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

A. Vermeulen, P. Ragaert, B. De Meulenaer
and F. Devlieghere

PredOxyPack O_2
Predicting Oxygen in Packaging

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INDUSTRY

65 members

RESEARCH INSTITUTES / NETWORK ORGANISATIONS

Filling systems

Food products

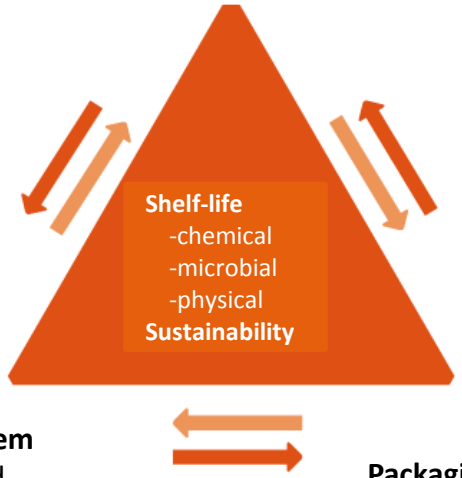
Gasses

Packaging materials

Resins

Distribution

Food products
-composition
-pH
-aw



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

Packaging material
-barrier
-active
-passive
-closure systems

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PredOxyPack O_2
Predicting Oxygen in Packaging

Advice

Research

Training

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Publications

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Advice

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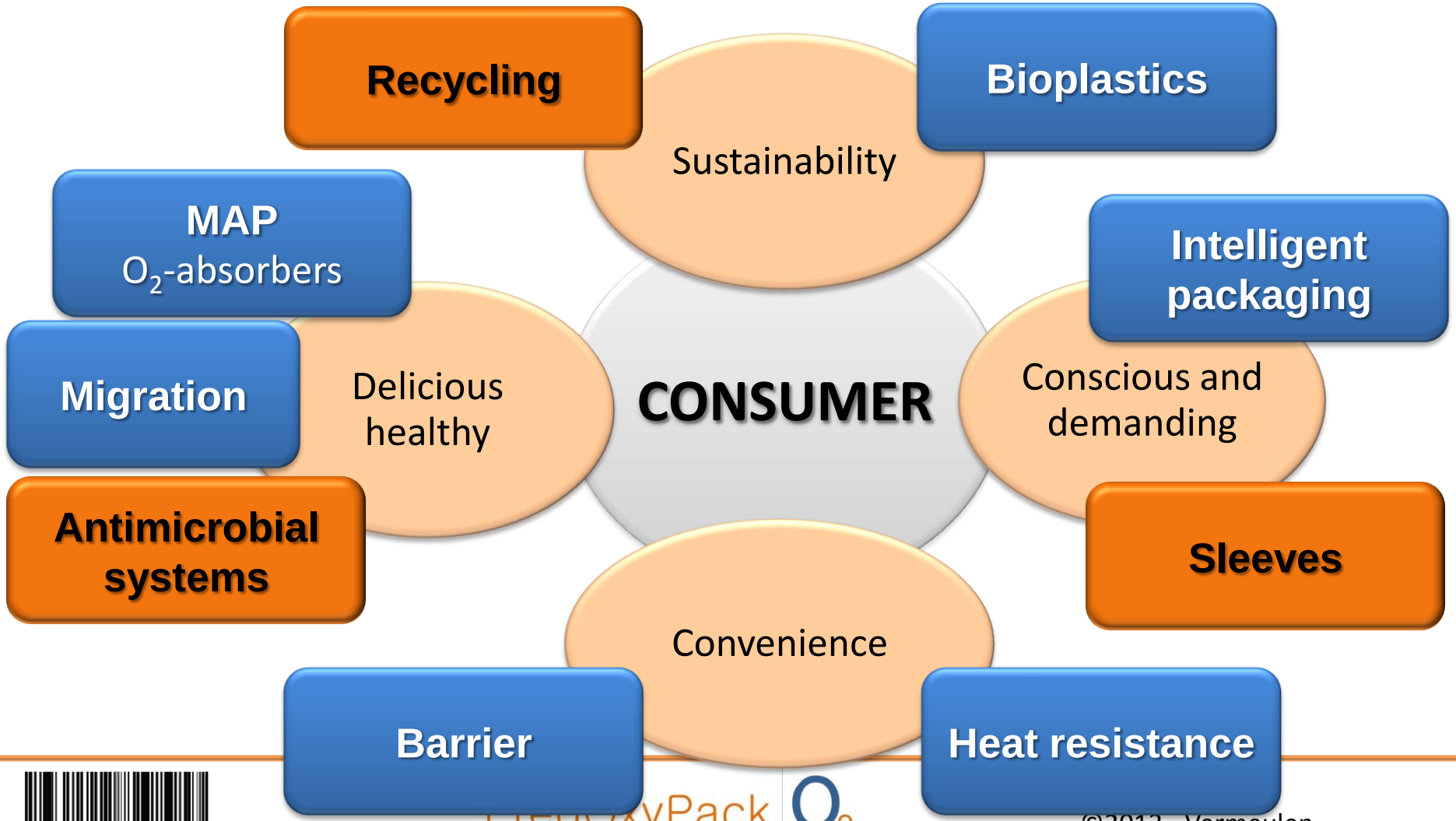
Activities Pack4Food
Research projects



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PredOxyPack O_2
Predicting Oxygen in Packaging

Trends in food

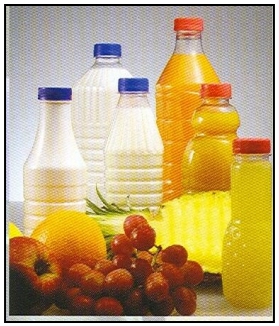
- Mild preservative techniques
- Less use of chemical preservatives (e.g. benzoic acid)
- Reduction in fat, sugar and salt

Stability of food?

