Coupling phenomenological model of expansion with mechanical model of starchy products extrusion (Projet AIC 'QualExp')

Magdalena Kristiawan, Guy G. Della Valle, Kamal Kansou

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

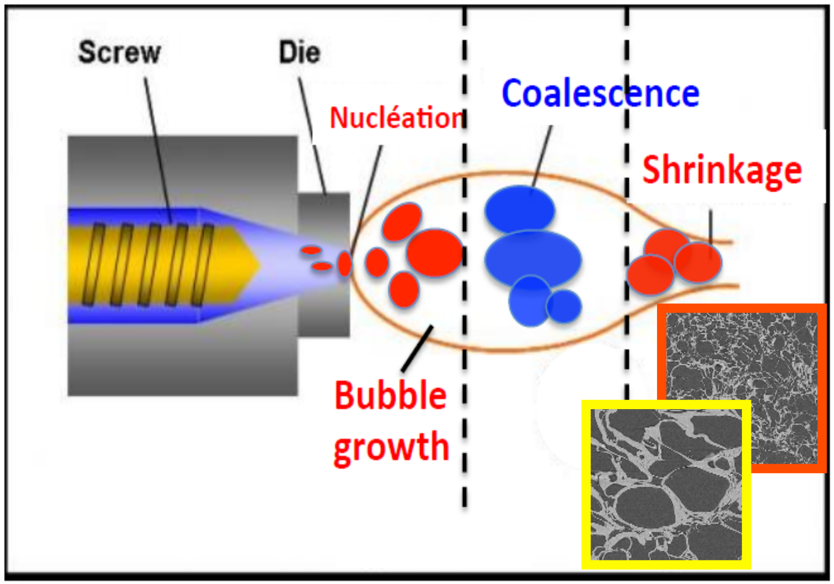
To build **a phenomenological model of expansion by extrusion** that allows to predict foam structure from process variables and material properties.

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

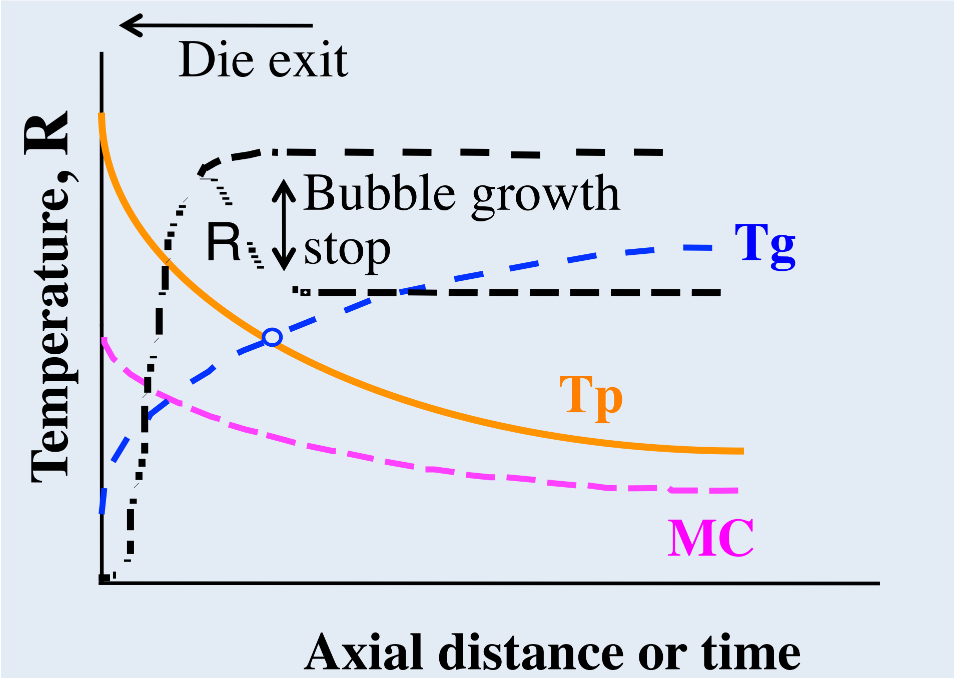
Acquisition of texture



The bubble growth stops (setting) at Tp > Tg + ….°C

Tg: 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%, Tp°C, SME kWh/t, $\eta(\dot{\Upsilon})$, $\eta(\dot{\varepsilon})$)

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

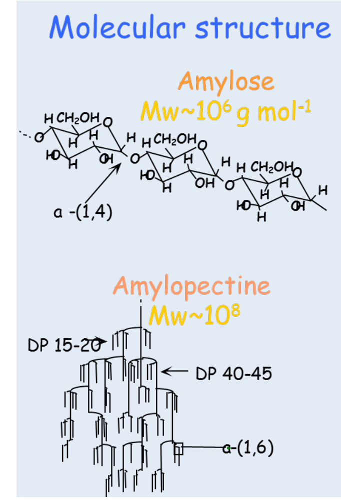
- **Experimental data: Extrusion of maize starch**

