eRefinery

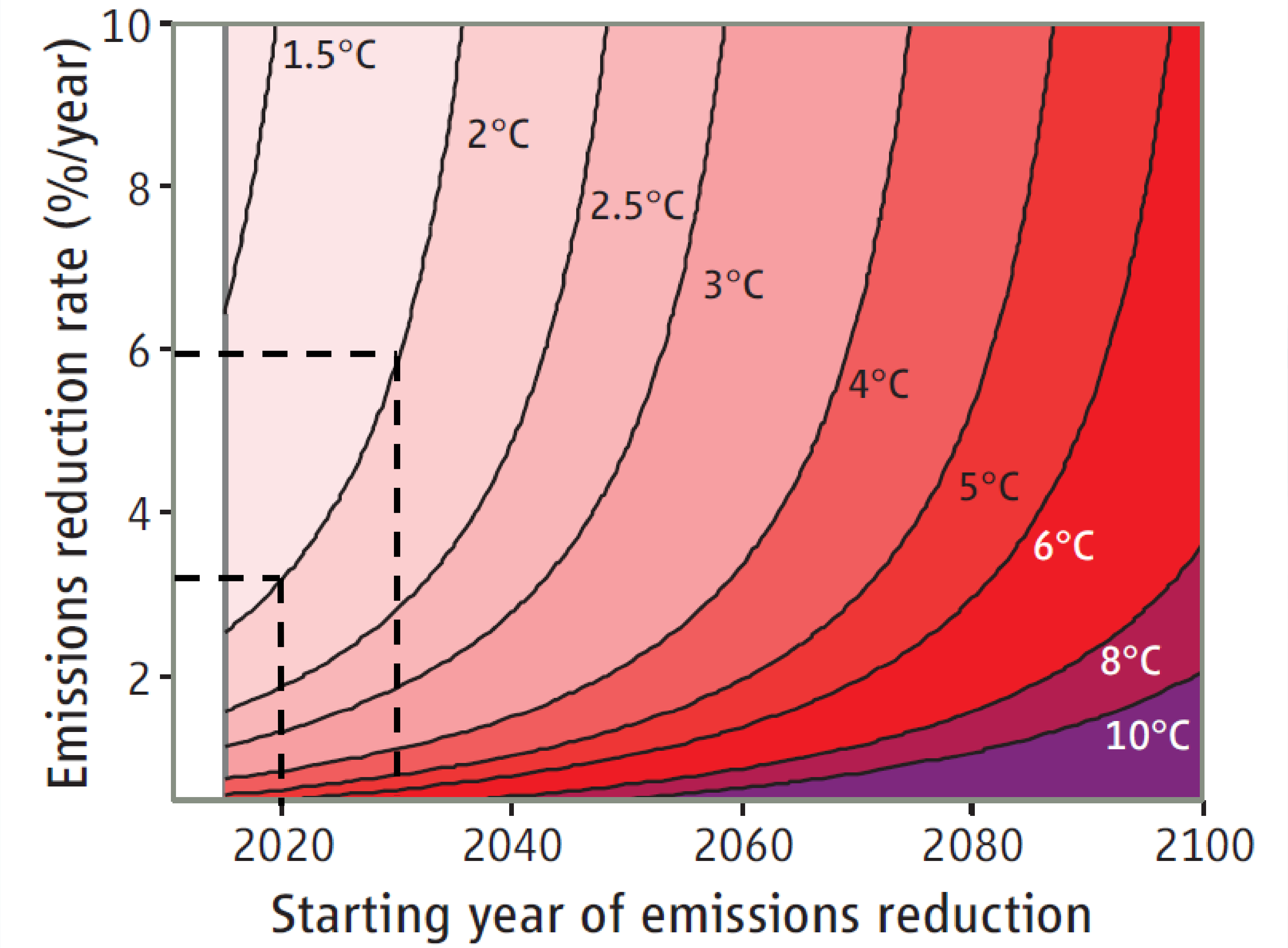
Towards sustainable production of chemicals and fuels

