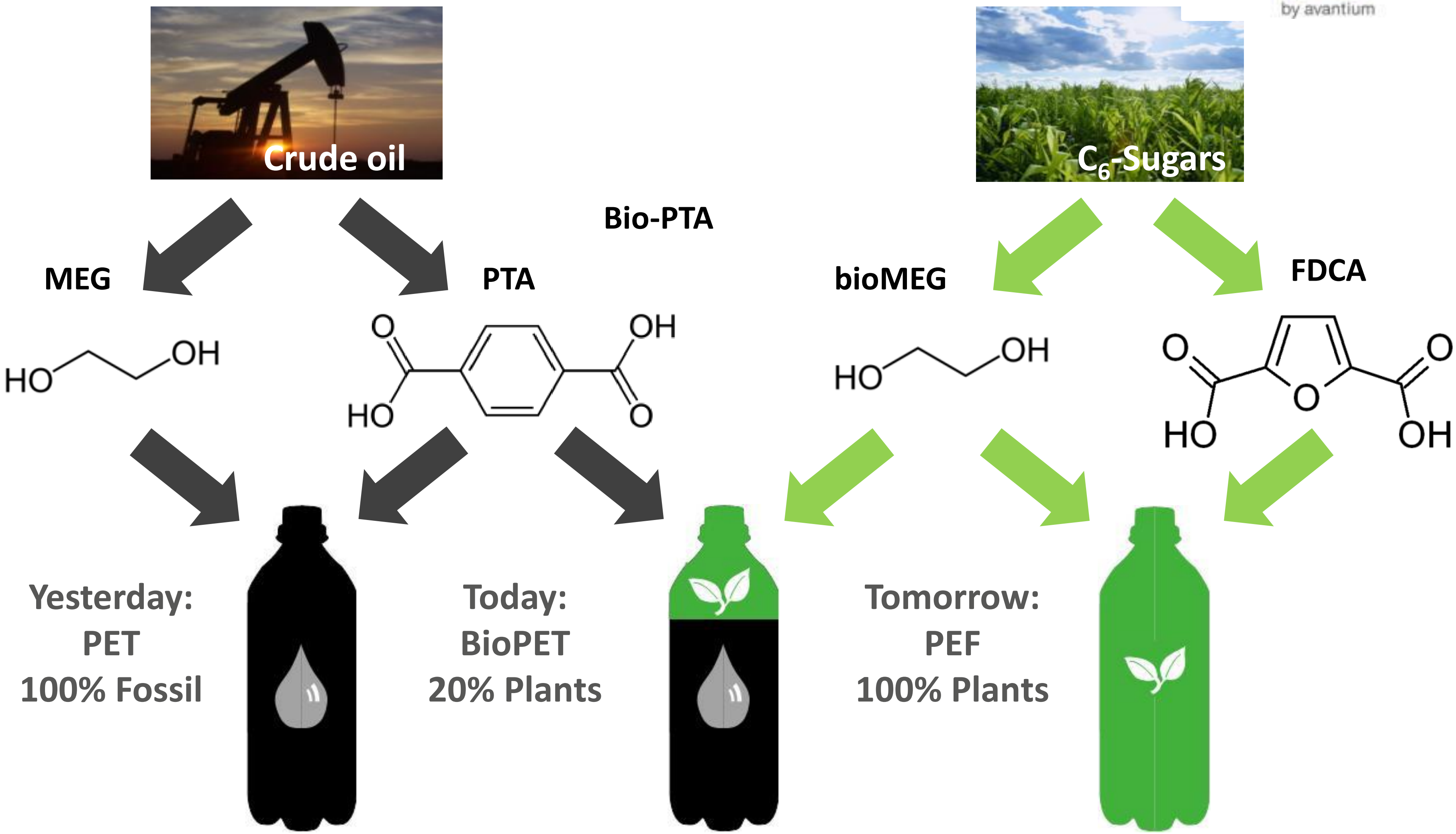
PET: Meeting the demand – The options



Bio-PET or PEF ?

1 on 1 replacement of fossil building blocks by green equivalents

Mid/long term potential has to be cost competitive versus existing oil-based routes:
nothing gained except 'being green'

Introduction of new monomers such as FDCA

Mid/**long** term potential has to be cost competitive
or better processing/ performance versus oil-based alternatives

Select the right target
Elemental Feedstock composition

	Crude oil	carbohydrate (glucose)
C	85-90%	40%
H	10-14%	7%
O	0-1.5%	53%

Oil (C_xH_y) —CATALYST PROCESS→ chemicals ←CATALYST PROCESS— biomass ($C_xH_yO_z$)

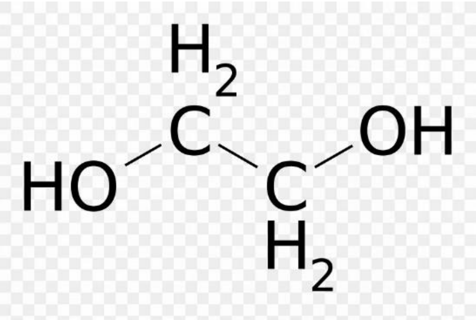
e.g. C_8H_{10} (p-Xylene; 91% C; 9% H)
"under functionalized"

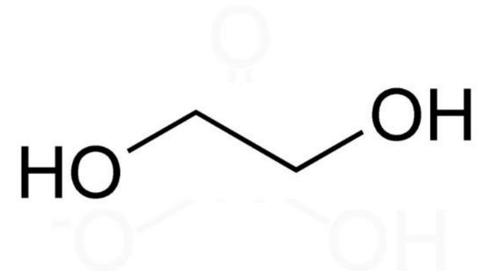
e.g. $C_6H_{12}O_6$ (glucose)
"over functionalized"

Functionalisation
O-introduction

(Depolymerisation &)
defunctionalisation (O-removal)

MEG from glucose





4 steps (= 4 plants !) from glucose to ethylene glycol

$$(C_6H_{10}O_5)_x \xrightarrow[+\ xH_2O]{\text{enzymes}} C_6H_{12}O_6 \xrightarrow{\text{enzymes}} 2CH_3CH_2OH + 2CO_2$$

Starch — Glucose — Ethanol

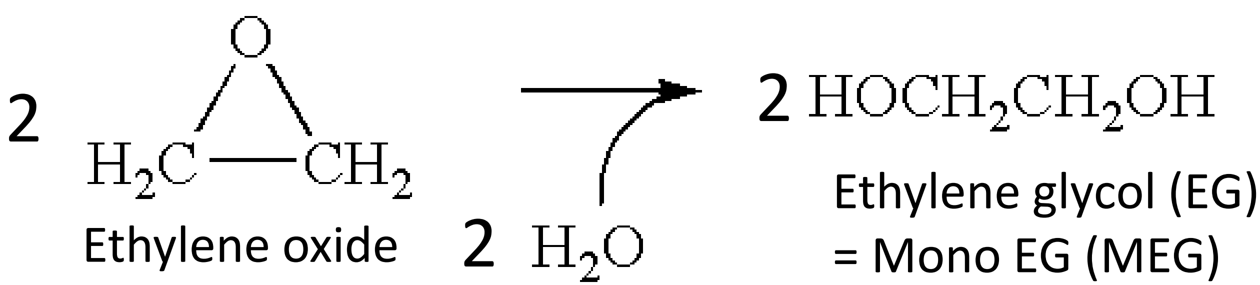
4 steps (= 4 factories !) from glucose to ethylene glycol

$$(C_6H_{10}O_5)_x \xrightarrow[+\,xH_2O]{\text{enzymes}} C_6H_{12}O_6 \xrightarrow{\text{enzymes}} 2CH_3CH_2OH + 2CO_2$$

Starch — Glucose — Ethanol

$$2\,CH_3CH_2OH \xrightarrow{-\,2\,H_2O} 2\,CH_2{=}CH_2 \longrightarrow$$

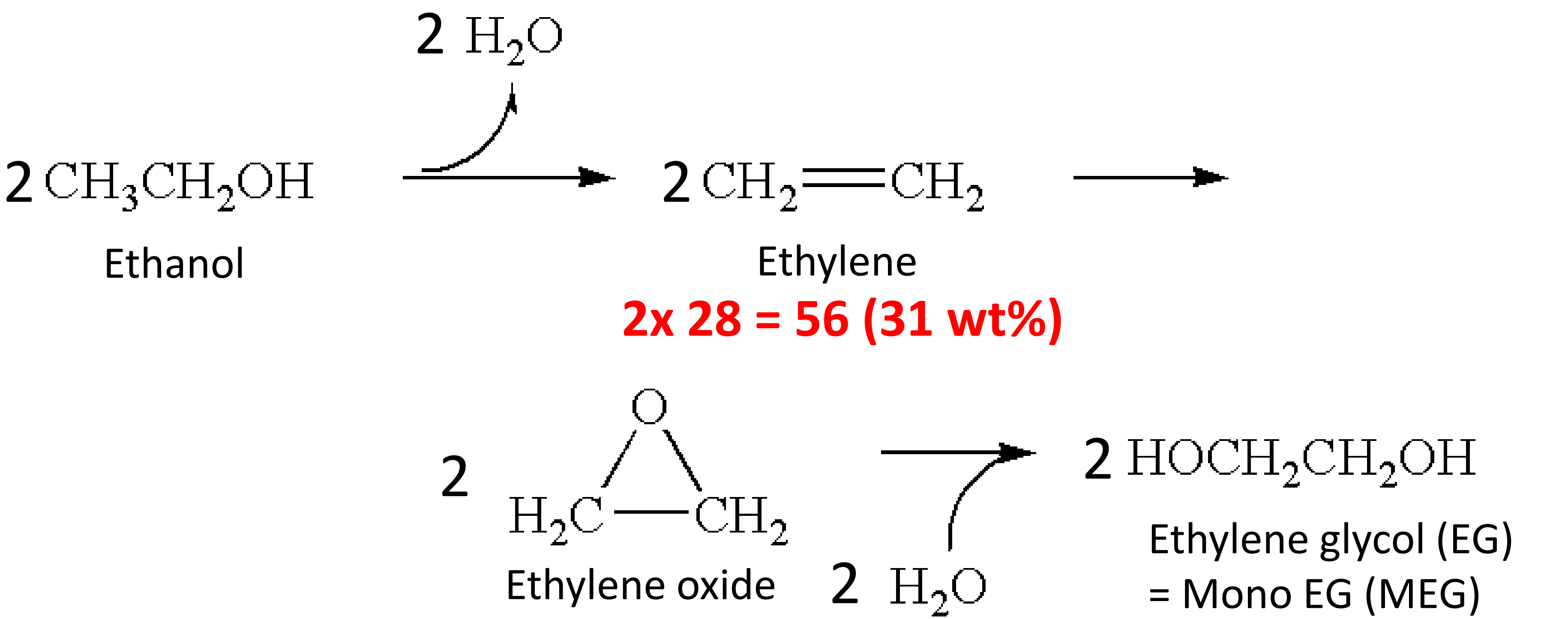
Ethanol — Ethylene



4 steps (= 4 plants !) from glucose to ethylene glycol

$$(C_6H_{10}O_5)_x \xrightarrow[+\,xH_2O]{\text{enzymes}} C_6H_{12}O_6 \xrightarrow{\text{enzymes}} 2CH_3CH_2OH + 2CO_2$$

Starch	Glucose	Ethanol	CO_2
$(162)_x$	**180**	**2x 46 = 92 (51 wt%)**	**2x 44 = 88**



2x 28 = 56 (31 wt%)

2x 44 = 88 (49 wt%)

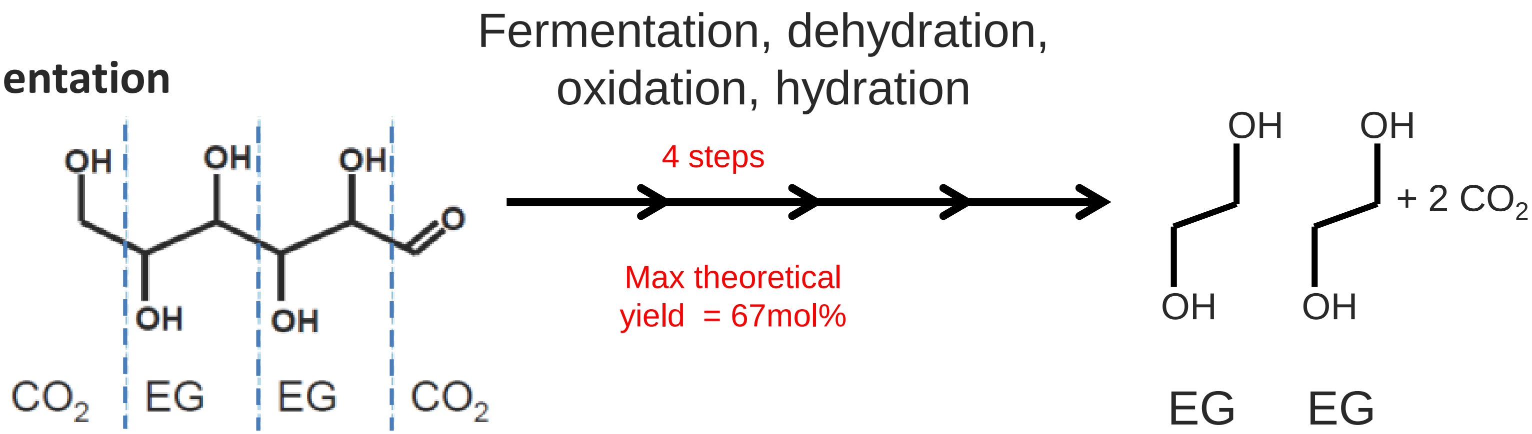
2x 62 = 124 (69 wt%)

RAY technology: Superior Carbon Efficiency

Superior economics

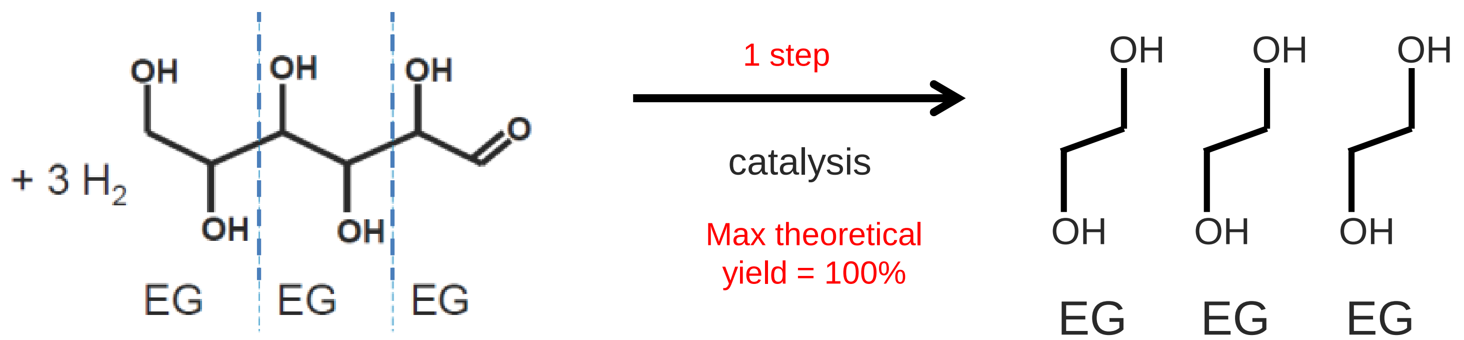
Current commercial production of bio-based MEG