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

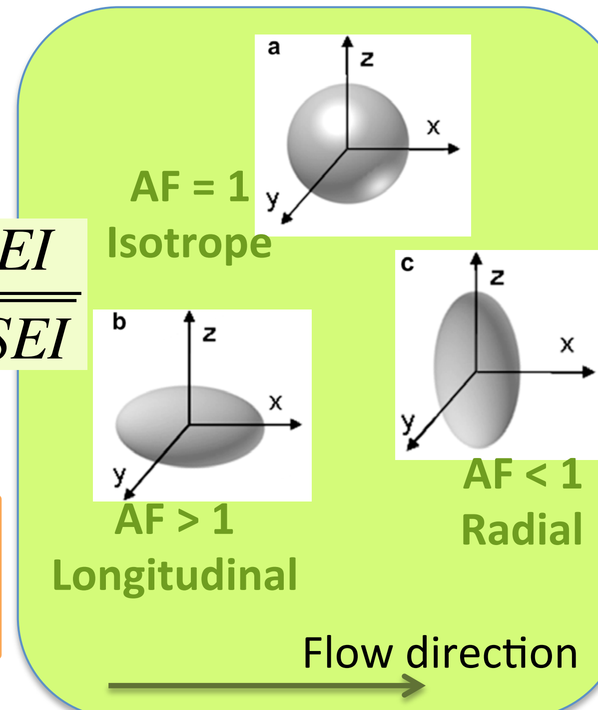
  – **Input variables: (400 points)**
    - Amylose (0 – 70%) (**E'(T_α)**); Plasticizer: Water % (MC)
    - T°C of product at die exit (Tp), SME kWh/t, shear viscosity

  – **Output variables**
    - Macrostructure
      - Volumetric Expansion Indices (VEI) **(VEI=LEI x SEI)**
      - Radial Expansion Indices (SEI)
      - Longitudinal Expansion Indices (LEI)
      - **Anisotropy Factor (AF)**
    - Cellular structure
      - Mean cell size (MCS) (mm)
      - Mean cell wall thickness (MWT) (µm)
      - **Fineness**

