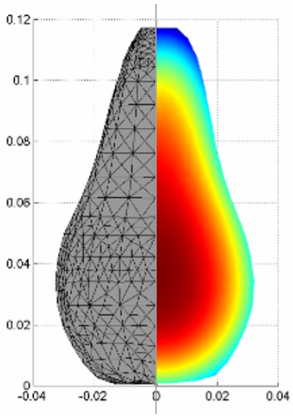
The Pear Project
Solving a macroscale respiration–diffusion model
Academic Year 2018–2019

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 in the pear 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.

The exchange of metabolic gases, such as oxygen and carbon dioxide, is crucial to maintain normal *metabolic/physiological* functioning. It is therefore important to understand how these gases are transported and distributed within the fruit structure in order to slow down the ripening of the fruit while preventing the fruit to go bad by lack of oxygen.

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: You develop and implement numerical solutions of a macroscale respiration–diffusion system for metabolic gas exchange in pears using the Finite Element Method. The programming and simulation has to be done in C++/Fortran. Code verification/testing against analytical solutions of simplified models.

Stationary axis-symmetric 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.

The model under study consists of a set of two coupled non–linear reaction–diffusion equations in a stationary regime, defined on a two-dimensional bounded spatial domain $\Omega \subset \mathbb{R}^2$; that is,

$$\begin{cases} \nabla \cdot \left(r \begin{pmatrix} \sigma_{u,r} & 0 \\ 0 & \sigma_{u,z} \end{pmatrix} \nabla C_u(r,z) \right) &= r\, R_u(C_u(r,z), C_v(r,z)) \\ \nabla \cdot \left(r \begin{pmatrix} \sigma_{v,r} & 0 \\ 0 & \sigma_{v,z} \end{pmatrix} \nabla C_v(r,z) \right) &= -r\, R_v(C_u(r,z), C_v(r,z)) \end{cases} \quad \text{for} \quad (r,z) \in \Omega, \tag{1}$$

where $C_u(r,z)$ and $C_v(r,z)$ represent the oxygen and carbon dioxide concentration, respectively. The spatial coordinates are denoted by r, z with $(r,z) \in \Omega$. Furthermore, gas diffusion is assumed to be anisotropic, with $\sigma_{u,r}, \sigma_{u,z}$ representing the given diffusion coefficients of oxygen in the directions r and z (and analogously $\sigma_{v,r}, \sigma_{v,z}$ for carbon dioxide). The boundary conditions are a mixed type of conditions at the boundary $\Gamma := \Gamma_1 \cup \Gamma_2$, where Γ_1 is the vertical axis of the pear, and Γ_2 is its boundary with

the outer environment. Denoting by $\vec{n}(r,z)$ the outward normal vector at position (r,z), the boundary conditions read

$$\begin{cases} -\vec{n}(r,z)\cdot\left(\begin{pmatrix}\sigma_{u,r} & 0\\ 0 & \sigma_{u,z}\end{pmatrix}\nabla C_u(r,z)\right) &= \varrho_u\ (C_u(r,z)-C_u^*(r,z)) \\ -\vec{n}(r,z)\cdot\left(\begin{pmatrix}\sigma_{v,r} & 0\\ 0 & \sigma_{v,z}\end{pmatrix}\nabla C_v(r,z)\right) &= \varrho_v\ (C_v(r,z)-C_v^*(r,z)) \end{cases} \quad \text{for} \quad (r,z)\in\Gamma, \tag{2}$$

where C_u^* and C_v^* are given functions. In particular, we have that $(C_u^*(r,z), C_v^*(r,z)) = (0,0)$ on Γ_1 and $(C_u^*(r,z), C_v^*(r,z)) = (C_{u\text{amb}}, C_{v\text{amb}})$ on Γ_2. The gas exchange between cells at the boundary of the pear and the environment is modelled by convective mass transfer, where $C_{u\text{amb}}$ and $C_{v\text{amb}}$ are the ambient oxygen and carbon dioxide concentrations and ϱ_u and ϱ_v are the given convective mass transfer coefficients of oxygen and carbon dioxide, which take the pear skin resistance to diffusion into account. Since we assume the symmetry of the solution w.r.t. the vertical axis, it is natural to impose a null flux across Γ_1.

The following equations describe the respiration kinetics $R_u(C_u(r,z), C_v(r,z))$ and $R_v(C_u(r,z), C_v(r,z))$

$$\begin{cases} R_u(C_u,C_v) &= \dfrac{V_{mu}C_u}{(K_{mu}+C_u)\left(1+\dfrac{C_v}{K_{mv}}\right)} \\ R_v(C_u,C_v) &= r_q\, R_u(C_u,C_v) + \dfrac{V_{mfv}}{1+\dfrac{C_u}{K_{mfu}}} \end{cases} \tag{3}$$

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.

