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Coupling phenomenological model of expansion with mechanical model of starchy products extrusion: **Projet AIC-QualExp**

Magdalena KRISTIAWAN (BIA-MC2)

Problème d'application concerné: *Itinéraire multi-étape & couplage de modèle*

Recall of Objectives

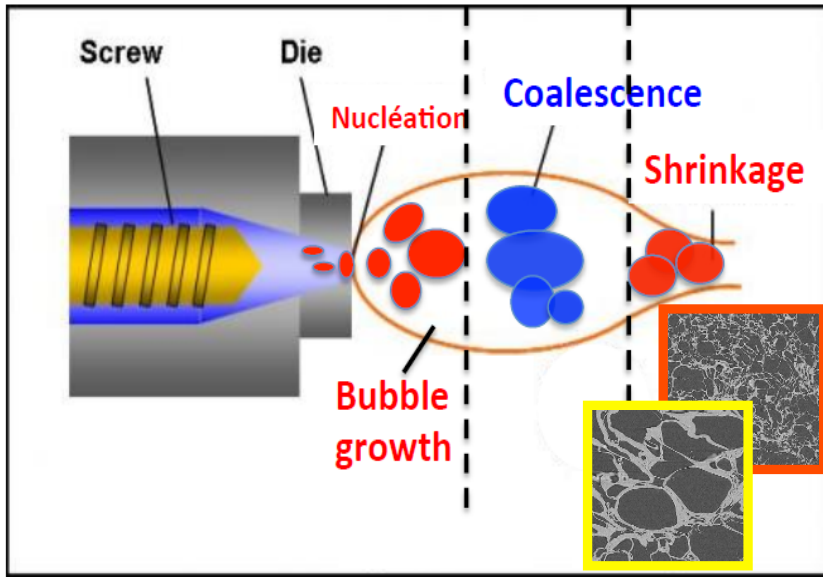
To build **a phenomenological model of expansion by extrusion** that allows to predict foam structure from process variables and material properties.

Delivrables

- 1/ **Phenomenological model of expansion** by extrusion for predicting **macro and cellular structure** of starchy solid foam.
- 2/ **Coupling** this phenomenological model with **mechanical model of extrusion** (Ludovic[®] software)

Context: **Expansion** by extrusion

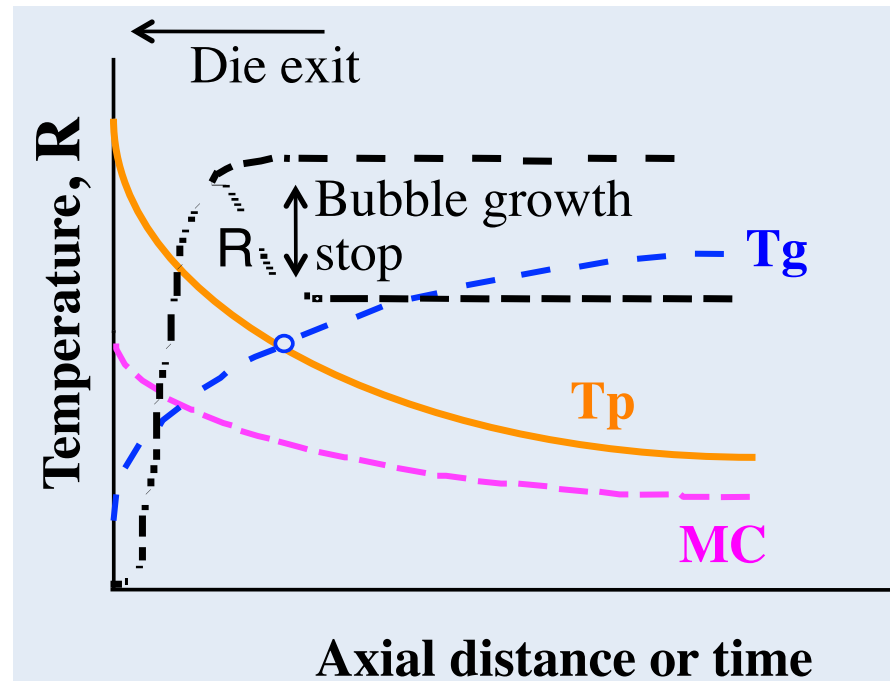
Acquisition of texture



The bubble growth stops (setting)
at $T_p > T_g + \dots ^\circ\text{C}$

T_g : glass transition temperature

State diagram



Applications

- Innovative starchy foods, with modulated shape and digestibility
- Starch based shape memory biopolymers for medical devices

Partners : BIA, I2M, externals

- **M. Kristiawan** :
Modeling implementation
- **B. Vergnes (CEMEF-MinesParisTech)** :
Extrusion and plastic foam manufacturing
- **G. Della Valle** :
Expertise on extrusion, rheology, process modeling
- **Ch. David /L. Ratte (SCC)** :
Software development for extrusion (Ludovic®)
- **L. Chaunier** :
Expertise on extrusion, experiments & physics measurements
- **Allaf / V. Sobolik (ULR)** :
Expansion by instant pressure drop, rheology, fluid mechanics
- **K. Kansou** :
Qualitative modeling and reasoning
- **A. Ndiaye** :
Qualitative modeling and reasoning
- **C. Fernandez** :
Software development for Knowledge Base System: Qualis©; Make Book



Methods and Resources

Modeling

Phenomenological models of **bubble growth** (+ nucleation, coalescence, setting, shrinkage) in a **viscoelastic** biopolymer matrix **in the transition state from rubbery to solid phase.**

Macro and **Cellular** structure = f (Water%, T_p °C, SME kWh/t, $\eta(\dot{\gamma})$, $\eta(\dot{\epsilon})$)

