Extraction of Phenolic Compounds from Grape Fruit. A Comparison between a 3D FEM Model and Experimental Results.

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Why are Wine Producers Interested in Improving the Extraction of Phenols from Grape Skin and Incorporating them into the Wine?

- Polyphenols designate a broad family of bio-molecules such as anthocyanins, flavonoïds, caratenoïds...
- They are very healthy compounds (antioxidative and anticancerogeneous);
- They give red and rosé wines some caracteristics such as colour, bitterness and astringency;
- They are mainly present in fruits and vegetables;

Why Does this Work Focus on Anthocyanins, their Extraction from the Grape Skin and their Incorporation into the Wine?

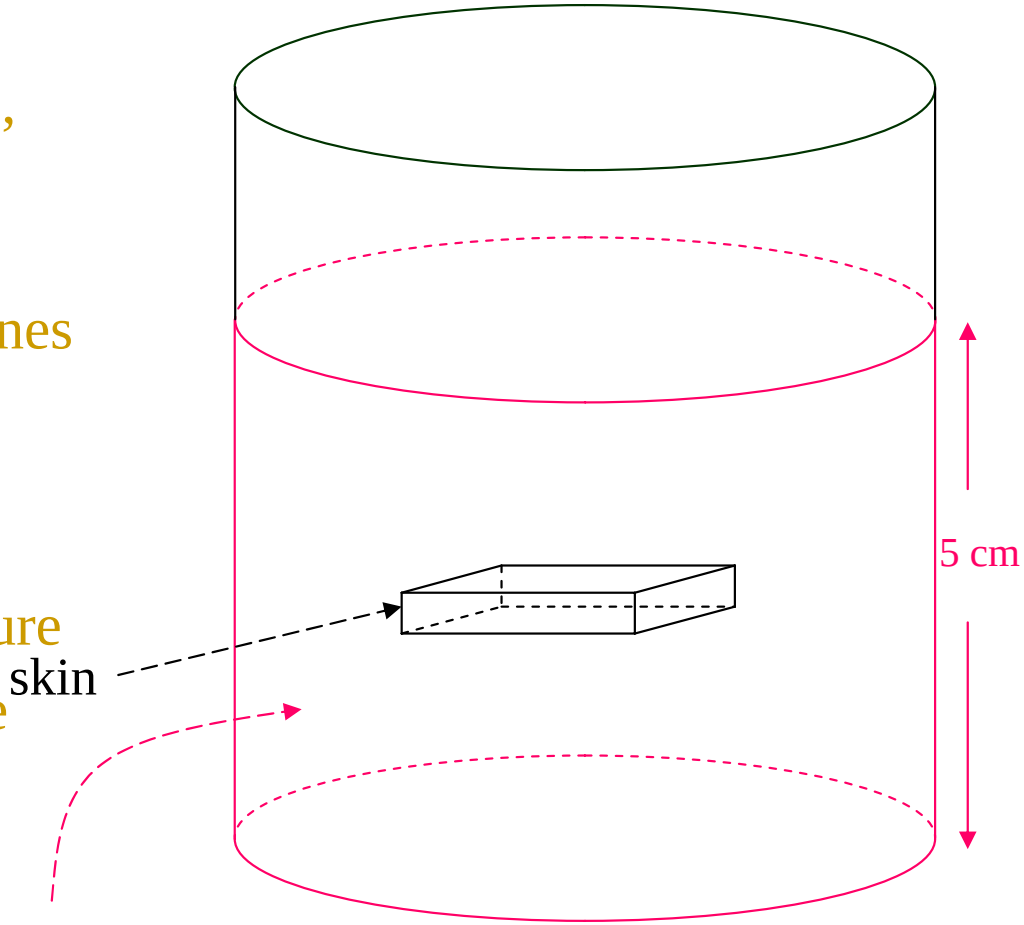
- Anthocyanins are the main phenolic compounds present in grape berries;
- Anthocyanins are located in the skin and the pips;
- Yet little is known about
  - distribution over the skin.
  - the mechanism of extraction from the grape skin and incorporation into the wine