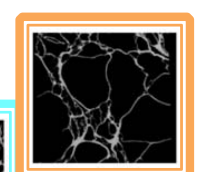
X-Ray tomography



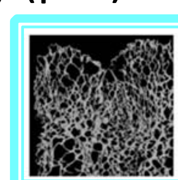
$$AF = \frac{LEI}{\sqrt{SEI}}$$



Coarse



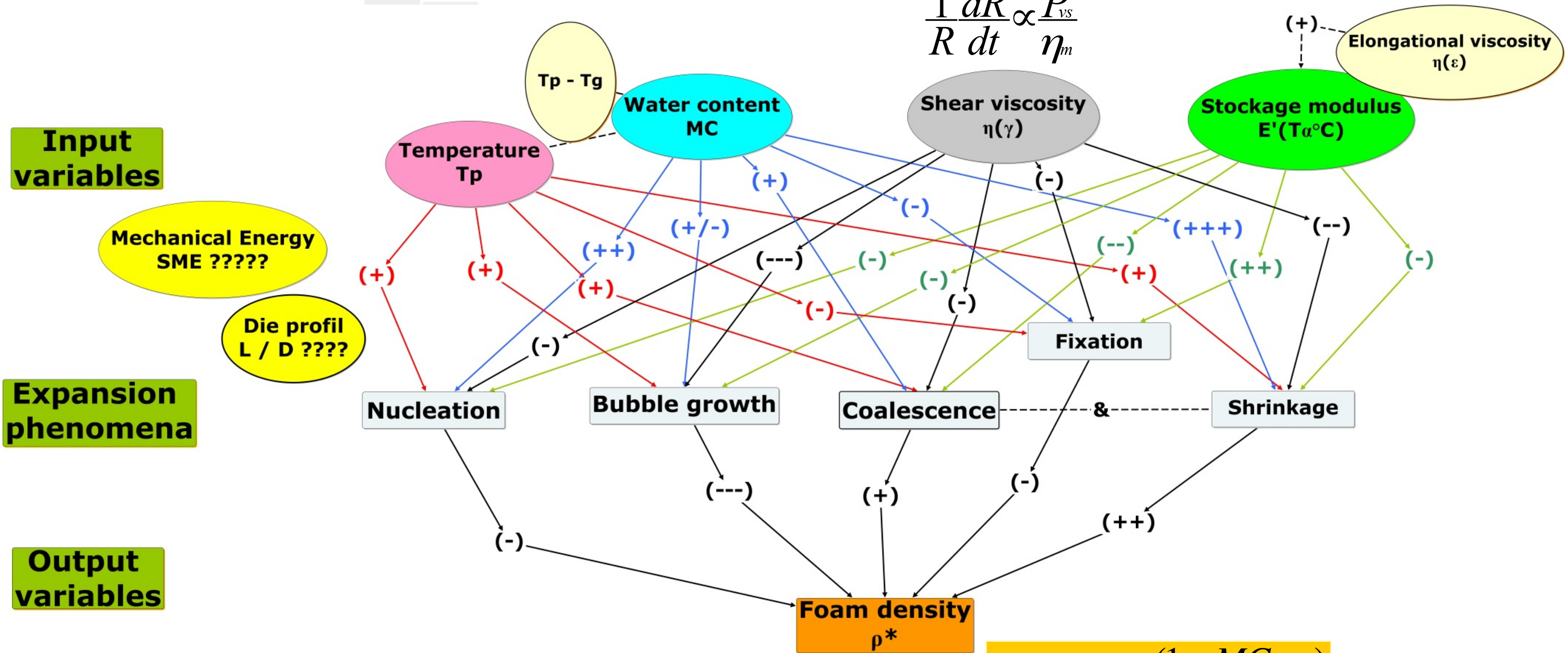
Fine



Results

Concept map: Phenomenological model of expansion

$$\frac{1}{R}\frac{dR}{dt} \propto \frac{P_{vs}}{\eta_m}$$



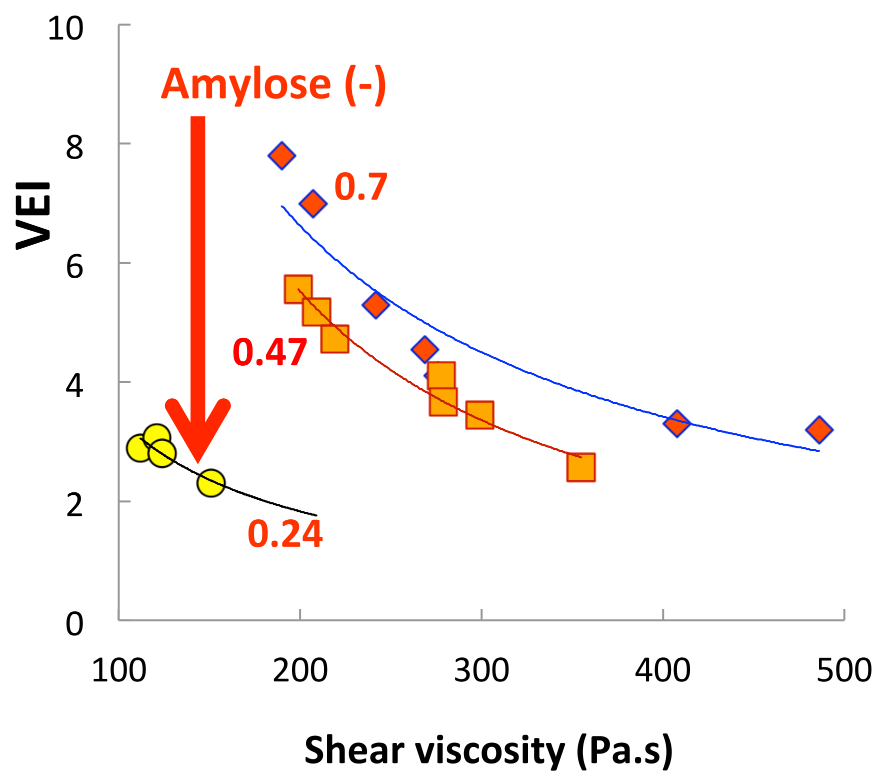
$$VEI = \frac{\rho_{melt}(1 - MC_{melt})}{\rho^{*}(1 - MC_{foam})}$$

$$VEI \approx [MC/MC_o]^x \otimes [Tp/Tp_o]^y \otimes [\eta(\dot{\gamma})/\eta_o(\dot{\gamma})]^z \otimes [E'(T_\alpha)/E_o'(T_\alpha)]^t$$

Volumetric expansion indices VEI

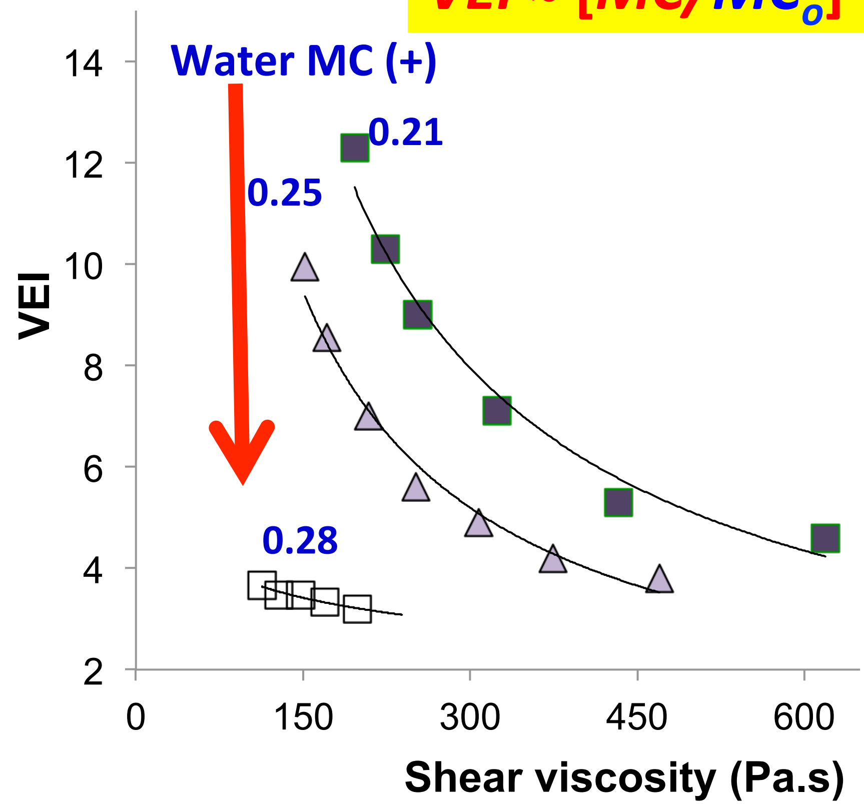
$$VEI = \frac{\rho_{melt}(1 - MC_{melt})}{\rho^{*}(1 - MC_{foam})}$$