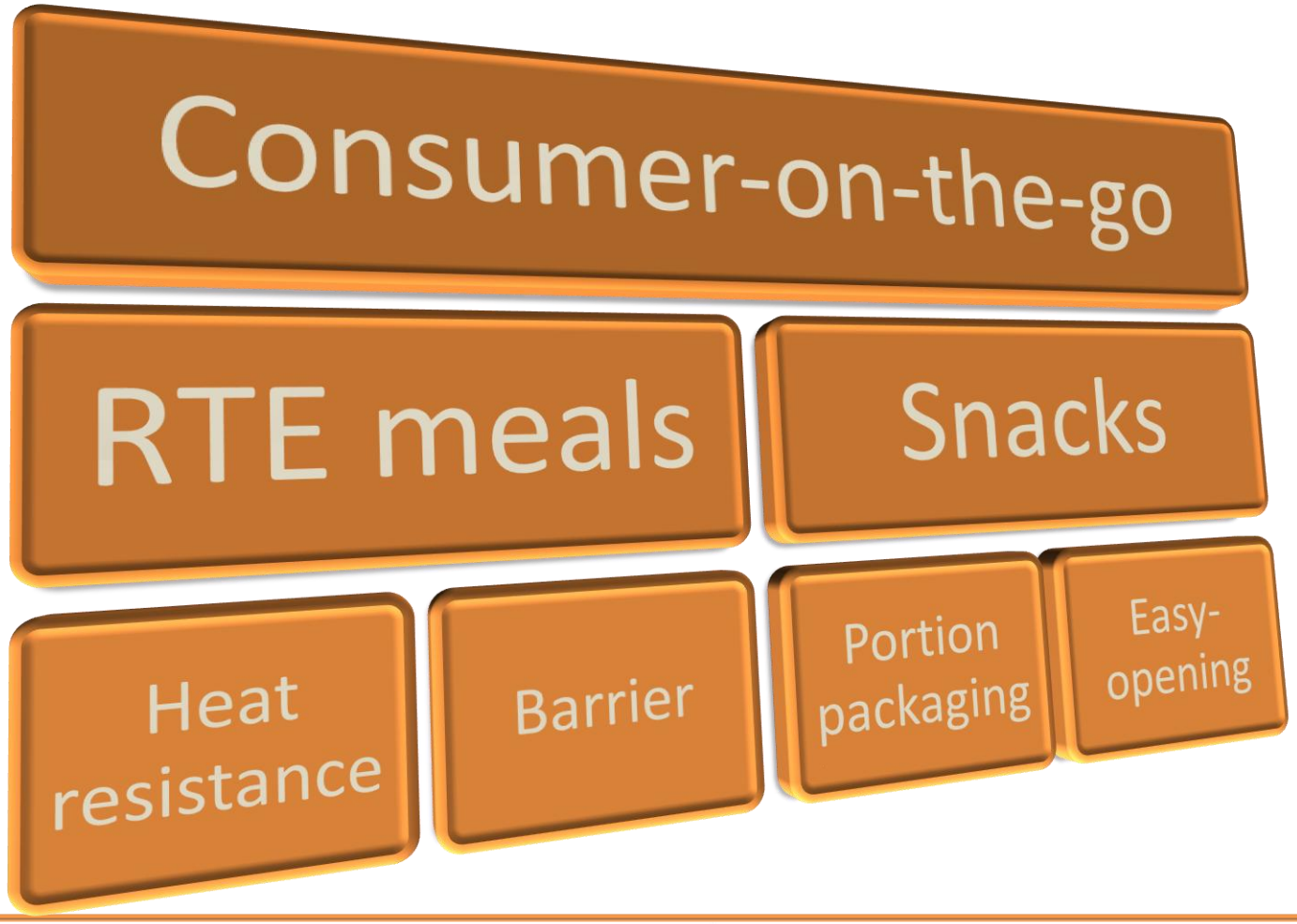
Importance of packaging

Trends in packaging

- Sustainability
  - Recycled materials
  - Light weight packaging
  - Monolayer packages
  - Waste management



Trends in packaging



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-organsims

- Discoloration reaction: bv. browning

Avoiding O_2 remains very important

Residual O_2 must be as low as possible.