Van CO_2, water en electriciteit naar ethyleen

Bernard Dam, Chemical Engineering, TU Delft

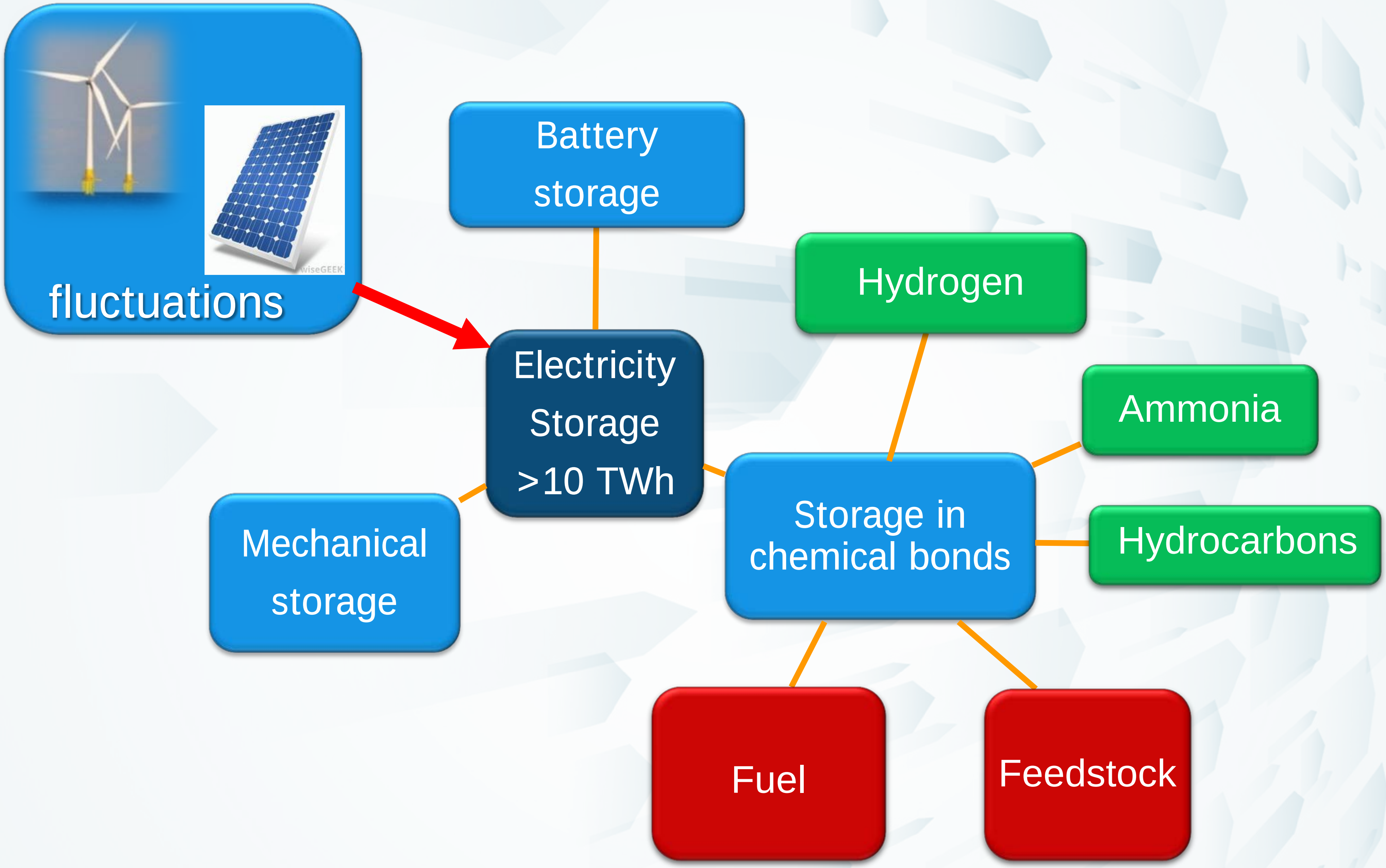
TU Delft

REDUCTION OF WORLD CO_2-EMISSIONS NEEDS TO START SOON



Science (2013) vol339

A sustainable energy system



Chemical industry cannot rely only on recycling and biobased feedstock


MILIEU EN KLIMAAT

De Botlek moet om, en zo snel mogelijk

De verduurzaming van de chemie en de energiesector schiet tekort. Vier Delftse wetenschappers buigen zich over de manier waarop de (petro)chemie moet vergroenen. Volgens de een is het vijf voor twaalf, volgens de ander is het al te laat. Voor de raffinaderijen in de Botlek is het erop of eronder. Het advies: hou verschillende potjes op het vuur, want voor één aanpak kiezen is gevaarlijk. 'We moeten als een gek fundamenteel onderzoek gaan doen.'

PAGINA 18


Wim Haije
Onderzoeker aan de faculteit werktuigbouwkunde, TU Delft


Paulien Herder
Hoogleraar energiesystemen, TU Delft


Ruud van Ommen
Hoogleraar product- en process-engineering, TU Delft


Bernard Dam
Hoogleraar fundamenteel onderzoek elektrochemie, TU Delft

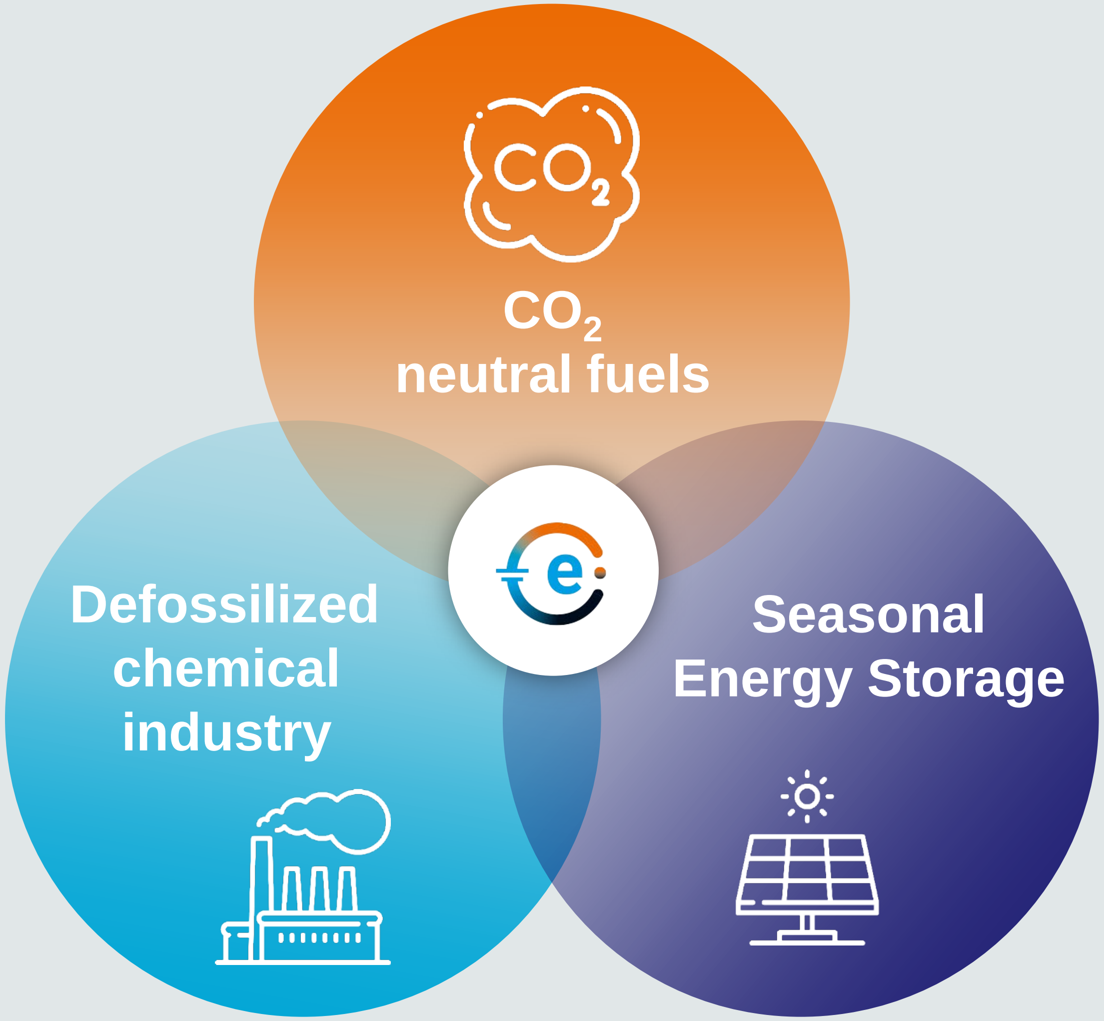
Industrial energy consumption NL:
1075 PJ/year of which ~50% non-energetic


e-Refinery
Towards sustainable production of chemicals and fuels
TU Delft
OTEC
e-Refinery

TU Delft

VISION

To accelerate the transition towards sustainable production of chemicals and fuels.