Observe that assuming the symmetry of the solution w.r.t. the vertical axis of the pear, the solution on the whole pear volume can be obtained as the rotation of the solution defined on Ω.

Tasks

You have to elaborate a numerical approximation for the steady state solution of the model. This has to be carried out using the Finite Element Method. In the development of the project you are free to choose among different languages, such as C++ or Fortran, but please consider the following points:

- You can generate the mesh using any existing free libraries that you will find on the web.
- You have to implement the finite element system from scratch, but you are free to solve the resulting linear and non-linear systems using existing libraries.
- You need to prove the correctness of your numerical method: for this purpose you also need to consider a simplified version of the provided model, for which you are able to find the analytical solution, and compare this with its numerical solution. (Hint: consider the pear as a sphere and use then spherical coordinates, then "play" with the terms R_u, R_v to make them simpler).
- You need to perform all the simulations proposed on the last page of this assignment.

Hints for the FEM implementation

- Consider a triangulation of the domain, i.e., $\Omega = \bigcup_{t\in T} \Omega_t$, which consists of M vertices $P_i \in \Omega \subset \mathbb{R}^2$ for $i = 1, \dots, M$. Then use (linear) basis functions $\varphi_i(r, z)$ with $\varphi_i(P_j) = \delta_{i,j}$ to approximate the quantities C_u and C_v; that is,

$$C_u(r,z) \approx C_u^M(r,z) := \sum_{j=1}^{M} c_i\, \varphi_i(r,z), \qquad C_v(r,z) \approx C_v^M(r,z) := \sum_{i=1}^{M} c_{M+i}\, \varphi_i(r,z).$$

- Defining the quantities $\vec{q}_u(r,z)$ and $\vec{q}_v(r,z)$ via

$$\vec{q}_u(r,z) = r \begin{pmatrix} \sigma_{u,r} & 0 \\ 0 & \sigma_{u,z} \end{pmatrix} \nabla C_u(r,z), \qquad \vec{q}_v(r,z) = r \begin{pmatrix} \sigma_{v,r} & 0 \\ 0 & \sigma_{v,z} \end{pmatrix} \nabla C_v(r,z),$$

  the weak formulation of (1) with test function $\varphi : \Omega \to \mathbb{R}$ reads

$$\begin{cases} \int_\Omega (\nabla \cdot \vec{q}(r,z))\ \varphi(r,z)\,\mathrm{d}\Omega &= \int_\Omega r\, R_u(C_u(r,z), C_v(r,z))\, \varphi(r,z)\,\mathrm{d}\Omega, \\ \int_\Omega (\nabla \cdot \vec{q}(r,z))\ \varphi(r,z)\,\mathrm{d}\Omega &= -\int_\Omega r\, R_v(C_u(r,z), C_v(r,z))\, \varphi(r,z)\,\mathrm{d}\Omega \end{cases}. \tag{4}$$

  Employing a divergence theorem; that is,

$$\int_\Omega (\nabla \cdot \vec{q}(r,z))\ \varphi(r,z)\,\mathrm{d}\Omega = -\int_\Omega \vec{q}(r,z) \cdot \nabla\varphi(r,z)\,\mathrm{d}\Omega + \int_\Gamma (\vec{n}(r,z) \cdot \vec{q}(r,z))\ \varphi(r,z)\,\mathrm{d}\Gamma,$$

  for the vector fields $\vec{q}_u(r,z)$ and $\vec{q}_v(r,z)$ to (4) yields the following form

$$\begin{aligned} &\int_\Omega \vec{q}_u(r,z) \cdot \nabla\varphi(r,z)\,\mathrm{d}\Omega + \int_\Omega r\, R_u(C_u, C_v)\, \varphi(r,z)\,\mathrm{d}\Omega + \int_\Gamma r\, \varrho_u\ (C_u(r,z) - C_u^*(r,z))\ \varphi(r,z)\,\mathrm{d}\Gamma = 0 \\ &\int_\Omega \vec{q}_v(r,z) \cdot \nabla\varphi(r,z)\,\mathrm{d}\Omega - \int_\Omega r\, R_v(C_u, C_v)\, \varphi(r,z)\,\mathrm{d}\Omega + \int_\Gamma r\, \varrho_v\ (C_v(r,z) - C_v^*(r,z))\ \varphi(r,z)\,\mathrm{d}\Gamma = 0. \end{aligned}$$

  Using the basis functions φ_i as test functions φ, the above system yields a system of linear equations which can be solved to obtain the coefficient vector $\mathbf{c} \in \mathbb{R}^{2M}$ of the approximations C_u^M and C_v^M.

