \quad \text{on } \ \Gamma_1 \ , \ t > 0.$$

$$\left\{\begin{array}{rcl} -D_{u_r} r \dfrac{\partial C_u}{\partial r} n_r - D_{u_z} r \dfrac{\partial C_u}{\partial z} n_z & = & 0 \\ -D_{v_r} r \dfrac{\partial C_v}{\partial r} n_r - D_{v_z} r \dfrac{\partial C_v}{\partial z} n_z & = & 0 \end{array}\right. \quad \text{on } \ \Gamma_2 \ , \ t > 0.$$

where $C_u \equiv C_u(r, \theta, z) \equiv C_u(r, z)$ and $C_v \equiv C_v(r, \theta, z) \equiv C_v(r, z)$ are independent of θ and represent the oxygen and carbon dioxide concentration, respectively. The spatial (cylindrical) coordinates are denoted by $r, \theta, z \in \Omega$, and $t \in \mathbb{R}$ is the time. Gas diffusion is assumed to be different (higher) in the axial direction compared to that in the radial direction, with D_{u_r}, D_{u_z}, D_{v_r} and D_{v_z} apparent radial and axial diffusivities of oxygen and carbon dioxide in pear tissue, respectively.

Gas exchange between cells at the boundary of the pear and the environment is modelled by convective mass transfer, with C_{uamb} and C_{vamb} ambient oxygen and carbon dioxide concentrations; n_r and n_z are the radial and axial components of the outward normal to the surface Γ; Γ_1 denotes the curved pear boundary, Γ_2 is the axis of symmetry; and $h_u$and h_v are the convective mass transfer coefficients of oxygen and carbon dioxide, which take into account the pear skin resistance to diffusion.

As mentioned before, the following equations describe the respiration kinetics $R_u(C_u, C_v)$ and $R_v(C_u, C_v)$, respectively:

$$\left\{\begin{array}{rcl} R_u(C_u, C_v) & = & \dfrac{V_{mu} C_u}{(K_{mu} + C_u)\left(1 + \dfrac{C_v}{K_{mv}}\right)} \\ R_v(C_u, C_v) & = & r_q \ R_u(C_u, C_v) + \dfrac{V_{mfv}}{1 + \dfrac{C_u}{K_{mfu}}} \end{array}\right.$$

with V_{mu} the maximum oxygen consumption rate, K_{mu} the Michaelis-Menten constant for oxygen consumption, K_{mv} the Michaelis-Menten constant for non-competitive carbon dioxide inhibition, r_q the respiration quotient, V_{mfv} the maximum fermentative carbon dioxide production rate, and K_{mfu} the Michaelis-Menten constant of oxygen inhibition on fermentative carbon dioxide production.

Model parameters

Diffusivities

* Radial and axial diffusivity of oxygen in pear tissue

$$D_{u_r} = 2.8 \times 10^{-10} \text{ m}^2/\text{s} \quad , \quad D_{u_z} = 1.10 \times 10^{-9} \text{ m}^2/\text{s}$$

* Radial and axial diffusivity of carbon dioxide in pear tissue

$$D_{v_r} = 2.32 \times 10^{-9} \text{ m}^2/\text{s} \quad , \quad D_{v_z} = 6.97 \times 10^{-9} \text{ m}^2/\text{s}$$

Respiration kinetic parameters

* Maximum oxygen consumption rate

$$V_{mu} = V_{mu,ref} \exp\left[\frac{E_{a,vmu,ref}}{R_g}\left(\frac{1}{T_{ref}} - \frac{1}{T}\right)\right]$$

  with T_{ref} a reference temperature (in degree Kelvin), T the actual temperature (in degree Kelvin) and $R_g = 8.314$ J/(mol K) the universal gas constant.

  - Maximum oxygen consumption rate at $T_{ref} = 293.15$ K ($= 20^o$C):

    $V_{mu,ref}$: 2.39×10^{-4} mol/(m^3 s).

