COMSOL
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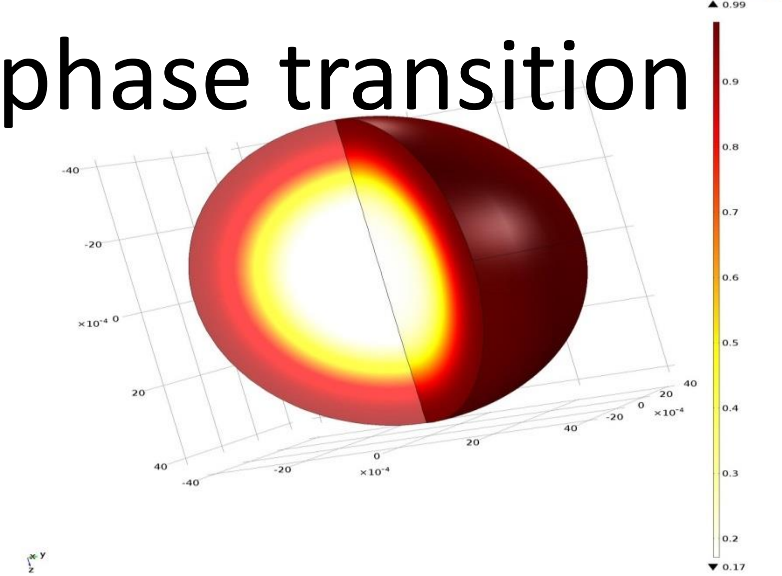
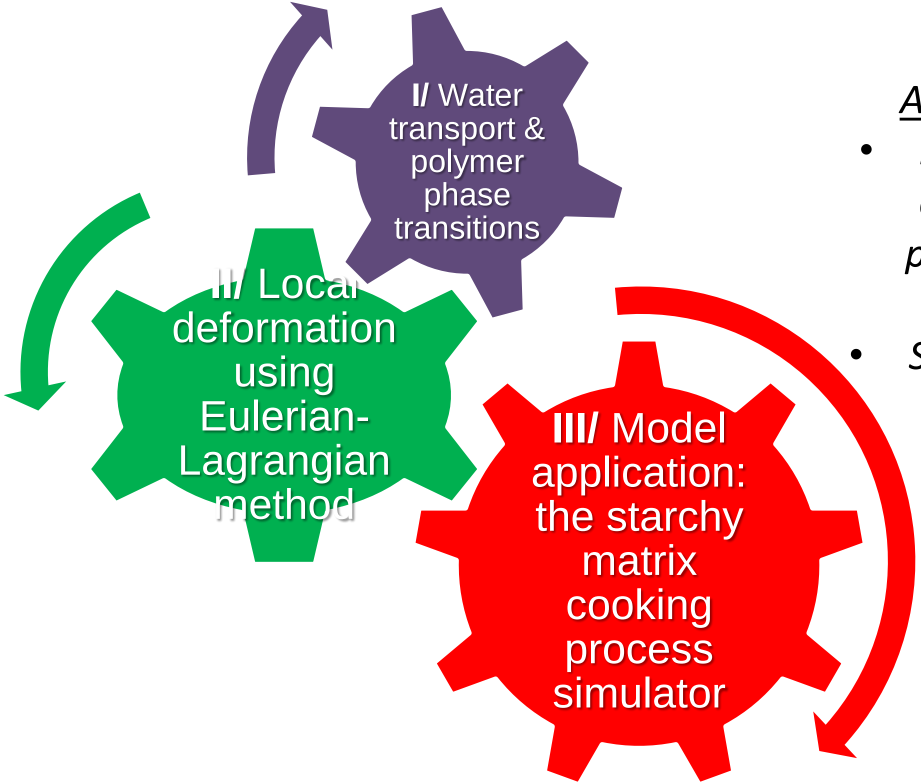
2015 GRENOBLE

A model coupling water transport with local deformation and polymer phase transition



Dr. Aurélien Briffaz, CIRAD / QualiSud Research Unit, Montpellier (France)

Structure of my presentation



I/ Water transport & polymer phase transitions

II/ Local deformation using Eulerian-Lagrangian method

III/ Model application: the starchy matrix cooking process simulator

<u>Assumptions</u>:

