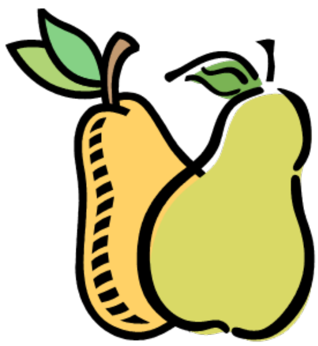
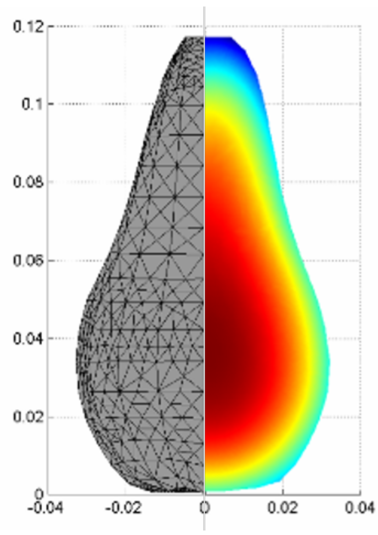
The Pear Project
Solving a macroscale respiration–diffusion model
2016 – 2017



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. Code verification/testing against analytical solutions of simplified models.

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 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.

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.

Tasks

The students 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++, Fortran and Python, but please consider the following points:

- The provided model is three-dimensional and it is described by means of Cartesian coordinates; please consider that the stationary solution of the model has the axisymmetric property, so you can implement a problem with a lower dimension;
- You can generate the mesh using any existing free libraries that you will find in the web;
- You have to implement the finite element system from scratch, but you are free to solve it using existing libraries;
- You need to prove the goodness 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).

References

1. Lammertyn, J., Scheerlinck, N., Jancsók, P., Verlinden, B., Nicolaï, B., 2003. A respiration-diffusion model for Conference pears I: model development and validation. Postharvest Biolology and Technology, 30, 29–42.
2. Lammertyn, J., Scheerlinck, N., Jancsók, P., Verlinden, B., Nicolaï, B., 2003. A respiration-diffusion model for Conference pears II: Simulations and relation to core breakdown. Postharvest Biolology and Technology, 30, 29–42.
3. Ho, Q.T., Verboven, P., Verlinden, B.E., Lammertyn, J., Vandewalle, S., Nicolaï, B.M., 2008. A continuum model for metabolic gas exchange in pear fruit. PLoS Computational Biology, 4(3), e1000023.

Background literature

1. Franck, C., Lammertyn, J., Ho, Q.T., Verboven, P., Verlinden, B., Nicolaï, B.M., 2007. Browning disorders in pear fruit. Postharvest Biolology and Technology, 43, 1–13.
2. Ho, Q.T., Verlinden, B.E., Verboven, P., Vandewalle, S., Nicolaï, B.M., 2006. A permeation-diffusion-reaction model of gas transport in cellular tissue of plant materials. Journal of Experimental Botany, 57, 4215–4224.

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.

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.