Fermentation



Avantium RAY process

Hydrogenolysis



Back of the envelope – best case atom efficiency

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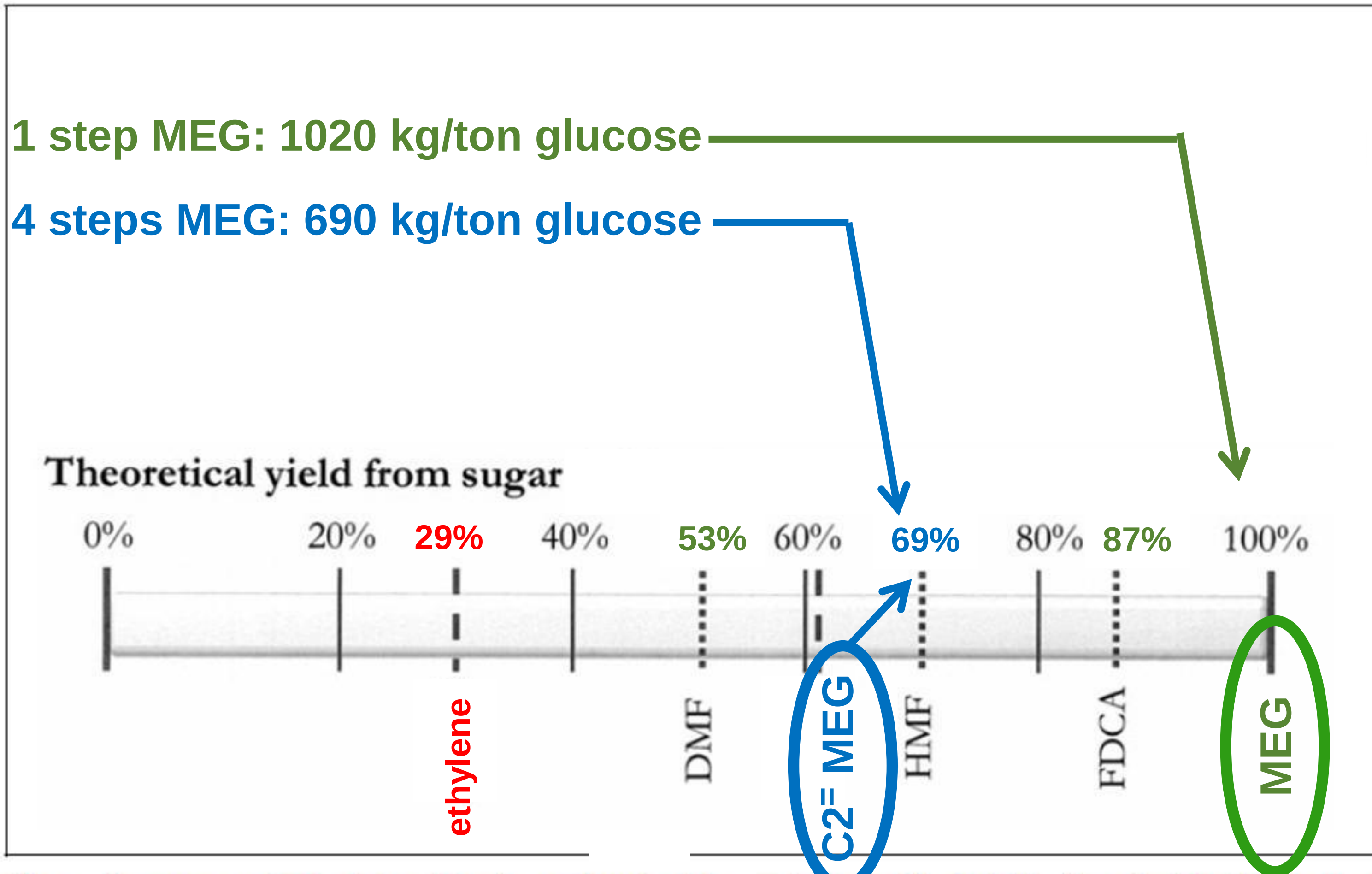


Fig. 3. Oxygen content of feedstocks and materials, and theoretical yield of materials from sugar

pX = p-xylene; C2 = ethylene

Very basic "back of the envelope" economics glucose → chemicals intermediate scale process (100kt/y) new technology

avantium

- Count # chemical conversion steps: €100/step + €100 per purification/ solvent swap (€50 in case of mature technology step) (*)
- Estimate realistic yield Y in commercial process
- Evaluate mass loss per mol of product
- Assume €350/ton for feedstock (long term large scale contracts)
- Calculate feedstock required per ton final product:

  100/Y x 180/ MW P

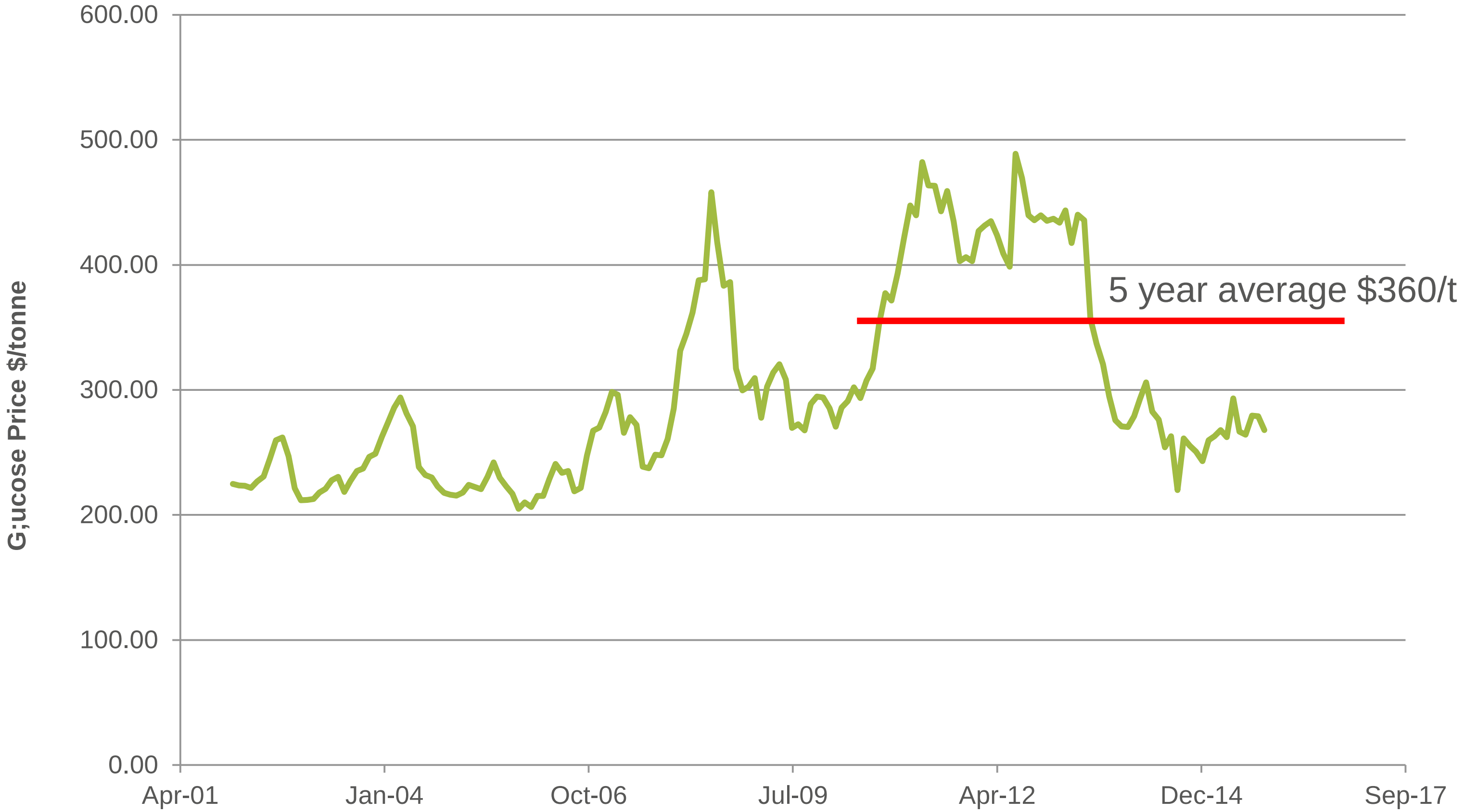
4 step ethylene glycol with all steps Y = 95% after purification:
Feedstock required per ton MEG: 100/81 x 180/124 = 1.79 ton
Production cost: 1.79 x €350 + €250*** + €250*** = €527 + €600 = **€1127 / ton**

Ethylene: 2 steps with Y = 90%
Feedstock required per ton ethylene: 100/90 x 180/56 = 3.57 ton
Production cost: 3.57 x €350 + €150* + €150* = €1250 + €300 = **€1550 / ton**

RAY™ 1 step ethylene glycol with Y = 70% after purification:
100/70 x 180/186 = 1.38 ton
Production cost: 1.38 x €350 + €100 + €100 = **€683 / ton + side product credits**

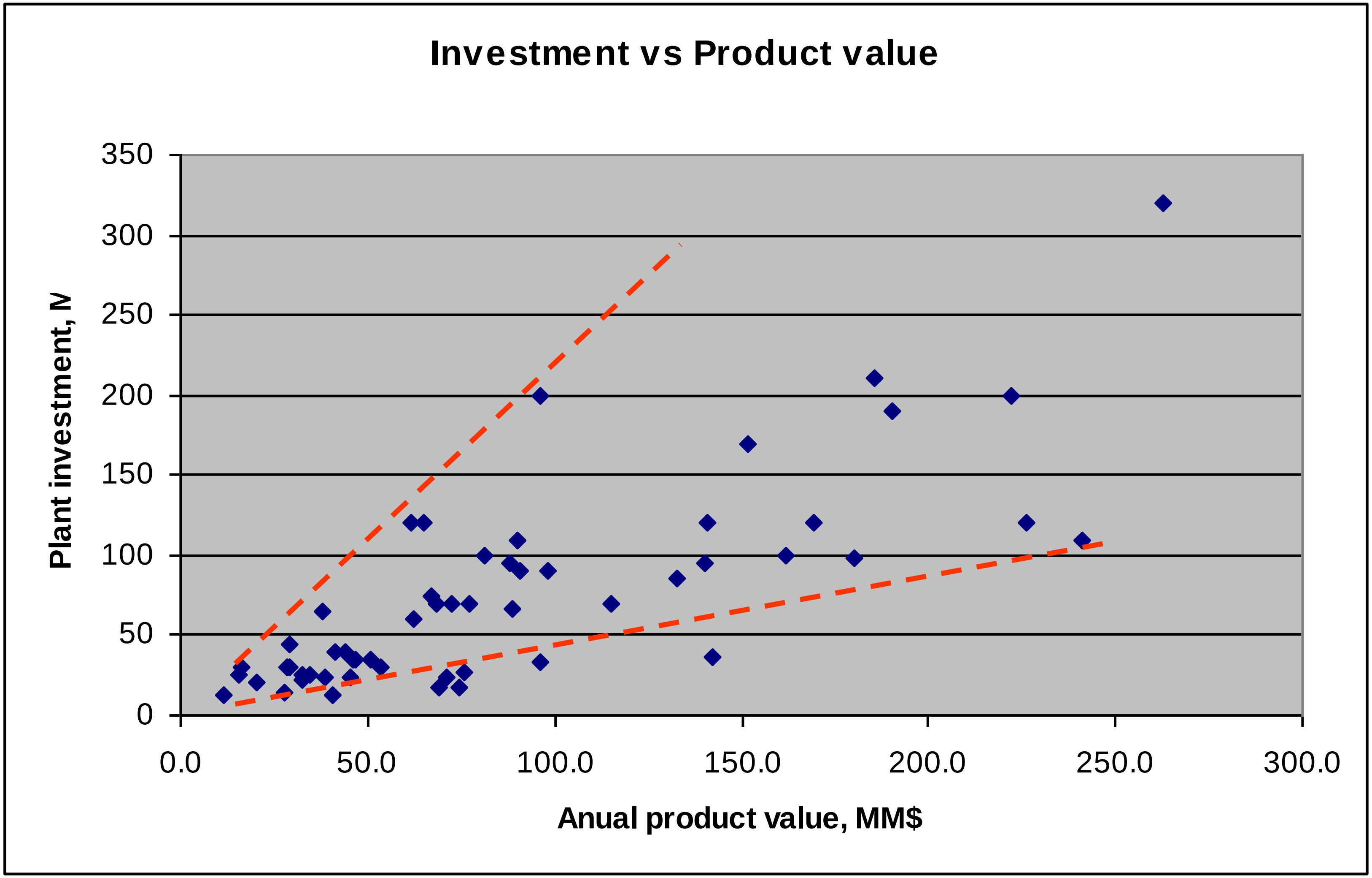
Glucose (from corn)

Glucose Price Estimate (Commercial US)



Prices were calculated using historical data for corn & co-products, typical yields for dextrose and co-products and a processing fee that could reasonably be negotiated by a large dextrose consumer.

Historical CAPEX versus annual product value

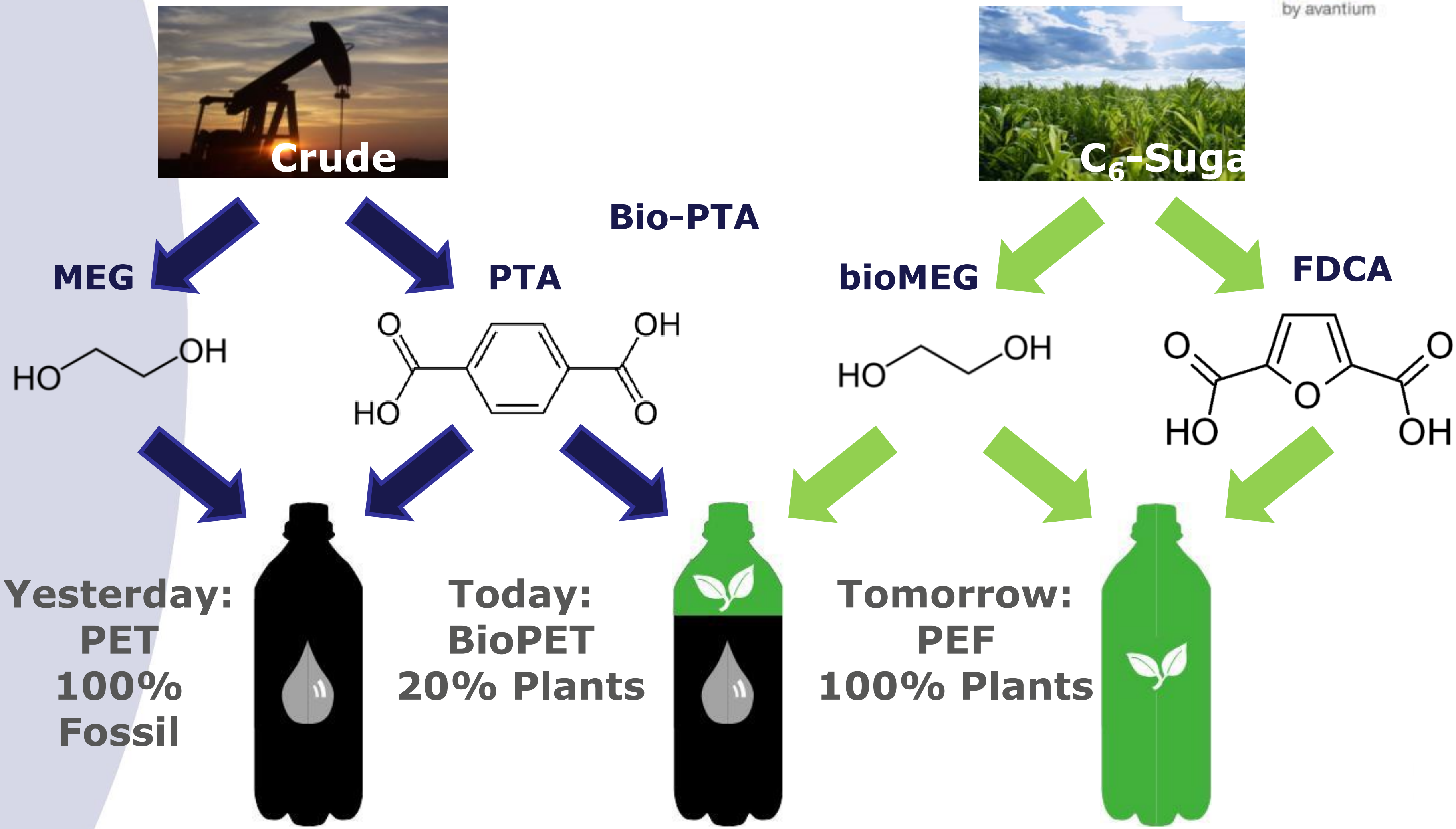


Source: F Dautzenberg (Serenix)

More detailed first pass techno-economics (Feasibility phase) – phys prop & factor model

	A	B	C	D	E	F	G	H	I	J	K	L	M
15						Consumption				Annual Cost		Unit Cost	
16				Cost/Unit		Factor				M$		$/T	%
17	**Raw Materials**												
18		Ethylbenzene		$410.00	$/MT	1.05	T/MT			$215,250		$430.50	
19													
20													
21									**Total Raw Materials**	**$215,250**		**$430.50**	72.2
22													
23	**Catalysts and Chemicals**												
24		Dehydr.cat		14500	$/cuM	0.00014	cuM/MT			1015		$2.03	
25		NSI Inhibitor		6.30	$/kg	0.44	kg/MT			1386		$2.77	
26		TBC Inhibitor		9.50	$/kg	0.02	kg/MT			95		$0.19	
27													
28									**Total Catalysts and Chemicals**	**$2,496**		**$4.99**	0.8
29													
30	**Utilities**												
31		Electricity		0.045	$/KWH	26.0	kWh/MT			585		$1.17	
32		Fuel		2.50	$/MMBTU	0.32	MMBTU/MT			400		$0.80	
33		Boiler feed water		1.60	$/Mgal	0.00	Mgal/MT			0		$0.00	
34		Cooling water		0.08	$/Mgal	24.57	Mgal/MT			983		$1.97	
35		HP Steam		4.40	$/Mlb	1.65	Mlb/MT			3630		$7.26	
36		MP Steam		4.20	$/Mlb	0.24	Mlb/MT			504		$1.01	
37		LP Steam		3.60	$/Mlb	5.05	Mlb/MT			9090		$18.18	
38													
39									**Total Utilities**	**$15,192**		**$30.38**	5.1
40													
41													
42	**Fixed Costs**												
43						Basis							
44		Operators		12			210	M$/YR		2520		$5.04	
45		Supervision		1	shift positions, each &		255	M$/YR		255		$0.51	
46		Maintenance		5	% ISBL +	3	% OSBL			7840		$15.68	
47		Plant Overhead		80	% operating labor +		20	% maint.		3788		$7.58	
48		Taxes & Insurance		2	% of fixed capital					3360		$6.72	
49									**Total Fixed costs**	**$17,763**		**$35.53**	6.0
50													
51									**OPERATING COSTS**	**$250,701**		**$501.40**	84.1
52													