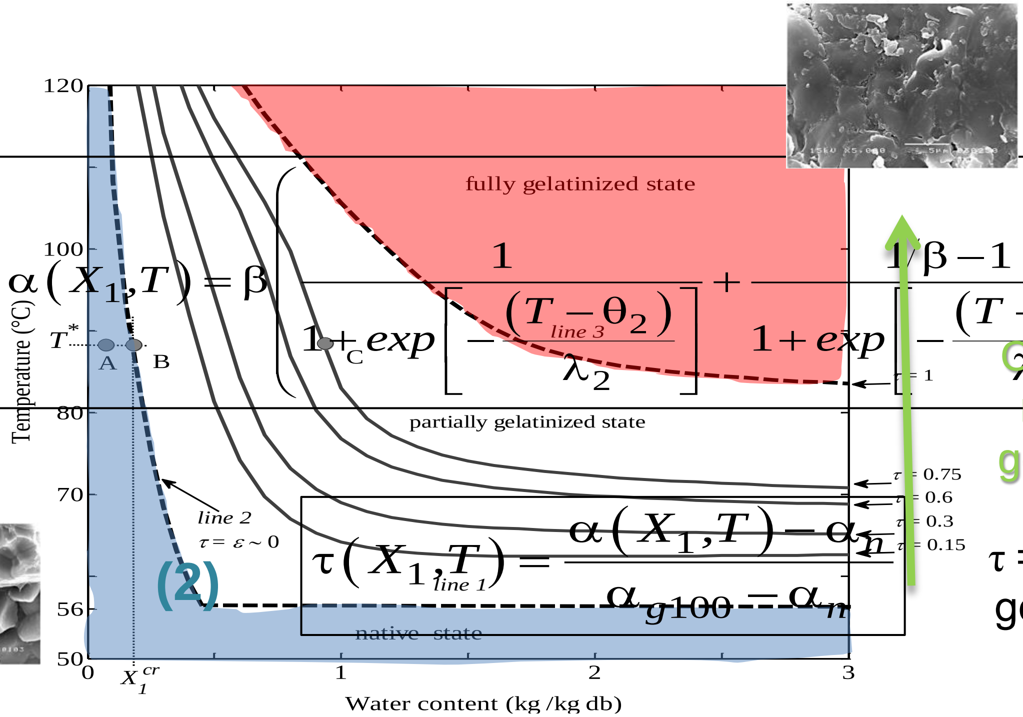
- *binary mixture of starch (solid phase) « s » and water « w »*
- *Spherical object*

I/ Water transport depending on polymer thermal transitions

I.1/ State diagram of starch

(1)

$$\alpha(X_1,T)=\beta\left(\frac{1}{1+exp\left[-\frac{(T-\theta_2)}{\lambda_2}\right]}+\frac{1/\beta-1}{1+exp\left[-\frac{(T-\theta_1)}{\lambda_1}\right]}\right)$$



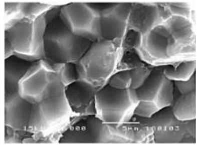
(2)

