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

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Recall of Objectives

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

**Deliverables**

- 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**

- **Screw**
- **Die**
- **Coalescence**
- **Shrinkage**
- **Bubble growth**

The bubble growth stops (setting) at \( T_p > T_g + \ldots ^\circ C \)

**Tg:** glass transition temperature

**State diagram**

- **Die exit**
- **Temperature, \( R \)**
- **Bubble growth stop**
- **Axial distance or time**
- **\( T_g \)**
- **\( T_p \)**
- **MC**
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, η(\dot{\gamma}), η(\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%) ($E'(T_\alpha)$); 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
    - Mean cell size (MCS) (mm)
    - Mean cell wall thickness (MWT) ($\mu$m)

**X-Ray tomography**

AF = 1
Isotrope

AF > 1
Radial

AF < 1
Longitudinal

Flow direction
Results
Concept map: Phenomenological model of expansion

\[ \text{VEI} \approx \left( \frac{\text{MC}}{\text{MC}_o} \right)^x \otimes \left( \frac{T_p}{T_{p_o}} \right)^y \otimes \left[ \frac{\eta(\gamma)}{\eta_0(\gamma)} \right]^z \otimes \left[ \frac{E'(T_\alpha)}{E_0'(T_\alpha)} \right]^t \]
Volumetric expansion indices VEI

\[ VEI \approx \left[ \frac{E'(T\alpha)}{E_o'(T\alpha)} \right]^t \]

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

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

\[ VEI \approx \left[ \frac{MC}{MC_o} \right]^x \]

Séminaire InCoM – 9-10 Avril 2014
The cellular structure can be deduced from the knowledge of anisotropy.

Cellular fineness ($F$):

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

- $F < 1 \rightarrow$ Coarse
- $F > 1 \rightarrow$ Fine

$\text{MWT}$ in $\mu$m; $\text{MCS}$ in mm
Scaling down: from *macroscopic* (anisotropy, AF) to *microscopic* (cellular structure, Fineness)

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

- **F** < 1 → Coarse
- **F** > 1 → Fine

*MWT in μm; MCS in mm*

**AF** = \( \frac{\text{LEI}}{(\text{SEI})^{1/2}} = \frac{\text{VEI}}{(\text{SEI})^{3/2}} \)

**R^2 = 0.69135**

**Fineness of cellular structure, F (microscopic)**
Ludovic's INPUT

Product properties
- Water content MC
- Thermal characteristics of solid and melt

Processing parameters
- Temperature profile °C (Barrels, screw and die)
- Screw rotation speed N rpm
- Feed flow rate Q

Extruder parameters
- L/D: D(-)
- Restrictive screw elements

Melt shear viscosity model
- Power law
  \[ \mu_{\text{shear}} = K \cdot \text{shear rate}^{(n-1)} \]

Influence (+)
- Thermal conductivity
- Heat capacity
- Density
- Fusion temperature
- Fusion enthalpy

Influences (-)

Melt viscosity

Temperature of product Tpd

Total specific mechanical energy SME

Mean residence time

Melt pressure

Ludovic's OUTPUT
f(axial length)

Influences (+)

« Ludovic®’s output variables = input of expansion model »
Extruder: Clextral BC 45 & Slit die

Amylose 0.7, Water 0.25, Tp 157°C, 224 kWh/t, 89 bar
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....
Integration of scientific knowledge

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

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

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

Water = 0.245, 185°C, 150 kWh/t, h die = 3 mm
If the Cells «more coarse » then MWT dist. « more heterogeneous »

If MCS (+) then MWT (+)