TU Delft

e-Refinery

RESEARCH

Scales

Micro
Electroconversion research

Meso
Reactor, process and system engineering

Macro
Life cycle analysis + societal embedding

Disciplines

- Power Engineering
- Catalysis
- Electrochemistry
- Materials science
- Transport Phenomena
- Reactor Engineering Process Intensification
- Process & Control
- Separation Technology
- Energy Technology & System Engineering
- System Integration & Societal Embedding

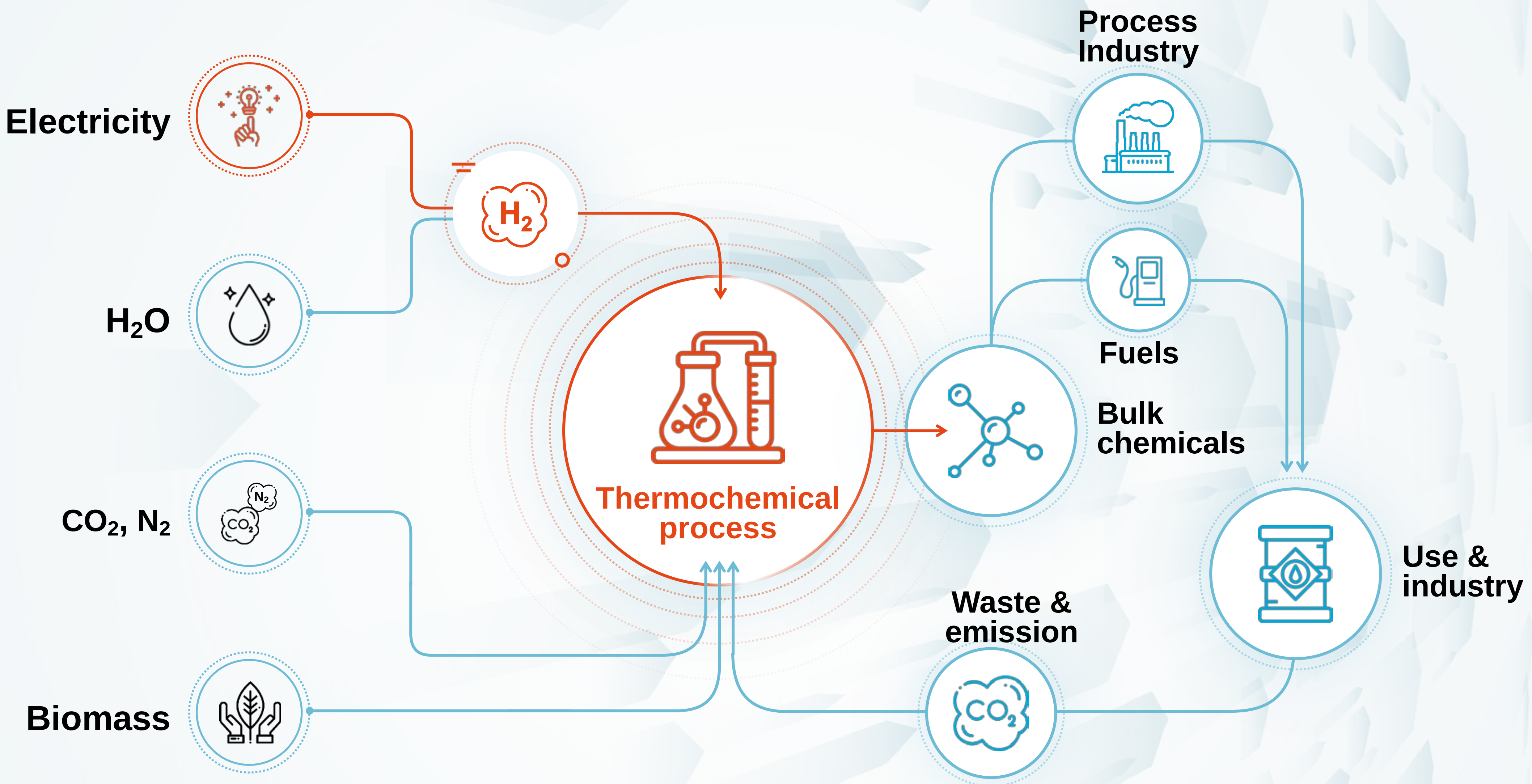
Research lines

- Indirect route
- Direct route

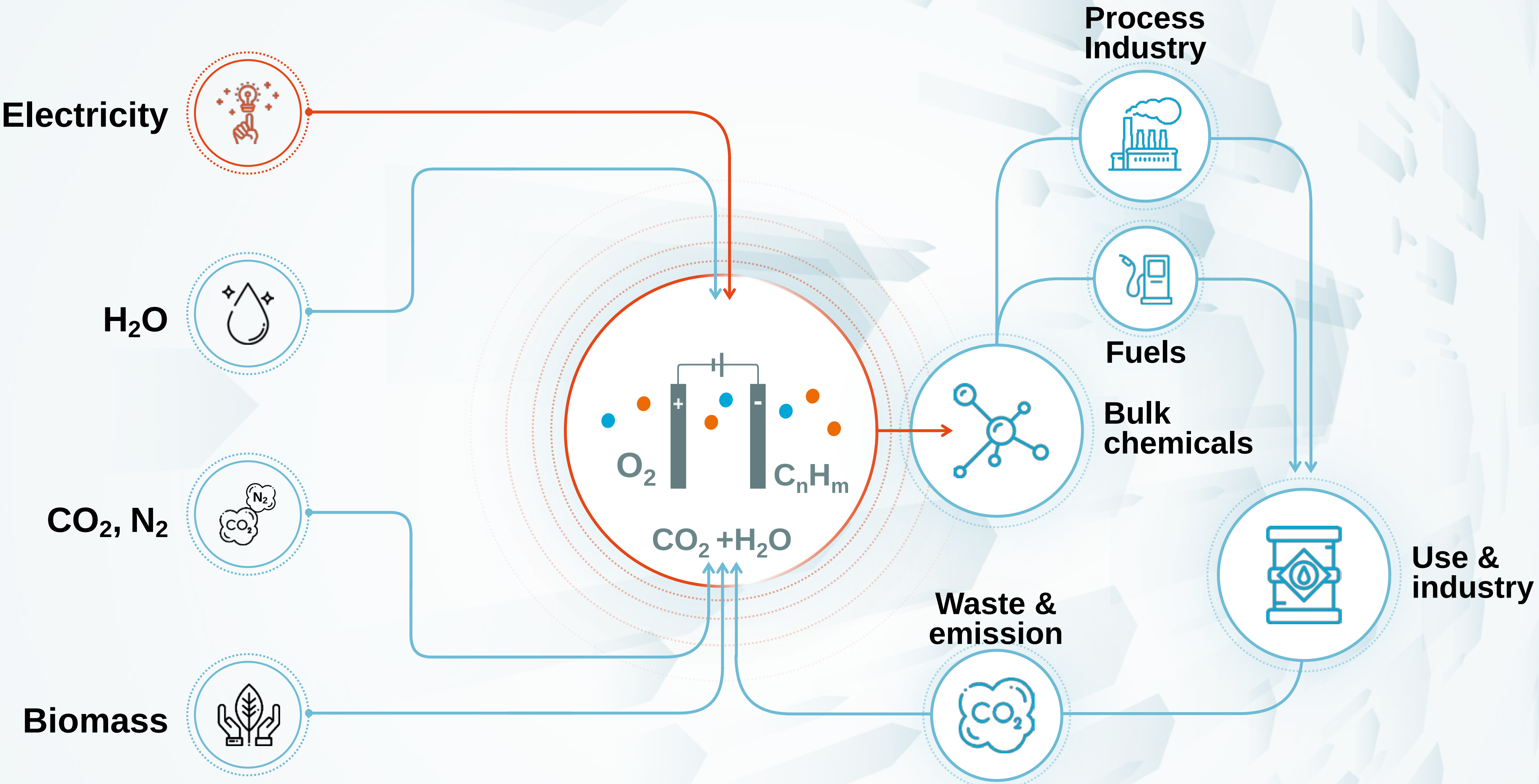
Base chemicals and fuels, such as CO, CH_4, C_2H_4, NH_3, etc.