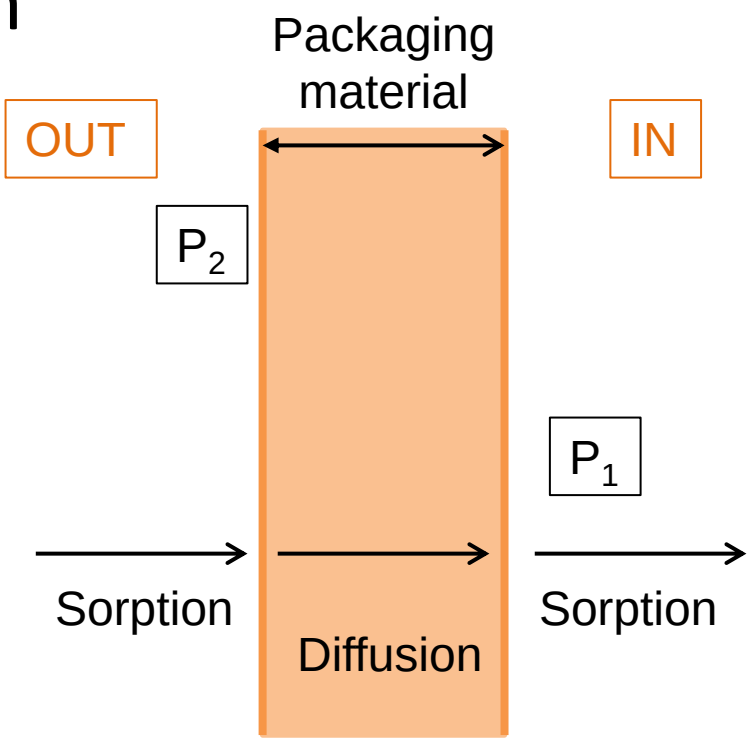
Determined by:

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

Permeability of packaging material

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

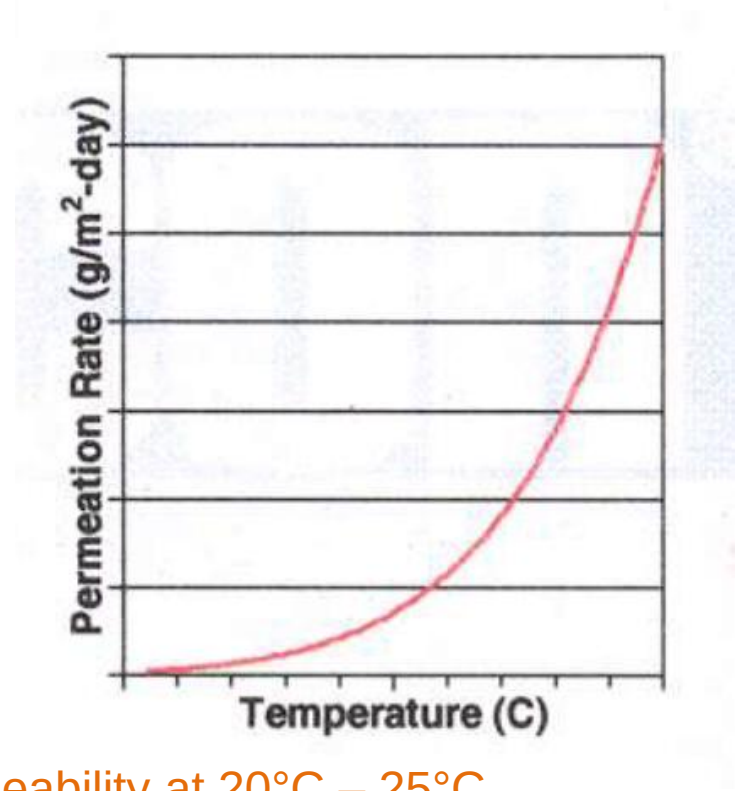
Permeability of packaging material

Polymeer	ml.25µm/m^2.d.atm		g.25µm/m^2.d	
	O_2 (min)	O_2 (max)	H_2O (min)	H_2O (max)
LDPE	6.500	8.500	10	20
HDPE	1.600	2.000	7	10
Cast PP	3.500	4.500	10	12
OPP	2.000	2.500	5	7
EVOH	0,5	0,5	1.000	1.000
PVdC	2	4	0,5	1,0
PA	50	75	300	400
PS	4.500	6.000	70	150
PET	100	150	15	20
Aluminium	0	0	0	0

Temperature

- Arrhenius relation between temperature and permeability

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



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

Polymer	**P** ($cm^3/(mil\ day\ 100\ in^2\ atm)$)	
	Dry, at 0% r.h.	*At 100% r.h.*
Polyvinyl alcohol	0·01	25·0
Uncoated cellulose	0·13	200·0
Nylon 6	1·0	5·0
Polyvinylacetate	55·0	150·0
Acrylonitrile–styrene copolymer	1·0	1·0
Polyester	7·0	6·0
HDPE	110·0	110·0

Peeters – Van Bree, IVPV course 2011-2012

Nature of the polymer

- Crystallinity

Effect of Polymer Crystallinity on Oxygen Permeability

Polymer	*% Crystallinity*	P_{O_2} *(cm³/(mil day 100 in² atm))*
LDPE	50	480
HDPE	80	110
Nylon 66, quenched	20	8·0
Nylon 66, annealed	40	1·5

