Multiscale Modelling Seminar – VTT – 5.02.2013

μFEM modelling of wood cell deformation under pulping-type dynamic loads

Stefania Fortino¹, Petr Hradil¹, Lauri Salminen²

¹TK2014 Service Life Management
²TK5103 Biofibre Processing
Generalities and objective

- Thermo-Mechanical (TM) pulping processes are very energy intensive (in the range of 2000 kWh/ton pulp). Small process improvements may give large benefits for the energy cost.

- New research results will provide benefits for biorefinery and, consequently, for industry of printing papers and package products.

- **Main objective of the research**: to decrease energy consumption during Thermo-Mechanical pulping.

- **Multidisciplinary approach**: Co-operation between research areas of Biofibre Processing and Materials Modelling is promising.
Refining by Thermo-Mechanical (TM) pulping

• Moist wood chips and dilution water are fed into the centre of the discs.

• The refining process is controlled by temperature, dilution water, plate gap and plate geometry.

• The plate gap temperature (120-160°C) profiles describe the refiner response to load increase.

• The principle of refiner is both to separate and to make more flexible the wood fibres. These are subjected to repeated compression and shear aimed to collapse the cells.

• The hardest and most consuming step during the process is the fibre cell wall opening.
Knowledge on geometry of wood cells
Microscale

- In the last decade knowledge on wood cell geometry, elasticity and chemistry has developed to such an extent (Salmén et al., Qing et al., Hofstetter et al.) that now progress necessitates on the intrawall deformation.

- To develop a μFEM computational tool reference experiments are needed.

Figure from De Magistris and Salmén, 2008
Reference experiments from the literature (De Magistris and Salmén, 2005-2008)
Modified Arcan device test

- Wood specimens in water at high temperature (T=50°C and T=90°C)
- Sequences of compression and/or compression+shear tests (1 mm/min); 40 min per each cycle
- Loading curves identify the less energy demanding case (area under the load curve is the work done)
Suggestions from small experimental tests to real refining process

Principle of time-temperature superposition → same conditions as the refiner

Table 2. The work done in the various cycles, Joule.

<table>
<thead>
<tr>
<th></th>
<th>comp (after comp)</th>
<th>comp (after s&amp;c)</th>
<th>comp (after s&amp;c and comp)</th>
<th>s&amp;c (after comp)</th>
<th>s&amp;c (after s&amp;c and comp)</th>
<th>comp (after comp and s&amp;c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>50°C</td>
<td>0.82</td>
<td>0.48</td>
<td>0.29</td>
<td>0.23</td>
<td>0.30</td>
<td>0.26</td>
</tr>
<tr>
<td>90°C</td>
<td>0.37</td>
<td>0.29</td>
<td>0.16</td>
<td>0.12</td>
<td>0.16</td>
<td>0.14</td>
</tr>
</tbody>
</table>

long, laborious and expensive experiments
µBio - computational tools for IMAGO/Bio

Parametric Script for Abaqus FEM code
(Fortino and Hradil, 2012)

- unit cell with early-transition-latewood zones and optional corners fillets;
- definition of contact between cell walls
- assignement of material properties and material orientations to the layers.

Variant of the hexagonal periodic microcell by Qing and Mishnaevsky (2009)
Microscale modelling - Definition of local coordinate system

**S1, S2, S3: secondary wall** (layers of unidirectional oriented fibrils, different orientations in each layer, varying with earlywood and latewood also)

**P: primary wall** (layer of randomly oriented fibres)

**M: matrix**

**Microfibril angles:**
- S1 layer: MFA=70°-90° to the tracheids axis (Brändström, 2002)
- S2 layer: MFA=30° juvenile earlywood (Bergander, 2001)
- S3 layer: MFA=50°

*Figure from Konnerth et al., 2010*
Microscale modelling – Material properties

Table 1. Chemical properties of the cell wall layers where \( w_i \) from Bergander (2001), \( p \) from Thuvander et al. (2002) and \( V_i \) - evaluated.

<table>
<thead>
<tr>
<th></th>
<th>Cellulose (%)</th>
<th>Hemicellulose (%)</th>
<th>Lignin (%)</th>
<th>Thickness (( \mu \text{m} ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( S_3 )</td>
<td>48</td>
<td>46</td>
<td>36</td>
<td>16</td>
</tr>
<tr>
<td>( S_2 )</td>
<td>50</td>
<td>48</td>
<td>31</td>
<td>19</td>
</tr>
<tr>
<td>( S_1 )</td>
<td>28</td>
<td>26</td>
<td>31</td>
<td>41</td>
</tr>
<tr>
<td>( P )</td>
<td>15</td>
<td>14</td>
<td>33</td>
<td>52</td>
</tr>
<tr>
<td>( M )</td>
<td>0</td>
<td>0</td>
<td>44</td>
<td>56</td>
</tr>
</tbody>
</table>

| \( \rho (\text{kg/m}^3) \) | 1550 | 1500 | 1300 |

Table 2. Elastic properties of hemicellulose, lignin and cellulose as applied to analytical models of wood fibres (Bergander 2001). \( E, G \) and \( v \) are the elastic moduli, the shear moduli and the Poisson’s ratios, respectively.