PET: Meeting the demand – The options



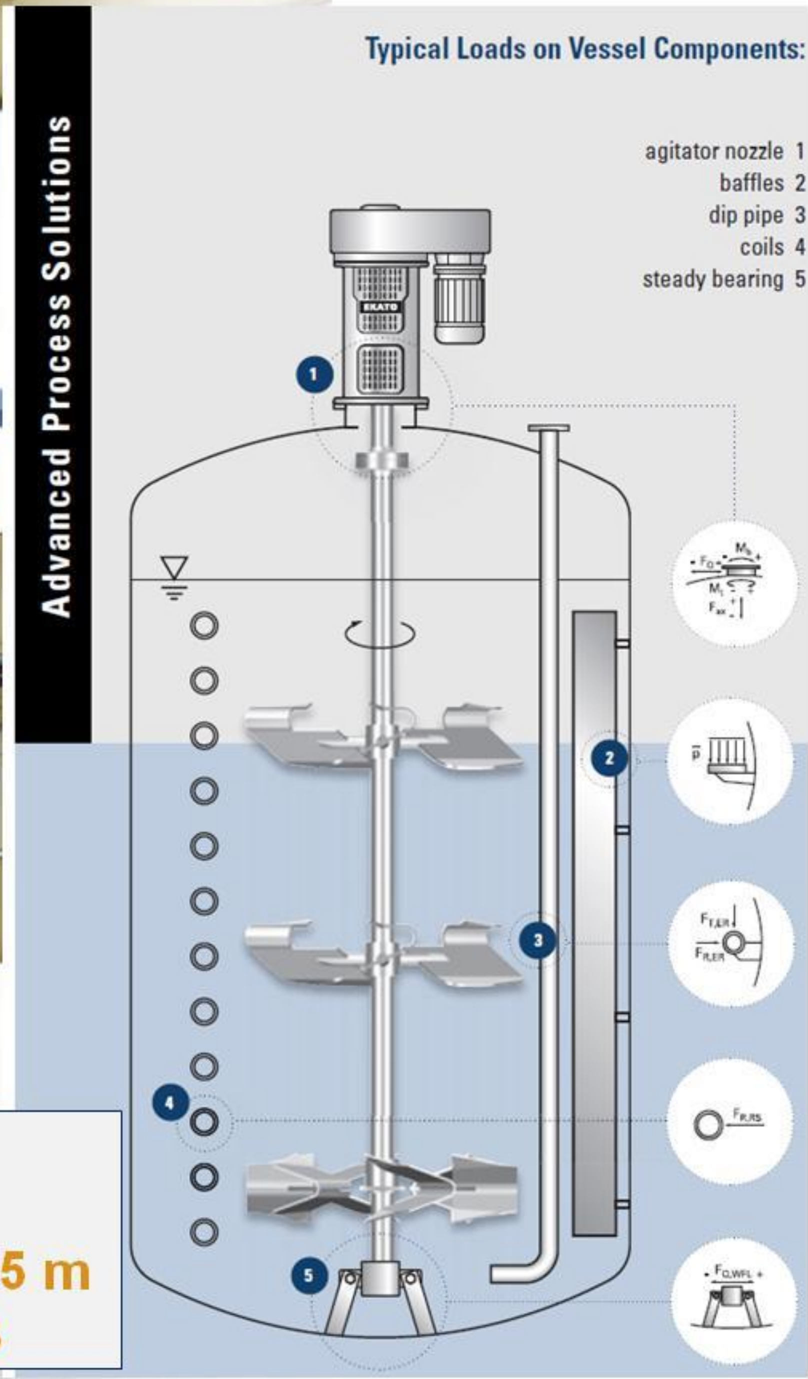
The stage: Some numbers
Terephthalic acid (TA): a commodity chemical

- Capacity in 2018: 65 Mt (6% growth per year)
- TA market value: €80 Billion

- In China, 1500 m^3 CSTR's are constructed with 1.5 million ton capacity.

2013
3MW
agitator

h = 20 m
d = 10 m
d(shaft) = 0.5 m
V = 1500 m3



Ekato slurry tank shaft with 20m length and 0.7m diameter

1. bio-based paraxylene

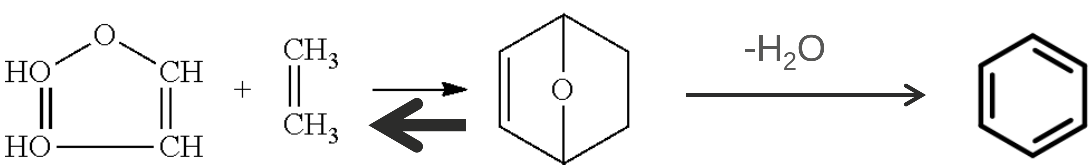
- Virent Inc. (Madison, WI). Aqueous phase reforming Hydrodeoxygenation of C5/C6 sugars to BTX. Theoretical hydrocarbon weight yield is 38%
- **Gevo Inc. (Englewood, CO)**
- Anellotech Inc. (Pearl River, NY)
- U of North Carolina at Chapel Hill (UNC)
- Origin Techn. (formerly Micromidas; West Sacramento, CA)
- **Avantium (Amsterdam) and The Coca-Cola Company (Atlanta, GA)**

Diels-Alder chemistry

- The reaction is an equilibrium

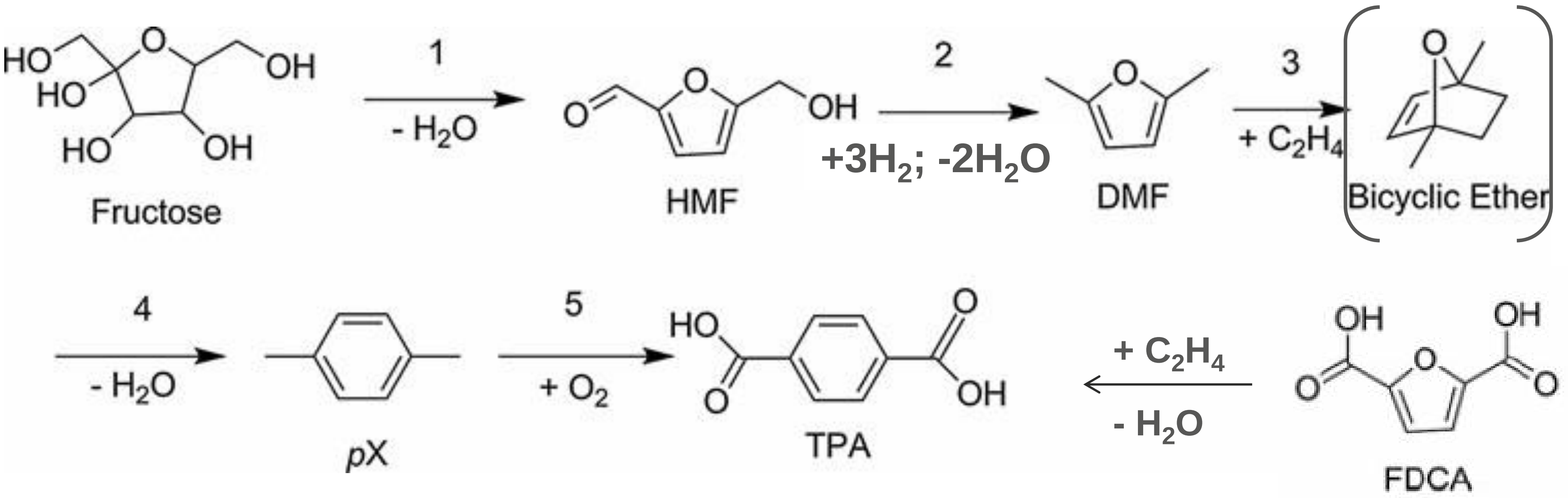
- Electron donating groups on diene
- Electron withdrawing groups on olefin

- The reverse reaction is called retro-Diels-Alder (rDA)
- The driving force for the DA is the enthalpy gain by forming σ-bonds
  – Low temperatures favor the DA
- The driving force for the rDA is the entropy gain from 1 to 2 molecules
  – Higher temperatures favor the rDA



- Ethylene unreactive at low p
- High T needed for dehydration
- Unsubstituted furan gives polymers

Avantium & Coca-Cola.
Diels Alder of furans with ethylene
1.5 C6 sugar needed per TPA at 100% yield



- WO2014/065657 (prio 10/2012)
- To PX: 88% yield of p-xylene (1 step for **3**&**4** !!);
- To PTA: 17% yield in 1 step from FDCA (>90% selective);
- Main challenge: best results obtained after 24 hrs at 200ºC

Back of the envelope – best case atom efficiency

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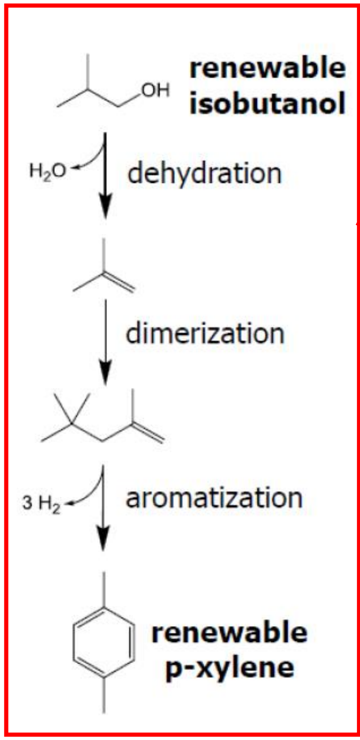

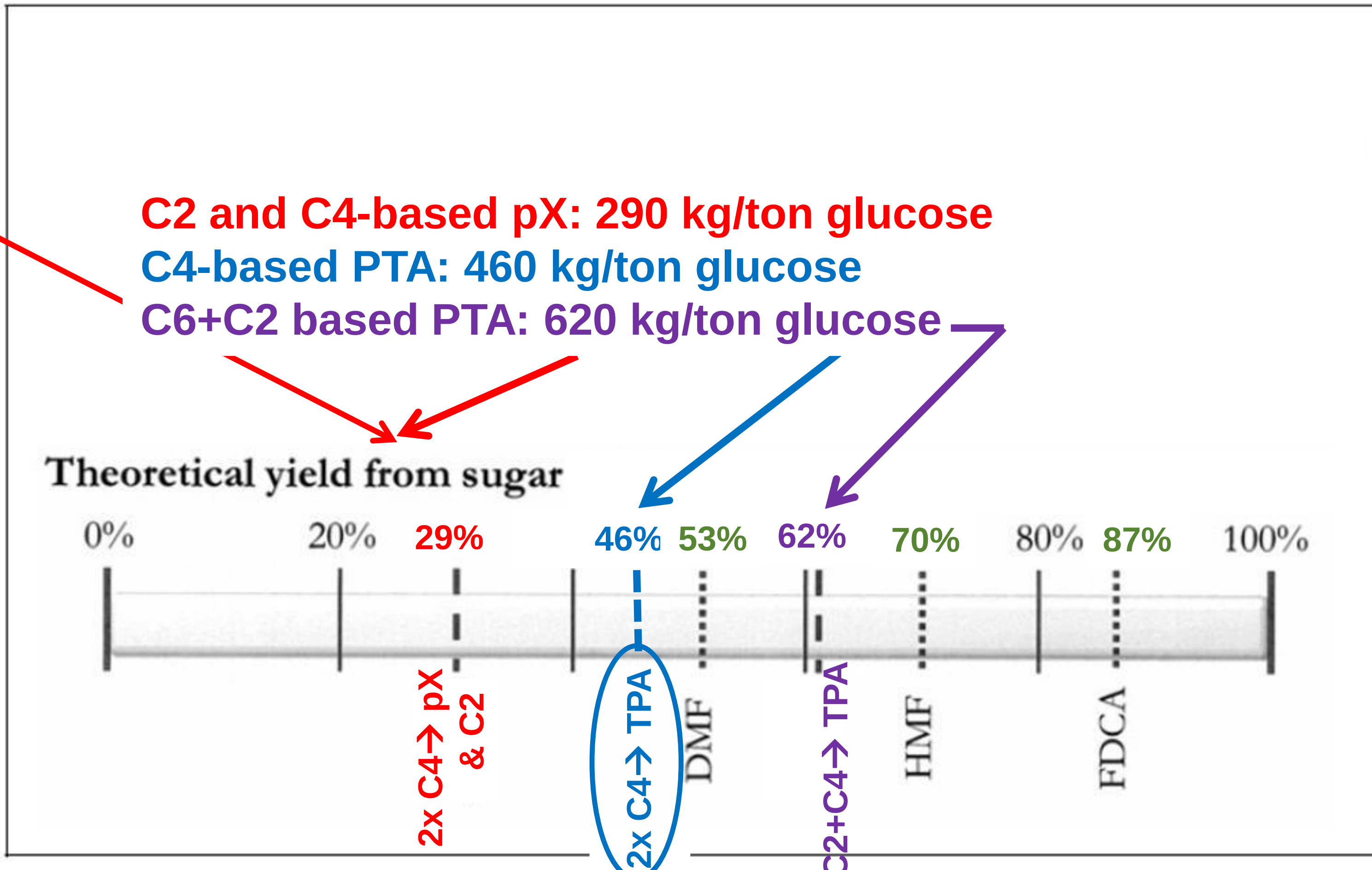

Fig. 3. Oxygen content of feedstocks and materials, and theoretical yield of materials from sugar