Peeters – Van Bree, IVPV course 2011-2012

Nature of the polymer

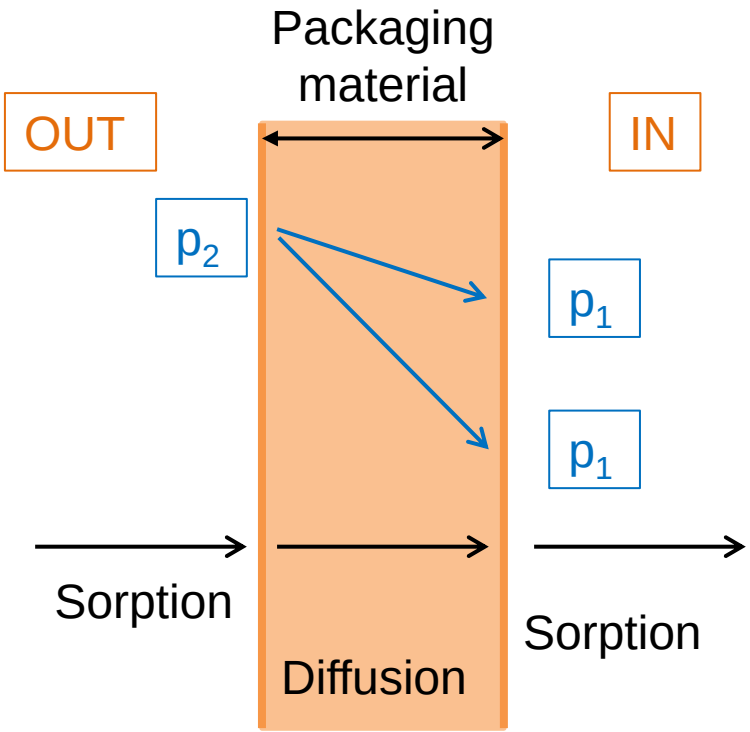
- Orientation

TABLE 5
Effect of Molecular Orientation on Oxygen Permeability

Polymer	*% Elongation*	P_{O_2} ($cm^3/(mil\ day\ 100\ in^2\ atm)$)
PP	0	150
	300	80
PS	0	420
	300	300
PET	0	10
	500	5
Styrene–acrylonitrile copolymer	0	1·0
	300	0·9

Peeters – Van Bree, IVPV course 2011-2012

Partial pressure and thickness



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

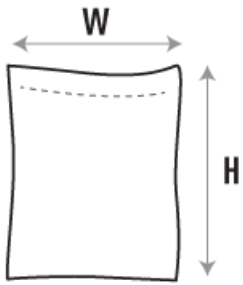
Can be used to…

- 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

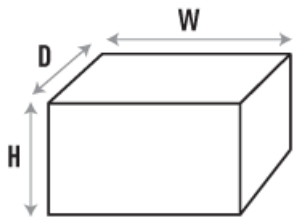
BUT it can not replace all permeability measurements!