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



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

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



Mapping of Anisotropy & Structure Cellular

Cellular fineness (F):

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

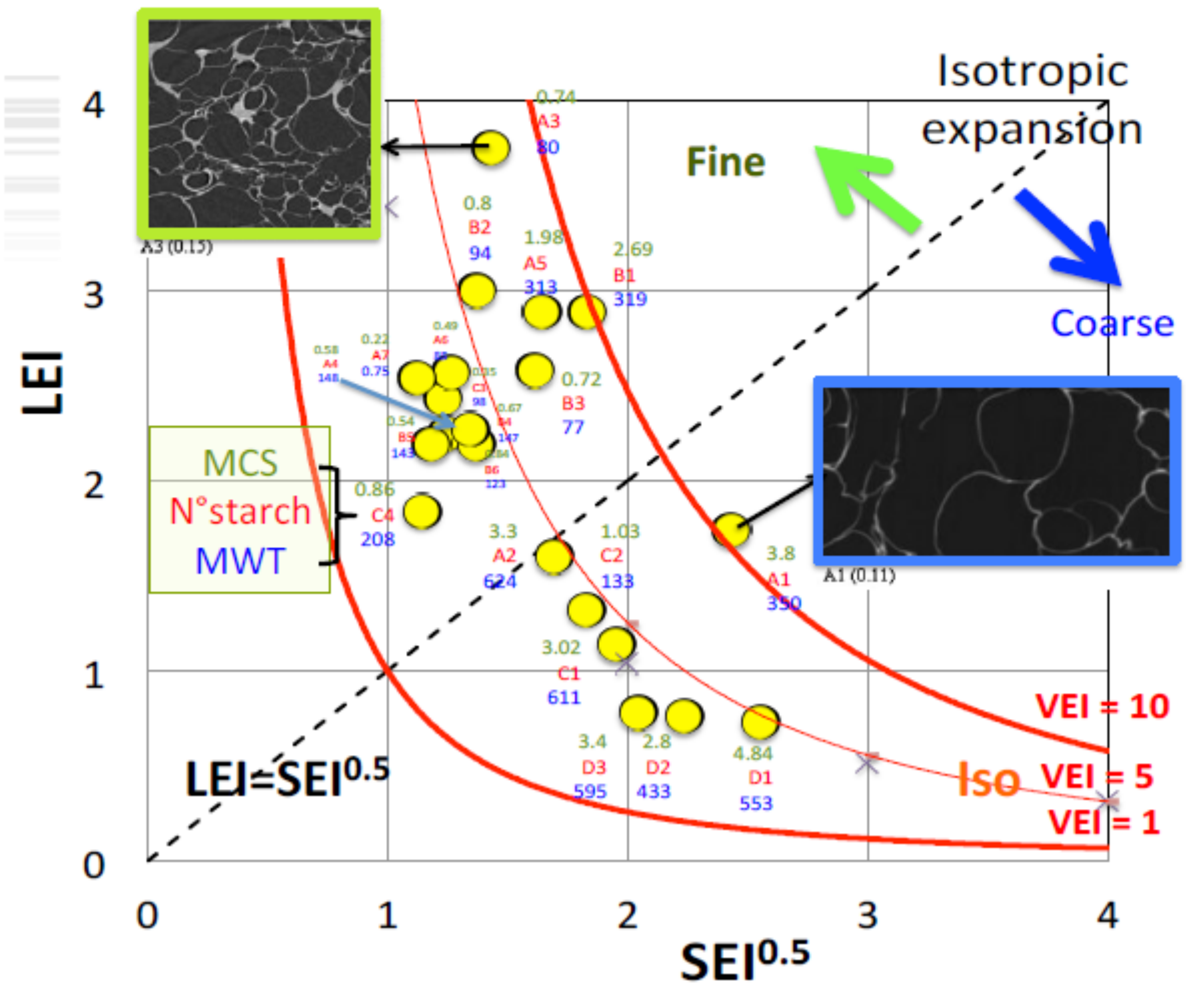
F < 1 → Coarse

F > 1 → Fine

MWT in µm; MCS in mm

The cellular structure can be deducted from the knowledge of anisotropy

Data from Babin et al. (2007)[2]