$$\tau(X_1,T)=\frac{\alpha(X_1,T)-\alpha_n}{\alpha_{g100}-\alpha_n}$$

Continuum from native to fully-gelatinized state

Double-sigmoid approach fitted on Differential Scanning Calorimetry (DSC) data

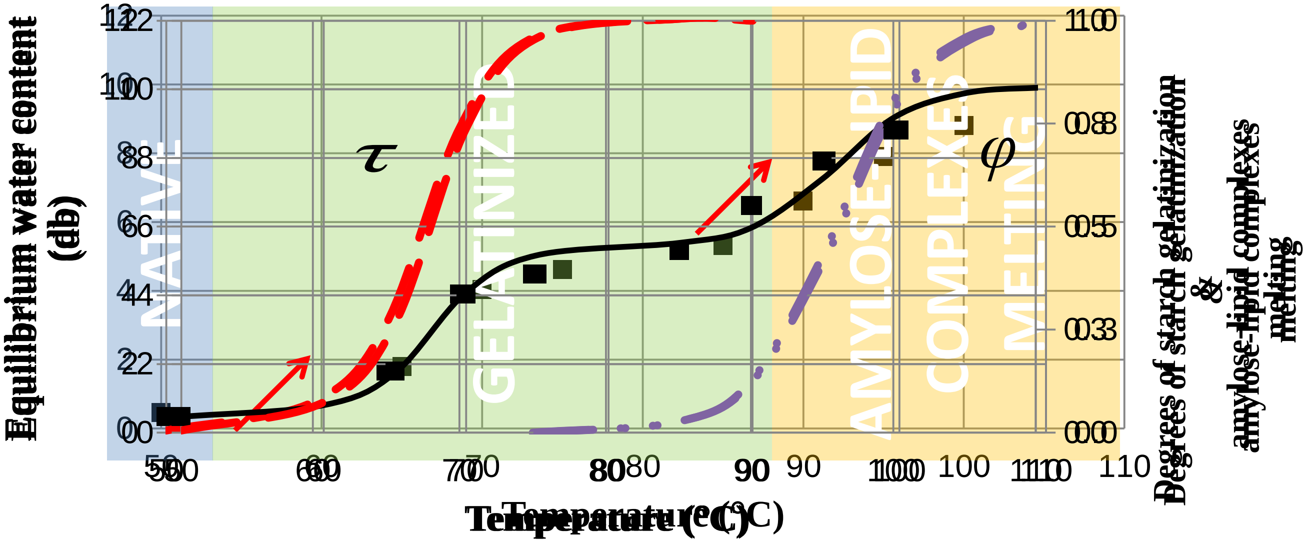
τ = degree of starch gelatinization (0−1)



SEM micrographs, Chungcharoen et al. (2015)

I.2/ Water content equilibrium associated with polymer state

$$X^{\infty}(T) = X_n^{\infty} \times (1-\tau) + X_g^{\infty} \times \tau + \left(X_f^{\infty} - X_g^{\infty} \right) \times \varphi \qquad (3)$$



I.3/ The two-water population concept

- Water absorption capacity X_1^{∞} is much higher for gelatinized starch (X_{1g}) than native starch (X_{1n})

PDE (5)

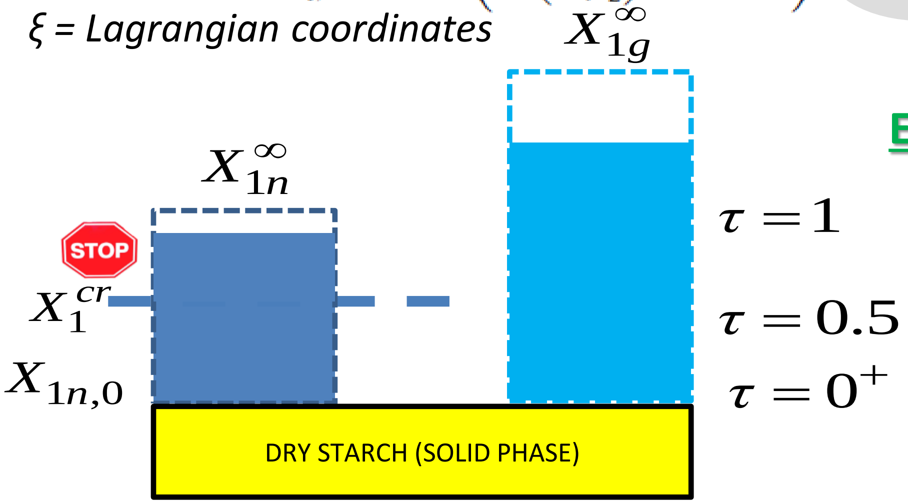
$$\left\{\begin{array}{l} \left(\frac{\partial X_{1n}}{\partial t}\right)_{\xi,t} = \frac{1}{\xi^2}\frac{\partial}{\partial \xi}\left(\xi^2\left(\frac{r^2\rho_2}{\xi^2\rho_2^0}\right)^2 D_{1n}\frac{\partial X_{1n}}{\partial \xi}\right) \\ \left(\frac{\partial X_{1g}}{\partial t}\right)_{\xi,t} = \frac{1}{\xi^2}\frac{\partial}{\partial \xi}\left(\xi^2\left(\frac{r^2\rho_2}{\xi^2\rho_2^0}\right)^2 D_{1g}\frac{\partial X_{1g}}{\partial \xi}\right) \quad X_{1n} \geqslant X_1^{cr} \end{array}\right.$$