TUDelft

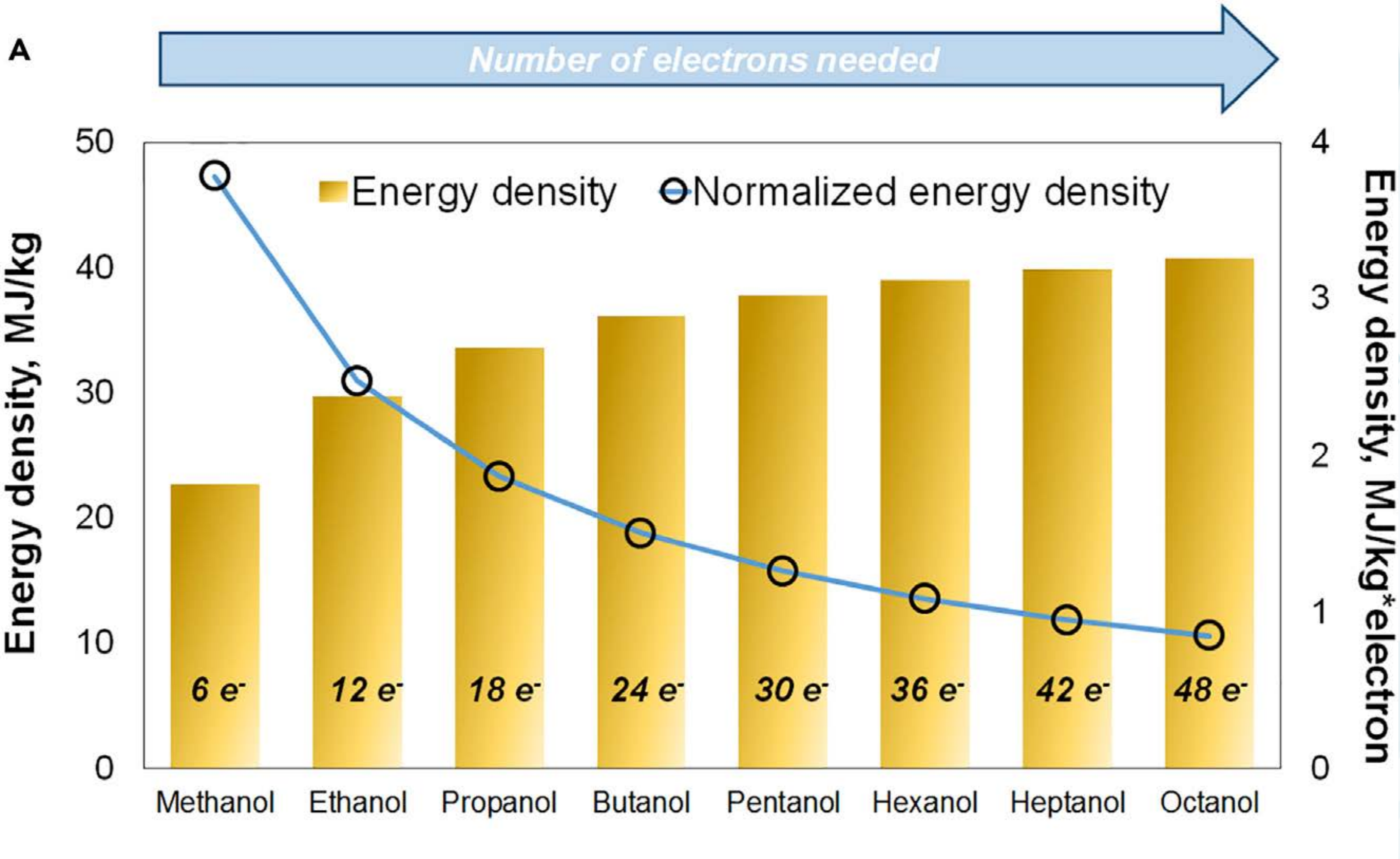
The indirect route



The direct route



Energy content per electron used (to make fuels)