This work aims at

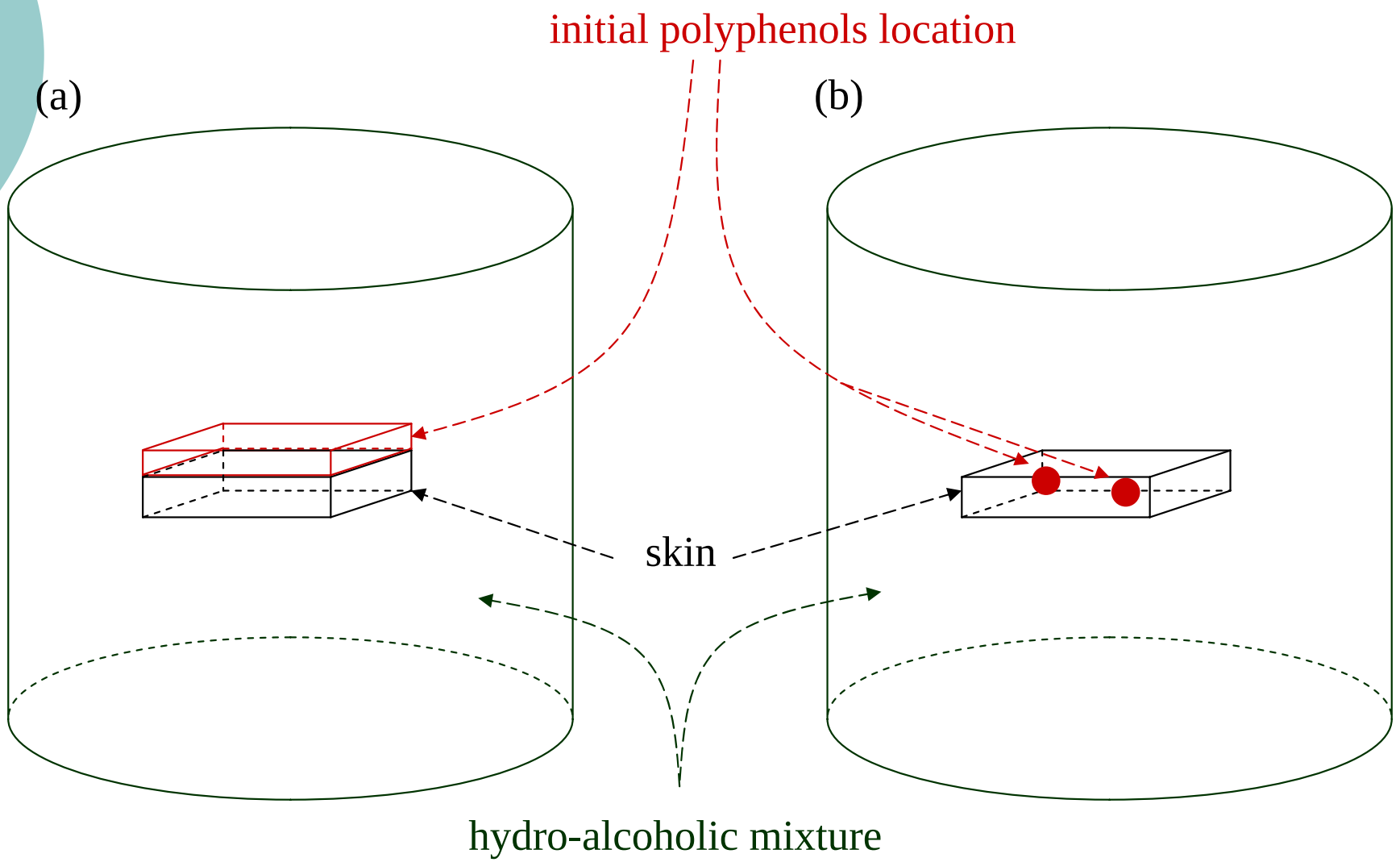
- Modelling the transfer from grape skin to alcoholic liquid using a three-dimensional Fickian-based-scheme;
- Comparing theoretical results to experimental ones.

The Experimental Design

- A hydro-alcoholic mixture was made with alcohol (12% ethanol), tartaric acid (3g/l) and SO_2 (100 mg/l);
- Grape berries came from grapevines monitored by our team;
- Some 1 cm x 0.5 cm x 0.15cm parallelepipeds of freshly peeled skins were plunged into the mixture
- Anthocyanins concentration were measured using absorbance spectrophotometric at 520 nm



Geometrical Modelling



Fickian-based Model and FEM Scheme

$$t = 0; c_1 = c_0$$

$$\frac{\partial c_1}{\partial t} = \nabla \bullet (D_1 \nabla c_1) \text{ inside } \Omega_1$$

$$D_1 \frac{\partial c_1}{\partial n} = D_2 \frac{\partial c_2}{\partial n} \text{ at } \Gamma_{12}$$

$$t = 0; c_2 = 0$$

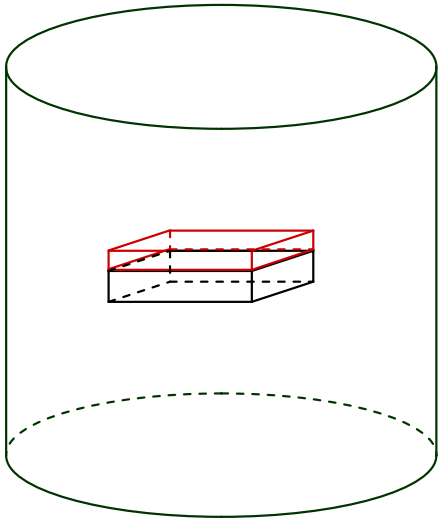
$$\frac{\partial c_2}{\partial t} = \nabla \bullet (D_2 \nabla c_2) \text{ inside } \Omega_2$$