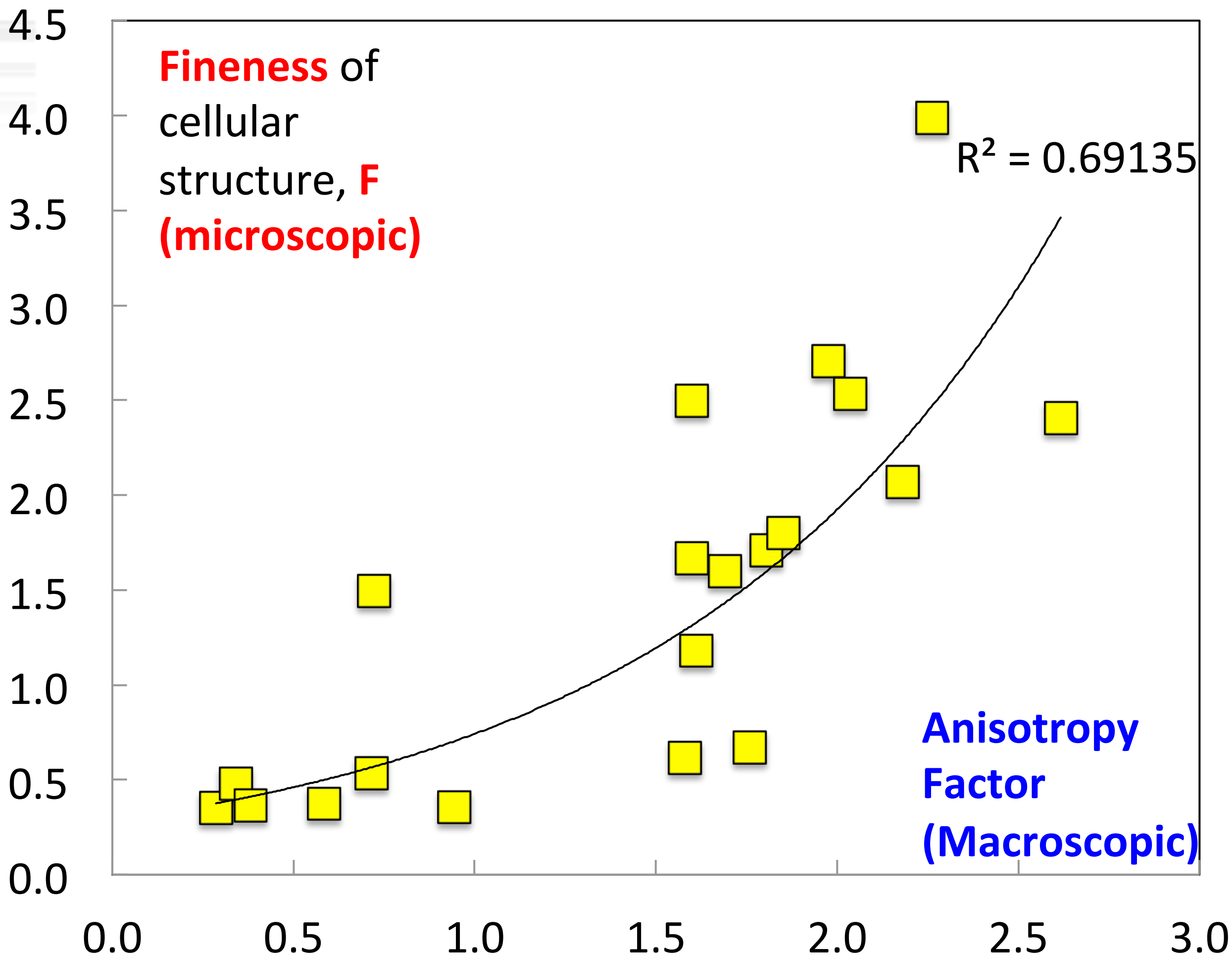
Scaling down: from macroscopic (anisotropy, AF) to microscopic (cellular structure, Fineness)