ξ = Lagrangian coordinates

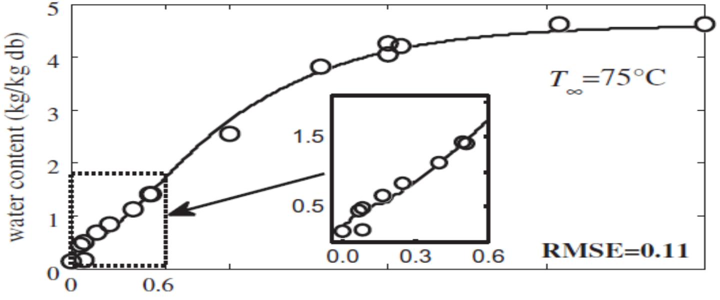
$$X_1 = X_{1n} + X_{1g} \qquad (4)$$

X1= Water content (dry basis)

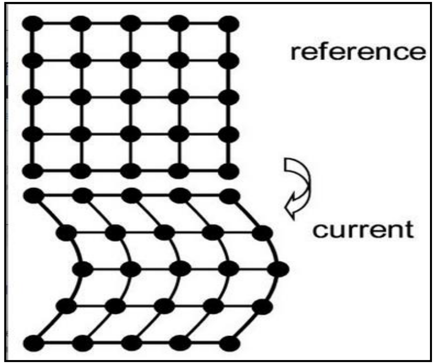
$$D_{1g} = D_{1g}^{*}(T) \times \tau \qquad (6)$$



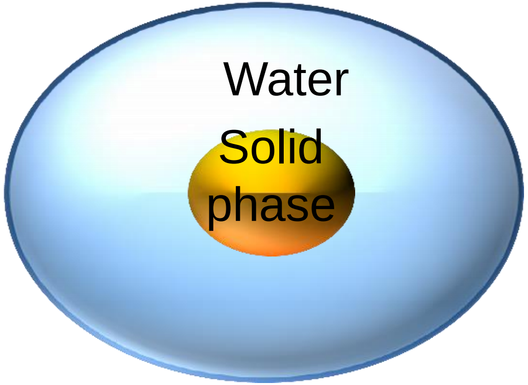
Experimental model validation:



II/ Local deformation using Eulerian-Lagrangian method



II.1/ Basic principles



- Two frames:

→ Eulerian (*r*,*t*)

→ Lagrangian (ξ,t)