Approach

1. Collection of scientific knowledge (SK)
2. Representation of knowledge (Concept map / causal graph)
3. Establishment of **phenomenological models of expansion**
 - 2/3 of experimental data: *Model establishment*
 - 1/3 of experimental data & scientific articles: *Model validation*
4. **Coupling mechanical model of extrusion (Ludovic®)** with **expansion models**
5. Simulation and validation with experiments

Experimental data: Extrusion of maize starch

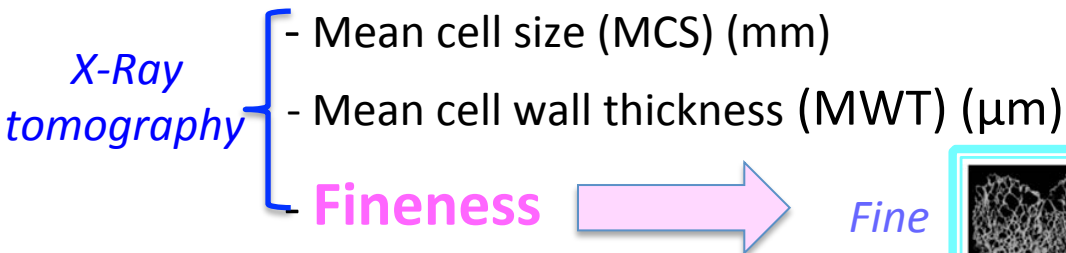
(Della Valle et al., 1996, 1997; Babin et al., 2007)

Input variables: (400 points)

- Amylose (0 – 70%) ($E'(T_\alpha)$); Plasticizer: Water % (MC)
- T°C of product at die exit (T_p), SME kWh/t, shear viscosity

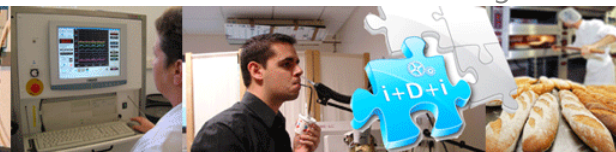
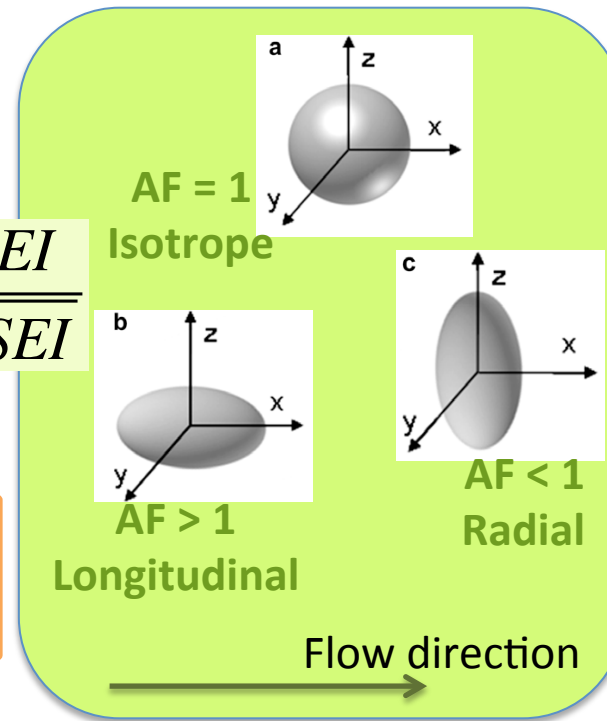
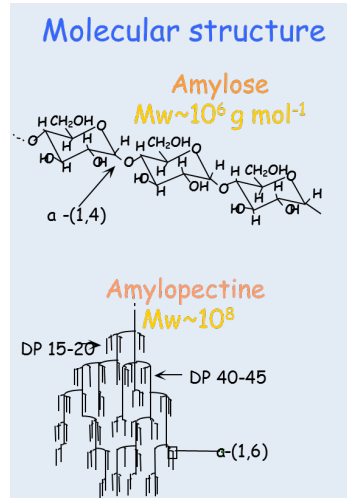
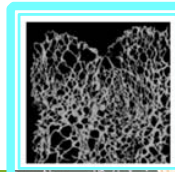
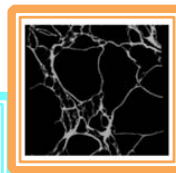
Output variables

- Macrostructure
 - Volumetric Expansion Indices (VEI) ($VEI = LEI \times SEI$)
 - Radial Expansion Indices (SEI)
 - Longitudinal Expansion Indices (LEI)
 - Anisotropy Factor (AF)
- Cellular structure