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

F < 1 → Coarse

F > 1 → Fine

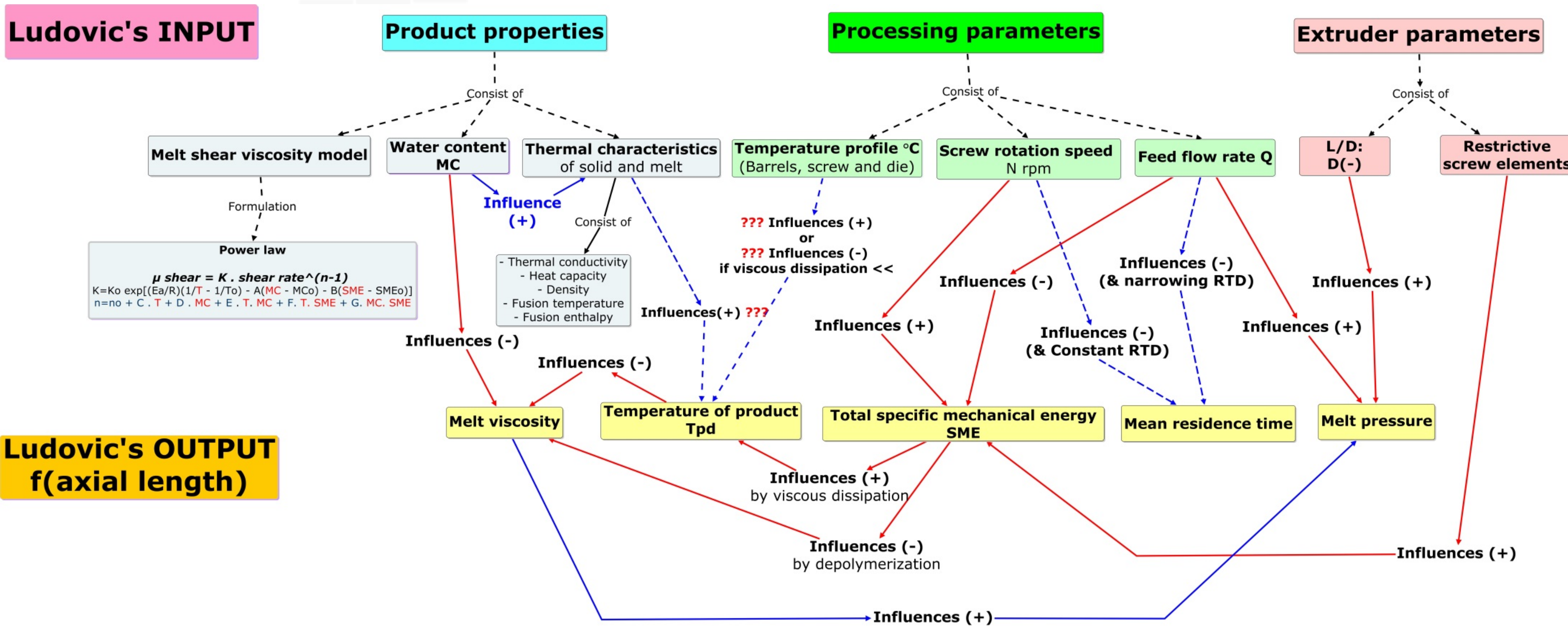
MWT in µm; MCS in mm



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

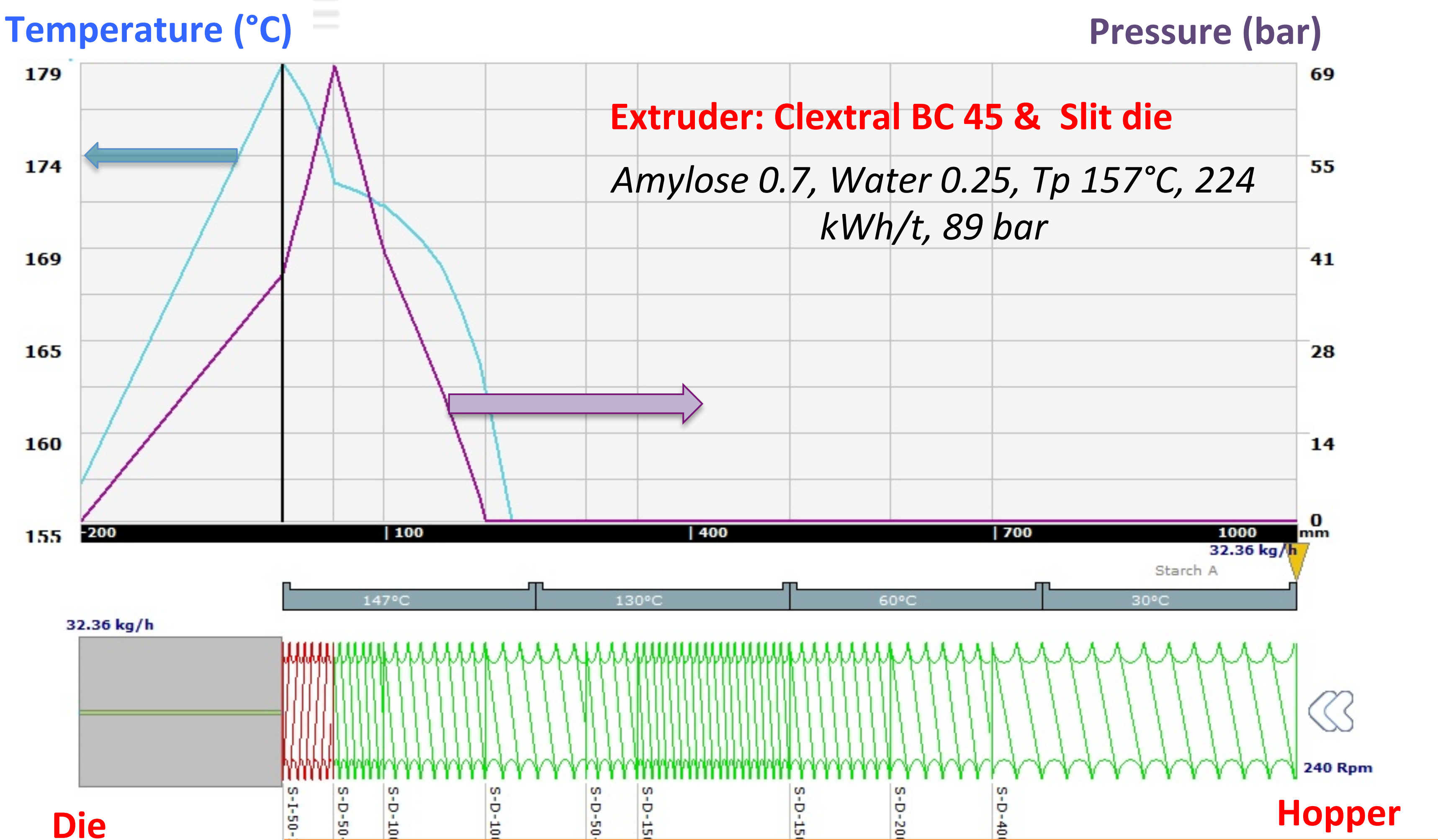
Concept map: Structure of Ludovic®

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



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

Flow parameters of extrusion process computed by Ludovic®