<table>
<thead>
<tr>
<th></th>
<th>Cellulose</th>
<th>Hemicellulose</th>
<th>Lignin</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E_1 ) (MPa)</td>
<td>134000</td>
<td>2700</td>
<td>2000</td>
</tr>
<tr>
<td>( E_2 ) (MPa)</td>
<td>27200</td>
<td>1300</td>
<td>1000</td>
</tr>
<tr>
<td>( G_{xy} ) (MPa)</td>
<td>4400</td>
<td>1100</td>
<td>760</td>
</tr>
<tr>
<td>( v )</td>
<td>0.1</td>
<td>0.2</td>
<td>0.3</td>
</tr>
</tbody>
</table>

**Properties for dry wood** (according to results by De Magistris and Salmén, this does not affect the results in terms of celle deformation)

**Laminate theory** – analytical methods from literature.

**Orthotropic elastic coefficients** for each layer are calculated by using the rule of mixture combined with a semi-empirical model from (Tsai and Hahn 1980).

<table>
<thead>
<tr>
<th>th</th>
<th>( E_1 ) (MPa)</th>
<th>( E_2 ) (MPa)</th>
<th>( E_3 ) (MPa)</th>
<th>( v_{12} )</th>
<th>( v_{13} )</th>
<th>( v_{23} )</th>
<th>( G_{12} ) (MPa)</th>
<th>( G_{13} ) (MPa)</th>
<th>( G_{23} ) (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>M</td>
<td>0.45</td>
<td>1144</td>
<td>1144</td>
<td>2340</td>
<td>-0.35</td>
<td>-0.63</td>
<td>890</td>
<td>890</td>
<td>890</td>
</tr>
<tr>
<td>P</td>
<td>0.15</td>
<td>10200</td>
<td>1580</td>
<td>10200</td>
<td>0.54</td>
<td>0.26</td>
<td>870</td>
<td>3910</td>
<td>1100</td>
</tr>
<tr>
<td>S1</td>
<td>0.225</td>
<td>2050</td>
<td>2050</td>
<td>41800</td>
<td>0.15</td>
<td>0.022</td>
<td>890</td>
<td>1330</td>
<td>1330</td>
</tr>
<tr>
<td>S2</td>
<td>2.4</td>
<td>3450</td>
<td>3450</td>
<td>70850</td>
<td>0.80</td>
<td>0.035</td>
<td>950</td>
<td>1910</td>
<td>1910</td>
</tr>
<tr>
<td>S3</td>
<td>0.045</td>
<td>3350</td>
<td>3350</td>
<td>68250</td>
<td>0.70</td>
<td>0.034</td>
<td>980</td>
<td>1890</td>
<td>1890</td>
</tr>
</tbody>
</table>
Dynamic analysis for cases of combined compression-shear loads
6 or 9 unit cells, hexagonal cell angle $\theta=30$ deg

Case 1: small shear, Arcan device set up with an angle $\alpha=17^\circ$

Case 2: large shear, $\alpha=35^\circ$

The group of 7 middle sub-cells is found to be representative for the deformation shape during loading

simulation in the elastic range
Simulation of the elastic response

De Magistris and Salmén, 2006
Combined compression and shear
Cell deformation of the first 6 earlywood rows
Simulation vs SEM images

**small shear**

De Magistris and Salmén, 2006

**large shear**

De Magistris and Salmén, 2006

brick-shape (mainly corner deformation), no collapse at 70% deformation

importance of the load direction for energy consuming!
Combined compression and shear

De Magistris and Salmén, 2006

\[ \sigma_y \text{ (TPa)} \]

\[ \mu\text{Bio} \]
Buckling modes under compression

S-shape (cells collapse by buckling of successive radial rows in earlywood, bending of tangential walls in latewood)
Appendix

Understanding of the effect high temperature and moisture content in wood

Hydro-Thermal model (IMAGO)

- Mass Conservation for Dry Air
  \[ \varepsilon \frac{\partial \rho_a}{\partial t} + \nabla \cdot \mathbf{J}_a = 0 \]
  - porosity
  - flux of air (diffusion + convection)
  - density of dry air

- Mass Conservation for Water (bound water, vapour)
  \[ \frac{\partial M}{\partial t} + \varepsilon \frac{\partial \rho_v}{\partial t} + \nabla \cdot (\mathbf{J}_b + \mathbf{J}_v) = 0 \]
  - moisture content
  - density of vapor
  - flux of bound (diffusion)
  - flux of vapor (diffusion + convection)

- Energy Conservation
  \[ q_c \frac{\partial T}{\partial t} = \nabla \cdot (K \nabla T + h_b \mathbf{J}_b + h_v \mathbf{J}_v + h_a \mathbf{J}_a) \]
  - temperature
  - hentalpies
  - heat capacity

Implementation in Uel subroutine/(Abaqus code)

High temperature (100-200 °C) from the lower surface ➔ peak of moisture content into the specimen
On-going and future work for µBio/IMAGO

- **Inelastic model** (plasticity in compression for wood cells) on going.

- Better assessment of **material properties for wet wood** by exploiting the Hydro-Thermal model for wood at high temperature.

- **Scratch tests at VTT** to understand the initial fracture mechanism and define criteria for disintegration of wood cells.

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**Energy saving requires:**
- certain ratios between compression/shear,
- suitable levels of moisture content and strain-rate,
- optimal orientation of woodchips in the refiner,
- .....