$$AF = \frac{LEI}{\sqrt{SEI}}$$

Coarse

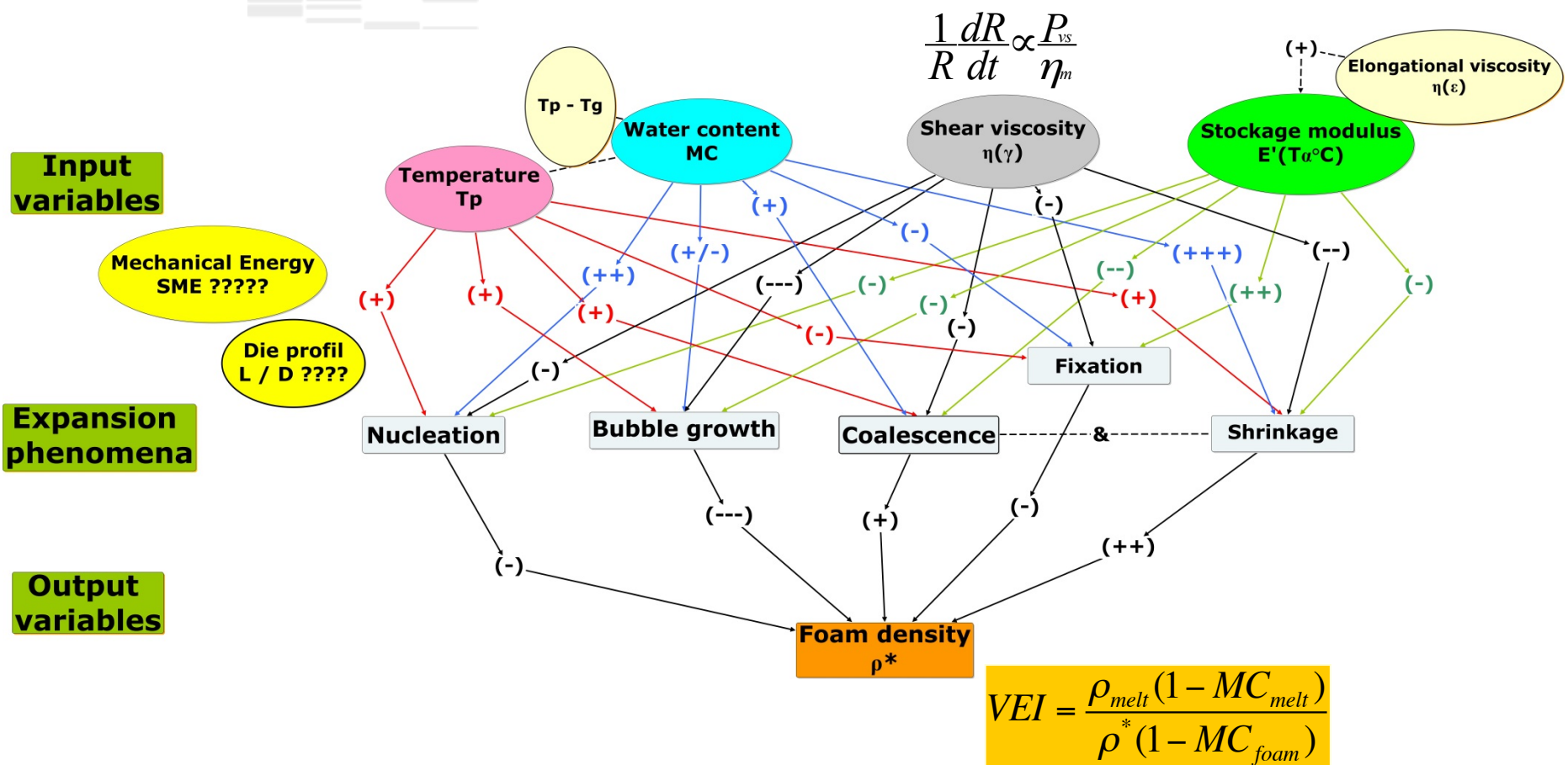




Results



Concept map: Phenomenological model of expansion



$$VEI \approx [MC/MC_0]^x \otimes [T_p/T_{p_0}]^y \otimes [\eta(\dot{\gamma})/\eta_0(\dot{\gamma})]^z \otimes [E'(T_\alpha)/E'_0(T_\alpha)]^t$$