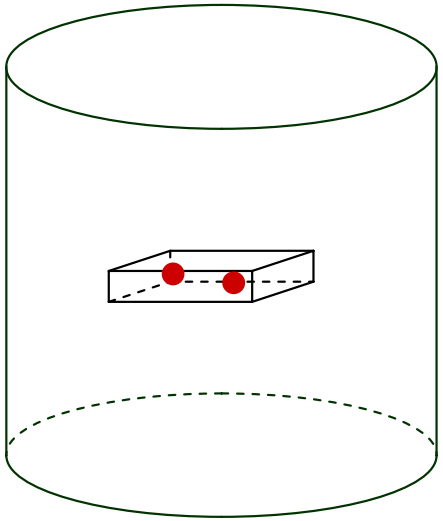
$$D_2 \frac{\partial c_2}{\partial n} = D_3 \frac{\partial c_3}{\partial n} \text{ at } \Gamma_{23}$$

$$t = 0; c_3 = 0$$

$$\frac{\partial c_3}{\partial t} = \nabla \bullet (D_3 \nabla c_3) \text{ inside } \Omega_3$$

$$\frac{\partial c_3}{\partial n} = 0 \text{ at } \Gamma_3$$





The 3D FE simulations were performed using version 3.4 of COMSOL Multiphysics™

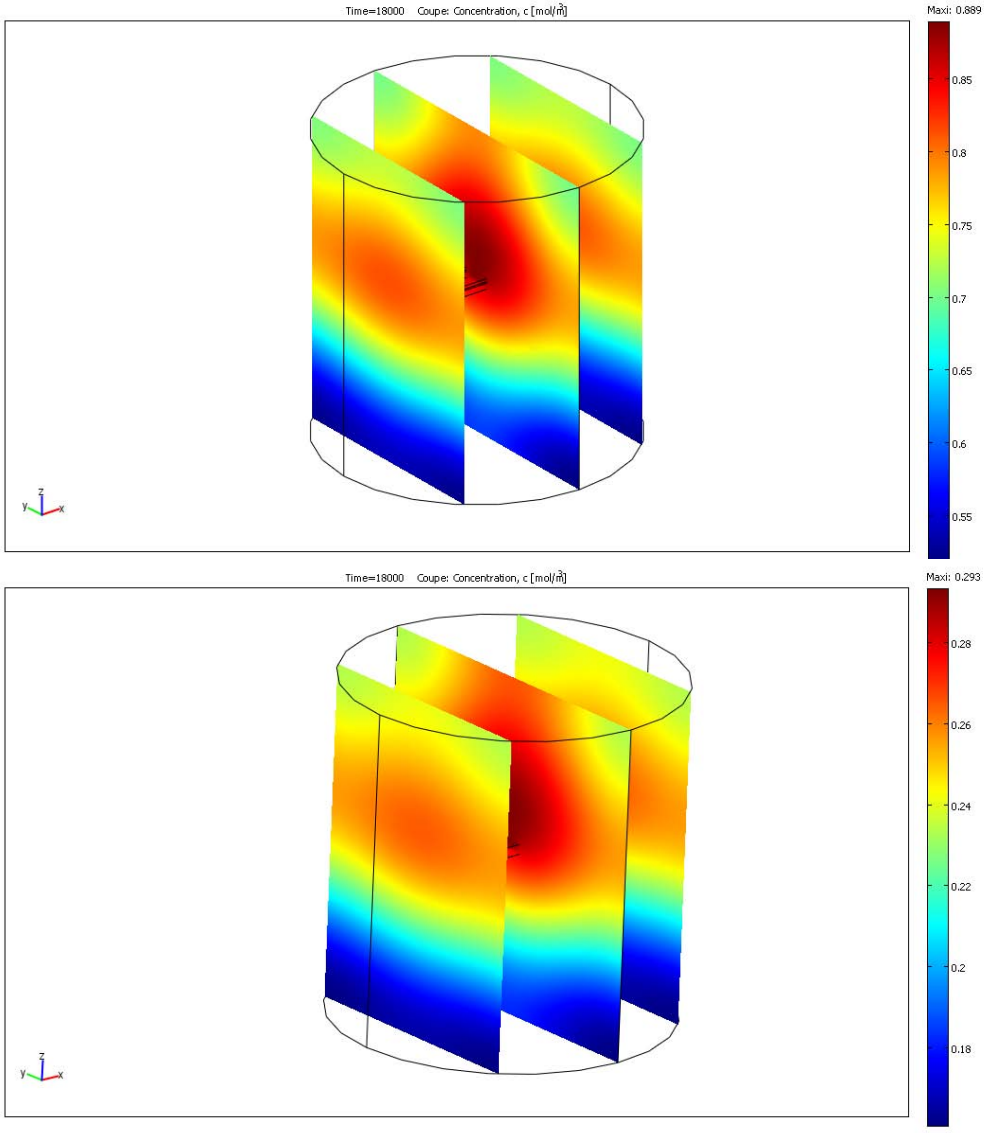
RESULTS

Iso-values of Anthocyanins Concentration

- At first glance, both distributions are comparable;

- The "candle flamed“ shape in the central horizontal plan is due to the little conductive character of the skin (D_2=5x10^{-10}m^2.s^{-1}) compared to hydro-alcoholic mixture (D_3=1x10^{-8}m^2.s^{-1});

- But the range of concentration in the second case is much smaller.



Concentration distribution drawn for t = 5 hours

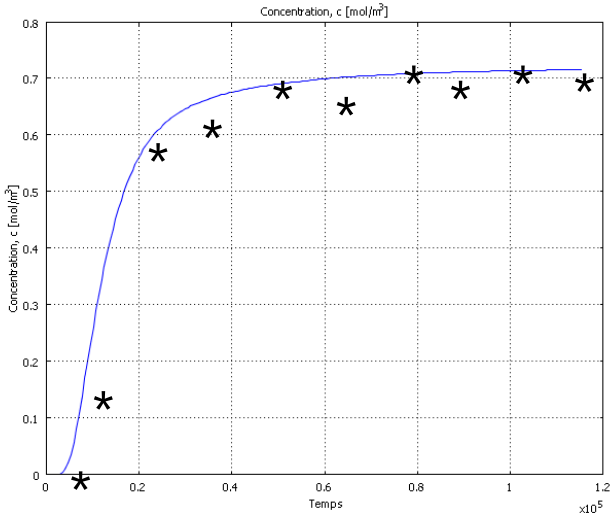