pX = p-xylene; C2 = ethylene

Back of the envelope – best case atom efficiency

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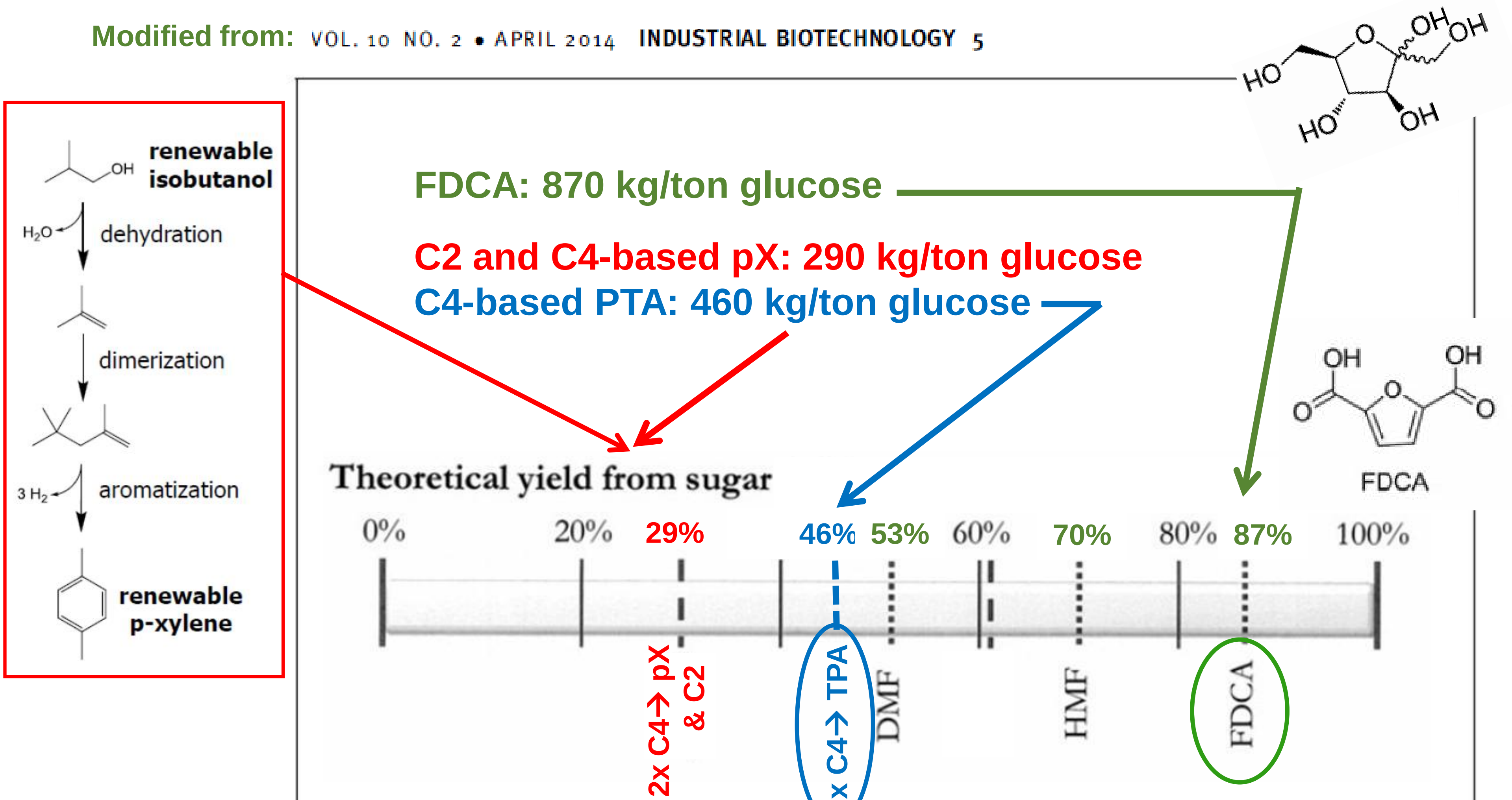
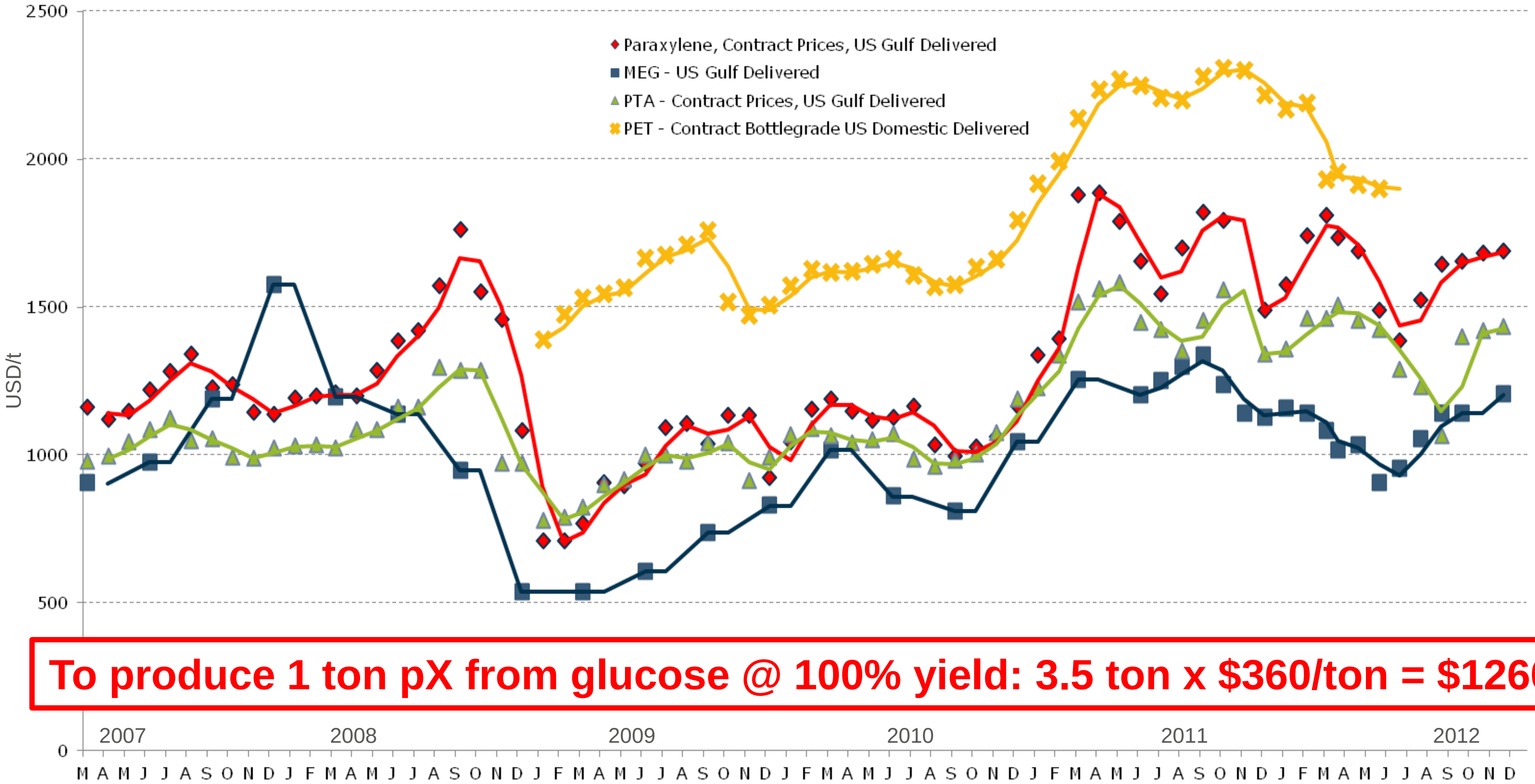


Fig. 3. Oxygen content of feedstocks and materials, and theoretical yield of materials from sugar

pX = p-xylene; C2 = ethylene

Paraxylene, PTA, MEG, PET



To produce 1 ton pX from glucose @ 100% yield: 3.5 ton x $360/ton = $1260

*Feedstock prices for US

Latest PET Prices Not available

Sources: ICIS Pricing; ICIS News

Sources: ICIS Pricing; ICIS News

Very basic "back of the envelope" economics glucose → chemicals intermediate scale process (100kt/y) new technology

avantium

- Count # chemical conversion steps: €100/step + €100 per purification/ solvent swap (€50 in case of mature technology step) (*)
- Estimate realistic yield Y in commercial process
- Evaluate mass loss per mol of product
- Assume €350/ton for feedstock (long term large scale contracts)
- Calculate feedstock required per ton final product:

  100/Y x 180/ MW P

4 + 2 step fructose/glucose to TPA (→HMF → DMF + bioethylene (from ethanol) → pX →TPA) with Y = 60% after purification:

Feedstock required per ton TPA: 100/60 x 180/142 = 1.80 x 116/142 (C6 fragm) = 1.47 ton

Feedstock required per ton ethylene: 100/90 x 180/56 = 3.57 x 26/142 (C2 fragm) = 0.65 ton

Feedstock required per ton TPA: 1.47 + 0.65 = 2.12 ton

Production cost: 2.12 x €400 + €450* + €450* = €848 + €900 = **€1748 / ton**

2 step fructose to FDCA with Y = 60% after purification:

Feedstock required per ton FDCA: 100/60 x 180/156 = 1.92 ton

Production cost: 1.92 x €400 + €200 + €200 = €769 + €400 = **€1169 / ton**

PEF

Catalysis

Foundational Technology and Expertise

Leading Systems and Services Provider for Catalyst R&D

Renewable Chemistries

Novel Chemical Technologies to Transform Renewable Carbon Into Chemical Building Blocks

DAWN® Technology: 2G glucose
RAY ® Technology: 1 step bio-MEG
VOLTA® Technology: e-chem

Renewable Polymers (formerly Synvina)

Polyesters

YXY® Technology: FDCA & PEF

Ticker: **AVTX**
Amsterdam & **Brussels**

HQ Amsterdam Science Park and Prodock Amsterdam (VOLTA)
ChemiePark Delfzijl (DAWN and MEKONG)
Chemelot (YXY)

100+
patent families

230

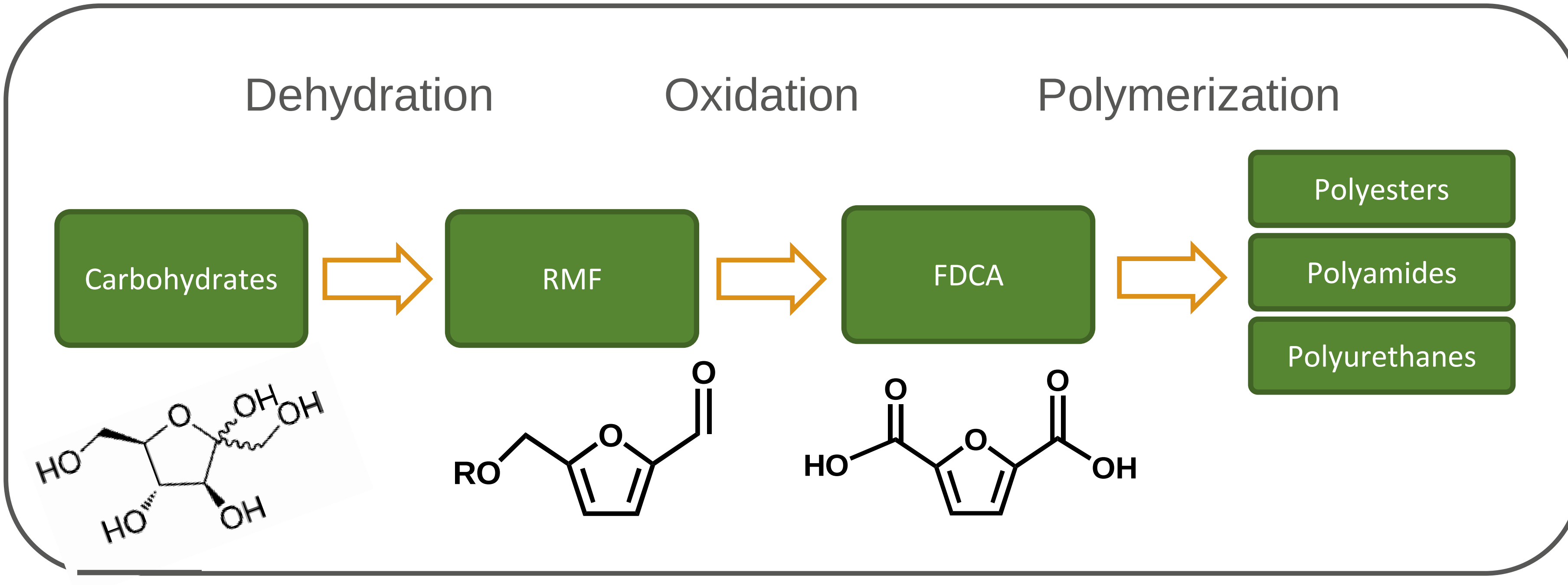
>75% scientists
20+ nationalities
30% female

Avantium Corporate Technology
UvA - Industrial Sustainable Chemistry

University of Amsterdam

Applied research with focus on sustainable polymers
With funding from EU, NWO, and Industry (e.g. Avantium, LEGO)

YXY Technology
Conversion



Maintaining Leadership

Upscaling our technology into world scale production

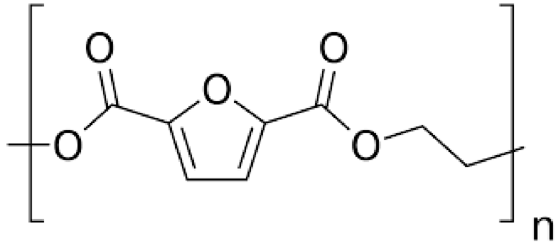
avantium

LAB-SCALE	PILOT PLANT SCALE	COMMERCIAL SCALE	INDUSTRIAL SCALE
2008	**2011 - now**	**2023**	**expected >2024**
Amsterdam	**Geleen (NL)**	**DELFZIJL (NL)**	**Licensee Site**
Kg's	Tons	5000 Tons	Industrial Scale
Innovative research	Technology development	Commercial launch of FDCA & PEF	Roll-out of FDCA & PEF at larger scale
			Licensing

1 | Commercial plant for proof of concept & market development

2 | Licensing to rapidly expand market

The Scope of FDCA & PEF



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APPLICATIONS OF FDCA

FDCA

- Polyesters (incl. PEF)
- Polyamides
- Polyurethanes
- Other polymers
- Chemical building blocks

APPLICATIONS OF PEF

PEF

- Bottle
- Thin Film
- Thermoform
- Fibers

1 | New molecule with countless applications

2 | PEF has the market size potential due to product properties

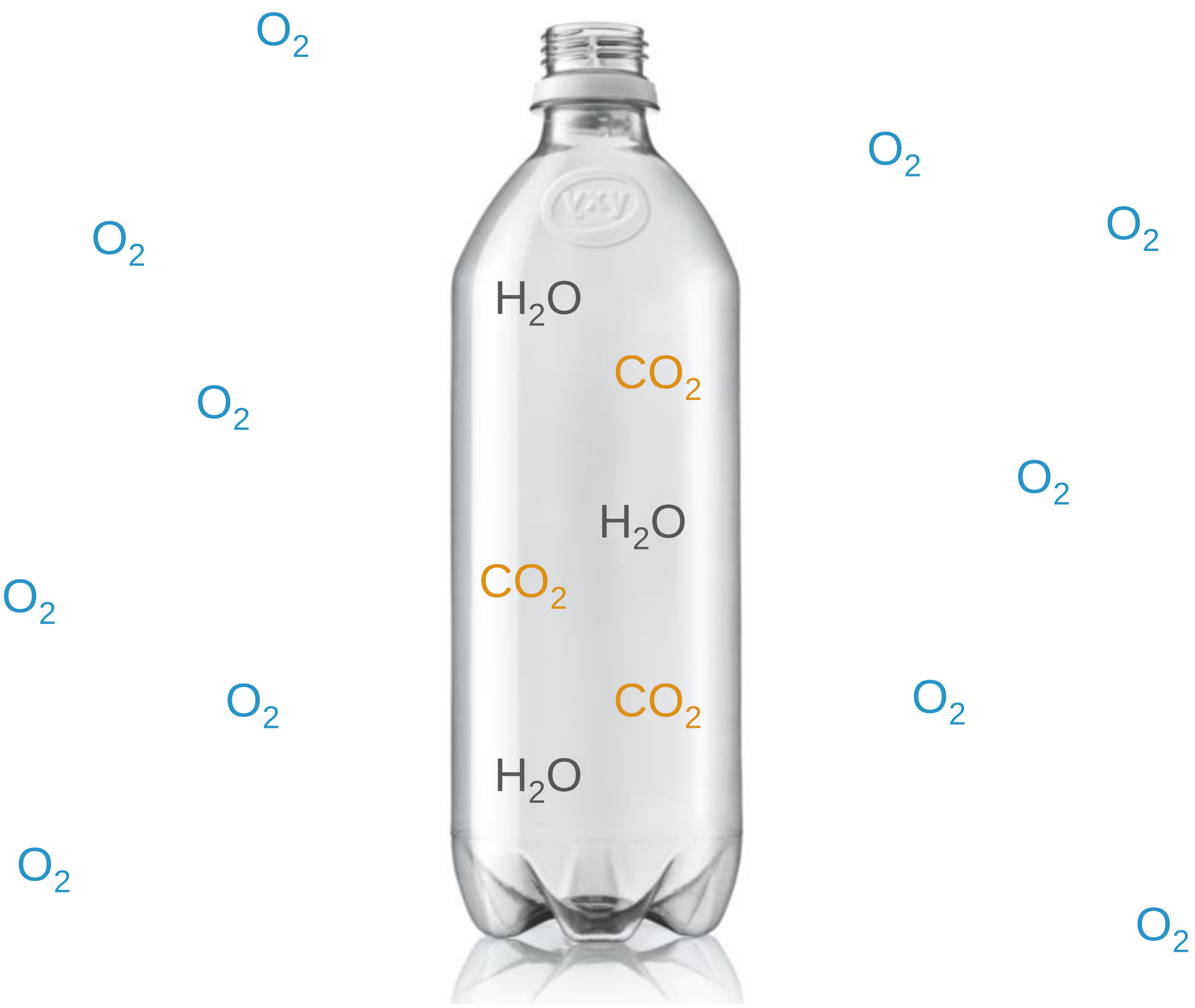
3 | Fulfilling market needs & trends

Pilot Plant – Chemelot Geleen (NL)

avantium

“Prove the process” & “Prove the products” (application development)

PEF has barrier !

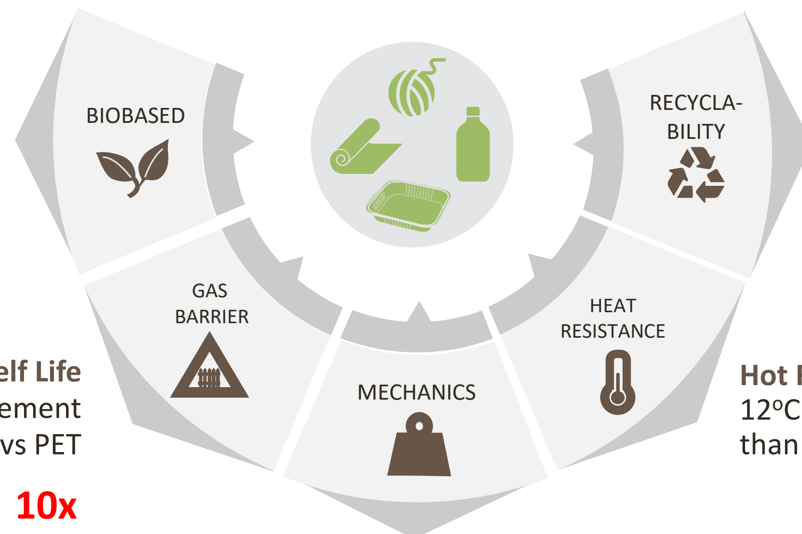


Why PEF?