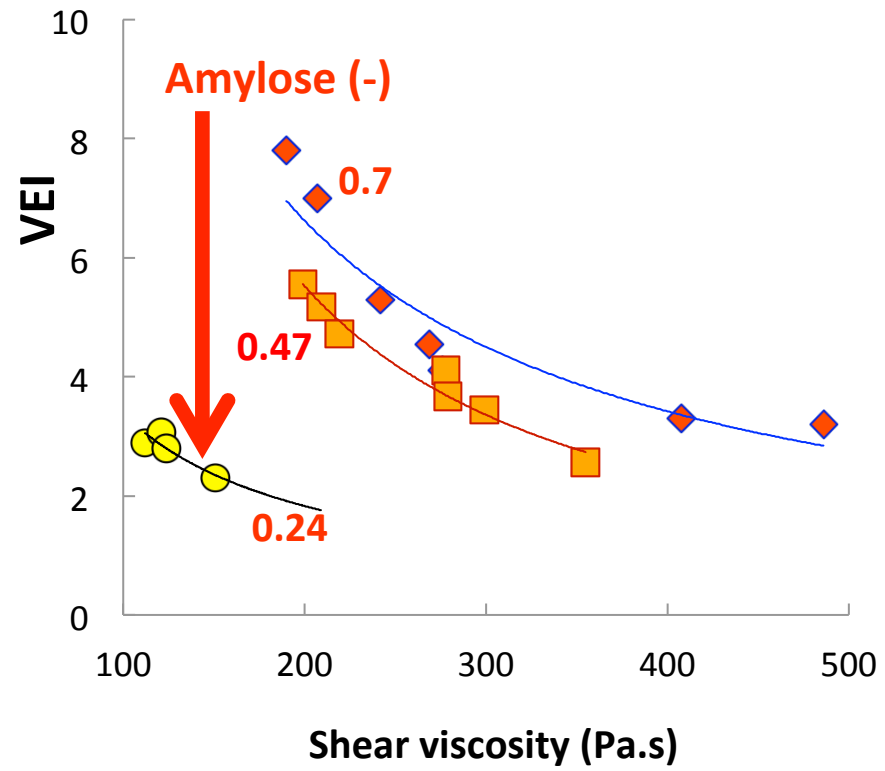


Volumetric expansion indices VEI

$$VEI = \frac{\rho_{melt} (1 - MC_{melt})}{\rho^* (1 - MC_{foam})}$$

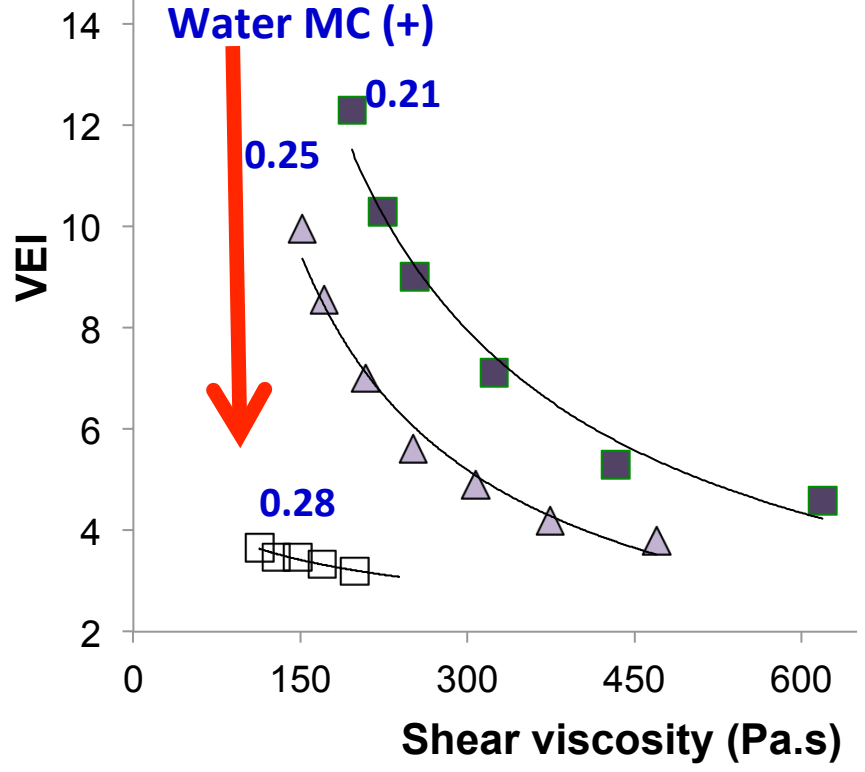
$$VEI \approx [E'(T_\alpha)/E'_o(T_\alpha)]^t$$

Water = 0.245, 185°C, 150 kWh/t, h die = 3 mm



Amylose 70%, 165°C, 200 kWh/t, h die = 3 mm

$$VEI \approx [MC/MC_o]^x$$



Data from Babin et al. (2007)²

Cellular fineness (F):

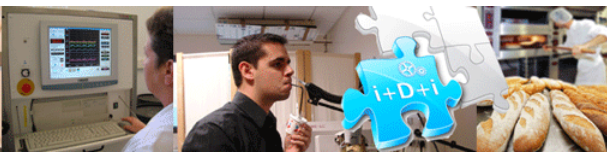
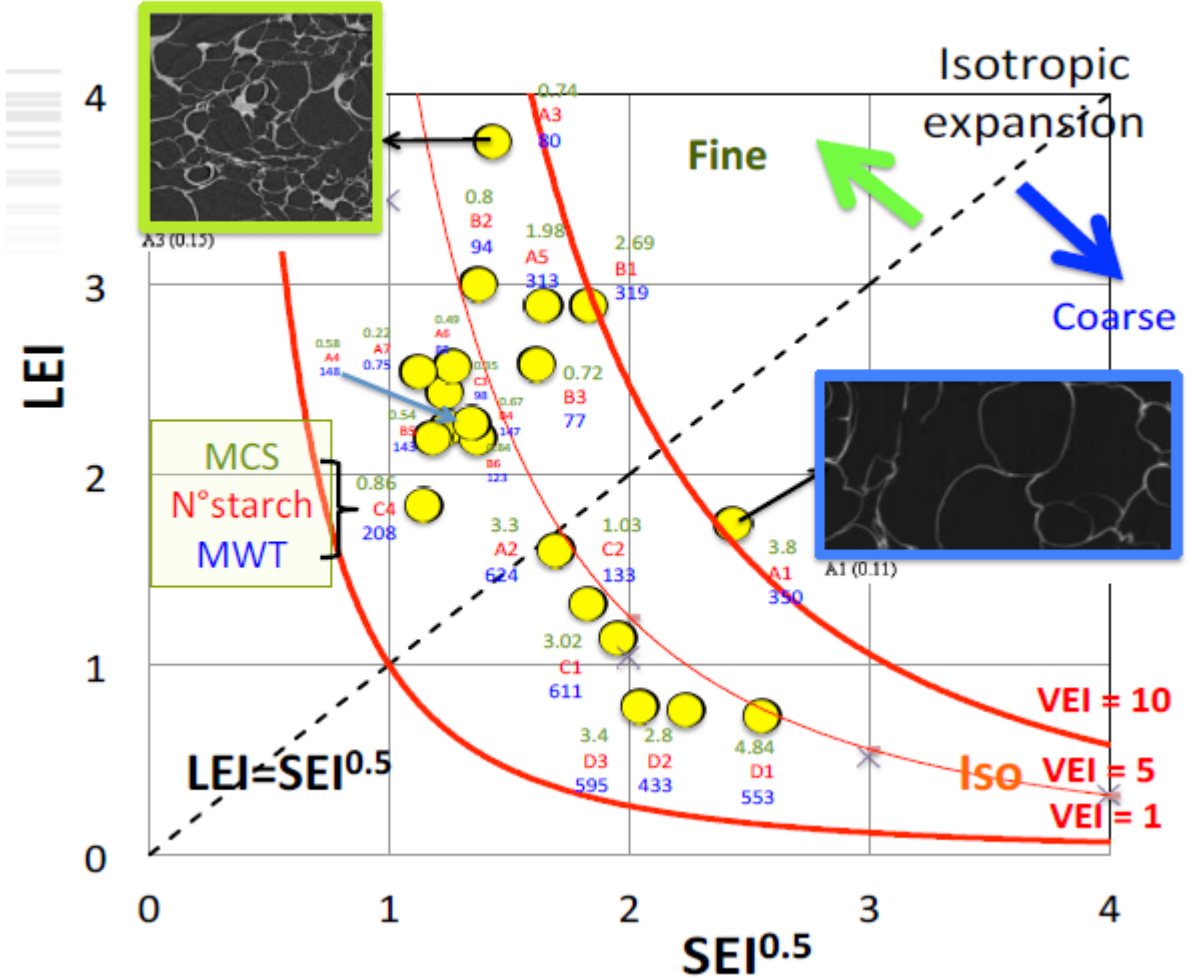
$$F = \sqrt{\frac{\left(\frac{250}{MWT}\right)^2 + \left(\frac{1}{MCS}\right)^2}{2}}$$