PredOxyPack: Input variables

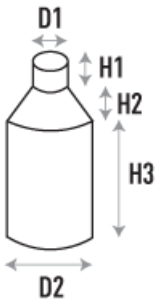
- Packaging configuration



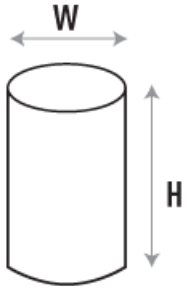
Bag



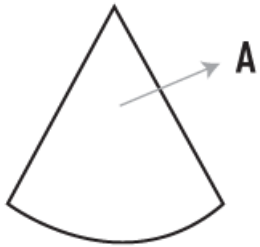
Tray



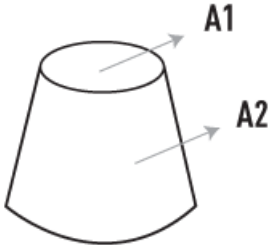
Bottle & cap



Cylinder

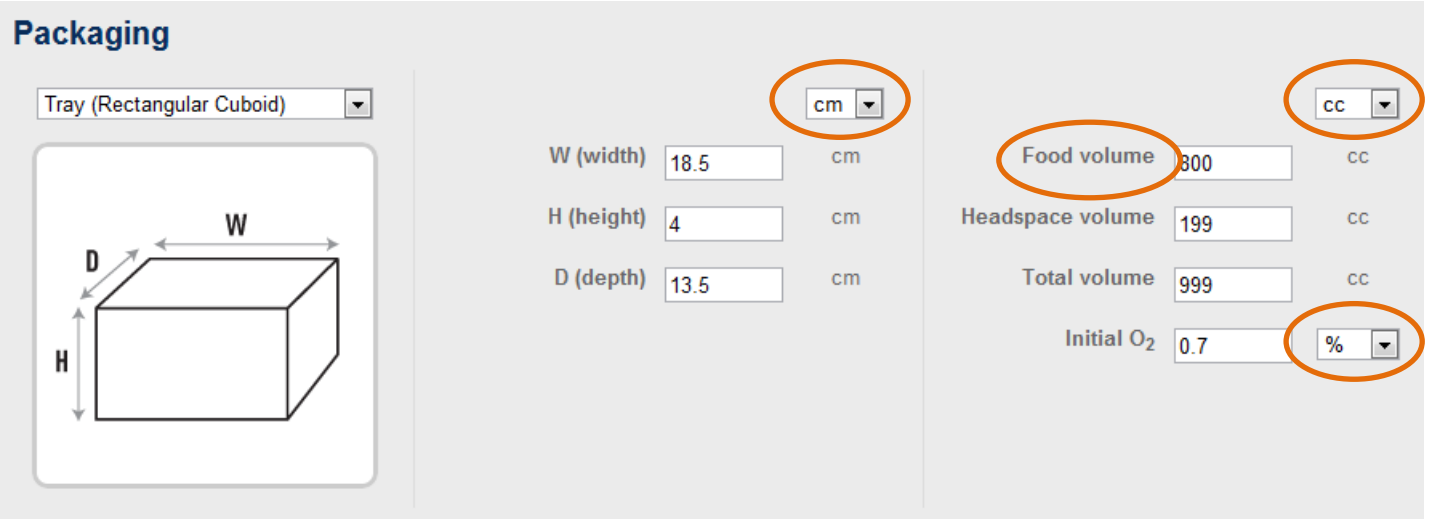


Custom 1



Custom 2

PredOxyPack: Input variables

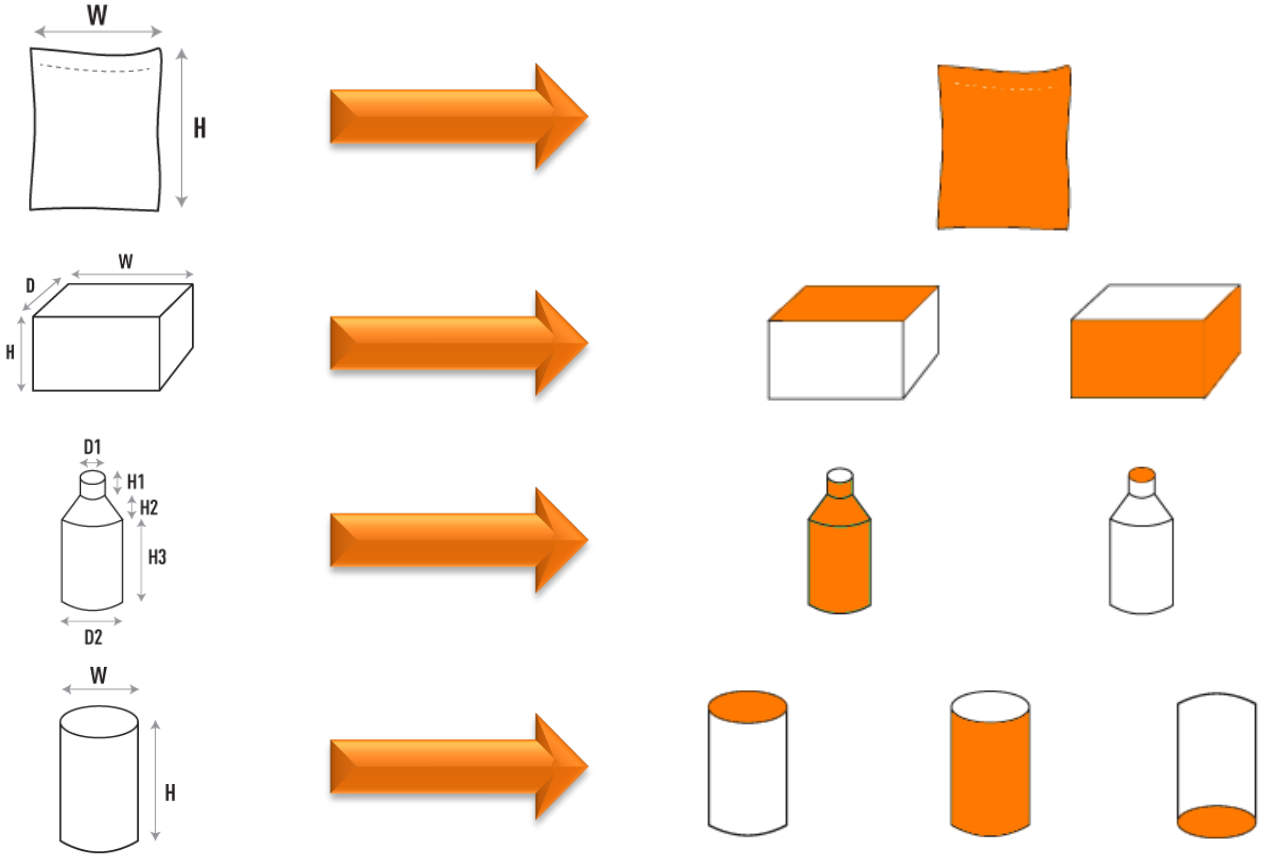


Dimensions configuration: choice of units (converter of units build in software)