Trends in packaging:

- **Sustainability**
- **Smaller servings**
- **Healthier drinks**
- **Cost reduction**

PEF



100% Biobased
Renewable material

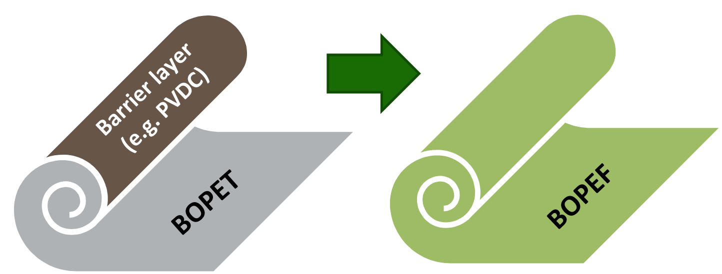
100% Recyclable
Using same steps as PET

Shelf Life Improvement Factor vs PET

O_2	10x
CO_2	6-10x
H_2O	3x

Hot Fill / Hot Serve
12°C higher T_g than PET

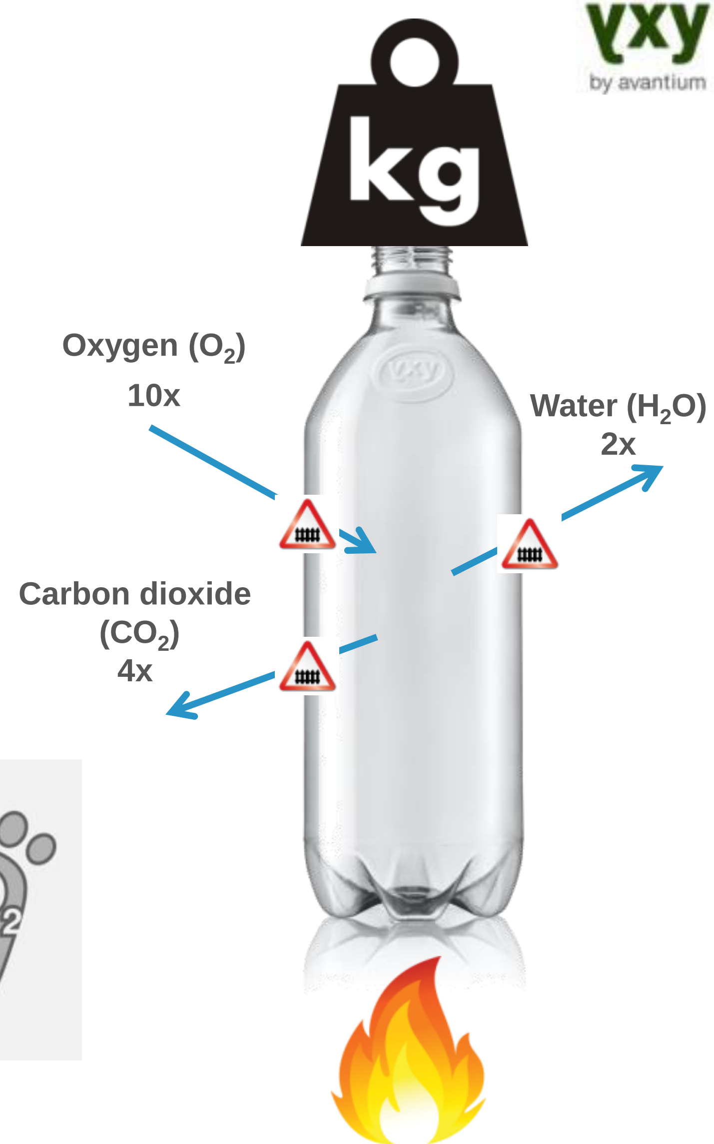
Light-weighting
60% higher modulus and strength than PET



PEF: the Next Generation Polyester

- Superior performance over PET:
  - O_2 barrier: 10x improvement
  - H_2O barrier: 2x improvement
  - CO_2 barrier: 4x improvement
- Improved Thermal Stability
  - Tg: ~88°C → 12°C higher than PET
- Excellent Mechanical Properties:
  - Tensile Modulus PEF : 1.6* PET

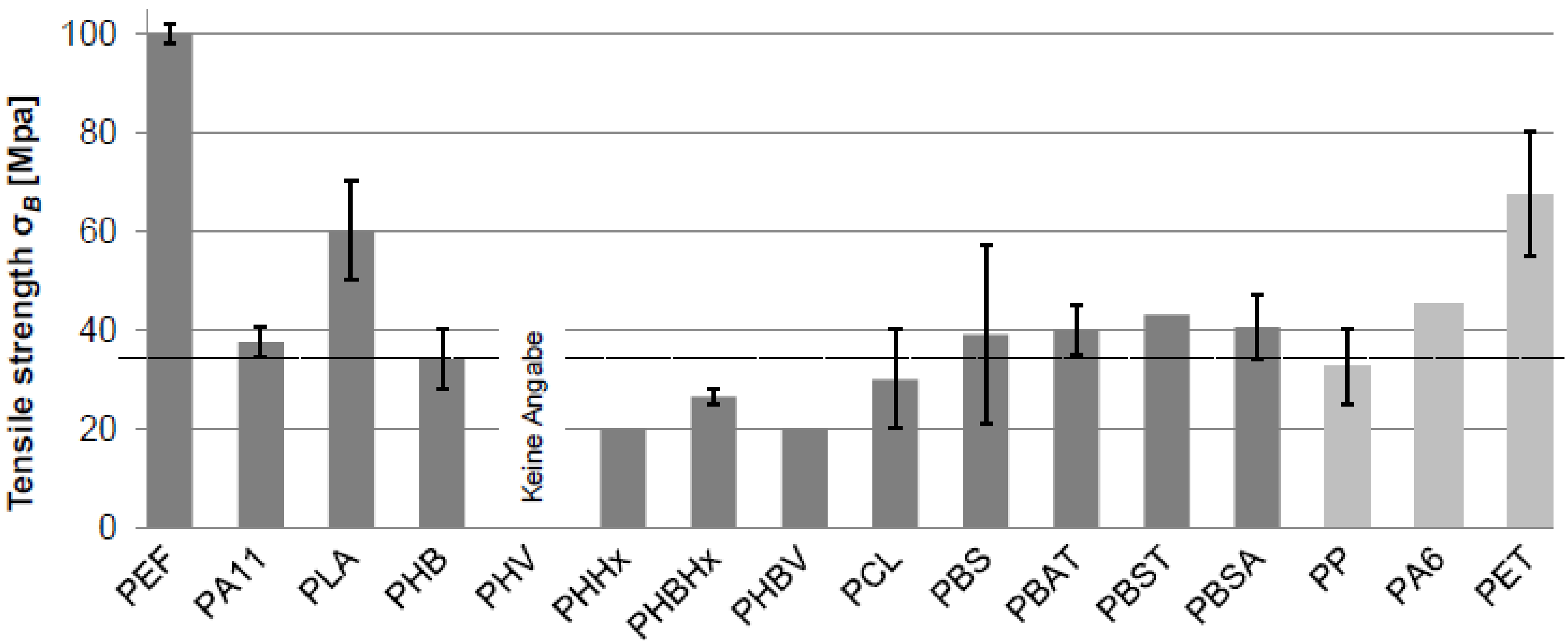
- Significant reduction in carbon footprint
  - 70% lower carbon emission
  - 65% lower NREU



Additional properties

- Improved Crystallization Behavior → No co-monomer needed to reduce crystallization rate.
- PEF exhibits well behaved stress-strain curves and strain hardening behavior.
- PEF rheology comparable with typical PET grades
- PEF heat distortion temperature is ~12°C higher than PET (77°C PEF vs 65°C for PET)
- Hydrolytic stability similar as PET
- Mechanical recycling including sorting demonstrated (similar to PET)
- Food Contact Safety studies finalized: positive EFSA opinion (2014)
- 65-70% reduction in NREU and CO2
- More reductions expected through process improvements

Tensile strength ISO 527-1/-2



Thesis Dolmans ITA, RWTH 2013

PEF Paper Bottle with PABOCO

- ✓ PABOCO is JV between BillerudKorsnäs and ALPLA.
- ✓ Avantium will provide fully plant-based recyclable bottle for Carlsberg.
- ✓ Thin layer of PEF will provide the Paper Bottle with high barrier. Mechanical properties from the paper.

PEF Market Traction in High-Value Applications

Multilayer packaging

Replace with single material PEF layers, reducing cost of packaging while enabling recycling

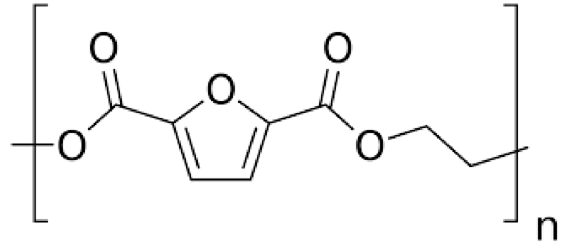
Enhanced bottles

PEF in small volume CSD/beer bottles or as barrier layer providing performance and enabling recycling

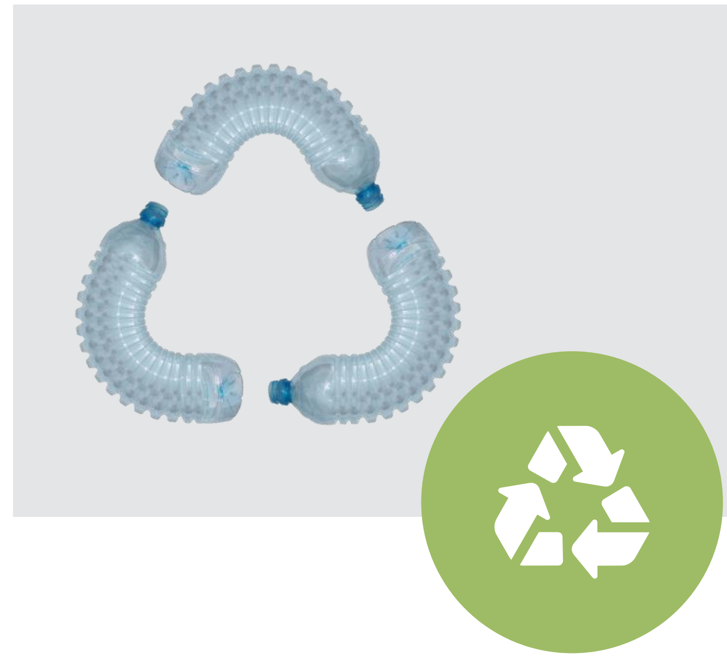
Optical film

Enable thinner LCD/OLED displays

Recycling



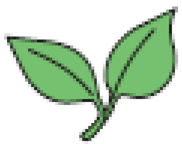
- Optimize end-of-life solutions for PEF polymer
- PEF to PEF recycling is similar to PET recycling
  - Mechanical & Chemical recycling
- PEF can be separated from PET by **IR sorting**
  - **Effect of PEF in rPET stream:**
    - PEF has significantly less impact on rPET than Nylon or PLA



→ European PET Bottle Platform (EPBP) has awarded interim approval to PEF Polyester in PET (up to 50kt/a)

http://www.epbp.org/download/319/interim-approval-synvinas-polyethylene-25-furandicarboxylate-or-pef

First PEF T-shirts of 100% recycled PEF bottles



100% Biobased

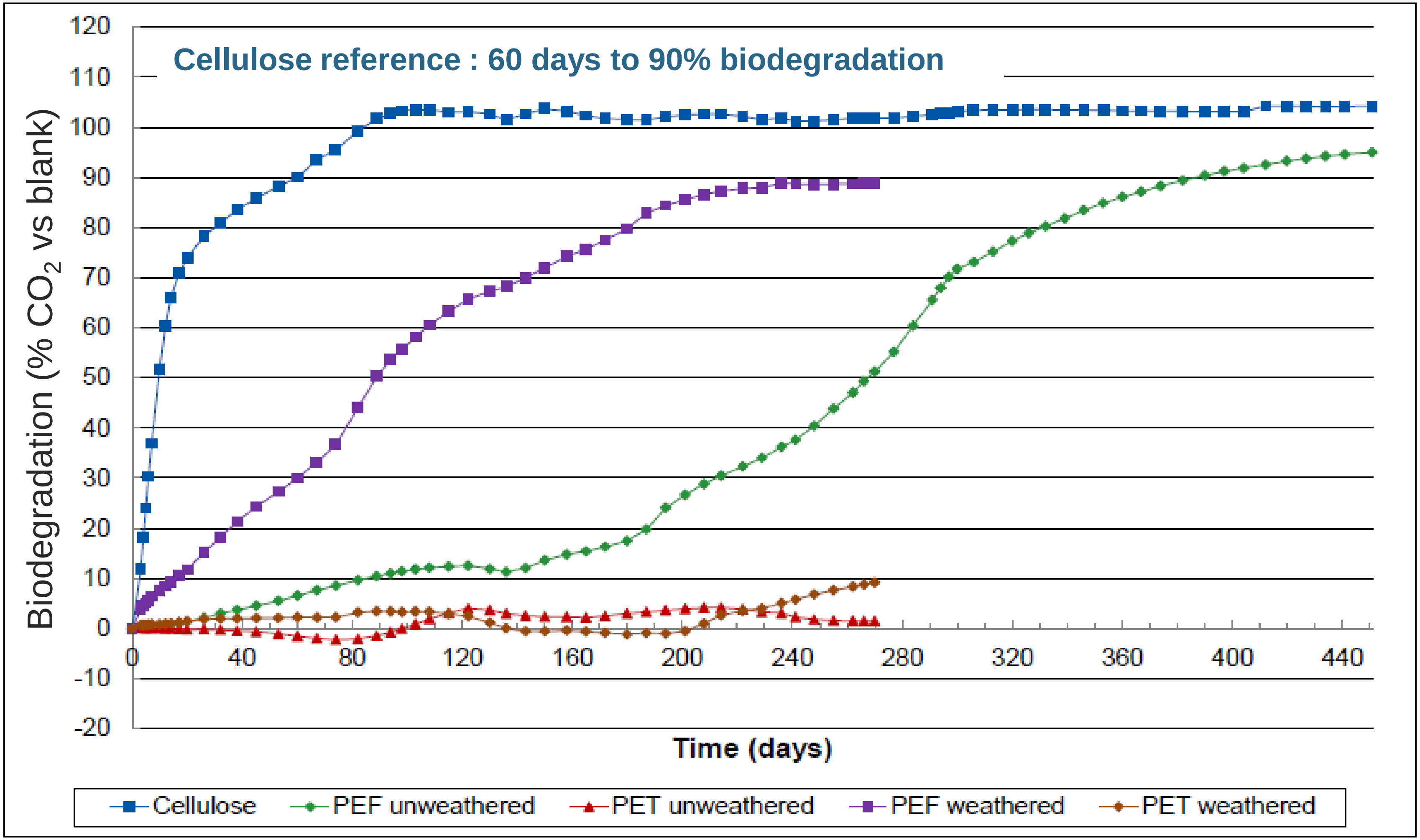
Conventional polyester spinning technology

Made from 100% Recycled PEF

Conventional polyester dyeing technology

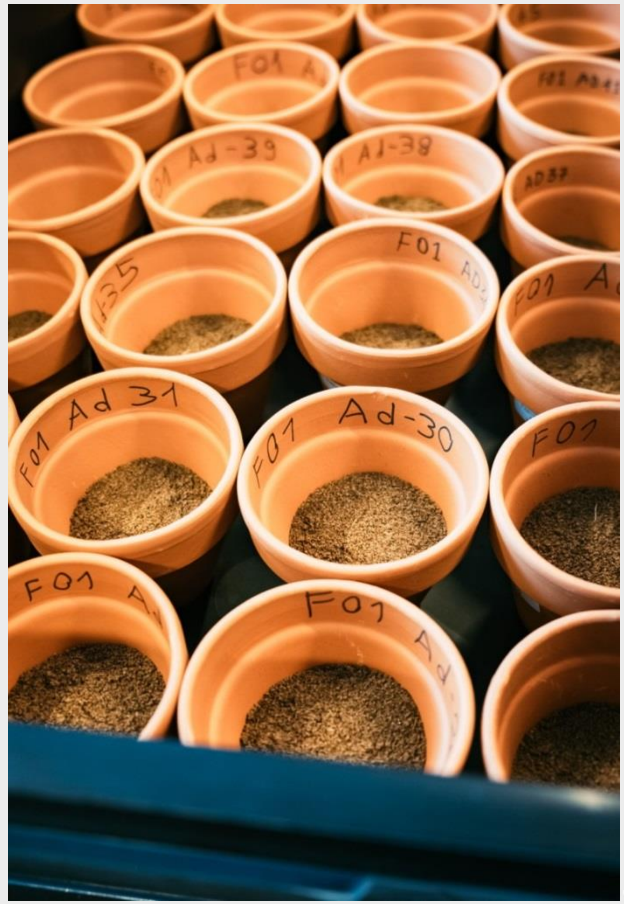
Biodegradation of PEF !!