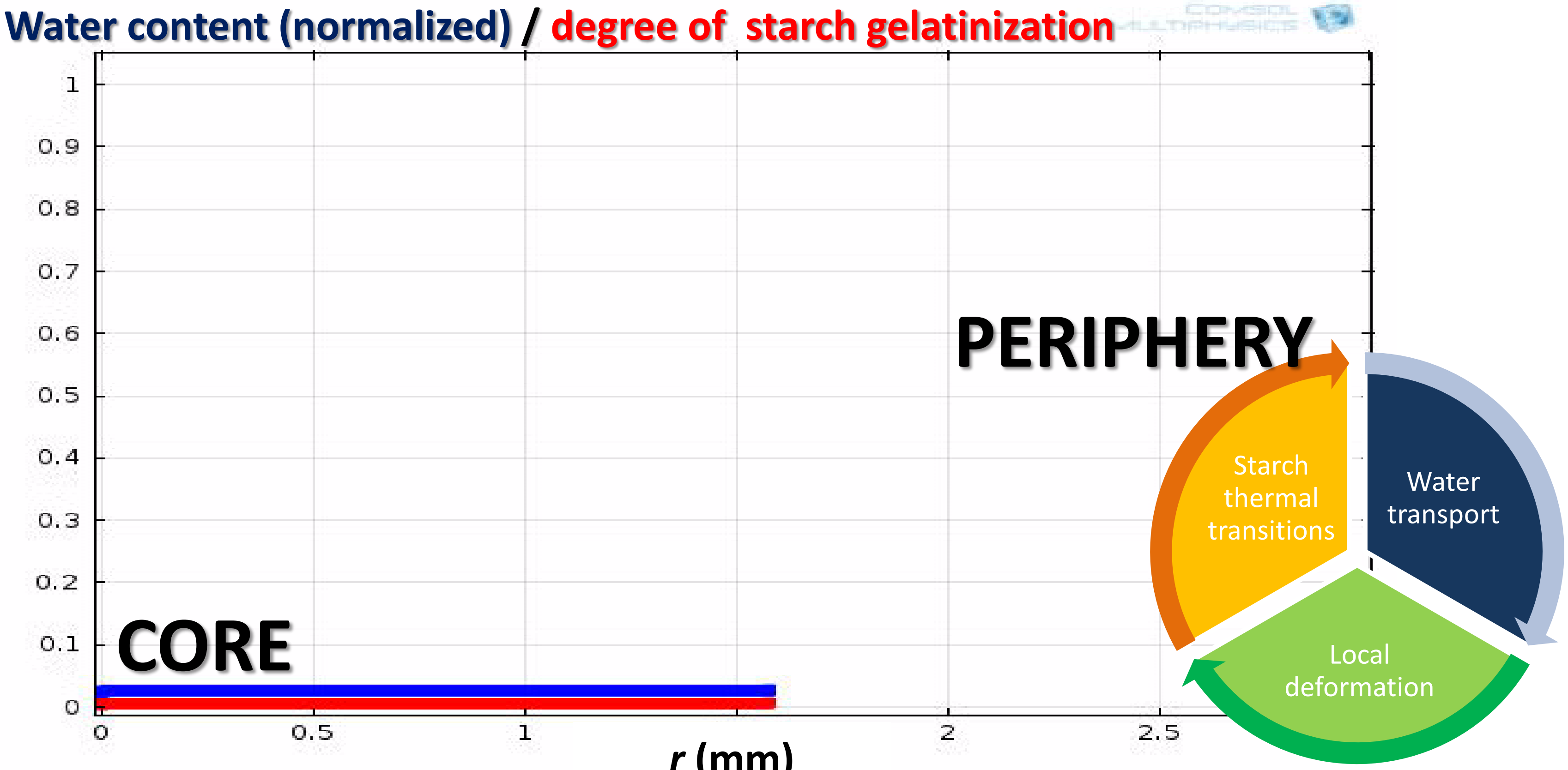
- Solid phase mass conservation between Eulerian and Lagrangian frames:

$$\boxed{\rho_2 r^2 dr = \rho_2^0 \xi^2 d\xi}$$ **PDE (7)**

- Integration of equation (7) gives local position:

$$\boxed{\xi(t) => r(t)}$$ **(8)**

II.2/ A local deformation related to local water flux density



CORE

PERIPHERY

Starch thermal transitions

Water transport

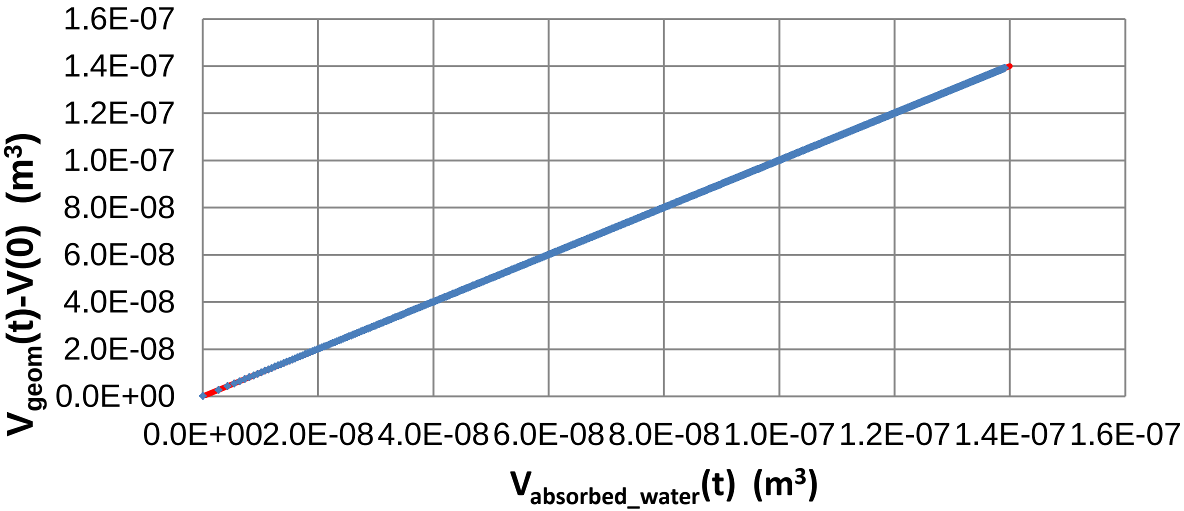
Local deformation

II.3/ A conservative approach

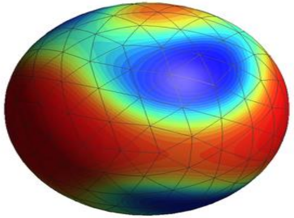
$$\boxed{\frac{d\left(\rho_{rice}V_{geom}\right)}{dt} \overset{?}{=} \underbrace{D_w \nabla_{r_{\max}}\left(X_1\rho_s\right)\times 4\pi r_{\max}^2}_{total\ water\ flux\left(kg_w.s^{-1}\right)}}$$

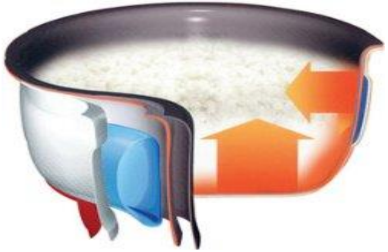
BODE (8)

Results for a 4h-simulation:

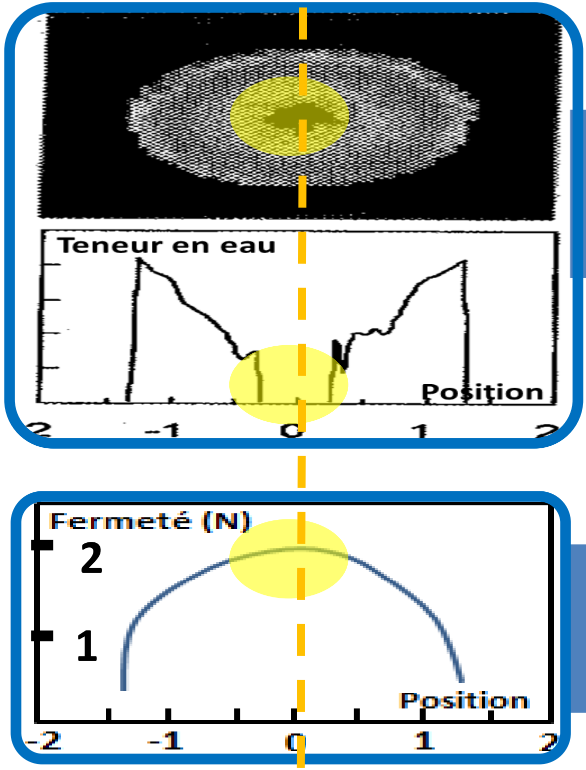


III/ Application: starchy cooking process simulation: case of rice





III.1/ Physicochemical properties & texture

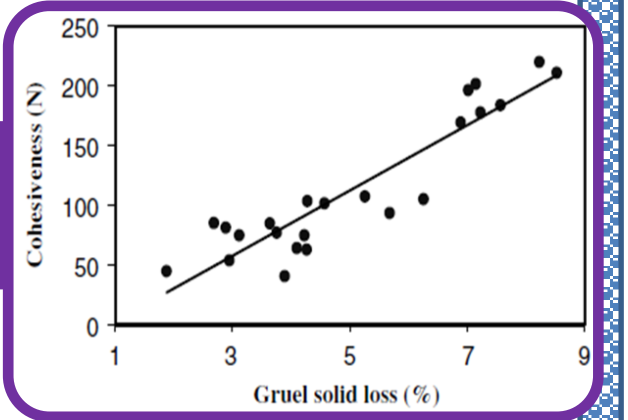


(Irie *et al.*, 2004)