Food volume should be filled in: headspace volume calculated by software

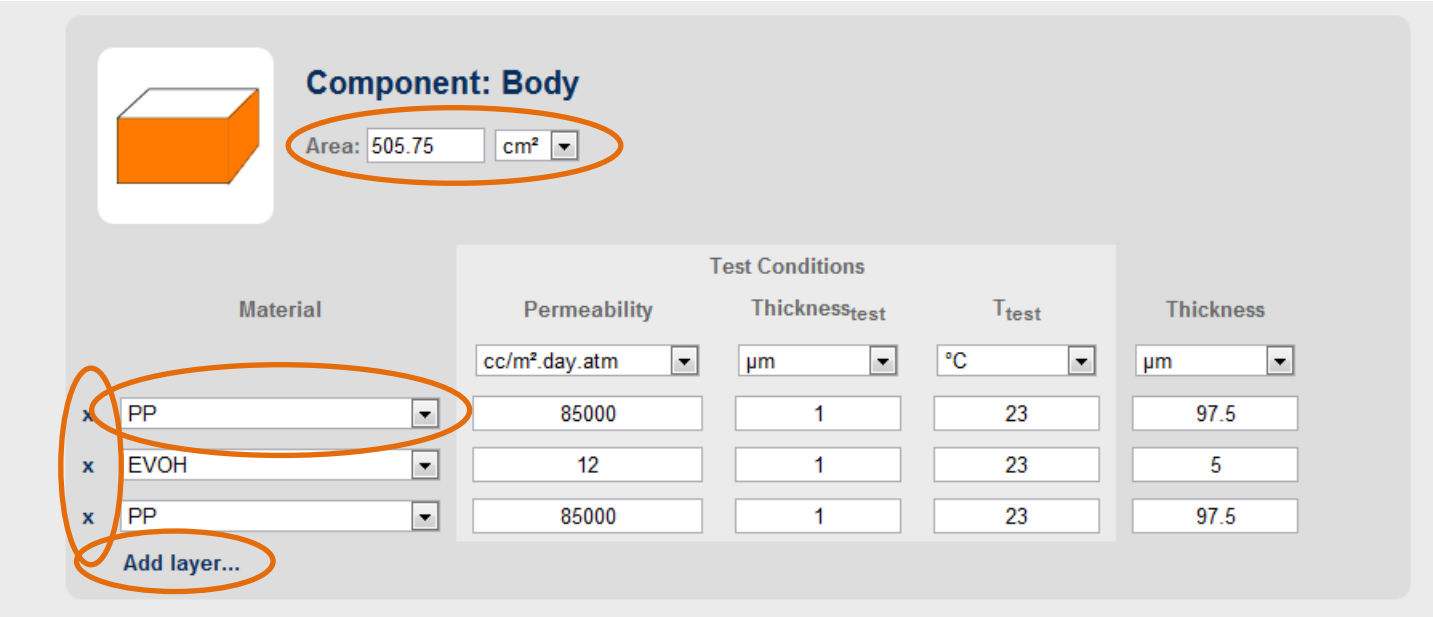
PredOxyPack: Input variables

- Different components of package



PredOxyPack: Input variables

- Packaging material: mono- and mulitlayer

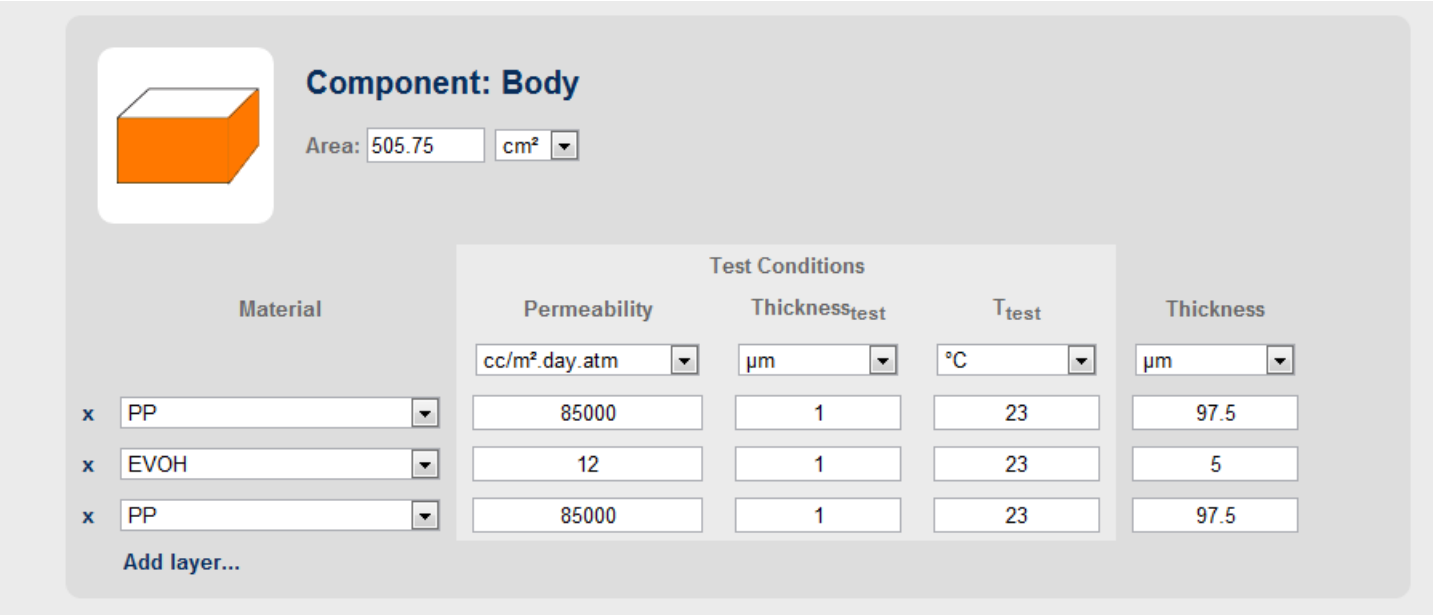


Contact surface: calculated by software

Adding and removing a layer from a multilayer

Material choice: drop down menu with most common material or custom (unknown)

PredOxyPack: Input variables



Component: Body

Area: 505.75 cm²

	Material	Test Conditions: Permeability	Test Conditions: $Thickness_{test}$	Test Conditions: T_{test}	Thickness
		cc/m².day.atm	µm	°C	µm
x	PP	85000	1	23	97.5
x	EVOH	12	1	23	5
x	PP	85000	1	23	97.5