-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

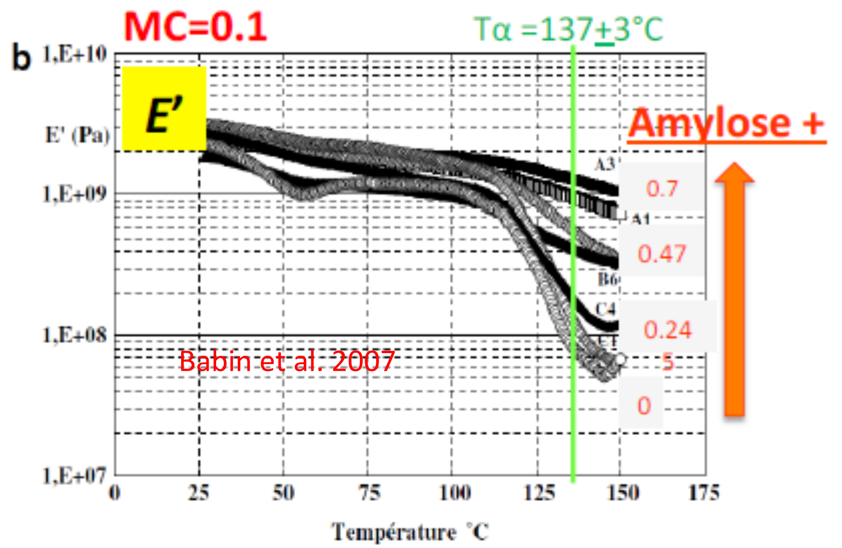
Perspective:

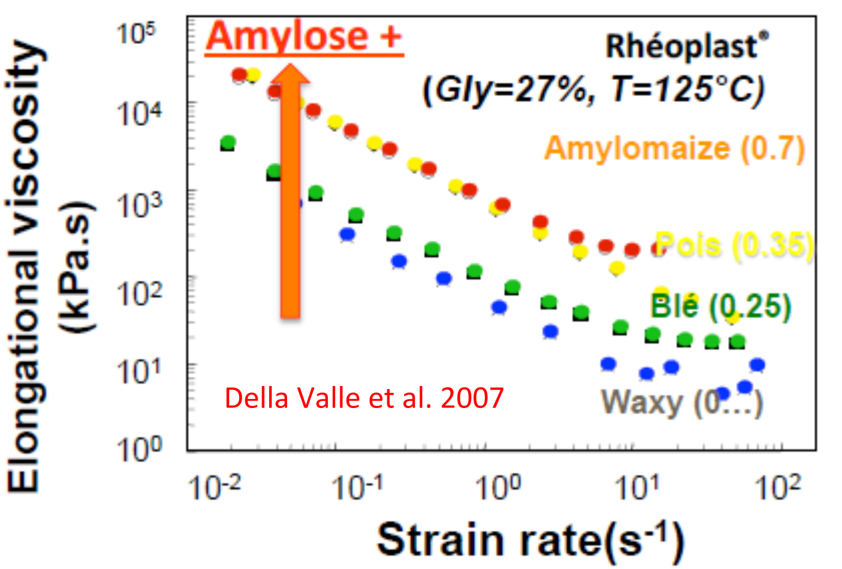
- Coupling mechanical model of extrusion (Ludovic®) with phenomenological models of expansion
- The new Ludovic®'s outputs: Macro and cellular structures of foams

Thank you for your attention

Discussion….

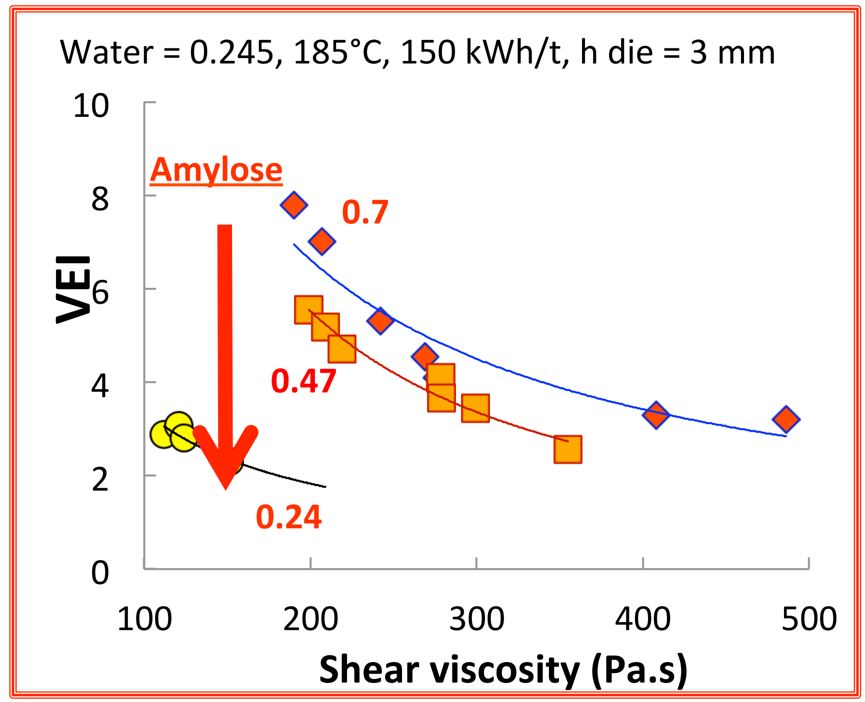
Elongational viscosity & $E'(T_\alpha)$ as f(Amylose%)