Note: the kinetics slows down with the number of electrons

Joule 2, 825–832

Some feasible CO_2 reduction reactions

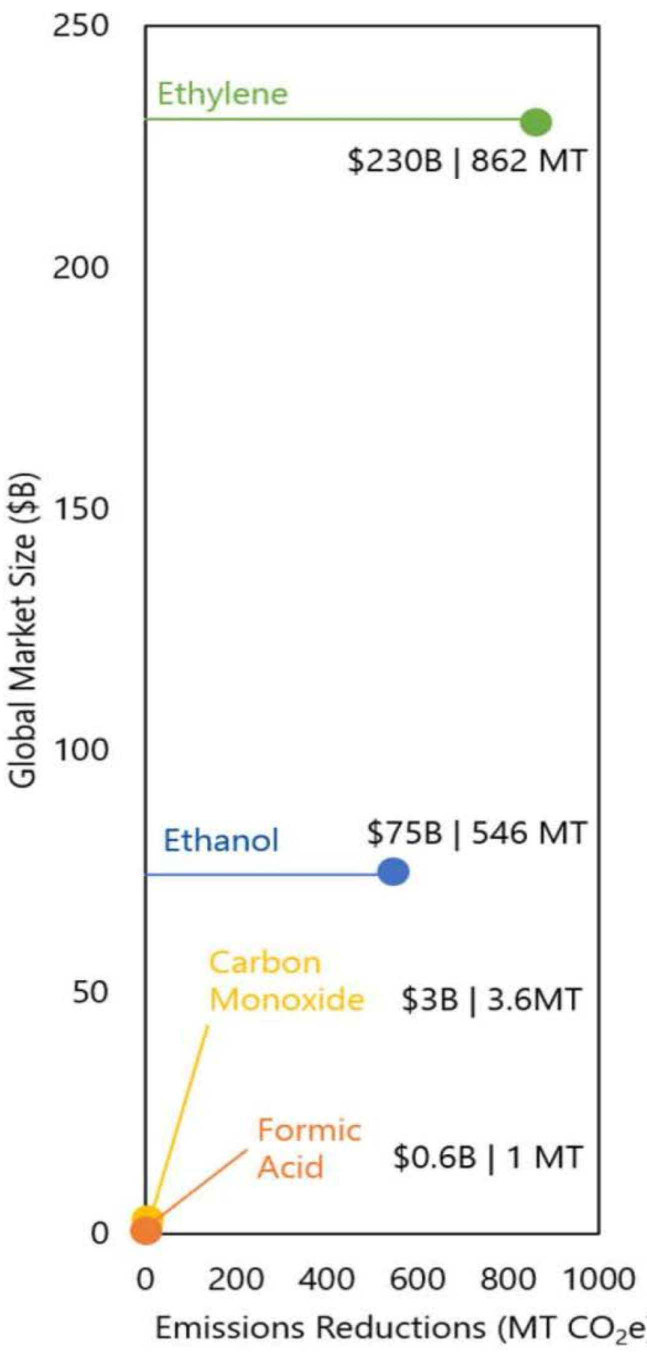
reaction	n	E°/V^a
$CO_2 \rightleftharpoons CO + 0.5O_2$	2	−1.33
$CO_2 + H_2O \rightleftharpoons HCOOH + 0.5O_2$	2	−1.43
$CO_2 + 2H_2O \rightleftharpoons CH_3OH + 1.5O_2$	6	−1.21
$CO_2 + 2H_2O \rightleftharpoons CH_4 + 2O_2$	8	−1.06
$2CO_2 + 3H_2O \rightleftharpoons C_2H_5OH + 3O_2$	12	−1.14
$2CO_2 + 2H_2O \rightleftharpoons C_2H_4 + 3O_2$	12	−1.15
$3CO_2 + 4H_2O \rightleftharpoons C_3H_7OH + 4.5O_2$	18	−1.13

Weber ACS Catal. 2019, 9, 946−950

TUDelft

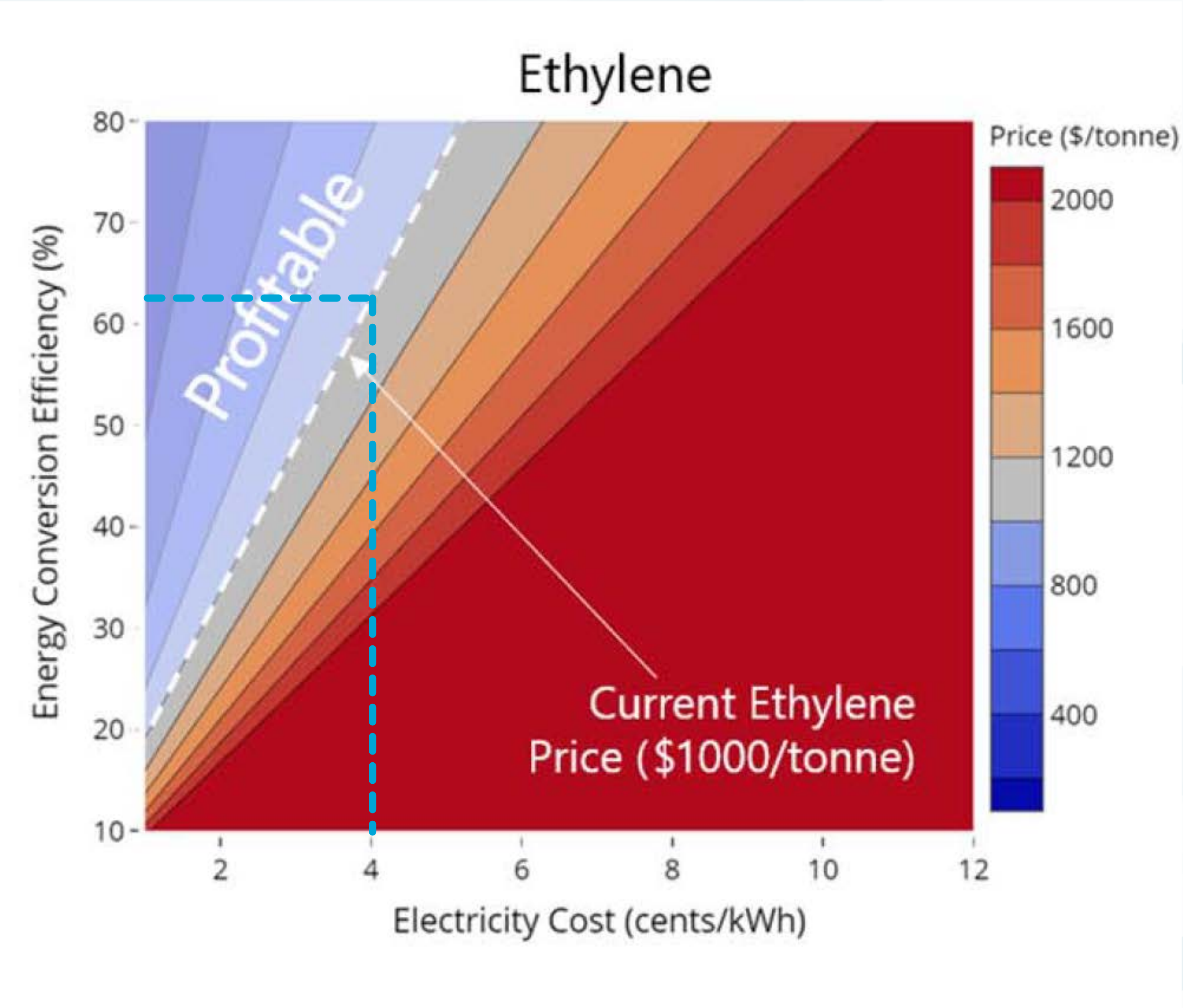
Let us focus on ethylene

- **Ethylene base material for plastic production**
- **Very large market (230 billion dollar)**
- **Very large emission reduction potential (863 MT)**