  - Activation energy for oxygen consumption:

    $E_{a,vmu,ref}$: 80200 J/mol.

* Maximum fermentative carbon dioxide production rate:

$$V_{mfv} = V_{mfv,ref} \exp\left[\frac{E_{a,vmfv,ref}}{R_g}\left(\frac{1}{T_{ref}} - \frac{1}{T}\right)\right].$$

  - Maximum fermentative carbon dioxide production rate at $T_{ref} = 293.15$K:

    $V_{mfv,ref}$: 1.61×10^{-4} mol/(m^3 s).

  - Activation energy for fermentative carbon dioxide production:

    $E_{a,vmfv,ref}$: 56700 J/mol.

* Michaelis-Menten constants and respiration quotient.

  - Michaelis-Menten constant for oxygen consumption:

    K_{mu}: 0.4103 mol/m^3.

  - Michaelis-Menten constant for non-competitive carbon dioxide inhibition:

    K_{mv}: 27.2438 mol/m^3.

  - Michaelis-Menten constant of oxygen inhibition on fermentative carbon dioxide production:

    K_{mfu}: 0.1149 mol/m^3.

  - The respiration quotient:

    r_q: 0.97.

Convective mass transfer coefficients

$$h_u = 7 \times 10^{-7} \text{ m/s} \quad , \quad h_v = 7.5 \times 10^{-7} \text{ m/s}.$$

Ambient conditions

* Atmospheric pressure

  $$p_{atm} = 101300 \text{ Pa}.$$

* Temperature

  $T = T_{cel} + 273.15$
  with T the temperature in degree Kelvin (K) and T_{cel} the temperature in degree Celsius (^{o} C).

* Ambient oxygen and carbon dioxide concentrations

$$\begin{aligned} C_{uamb} &= \frac{p_{atm}\ \eta_u}{R_g T} \\ C_{vamb} &= \frac{p_{atm}\ \eta_v}{R_g T} \end{aligned}$$

with p_{atm} (Pa) the atmospheric pressure, η_u and η_v the fraction (percentage) oxygen and carbon dioxide in the (controlled) atmosphere, respectively; R_g the universal gas constant (J/(mol K)); and T the ambient temperature in degree Kelvin (K).

Note: $0 \leq \eta_u \leq 1$, $0 \leq \eta_v \leq 1$.

Simulations

Compute steady-state oxygen and carbon dioxide concentration profiles for the following storage conditions.

Storage description	T_{cel}(^{o}C)	η_u (%)	η_v (%)
Orchard	25	20.8	0.04
Shelf life	20	20.8	0
Refrigerator	7	20.8	0
Precooling	-1	20.8	0
Disorder inducing	-1	2	5
Optimal CA	-1	2	0.7

Note: To compute C_{uamb} and C_{vamb} the fractions η_u and η_v should be numbers between 0 and 1.

References

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Background literature

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3. Ho, Q.T., Verboven, P., Verlinden, B.E., Herremans, E., Wevers, M., Carmeliet, J., Nicolaï, B.M., 2011. A three-dimensional multiscale model for gas exchange in fruit. Plant Physiology, 155, 1158–1168.

4. Ho, Q.T., Verboven, P., Verlinden, B.E., Schenk, A., Nicolaï, B.M., 2013. Controlled atmosphere storage may lead to local ATP deficiency in apple. Postharvest Biolology and Technology, 78, 103–112.

Useful handbook

1. Huebner, K.H., Thornton, E.A., Byrom, T.G., 1995. The finite element method for engineers. John Wiley and Sons, Inc.

Weblinks, short (lecture) notes/tutorials

- MeBioS – Biofluidics research, Department of Biosystems, KU Leuven
- Nikishkov, G. P. Introduction to the Finite Element Method. 2004 Lecture Notes.
- Cuneyt Sert. Finite Element Analysis in Thermofluids. Chapter 2: Formulation of FEM for One-Dimensional Problems.
- Gagandeep Singh, Short Introduction to Finite Element Method.