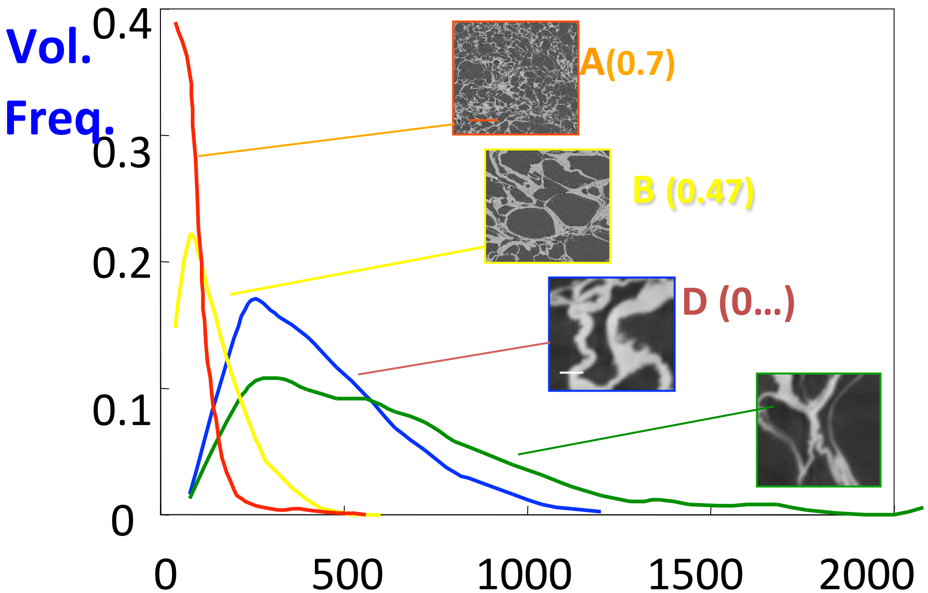
1) Variations of **$E'(T_\alpha)$** and $\eta(\dot{\varepsilon})$ with amylose% follow the **same pattern**

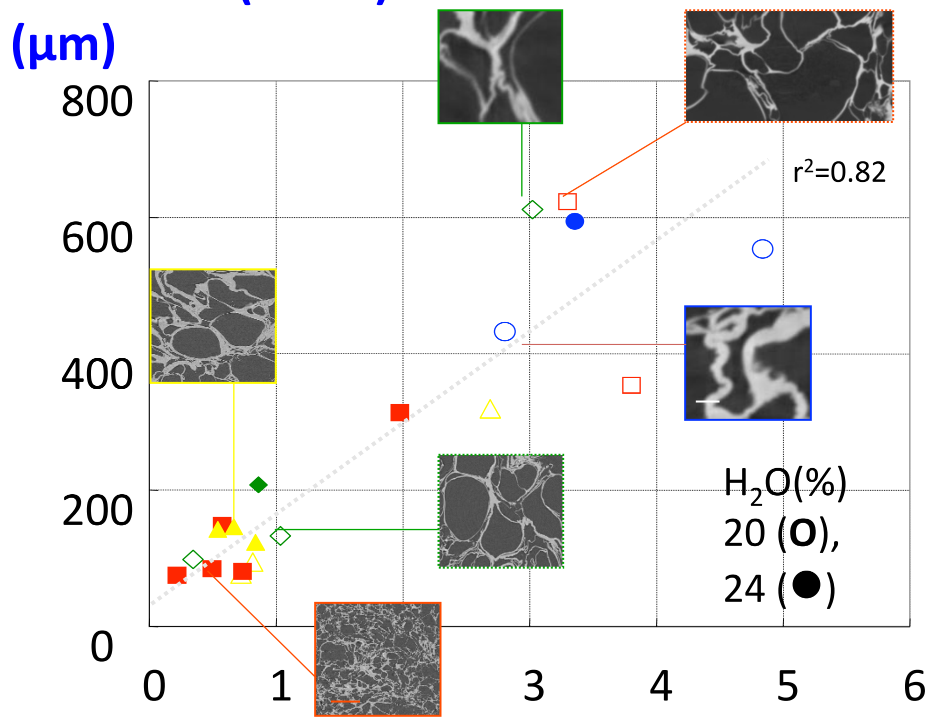
2) If E' (+) then Coalescence (-) & VEI (+)



Babin et al., 2007

Distribution of Cell Wall Thickness





If MCS (+) then MWT (+)

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