PredOxyPack®: How to predict the impact of the cold chain conditions on the oxygen barrier properties

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Pack4Food

INDUSTRY
65 members

RESEARCH INSTITUTES / NETWORK ORGANISATIONS

Filling systems
Food products
Gasses
Packaging materials
Resins

Distribution

Food products
- composition
- pH
- aw

Shelf-life
- chemical
- microbial
- physical
Sustainability

Filliing System
- standard
- clean
- ultraclean
- Hot fill
- Aseptic
- In packaging
- MAP

Packaging material
- barrier
- active
- passive
- closure systems

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Advice

Research

Training

Publications

Networking

www.Pack4Food.be
Activities Pack4Food
Research projects

- Recycling
- Bioplastics
- Intelligent packaging
- Sleeves
- Migration
- MAP O₂-absorbers
- Antimicrobial systems
- Barrier
- Heat resistance

Sustainability
Conscious and demanding
Convenience
Delicious healthy

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Trends in food

- Mild preservative techniques
- Less use of chemical preservatives (e.g. benzoic acid)
- Reduction in fat, sugar and salt

Stability of food?

Importance of packaging
Trends in packaging

• Sustainability
  – Recycled materials
  – Light weight packaging
  – Monolayer packages
  – Waste management
Trends in packaging

- Consumer-on-the-go
- RTE meals
- Snacks
  - Portion packaging
  - Easy-opening
- Heat resistance
- Barrier

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PredOxyPack
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Avoiding $O_2$ remains very important

$O_2$ in spoilage processes:

- **Chemical**: bv. fat oxidation, Vit C degradation, ...

- **Microbial**: bv. growth of spoilage and pathogenic micro-organisms

- **Discoloration reaction**: bv. browning
Avoiding $O_2$ remains very important

Residual $O_2$ must be as low as possible.

Determined by:

- At the moment of packaging
  - Filling concept (vacuum versus flushed)
- During shelf life:
  - Permeability of packaging material
  - The interaction with the food
Permeability of packaging material

Permeability is the combination of sorption and diffusion

P: partial pressure of the permeating component at inner and outer side
Permeability of packaging material

Permeability depends on:

- Polymer type
- Temperature
- Relative humidity
- Nature of the polymer (e.g. crystallinity, orientation, concentration of plasticizer,...)
- Thickness of the polymer
- Difference in partial pressure of gasses
## Permeability of packaging material

<table>
<thead>
<tr>
<th>Polymeer</th>
<th>ml.25µm/m².d.atm</th>
<th>g.25µm/m².d</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>O₂ (min)</td>
<td>O₂ (max)</td>
</tr>
<tr>
<td>LDPE</td>
<td>6.500</td>
<td>8.500</td>
</tr>
<tr>
<td>HDPE</td>
<td>1.600</td>
<td>2.000</td>
</tr>
<tr>
<td>Cast PP</td>
<td>3.500</td>
<td>4.500</td>
</tr>
<tr>
<td>OPP</td>
<td>2.000</td>
<td>2.500</td>
</tr>
<tr>
<td>EVOH</td>
<td>0,5</td>
<td>0,5</td>
</tr>
<tr>
<td>PVdC</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>PA</td>
<td>50</td>
<td>75</td>
</tr>
<tr>
<td>PS</td>
<td>4.500</td>
<td>6.000</td>
</tr>
<tr>
<td>PET</td>
<td>100</td>
<td>150</td>
</tr>
<tr>
<td>Aluminium</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Temperature

• Arrhenius relation between temperature and permeability

\[ P = P_{\text{ref}} \exp \left[ \frac{E_p}{R} \left( \frac{1}{T_{\text{ref}}} - \frac{1}{T} \right) \right] \]

Most technical sheets give permeability at 20°C – 25°C

Important difference if products are stored in refrigerated conditions
Relative humidity

### TABLE 8

Effect of Humidity on Oxygen Permeability

<table>
<thead>
<tr>
<th>Polymer</th>
<th>Dry, at 0% r.h.</th>
<th>At 100% r.h.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polyvinyl alcohol</td>
<td>0.01</td>
<td>25.0</td>
</tr>
<tr>
<td>Uncoated cellulose</td>
<td>0.13</td>
<td>200.0</td>
</tr>
<tr>
<td>Nylon 6</td>
<td>1.0</td>
<td>5.0</td>
</tr>
<tr>
<td>Polyvinylacetate</td>
<td>55.0</td>
<td>150.0</td>
</tr>
<tr>
<td>Acrylonitrile-styrene copolymer</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Polyester</td>
<td>7.0</td>
<td>6.0</td>
</tr>
<tr>
<td>HDPE</td>
<td>110.0</td>
<td>110.0</td>
</tr>
</tbody>
</table>
Nature of the polymer

• Crystallinity

<table>
<thead>
<tr>
<th>Polymer</th>
<th>% Crystallinity</th>
<th>( P_{O_2} ) (cm(^3)/ (mil day 100 in(^2) atm))</th>
</tr>
</thead>
<tbody>
<tr>
<td>LDPE</td>
<td>50</td>
<td>480</td>
</tr>
<tr>
<td>HDPE</td>
<td>80</td>
<td>110</td>
</tr>
<tr>
<td>Nylon 66, quenched</td>
<td>20</td>
<td>8.0</td>
</tr>
<tr>
<td>Nylon 66, annealed</td>
<td>40</td>
<td>1.5</td>
</tr>
</tbody>
</table>