Industrial Composting Conditions (in soil @ 58 °C)
With and without weathering (UV light)



- **PEF (weathered): 240 days to 90% biodeg. PEF (unweathered): 380 days to 90% biodeg.**
- No PET degradation observed (experiments stopped after 270 days)

multi year field trials started Q1 2019

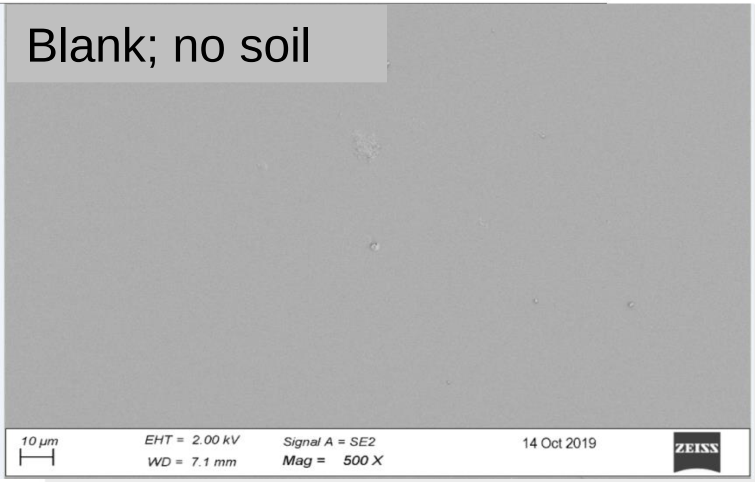


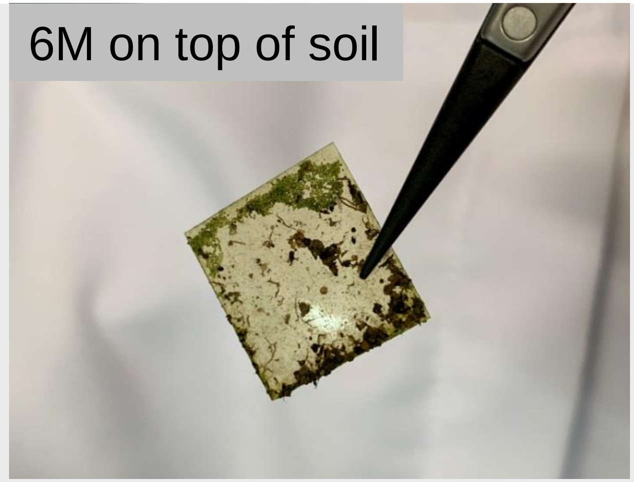
- Mass loss,
- surface change,
- Mol. weight changes
- micro-organism study

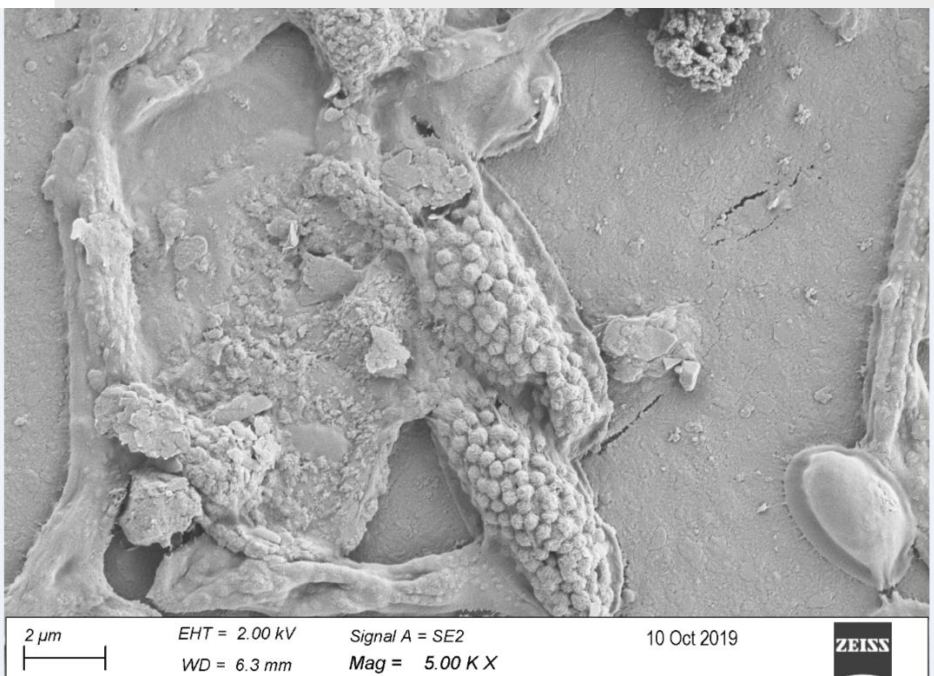
UNIVERSITY OF AMSTERDAM

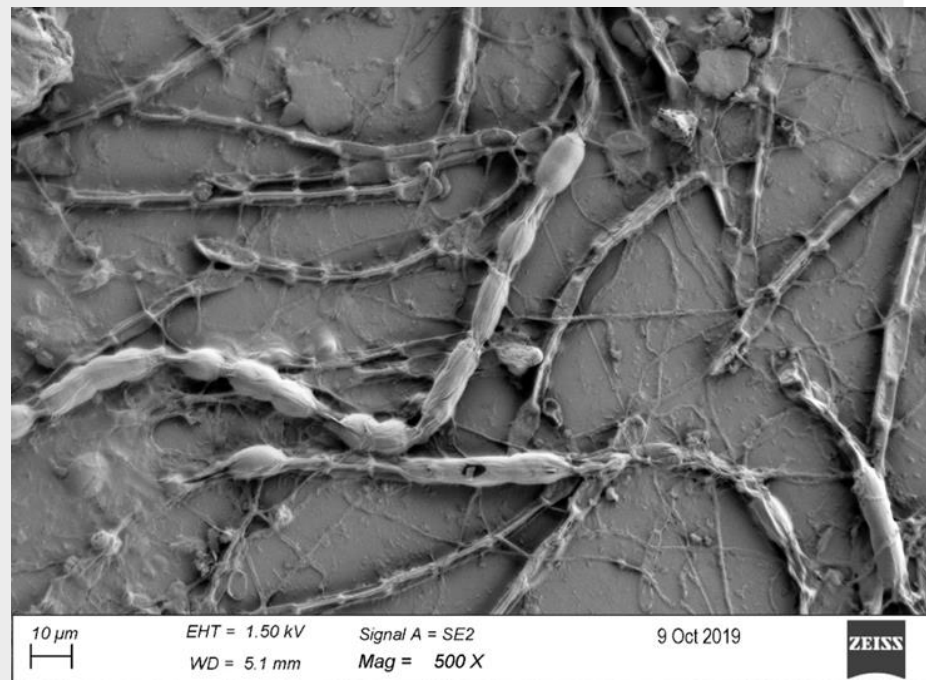
10 year field trials

Initial results (after 6 months) Amsterdam, Netherlands









Why is even slow biodegradation relevant

NOT as designed end-of-life option !!

Plastic fibres found in tap water around the world, study reveals

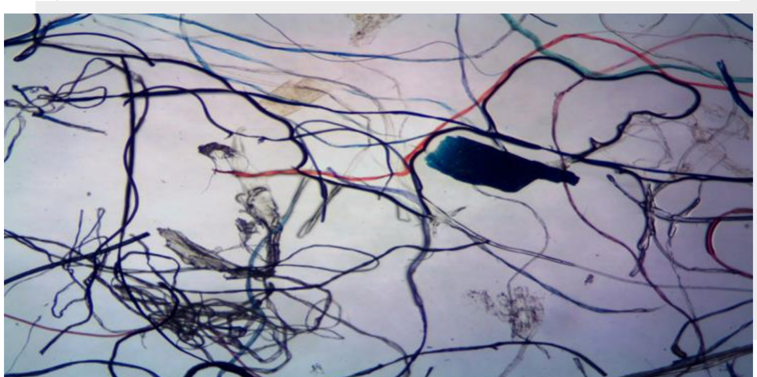
Exclusive: Tests show billions of people globally are drinking water contaminated by plastic particles, with 83% of samples found to be polluted

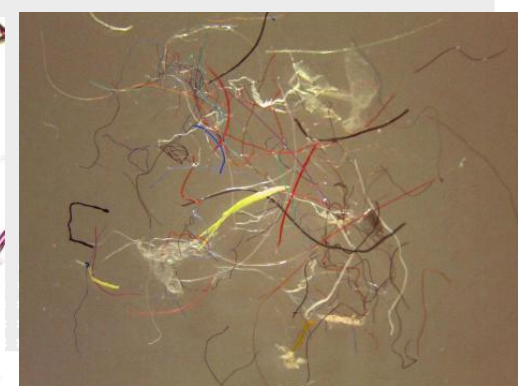
- We are living on a plastic planet. What does it mean for our health?

1.704

The average number of fibres found in each 500ml sample ranged from 4.8 in the US to 1.9 in Europe. Photograph: Michael Heim/Alamy

The Guardian

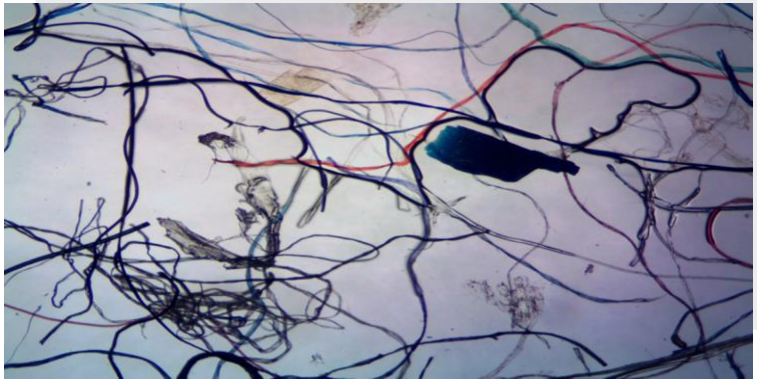


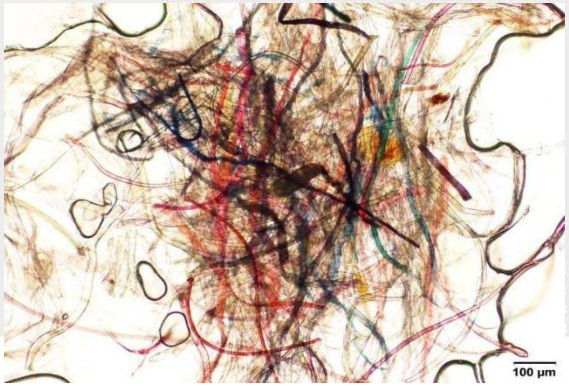


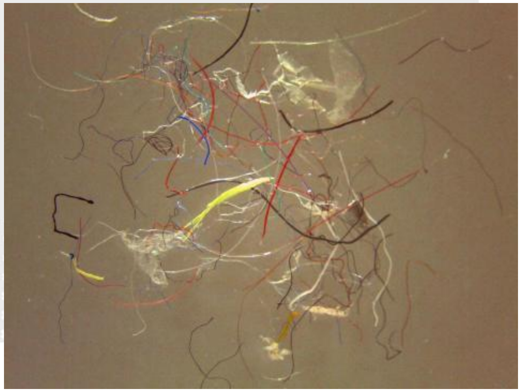
Why is even slow biodegradation relevant

NOT as designed end-of-life option !!

- Take PET fibers from washing textiles as example
  - If on average 1 million tons of PET fibers entered the environment every year since 1970 and degradation takes 500 years, we have 50 million tons of PET fibers in the environment today and >100 million tons in 2070.
  - If PEF degradation takes 5 years, we would have 5 million tons of PEF fibers in the environment today and also in 2070.





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electrochemistry platform

CO_2 as feedstock

Electrochemistry at Avantium

- In Nov 2016, **Avantium acquired Liquid Light Inc**, a Princeton 2009 start-up in which >$35M was invested by VC's to develop CO_2 to MEG
  G,

Let's Get it On: Avantium acquires Liquid Light

January 10, 2017 | Jim Lane

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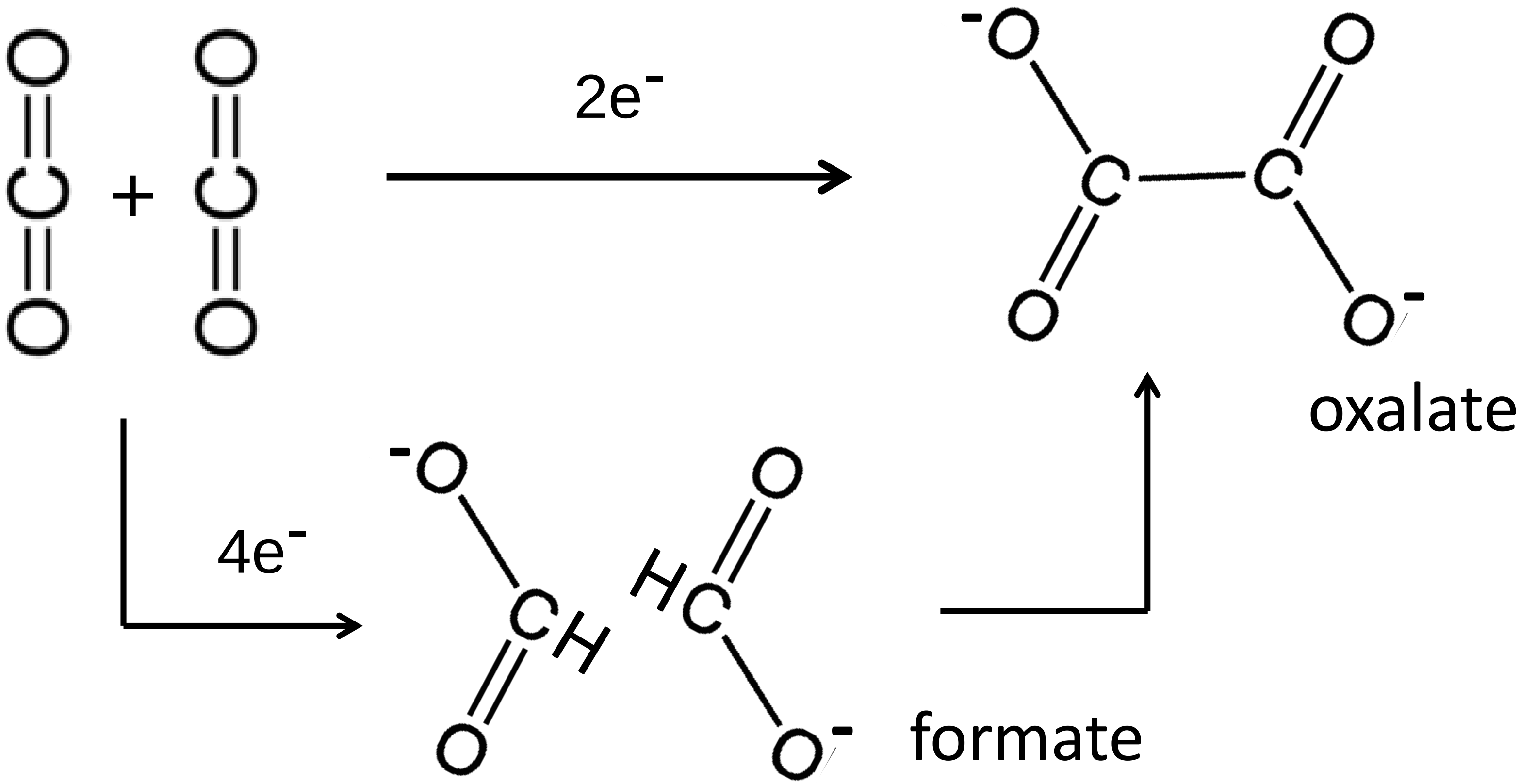
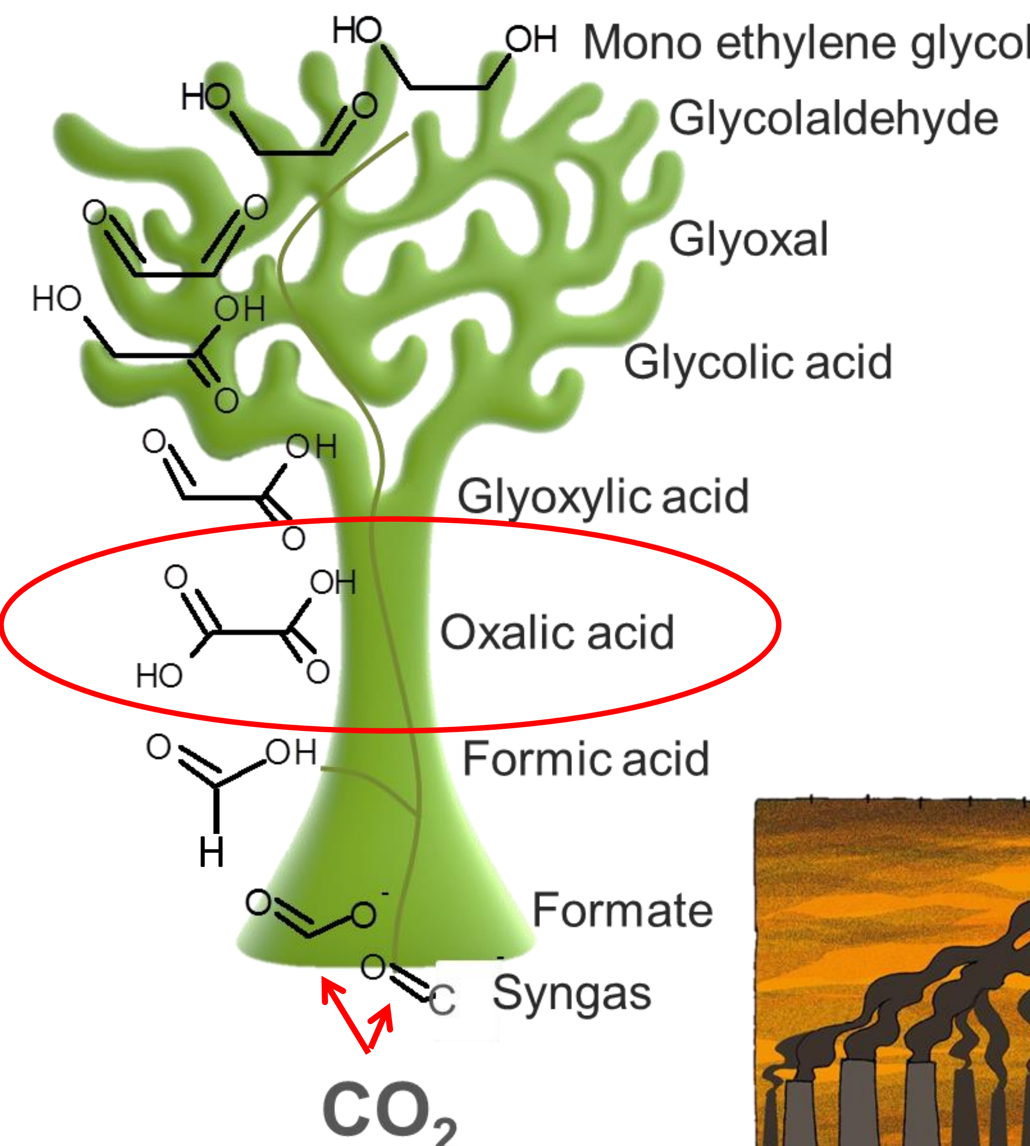
In the Netherlands, Avantium has acquired the assets of Liquid Light Inc, developer of a process technology to make major chemicals from low-cost, globally-abundant carbon dioxide (CO2). The acquisition combines the technologies of both Liquid Light and Avantium to develop a world leading electro-catalysis platform and to commercialize new process technologies using CO2 as feedstock to produce sustainable chemicals and materials.