De Luna *et al.*, *Science* **364**, eaav3506 (2019) 26 April 2019

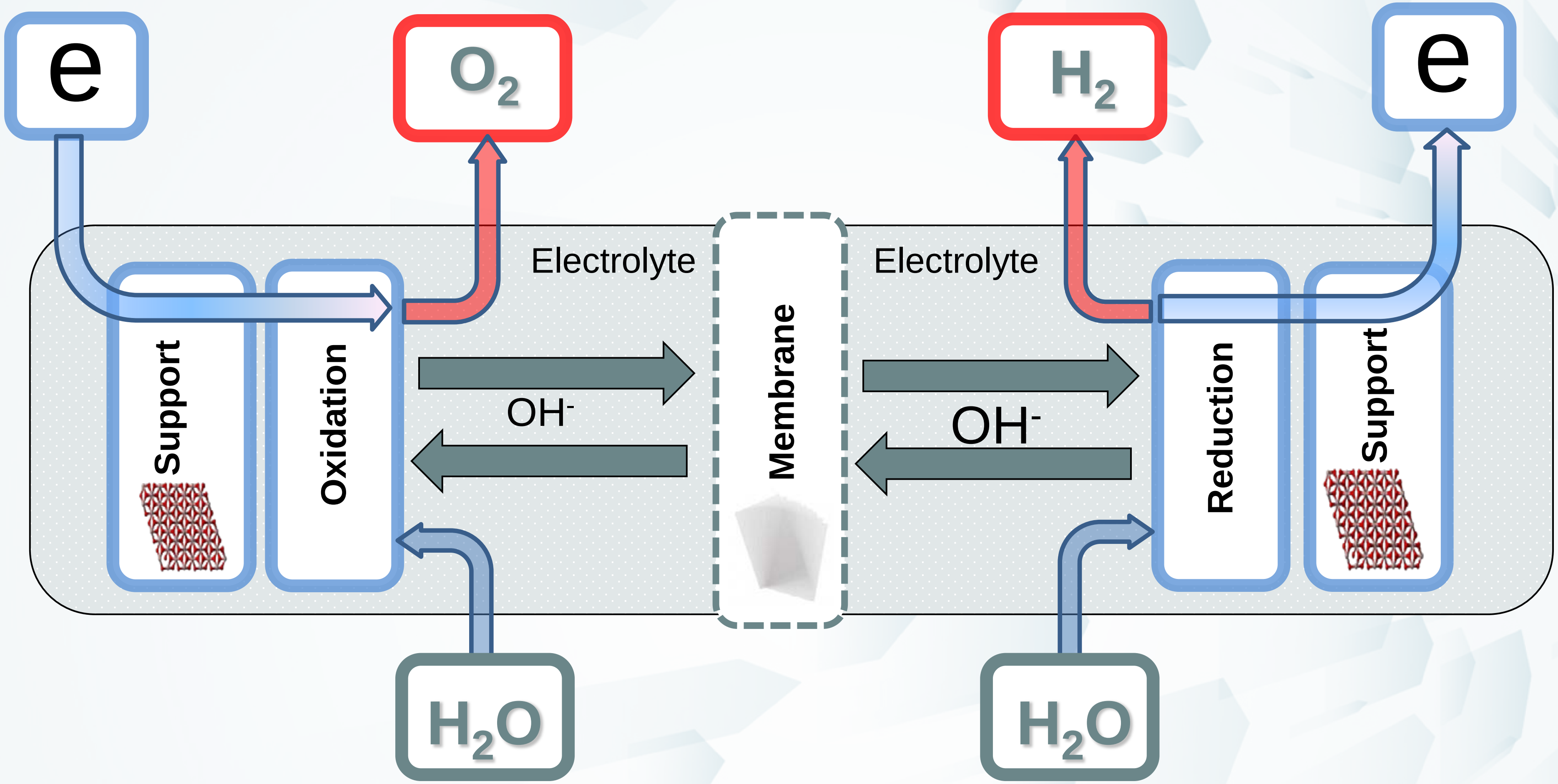
When is the electrochemical production profitable



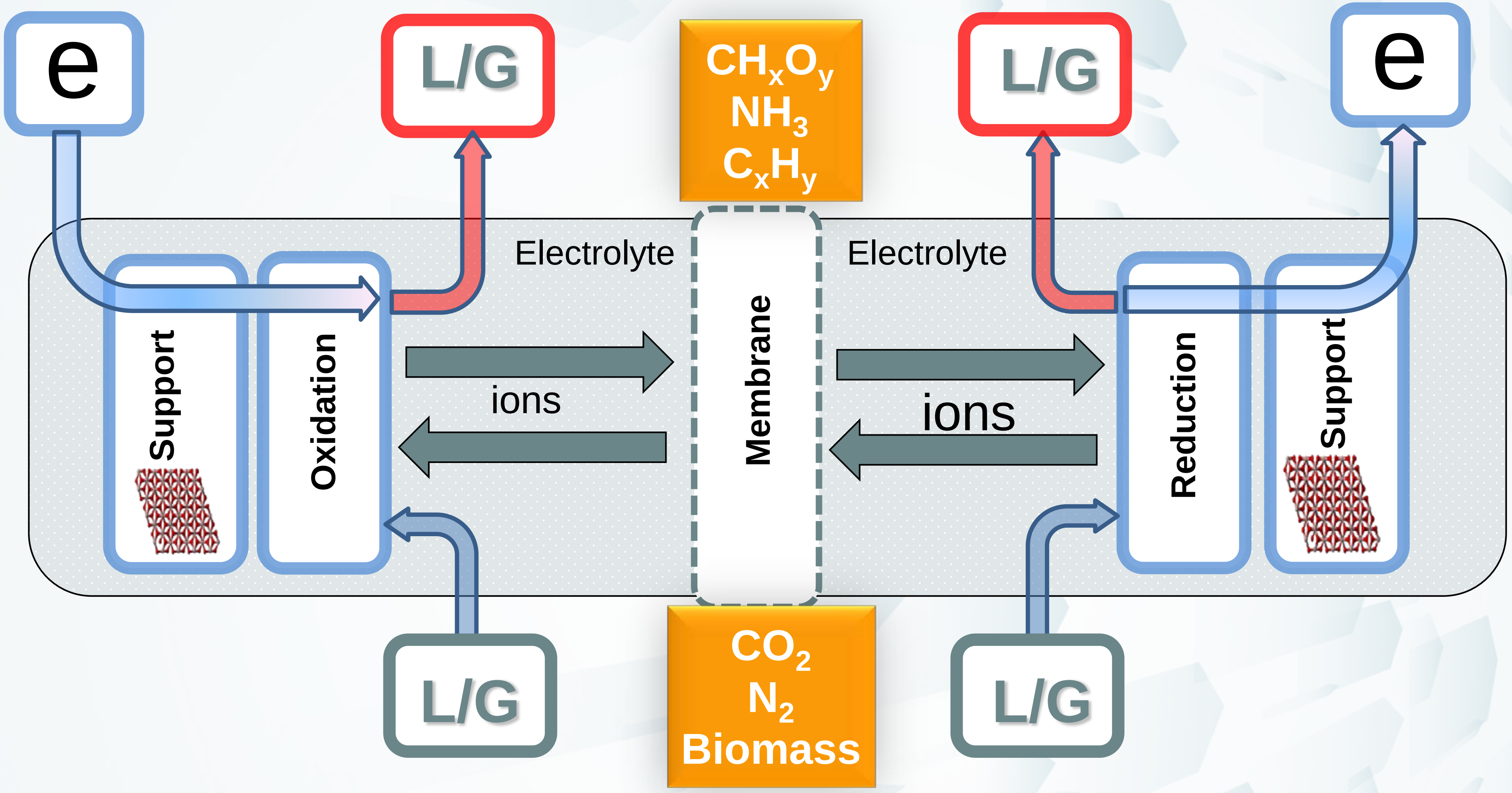
- DAC of CO_2 cost = $30/tonne
- Faradaic efficiency 90%
- Current density 500 mA/cm^2
- Electrolyser $300/kW