- As the functions R_u and R_v are non-linear w.r.t. the concentrations C_u, C_v, the above derivation implies that a non-linear equation of the form

$$\begin{pmatrix} K_u & 0 \\ 0 & K_v \end{pmatrix} \begin{pmatrix} \mathbf{c}_u \\ \mathbf{c}_v \end{pmatrix} - \begin{pmatrix} \mathbf{f}_u \\ \mathbf{f}_v \end{pmatrix} + \begin{pmatrix} \mathbf{H}_u(\mathbf{c}_u, \mathbf{c}_v) \\ \mathbf{H}_v(\mathbf{c}_u, \mathbf{c}_v) \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}$$

  must be solved to find the coefficients $\mathbf{c} = (\mathbf{c}_u, \mathbf{c}_v)$. Newton's method is a good strategy to solve this equation.

- Newton's method requires a starting value. For this initial value, you can, e.g., linearize the functions R_u, R_v in the original form (3) to obtain the starting values for the vector of coefficients $\mathbf{c} = (\mathbf{c}_u, \mathbf{c}_v)$ as the solution of a linear system of equations.

Weblinks, short (lecture) notes/tutorials

- Nikishkov, G. P. Introduction to the Finite Element Method. 2004 Lecture Notes.
- Gagandeep Singh, Short Introduction to Finite Element Method.

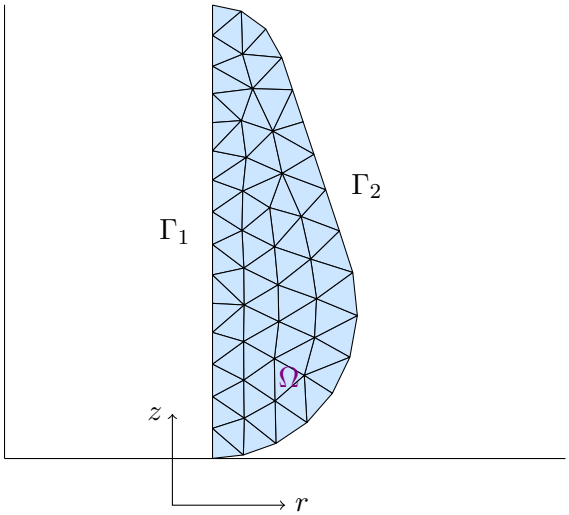


Figure 1: Mesh of the right half of a vertical section of a pear. We indicate with Ω the compact domain, with $\Gamma = \Gamma_1 \cup \Gamma_2$ its boundary. Γ_1 coincides with the vertical axis of the pear, while Γ_2 represents its boundary with the outer environment.

Model Parameters

Diffusivities

- Radial and axial diffusivity of oxygen in pear tissue:

$$\sigma_{u,r} = 2.8 \times 10^{-10} \text{ m}^2/\text{s}, \quad \sigma_{u,z} = 1.10 \times 10^{-9} \text{ m}^2/\text{s}$$

- Radial and axial diffusivity of carbon dioxide in pear tissue:

$$\sigma_{v,r} = 2.32 \times 10^{-9} \text{ m}^2/\text{s}, \quad \sigma_{v,z} = 6.97 \times 10^{-9} \text{ m}^2/\text{s}$$

Respiration kinetic parameters

- Maximum oxygen consumption rate:

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

  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):

$$V_{mu,\text{ref}} = 2.39 \times 10^{-4} \text{ mol}/(\text{m}^3 \text{ s})$$

  - Activation energy for oxygen consumption:

$$E_{a,vmu,\text{ref}} = 80200 \text{ J/mol}$$

- Maximum fermentative carbon dioxide production rate:

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

  - Maximum fermentative carbon dioxide production rate at $T_{ref} = 293.15$ K ($= 20^o$C):

$$V_{mfv,\text{ref}} = 1.61 \times 10^{-4} \text{ mol}/(\text{m}^3 \text{ s})$$

  - Activation energy for fermentative carbon dioxide production:

$$E_{a,vmfv,\text{ref}} = 56700 \text{ J/mol}$$

- Michaelis-Menten constants and respiration quotient:
  - Michaelis-Menten constant for oxygen consumption:

$$K_{mu} = 0.4103 \text{ mol/m}^3$$

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

$$K_{mv} = 27.2438 \text{ mol/m}^3$$

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

$$K_{mfu} = 0.1149 \text{ mol/m}^3$$

  - Respiration quotient:

$$r_q = 0.97$$

Convective mass transfer coefficients

$$\varrho_u = 7 \times 10^{-7} \text{ m/s}, \qquad \varrho_v = 7.5 \times 10^{-7}$$

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:

$$C_{u\text{amb}} = \frac{p_{atm}\ \eta_u}{R_g T}, \qquad C_{v\text{amb}} = \frac{p_{atm}\ \eta_v}{R_g T},$$

  with 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).

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 $C_{u\text{amb}}$ and $C_{v\text{amb}}$ the fractions η_u and η_v should be numbers between 0 and 1.