Water and starch gelatinization distributions

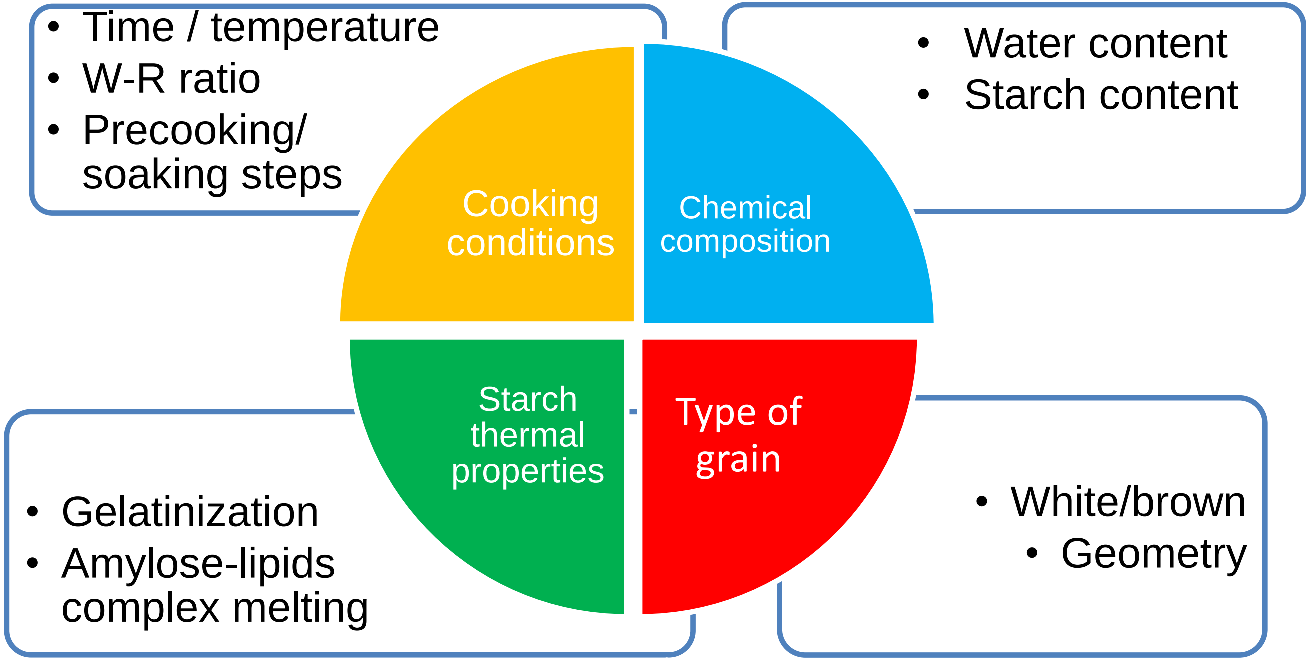
Correlation between solid losses and cooked rice stickiness

Instrumental hardness (compression test)



(Singh *et al.*, 2005)