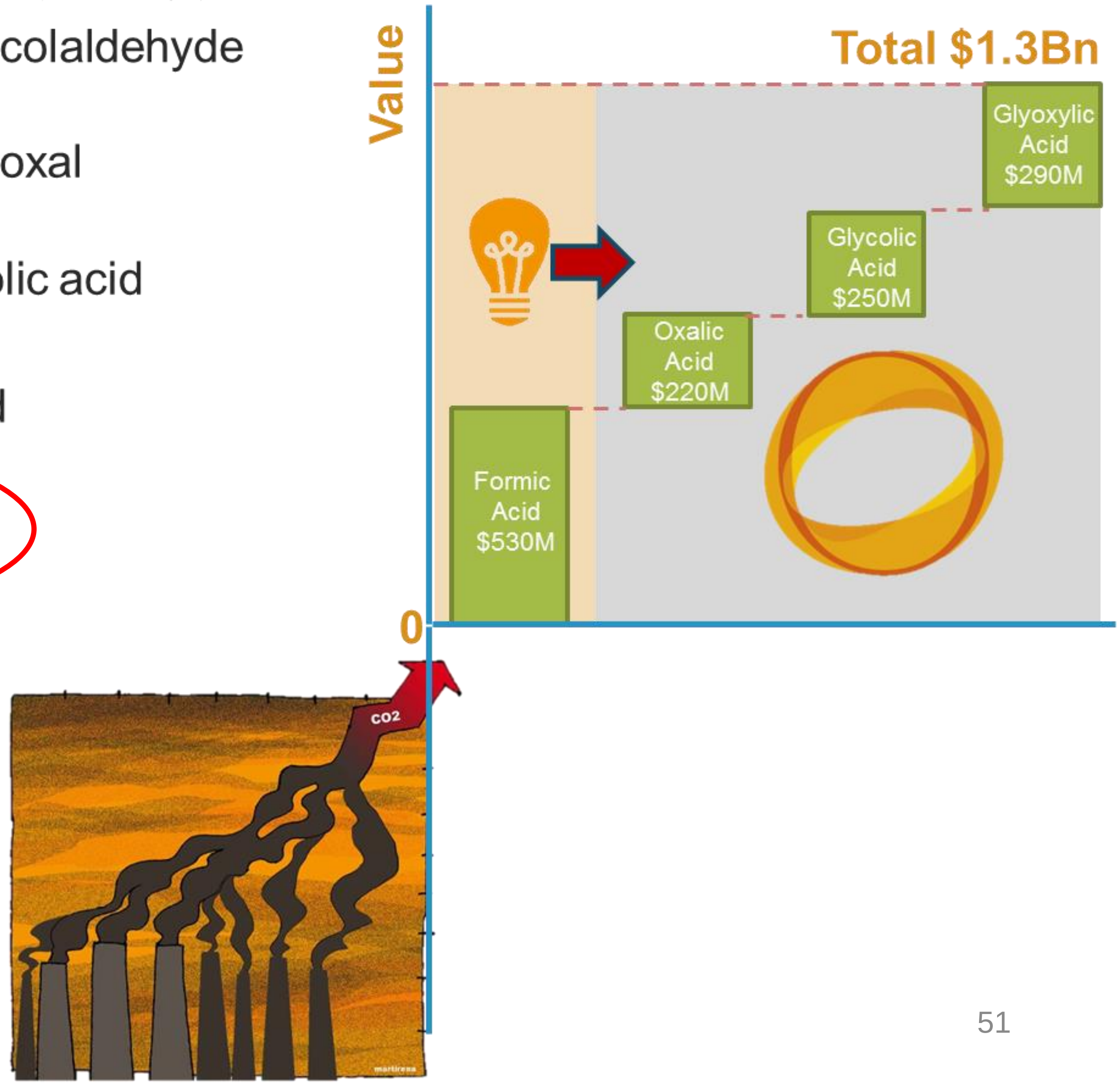
Liquid Light re-emerges from the dark

CO2 as feedstock



CO_2 to C2 - Platform Opportunity





CO_2 valorization (CCU) via electrochemical routes – Cost drivers.

- Atom efficiency (at 100% yield).
  - CO_2 to formate (HCOOH) and to oxalate (HOOC-COOH) ~ 100% weight retention
  - CO_2 to methanol (CH_3OH) ~ 73% weight retention
  - CO_2 to methane (CH_4) ~36% weight retention
- Number of electrons needed (see next slide).
  - Note that an 8 electron reduction at 36% atom efficiency (CO_2 to methane) requires 8/2 x 100/36 = 12 x more electrons (electricity) than a 2 electron reduction at 100% atom efficiency per ton of product produced.
- Faraday efficiency and overpotential
  - The efficiency of the electrons used for desired reaction (versus electrons going to side reactions and heat)
- Current Density (mA/cm2)
  - The productivity per area of electrode (= Capex ! > 200 mA/cm2 is typically required)

Very basic "back of the envelope" economics
electrochemistry: CO2 → chemicals
intermediate scale process (100kt/y) new technology

- Count # chemical conversion steps: €100/step + €100 per purification/ solvent swap (€50 in case of mature technology step) (*) and **€200/electrochemical step**)
- Estimate realistic yield Y in commercial process
- Evaluate mass loss per mol of product
- Assume €50/ton for feedstock (purification/ transport ?)
- **Assume 3500 kWh electricity for a 2 electron reduction of 1 ton of CO2**, Assume €0.05/kWh
- Calculate feedstock required per ton final product:

  100/Y x 180/ MW P

1 step CO2 to formate. Faradeic yield > 95%

Feedstock required per ton Formate: 100/95 x 44/45 = 1.03

Production cost: 1.03 x €50 + €175 + €200 + €100 = **€525**

2 x formate → oxalate; Y = 90%

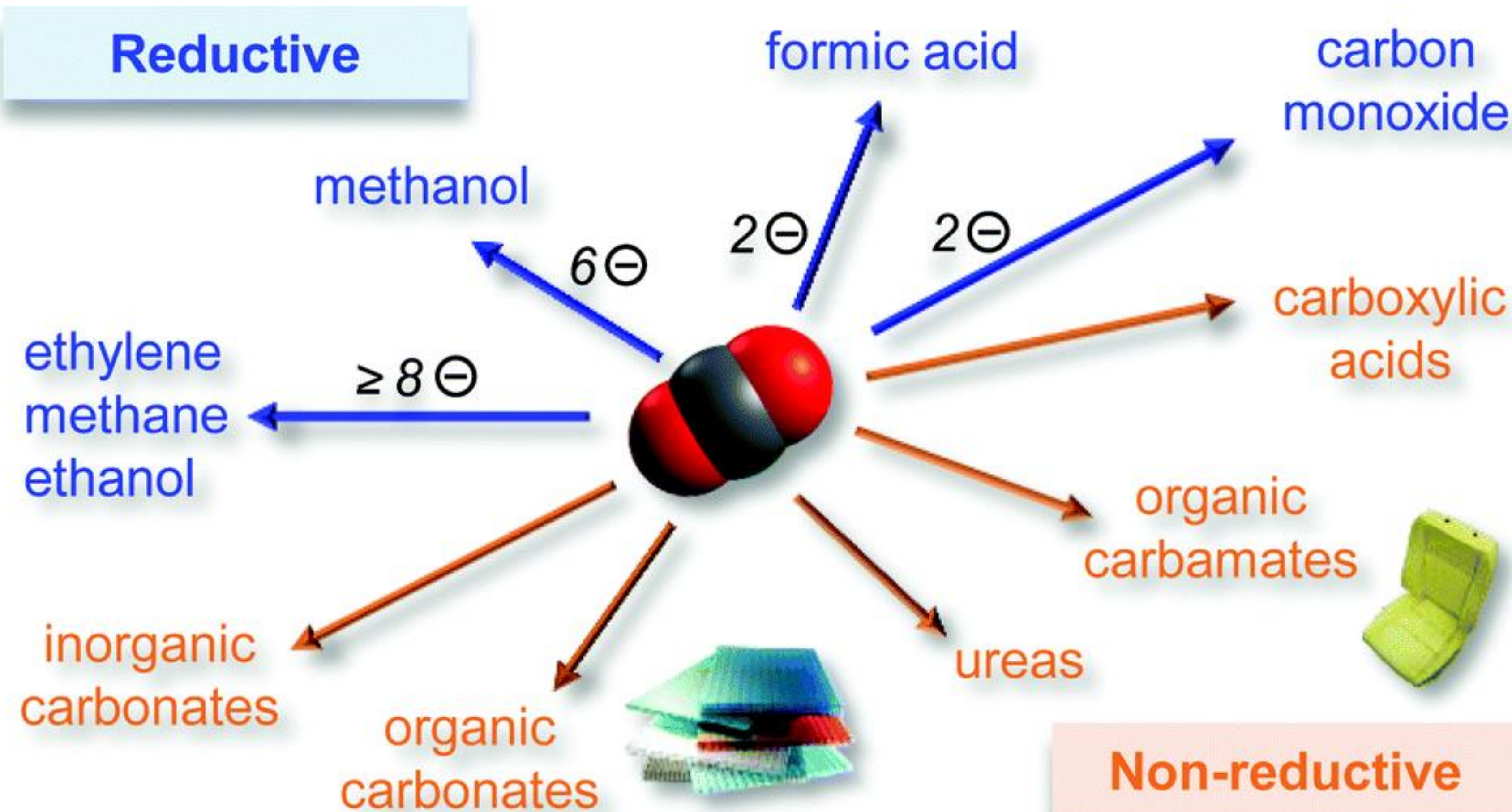
Production cost: (100/90 * 90/90 * €525) + 100 + 100 = €585 + 100 + 100 = **€785**

Oxalate → oxalic acid → MEG; Y = 90%

Production cost: (100/90 x 92/62 * €785) + €200 + €200 = €1295 + €200 + €200 = **€1695**