Mean Anthocyanins Concentration Versus Time (Theoritical and Experimental Results)

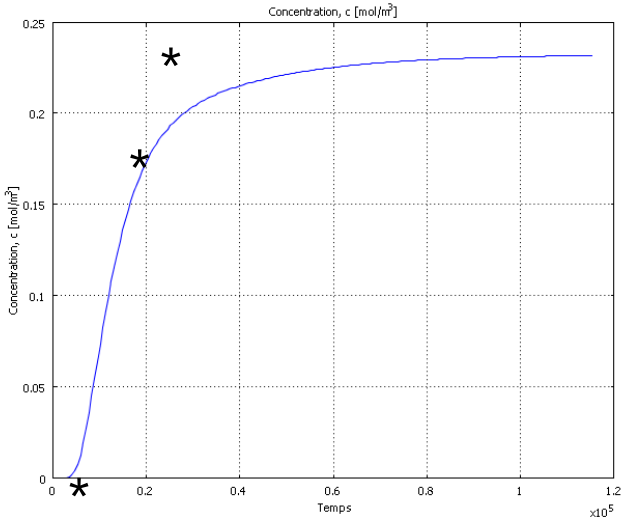
- The mean value is defined by :

$$\bar{c} = \frac{\int_V c \, \mathrm{d}\Omega}{V}$$

- It is fitted using

$$\bar{c} = \overline{c_0} + \Delta c \left(1 - e^{\frac{t - t_0}{\tau}} \right)$$





Mean Anthocyanins concentration (fitted data)

	Δc (mol/m^3)	t_0 (s)	τ (s)	*RSME* (mol/m^3)
Continuous Distribution	0.75	0.05e5	0.15e5	0.02
Discontinuous Distribution	0.23	0.05e5	0.19e5	0.5
Experimental Data	0.78	0.06e5	0.14e5	

$$RSME = \frac{1}{N}\sqrt{\sum_i (\bar{c}_i - \bar{c}_{iex})^2}$$

Conclusion

- Fickian-based Diffusion theory seems efficient to understand Anthocyanins extraction;
- Continuous distribution seems to be more consistent at this scale;
- These initial results will be confronted with experimentations involving a larger number of samples.

Thanks very much.

Please…
If You do drink,
Take Good Wine and …
Drink it modaretly.