III.2/ The rice cooking process simulator



- Time / temperature
- W-R ratio
- Precooking/ soaking steps

- Water content
- Starch content

Cooking conditions

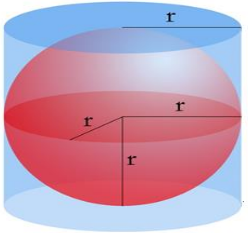
Chemical composition

Starch thermal properties

Type of grain

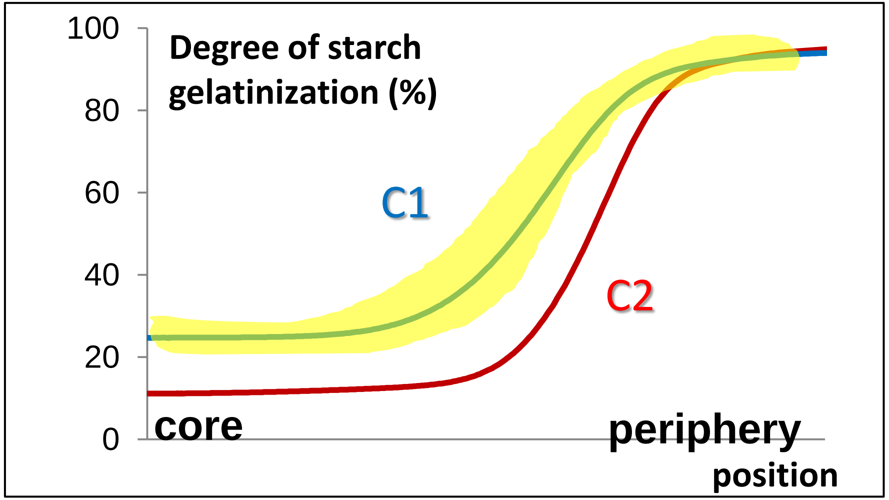
- Gelatinization
- Amylose-lipids complex melting

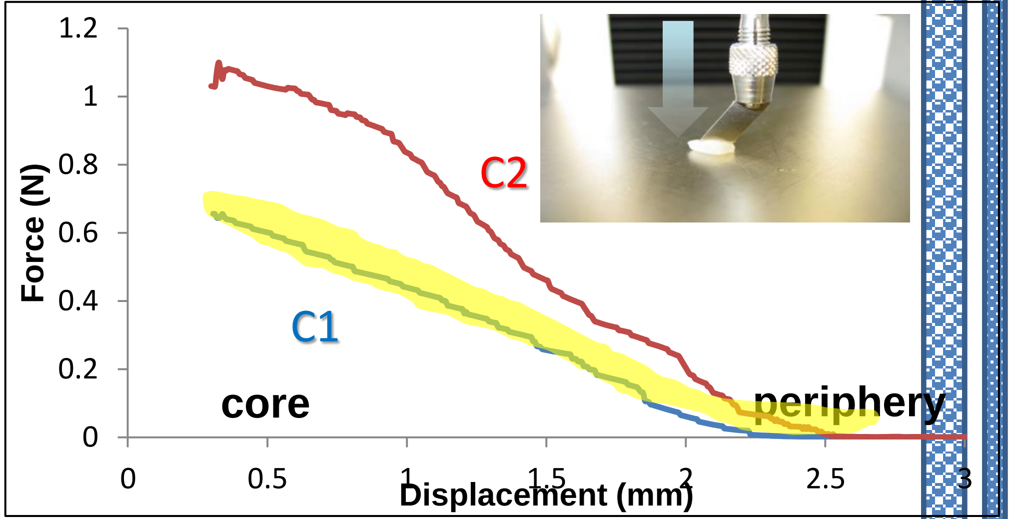
- White/brown
  - Geometry



III.3/ Ex: Impact of a precooking step on cooked rice firmness

Cooking route C_i	*WRR* (kg.kg^{-1} db)	Precooking step	Cooking step
C_1	2	55 °C/30 min	100 °C/15 min
C_2	2	X	100 °C/15 min





- => including a precooking step increases the degree of starch gelatinization and hence softens the cooked rice grain

Conclusion & Perspectives

1

- A mechanistic and generic model

- Coupling water transport, starch thermal transitions together with local deformation.
- Model validated in the case of rice cooking process.
- This approach can be applied to describe the behaviour of any deforming material whose phase change induces species transport property modifications.

2

- Design of tailored cooking scenarios

- Several meaningful model input parameters (geometry, φ-C, *T*(*t*), water-to-grain ratio, thermal properties of starch…).
- Model allowing to reach specific organoleptic (texture) targets (e.g. firmness and stickiness levels) to meet consumers' expectations.

3

- Creation of new models derived from this approach

- Describing plum drying with 3 compartments: stone, flesh and peel (see poster session).
- Describing the diffusion of multiple species with the consideration of mutual convective coupled and deformation (local + surface erosion).

Questions?

Thank you for your attention

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