F < 1 → Coarse

F > 1 → Fine

MWT in μm; MCS in mm

The cellular structure can be deduced from the knowledge of anisotropy



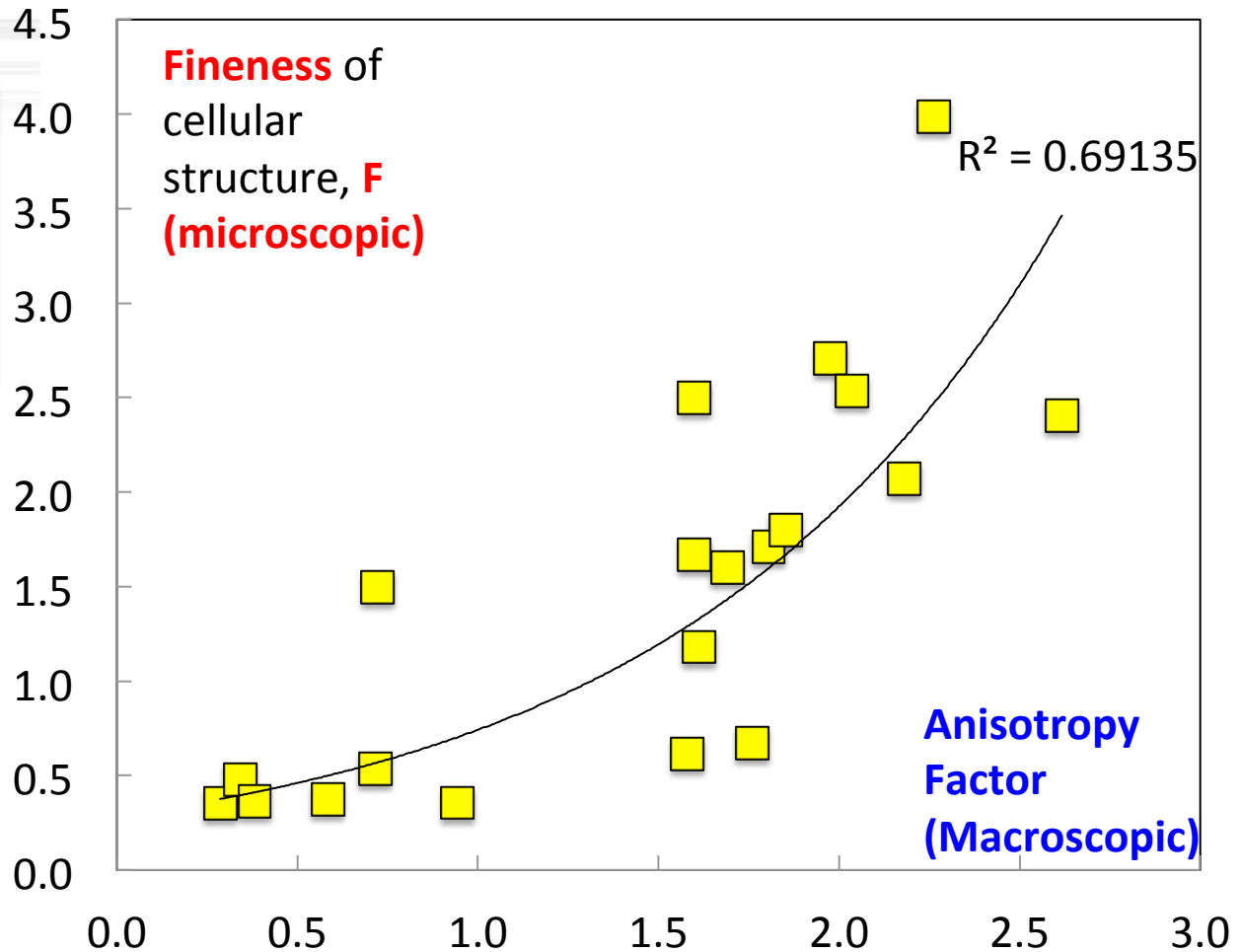
Scaling down: from macroscopic (anisotropy, AF) to microscopic (cellular structure, Fineness)

$$F = \sqrt{\frac{\left(\frac{250}{MWT}\right)^2 + \left(\frac{1}{MCS}\right)^2}{2}}$$