Peeters – Van Bree, IVPV course 2011-2012
Nature of the polymer

• Orientation

<table>
<thead>
<tr>
<th>Polymer</th>
<th>% Elongation</th>
<th>$\text{P}_\text{O}_2$ (cm$^3$/(mil day 100 in$^2$ atm))</th>
</tr>
</thead>
<tbody>
<tr>
<td>PP</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>150</td>
</tr>
<tr>
<td></td>
<td>300</td>
<td>80</td>
</tr>
<tr>
<td>PS</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>420</td>
</tr>
<tr>
<td></td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>PET</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td></td>
<td>500</td>
<td>5</td>
</tr>
<tr>
<td>Styrene–acrylonitrile</td>
<td></td>
<td></td>
</tr>
<tr>
<td>copolymer</td>
<td>0</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>300</td>
<td>0.9</td>
</tr>
</tbody>
</table>

Peeters – Van Bree, IVPV course 2011-2012
Partial pressure and thickness

Sorption Packing material Diffusion Sorption

$P_1$ $P_2$
Permeability of packaging material

Ideal material for MAP applications should have:

– High gas barrier
– High water vapor barrier
– Good mechanical strength
– Transparent (for some products)
– Low cost

Multilayers each with a specific function
Need for an easy-to-use software tool which allows the prediction of oxygen ingress for different packaging configurations, packaging materials and time-temperature profiles.
PredOxyPack

Can be used to...

– support the ‘translation’ of the OTR on the technical sheet
What does it mean exactly for your own packed product in
the specific storage conditions?

– optimize the packaging concept by comparing different
alternatives

– Fast screening on a large amount of packaging materials, by
which the amount of permeability measurements can be
decreased

**BUT it can not replace all permeability measurements!**
PredOxyPack: Input variables

• Packaging configuration

- Bag
- Tray
- Bottle & cap
- Cylinder
- Custom 1
- Custom 2
PredOxyPack: Input variables

Dimensions configuration: choice of units (converter of units build in software)

Food volume should be filled in: headspace volume calculated by software
PredOxyPack: Input variables

• Different components of package

[Diagram showing different geometric shapes with dimensions labeled: W, H, D, H1, H2, H3, D1, D2, W]
**PredOxyPack: Input variables**

- **Packaging material:** mono- and multilayer

<table>
<thead>
<tr>
<th>Component: Body</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Area:</strong> 505.75 cm²</td>
</tr>
</tbody>
</table>

**Material**

<table>
<thead>
<tr>
<th>Material</th>
<th>Permeability</th>
<th>Thickness$_{test}$</th>
<th>T$_{test}$</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>PP</td>
<td>85000</td>
<td>1</td>
<td>23</td>
<td>97.5</td>
</tr>
<tr>
<td>EVOH</td>
<td>12</td>
<td>1</td>
<td>23</td>
<td>5</td>
</tr>
<tr>
<td>PP</td>
<td>85000</td>
<td>1</td>
<td>23</td>
<td>97.5</td>
</tr>
</tbody>
</table>

Contact surface: calculated by software

Adding and removing a layer from a multilayer

Material choice: drop down menu with most common material or custom (unknown)
Material characteristics: (e.g. data on technical sheets)
- permeability: different units are foreseen in software
- Thickness$_{\text{test}}$: Thickness of the tested material
- T$_{\text{test}}$: Temperature at which permeability is determined
- Thickness: Actual thickness of the layer
**PredOxyPack: Input variables**

- **Time – temperature profile**

![Temperature Profile Diagram]

Time and temperature: choice of units

Amount of input steps is unlimited

Start simulation transfer to the output page

Save simulation input
PredOxyPack: input variables
PredOxyPack: output

Oxygen level in the headspace of the package

- Rood: 5 µm EVOH
- Blauw: zonder EVOH

Temperature Profile

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## PredOxyPack: output

### Packaging

<table>
<thead>
<tr>
<th>Geometry</th>
<th>W (width)</th>
<th>L (length)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bag</td>
<td>20 cm</td>
<td>30 cm</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Total Volume</th>
<th>Product Volume</th>
<th>Headspace Volume</th>
<th>Initial O₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>500 cc</td>
<td>400 cc</td>
<td>100 cc</td>
<td>2.4 %</td>
</tr>
</tbody>
</table>

**Component: Bag (1200 cm³)**

<table>
<thead>
<tr>
<th>Material</th>
<th>OTR</th>
<th>Thickness&lt;sub&gt;test&lt;/sub&gt;</th>
<th>Temperature&lt;sub&gt;test&lt;/sub&gt;</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>LDPE</td>
<td>210000 cc/m².day.atm</td>
<td>1 µm</td>
<td>23 °C</td>
<td>32 µm</td>
</tr>
<tr>
<td>LDPE</td>
<td>2100000 cc/m².day.atm</td>
<td>1 µm</td>
<td>23 °C</td>
<td>32 µm</td>
</tr>
</tbody>
</table>

**Temperature Profile**

<table>
<thead>
<tr>
<th>Part 1</th>
<th>Part 2</th>
<th>Part 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>14 days</td>
<td>21 days</td>
<td>5 days</td>
</tr>
<tr>
<td>7 °C</td>
<td>12 °C</td>
<td>21 °C</td>
</tr>
</tbody>
</table>
PredOxyPack: output
PredOxyPack: extra features

• Simulations can be saved and opened again in a next session

• O$_2$ evolution as a function of time can be saved in a CSV-file and imported in e.g. Excel

• A report of the simulations can be generated in pdf
PredOxyPack: user friendly

Important incorporated functions

- Automatic unit conversion
- Programmed configurations (surface and volume calculations)
- Easy ‘help’ function
- Comparison of 6 different series
- Monolayer as well as multilayers
- Permeability database: min, max and default values for OTR
- Graphical output of the results
- Summary of the input variables for each series underneath the graph
- Personal simulation database for the user