CCU: Using CO_2 as feedstock: electricity cost

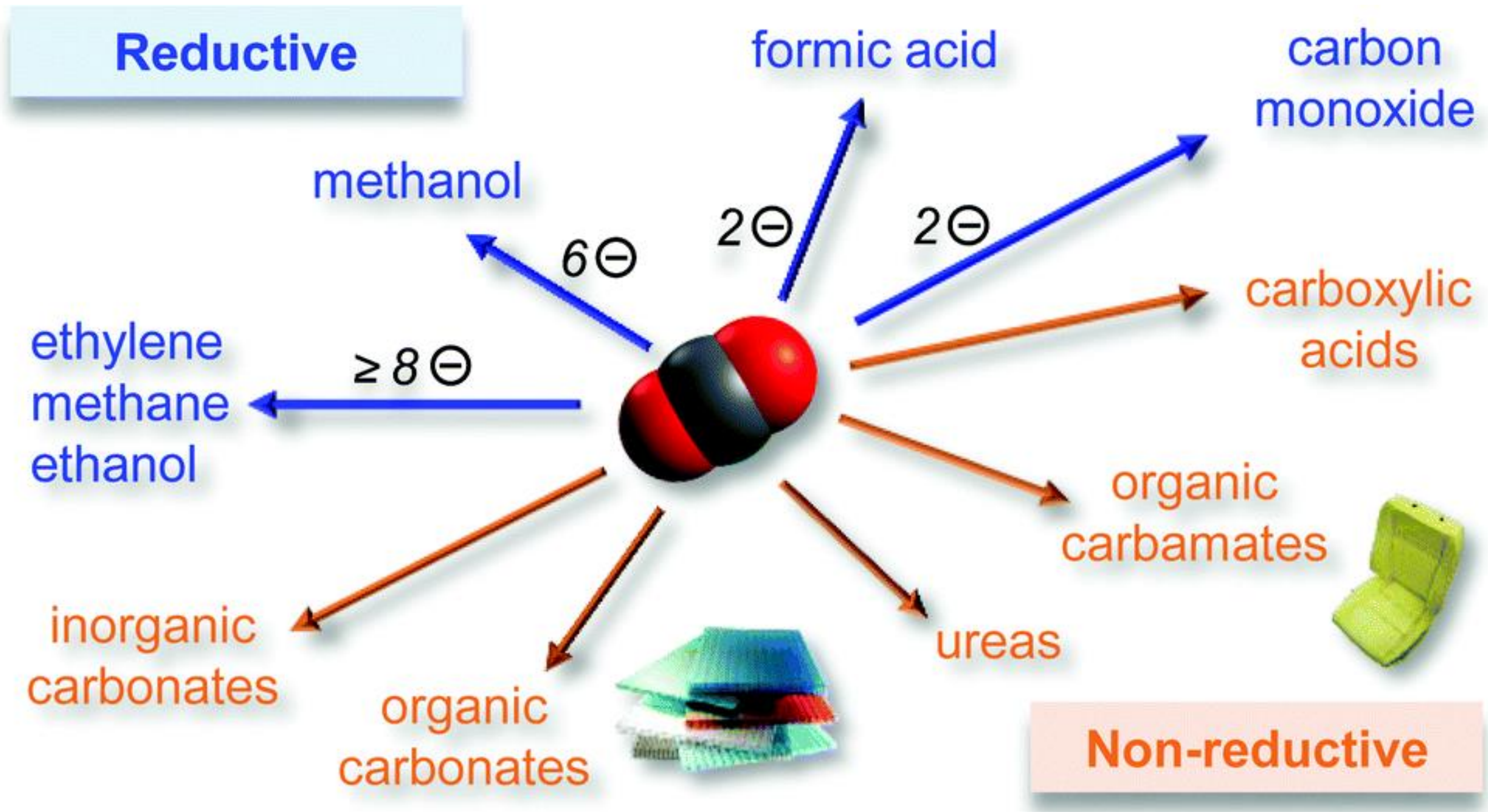
2e → €175/ton CO2
=€175/ton formate



CCU: Using CO_2 as feedstock: electricity cost

2e → €175/ton CO2
=€175/ton formate

2e → €175/ton CO2
= €280/ton CO



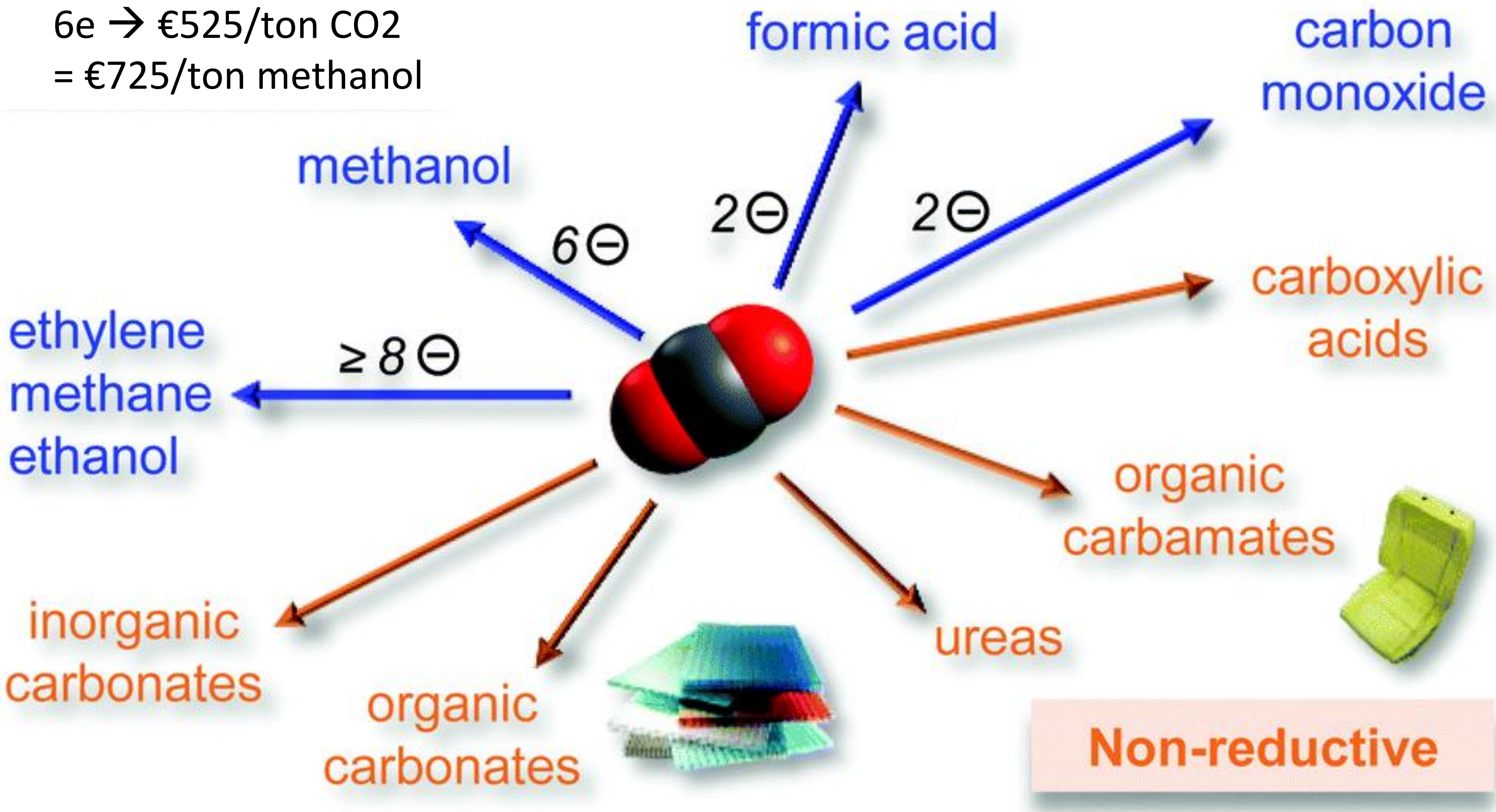
CCU: Using CO_2 as feedstock: electricity cost

avantium

2e → €175/ton CO2
=€175/ton formate

2e → €175/ton CO2
= €280/ton CO

6e → €525/ton CO2
= €725/ton methanol



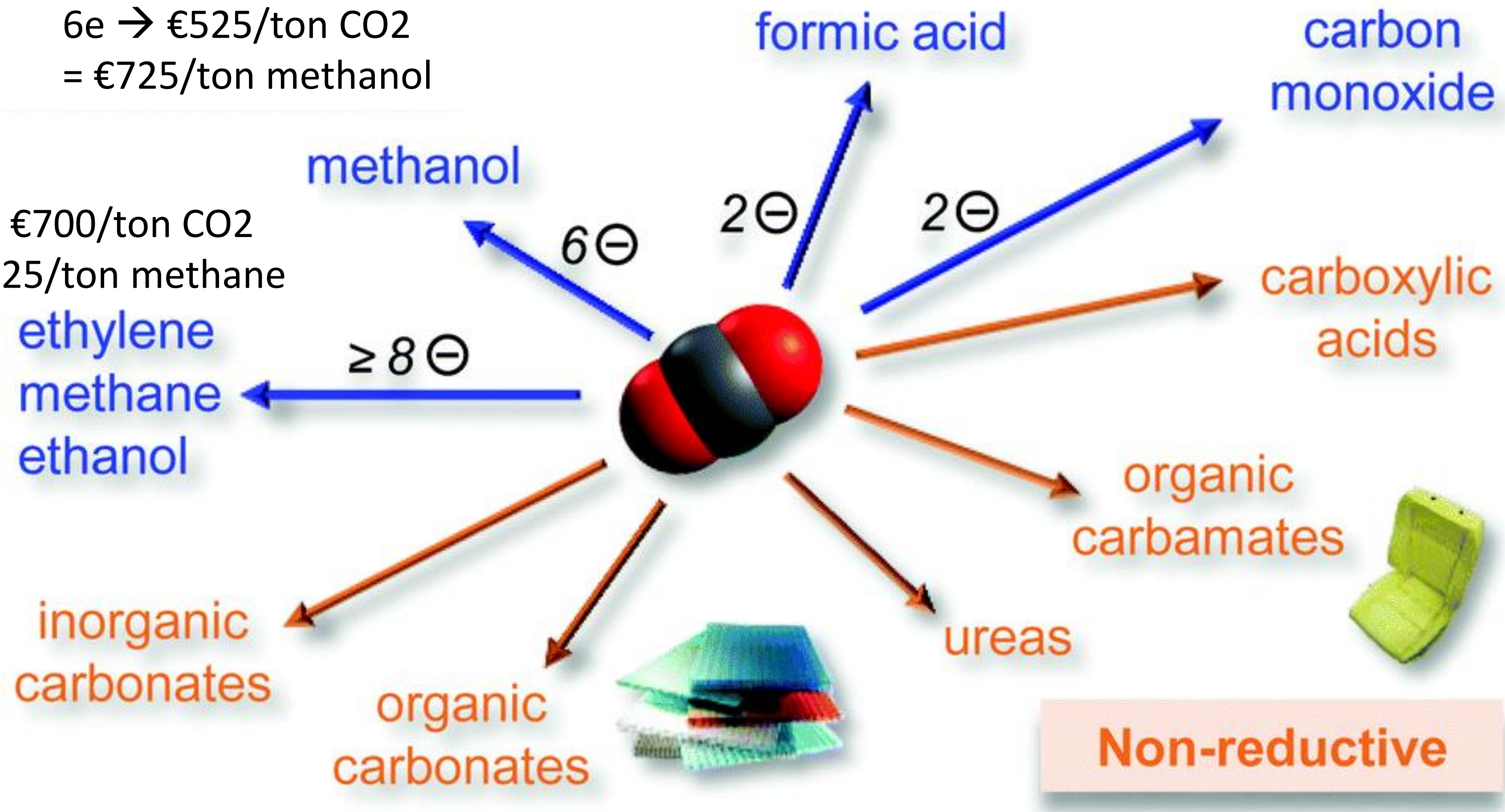
CCU: Using CO_2 as feedstock: electricity cost

2e → €175/ton CO2
=€175/ton formate

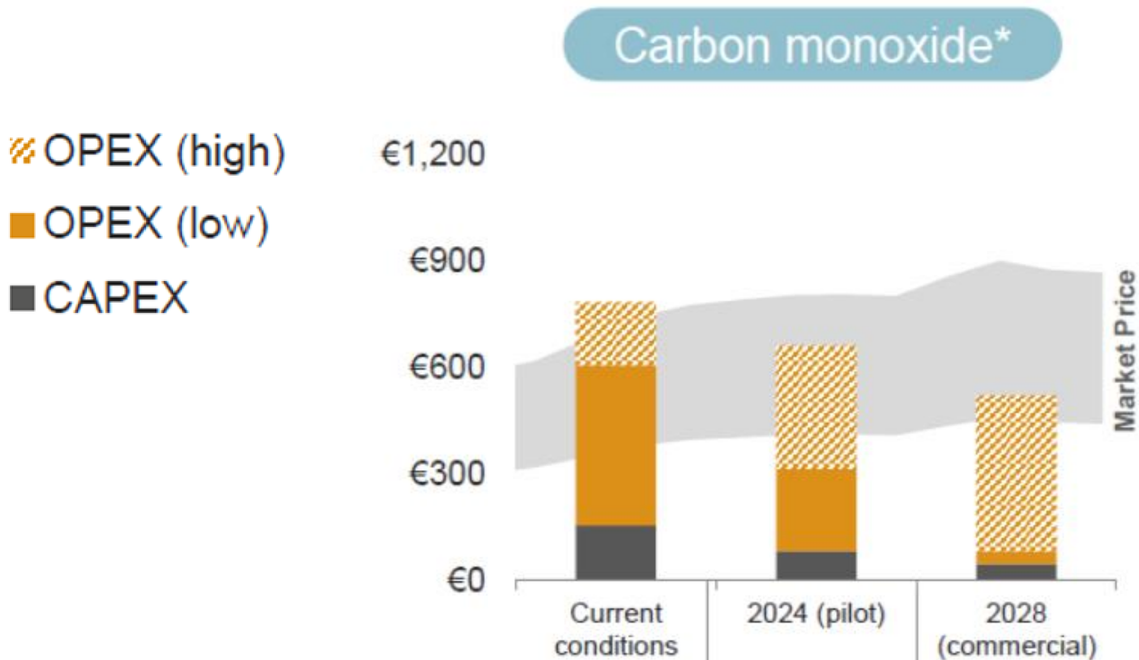
2e → €175/ton CO2
= €280/ton CO

6e → €525/ton CO2
= €725/ton methanol

8e → €700/ton CO2
= €1925/ton methane



CO business case



Key Assumptions	Current conditions	2024 (pilot)	2028 (commercial)
Cell costs (€/m^2)	5000	4000	3000
Electricity price (€/MWh)	30-50	20-50	10-50
CO_2 price (€/tonne)	50	0-50	(50)-0
Current density (A/m^2)	2000	3000	4000

Oxalic acid → glycolic acid (€3500/ton)
Glycolic acid (GA) polymers for biodegradable barrier film

- Glycolic acid – Lactic acid copolymers with 50-90% GA content for barrier film
- Increased barrier to O_2 and water vapor with increasing GA content
- Barriers even better than PEF !!
- Polymers with > 75% GA are Low Tg fully biodegradable polymers
- Polymers with higher LA content are industrially compostable

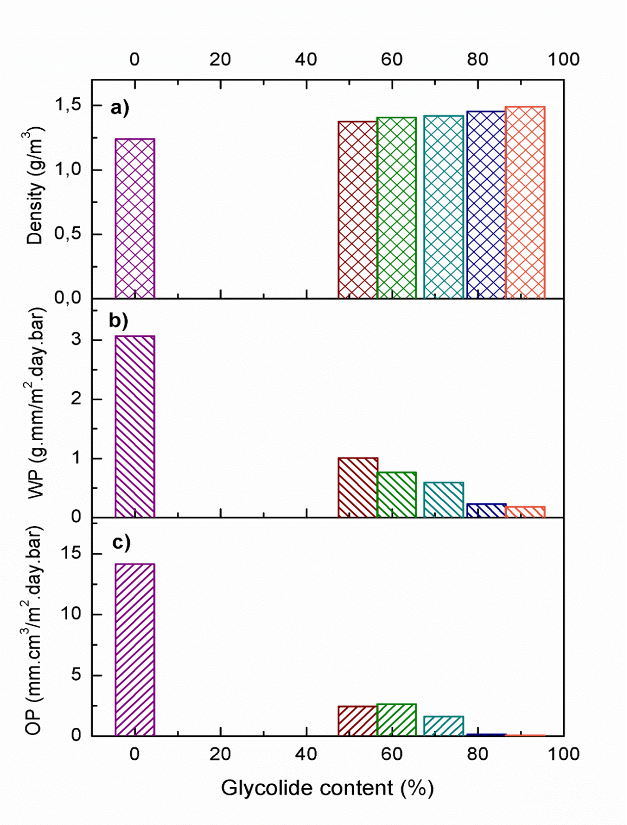
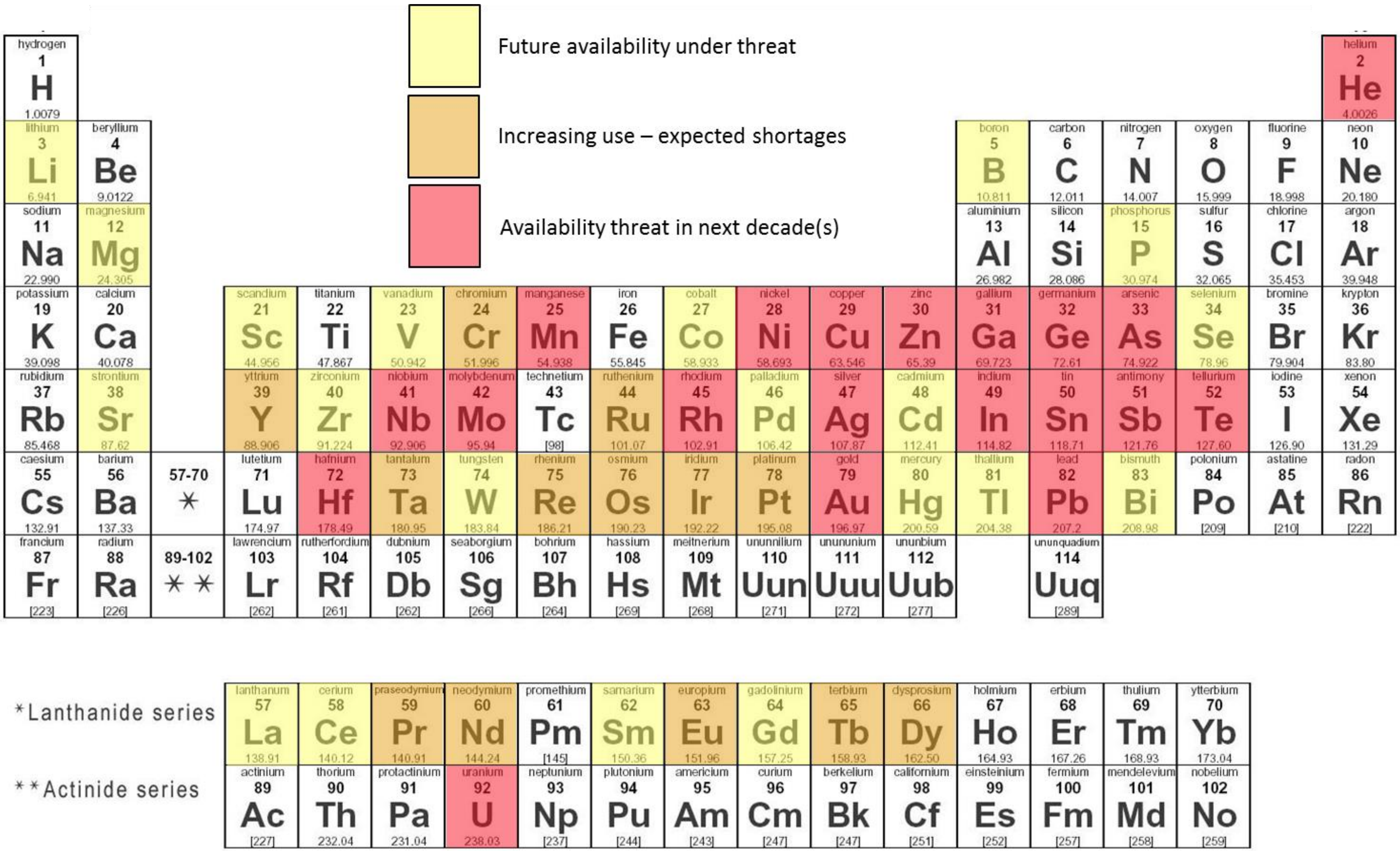


Figure 6. Density (a), oxygen permeability (b), and water permeability (c) (measured at 70% RH and 30 °C) as a function of glycolide content in PLGA copolymers.

Gruter et al. ACS Appl Pol Mat 2020

Elements regarded as critical against risk criteria of supply constraints, demand growth and geographical spread.



Is Chemistry a mature discipline from which radical innovation cannot be expected anymore ?

- Huge challenges ahead for chemistry to enable transition from linear to circular economy.
- **Our chemical future is in an embryonic stage !!**

- Biomass – biorefineries – biobased products: we are only at the beginning…
- CO_2 as feedstock
- Wind/Solar – Electrochemistry, energy storage,…
- Scarcity of elements: In, Ag, Sb, Pt, P…. → development of alternatives
- Many others…