$F < 1 \rightarrow$ Coarse

$F > 1 \rightarrow$ Fine

MWT in μm ; MCS in mm



$$AF = LEI / (SEI)^{1/2} = VEI / (SEI)^{3/2}$$



Concept map: Structure of Ludovic®

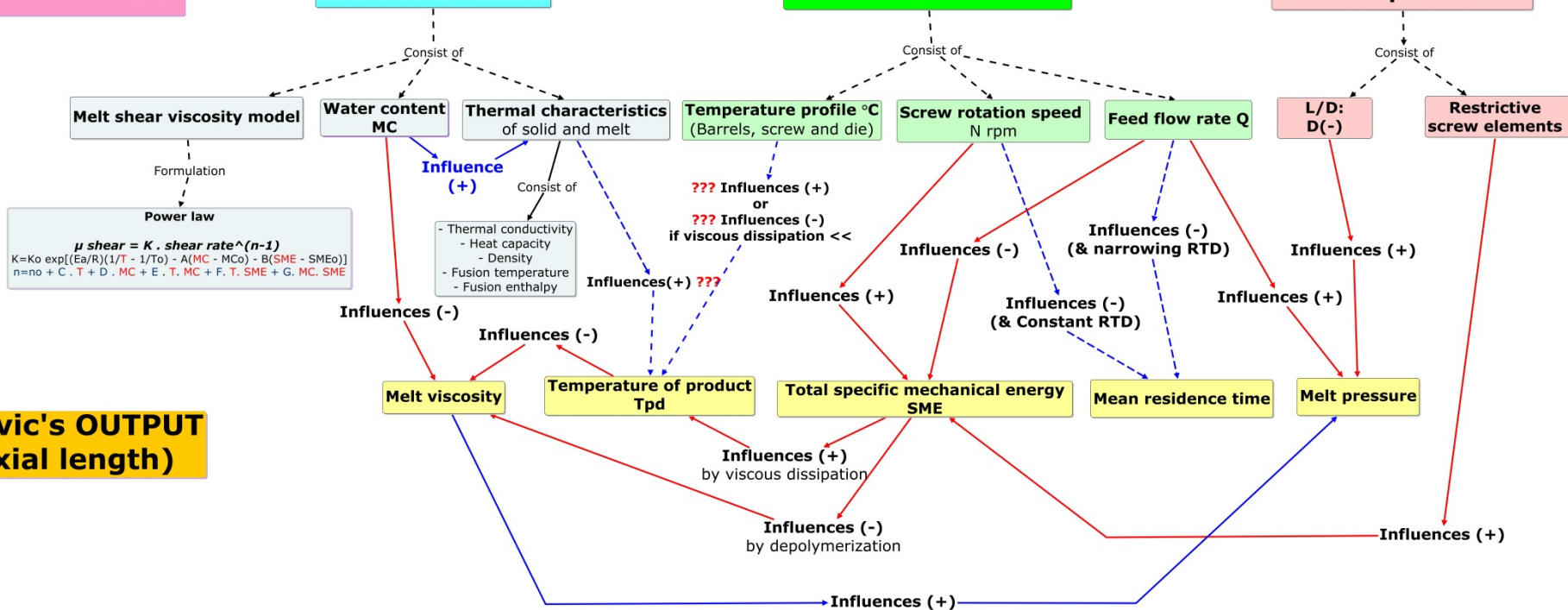
« Software for simulation of co-rotating twin-screw extrusion »

Ludovic's INPUT

Product properties

Processing parameters

Extruder parameters

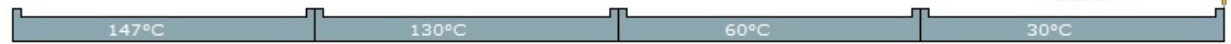
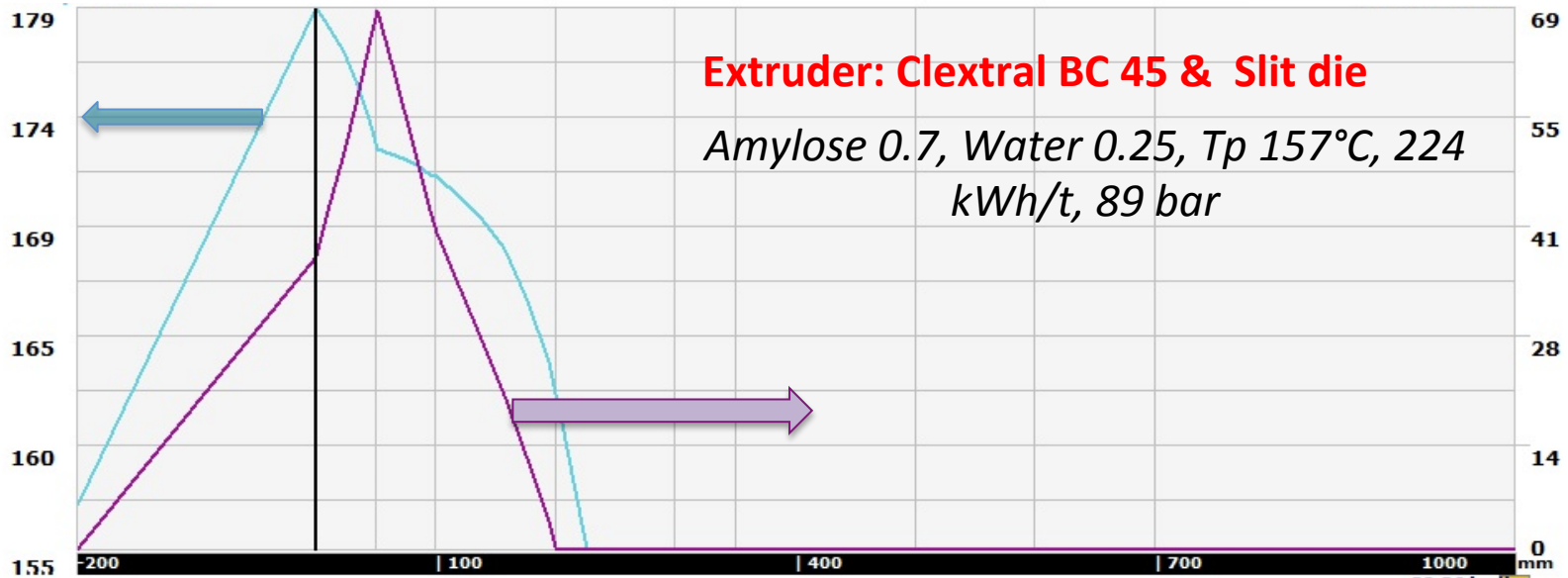


« Ludovic®'s output variables = input of expansion model »

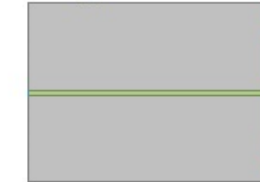
Flow parameters of extrusion process computed by Ludovic®

Temperature (°C)