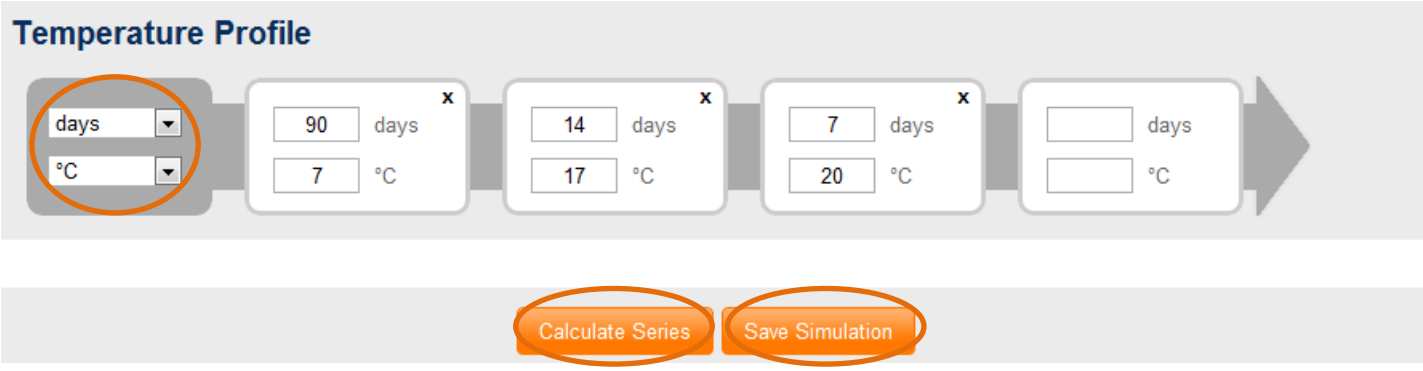
Add layer...

Material characteristics: (e.g. data on technical sheets)

- permeability: different units are foreseen in software
- $Thickness_{test}$: Thickness of the tested material
- T_{test} : Temperature at which permeability is determined
- Thickness: Actual thickness of the layer