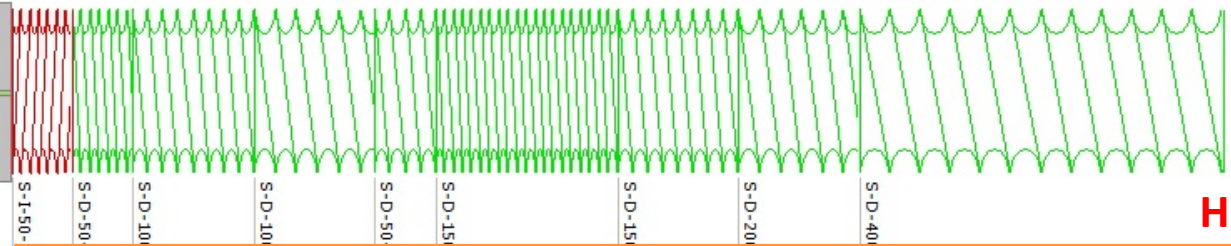
Pressure (bar)



32.36 kg/h



Die



Hopper

-15	15	25	35	25	15	25	35	50	pitch
50	50	100	100	50	150	100	100	300	length (mm)



Evaluation

Realized:

- Collection & integration of scientific knowledge
- Experiments on extrusion of starchy foams having shape memory
(the part of CR2 project, for familiarization with extrusion)
- Representation of knowledge
« Concept map with causalities »

On going:

- Establishment of phenomenological models of expansion

Perspective:

- Coupling mechanical model of extrusion (Ludovic[®]) with phenomenological models of expansion
- The new Ludovic[®]'s outputs: Macro and cellular structures of foams



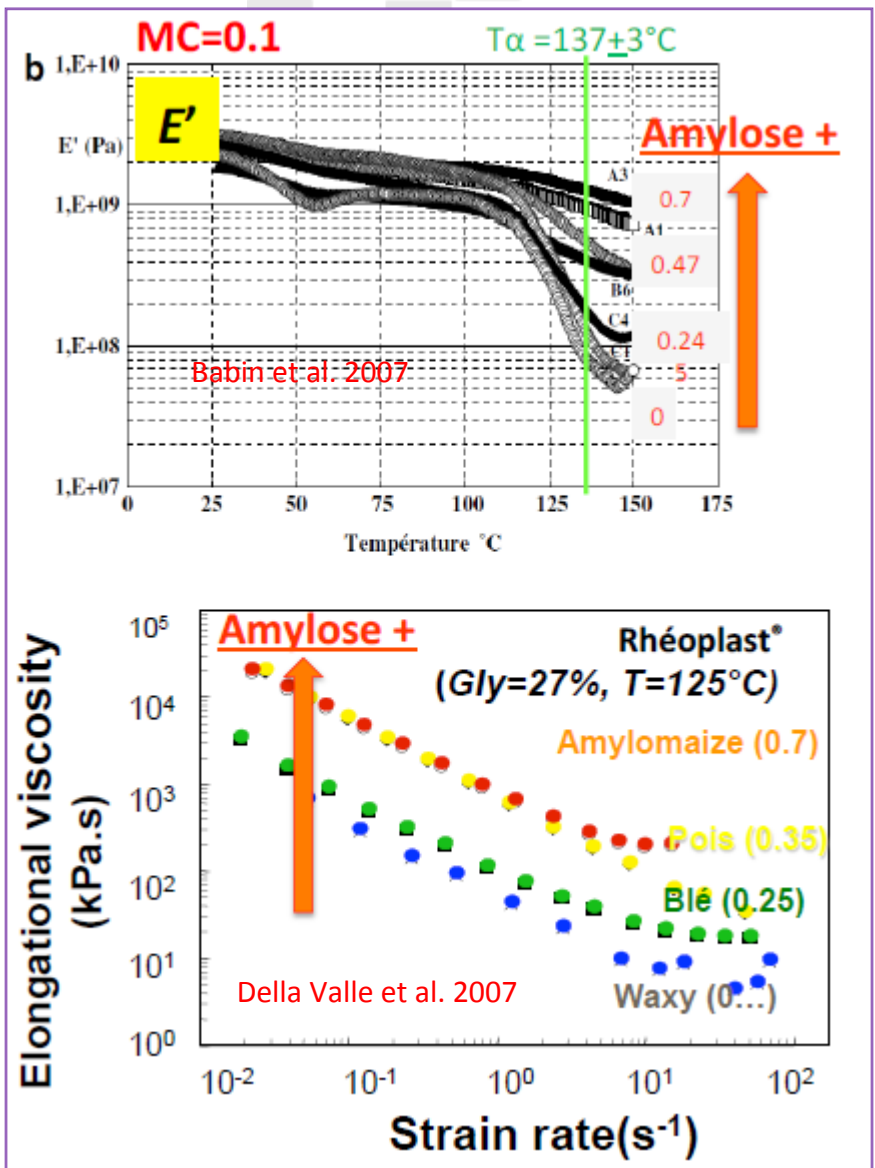


Thank you for your attention

Discussion...

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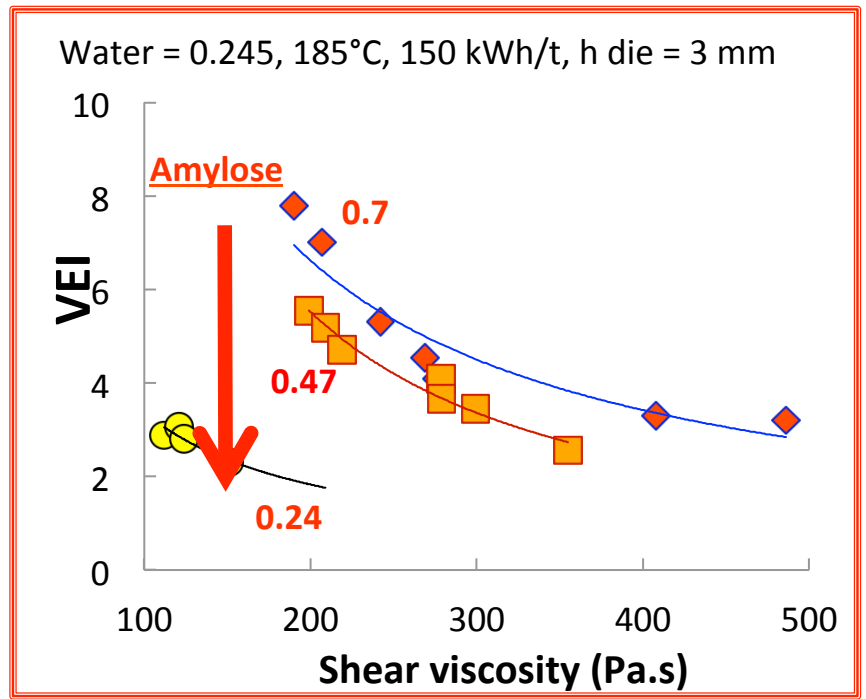




Elongational viscosity & $E'(T_{\alpha})$ as $f(\text{Amylose}\%)$

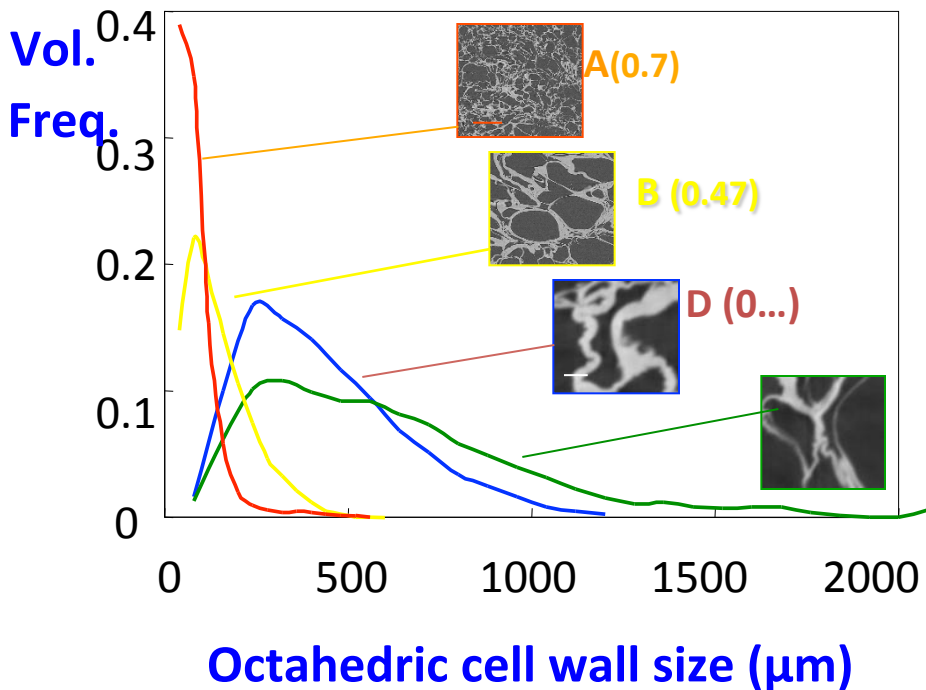
1) Variations of $E'(T_{\alpha})$ and $\eta(\dot{\epsilon})$ with amylose% follow the **same pattern**

2) If E' (+) then Coalescence (-) & VEI (+)



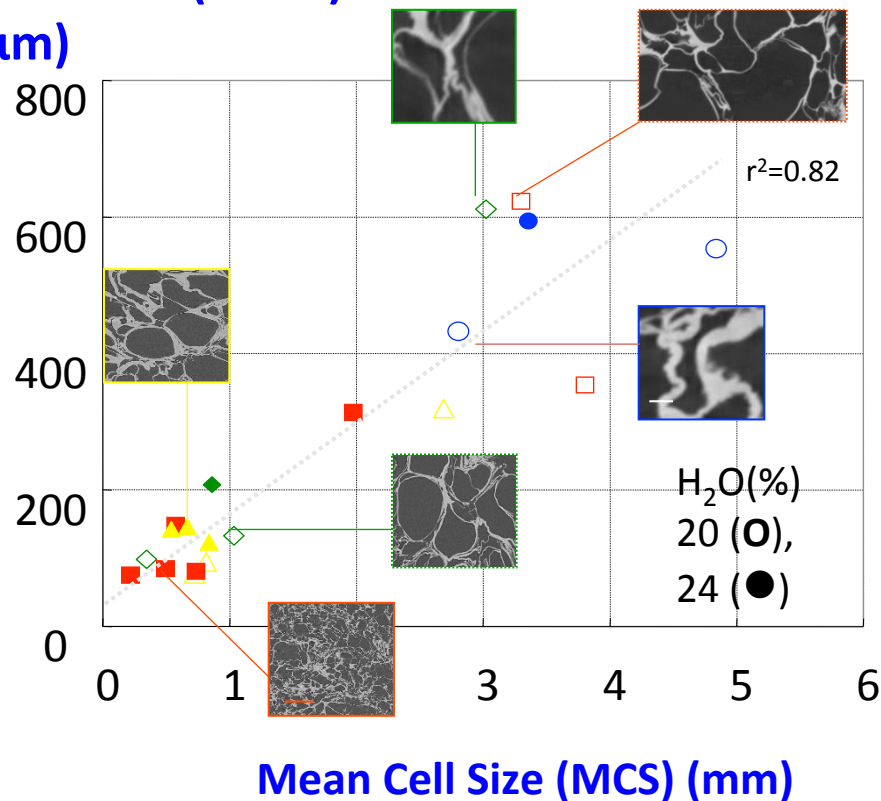
Babin et al., 2007

Distribution of Cell Wall Thickness



If the Cells « more coarse » then MWT dist. « more heterogeneous »

Mean Cell Wall Thickness (MWT) (μm)



If MCS (+) then MWT (+)