PredOxyPack: Input variables

- Time – temperature profile



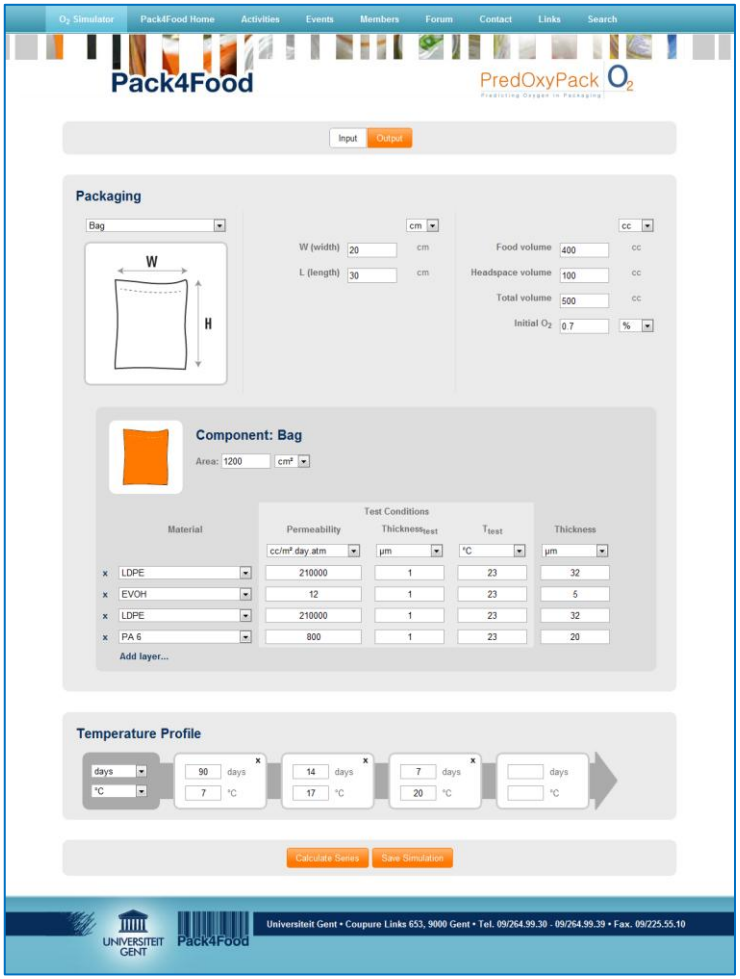
Time and temperature: choice of units

Amount of input steps is unlimited

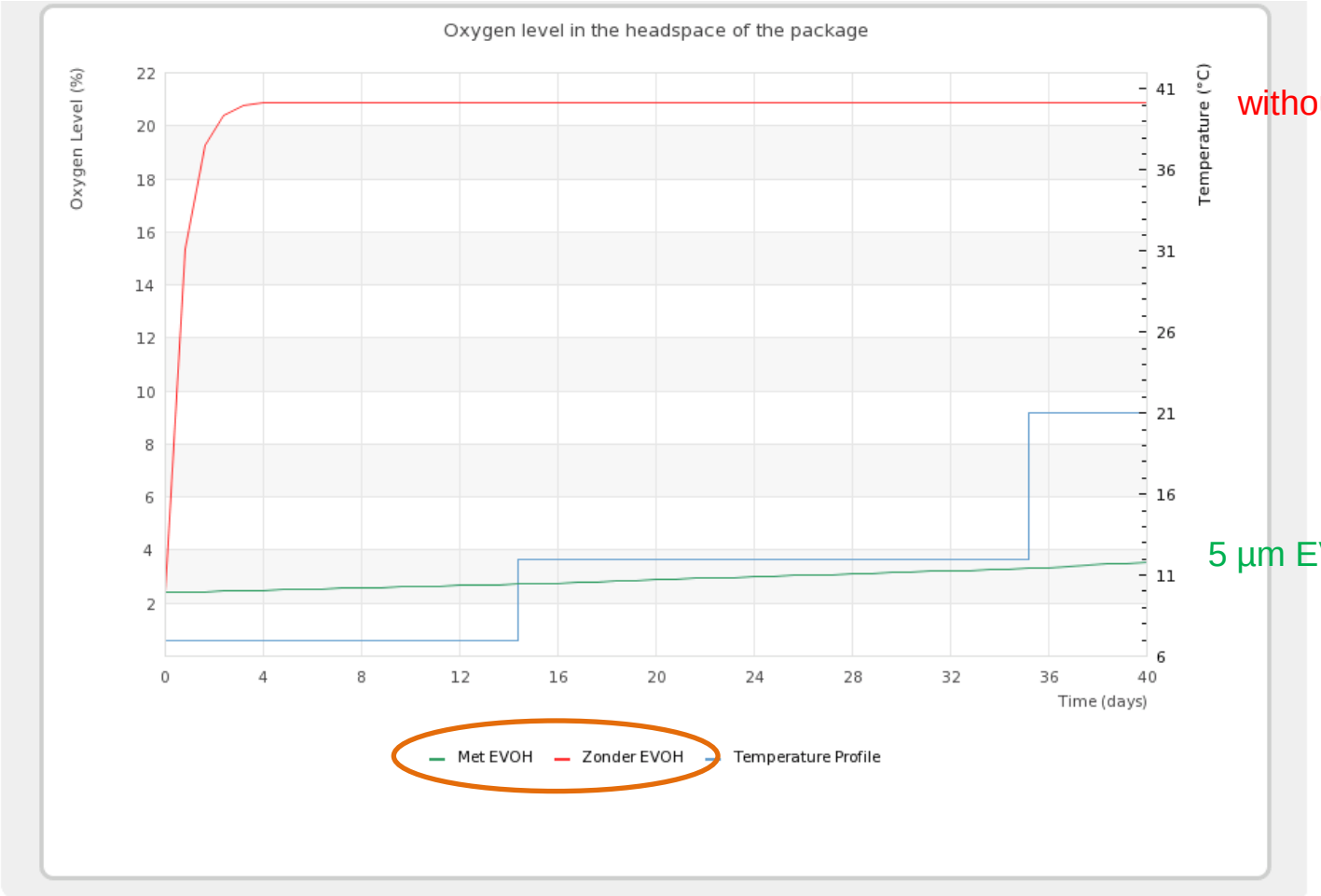
Start simulation transfer to the output page

Save simulation input

PredOxyPack: input variables



PredOxyPack: output



without EVOH

5 µm EVOH

PredOxyPack: output

rename selected series – clear all series

Met EVOH | Zonder EVOH

Packaging

Geometry	W (width)	L (length)
Bag	20 cm	30 cm

Total Volume	Product Volume	Headspace Volume	Initial O_2
500 cc	400 cc	100 cc	2.4 %

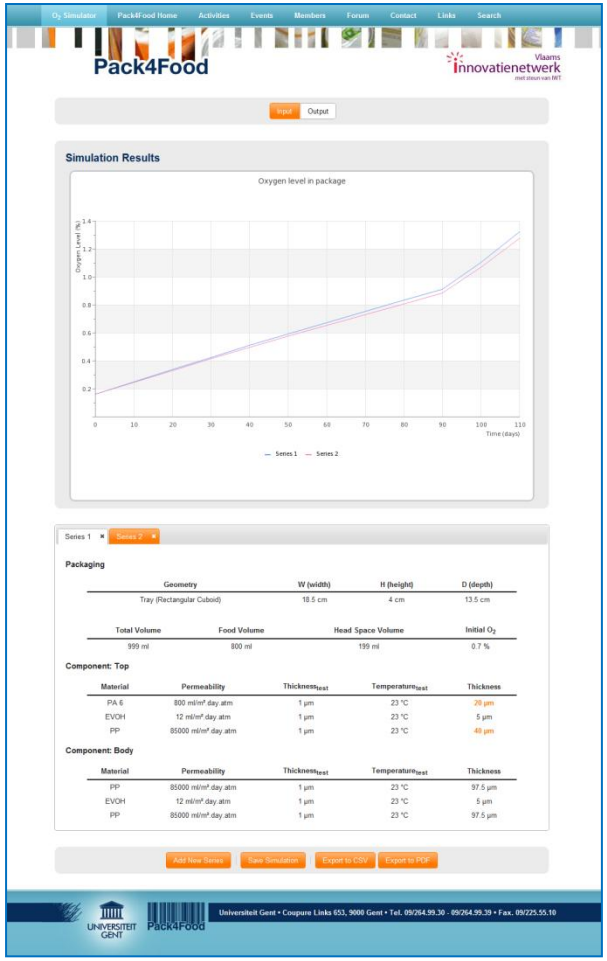
Component: Bag (1200 cm²)

Material	OTR	$Thickness_{test}$	$Temperature_{test}$	Thickness
LDPE	210000 cc/m².day.atm	1 µm	23 °C	32 µm
LDPE	**210000 cc/m².day.atm**	1 µm	23 °C	**32 µm**

Temperature Profile

Part 1	Part 2	Part 3
14 days	21 days	5 days
7 °C	12 °C	21 °C

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

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Pack4Food
Coupure Links 653
9000 Gent

Tel: +32 (0)9 264 99 30
Tel: +32 (0)9 264 99 39
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