De Luna *et al.*, *Science* **364**, eaav3506 (2019) 26 April 2019

Water electrolysis: the medium equals the feed

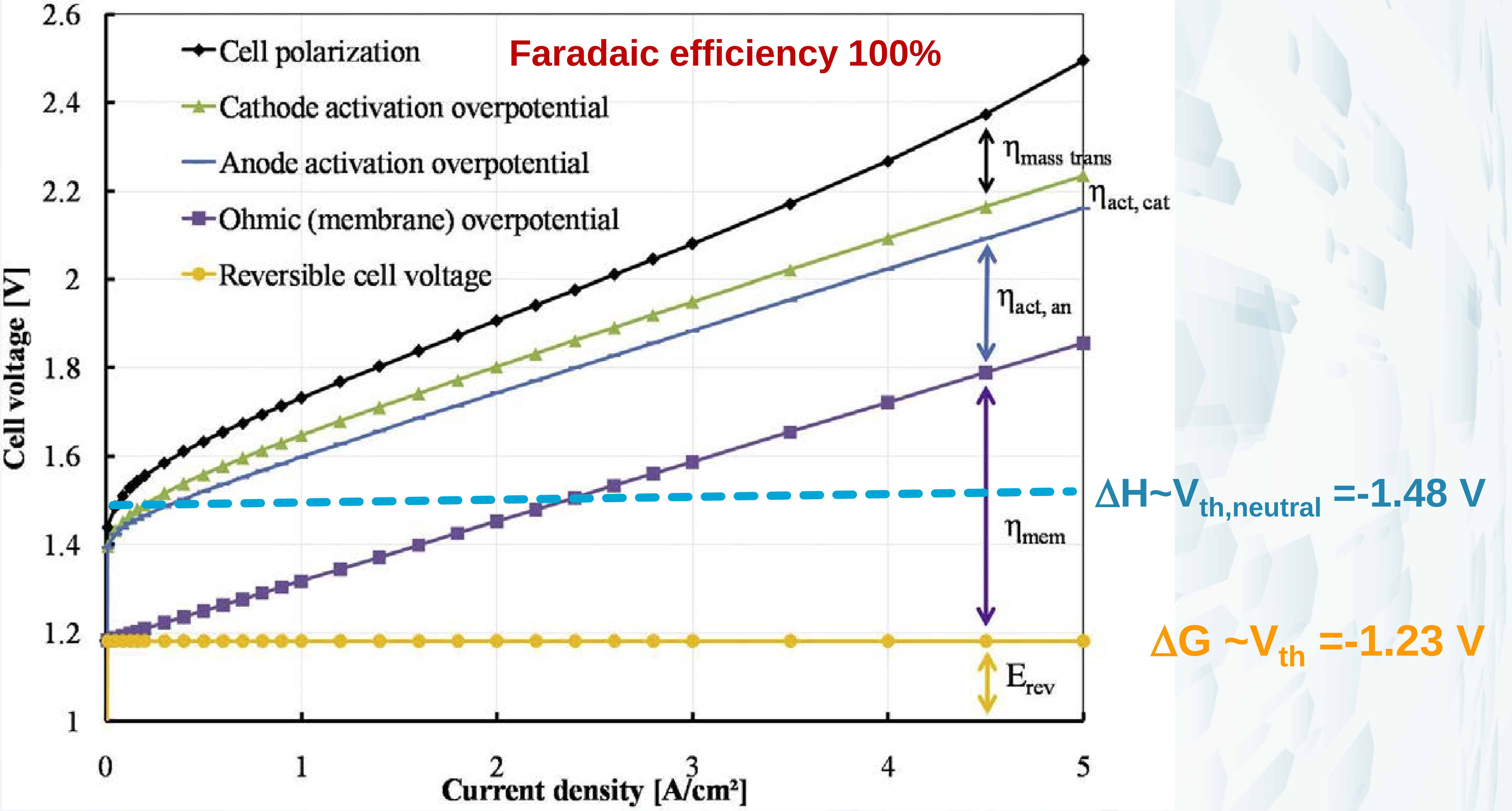


Electrolysis: the medium does not equal the feed

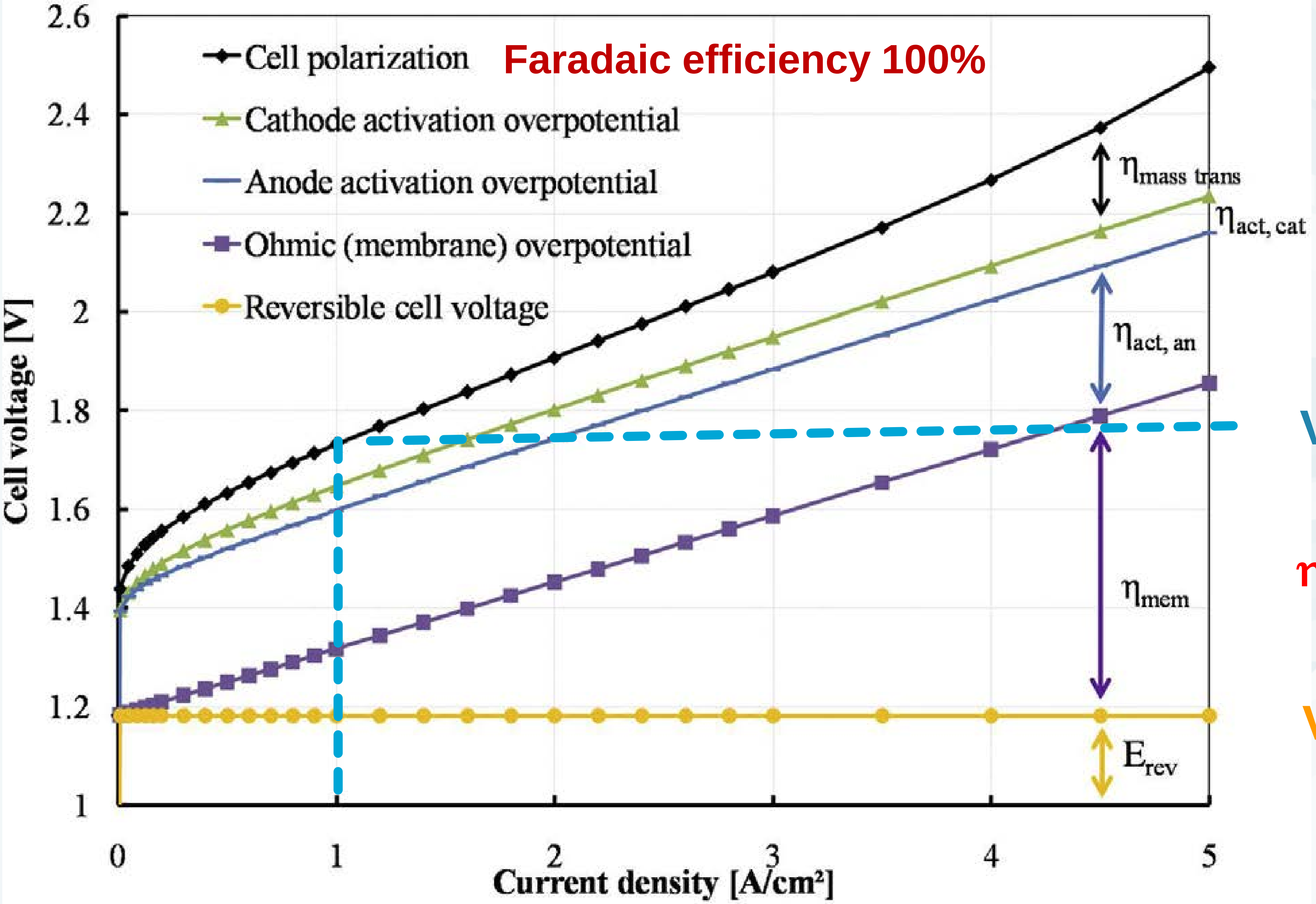


The nature of the feeds and products determines the reactor design

Typical losses water electrolysis



Typical losses water electrolysis



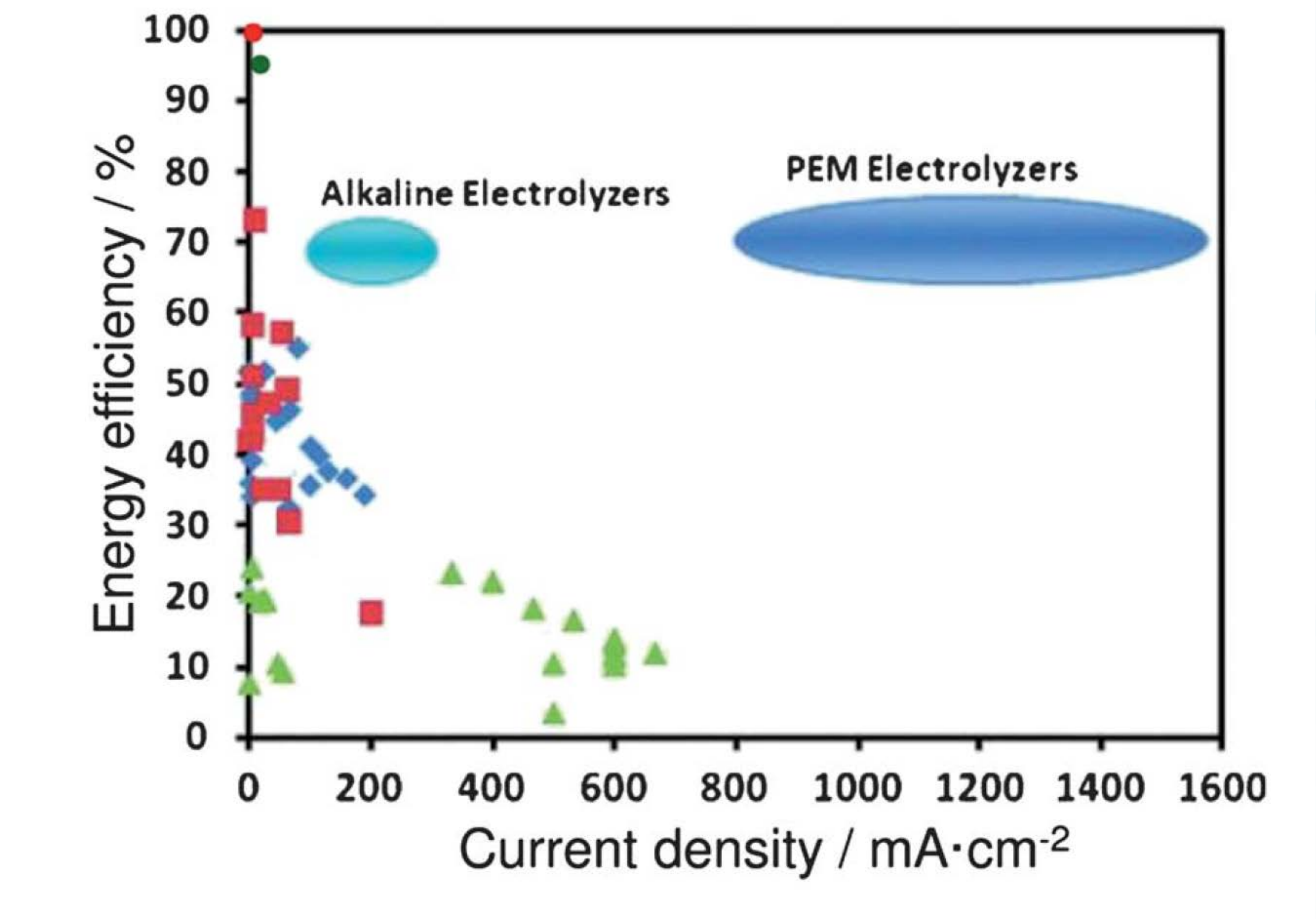
V_{op} ~-1.75 V

$\eta \sim V_{th} / V_{op} = 70\%$

V_{th} ~-1.23 V

IJHE 42 (2017) p25831

At high current density the efficiency of CO_2 conversion rapidly drops



Large scale implies: high current density + abundant materials

Energy Environ. Sci., 2013, **6**, 3112–3135 | **3121**

Some electrochemical reactions

Half-reactions:

$$12OH^- \rightarrow 3O_2 + 6H_2O + 12e^- \qquad -1.23\ V$$

$$12e^- + 2CO_2 + 8H_2O \rightarrow C_2H_4 + 12OH^- \qquad -0.08\ V$$

Sum reaction:

$$2CO_2 + 2H_2O \rightarrow C_2H_4 + 3O_2 \text{ with } \Delta G = 1331\ kJ/mol$$

Potential:

$$E = -\Delta G/nF = 1331kJ/\ (12*96485) = -1.15\ V$$

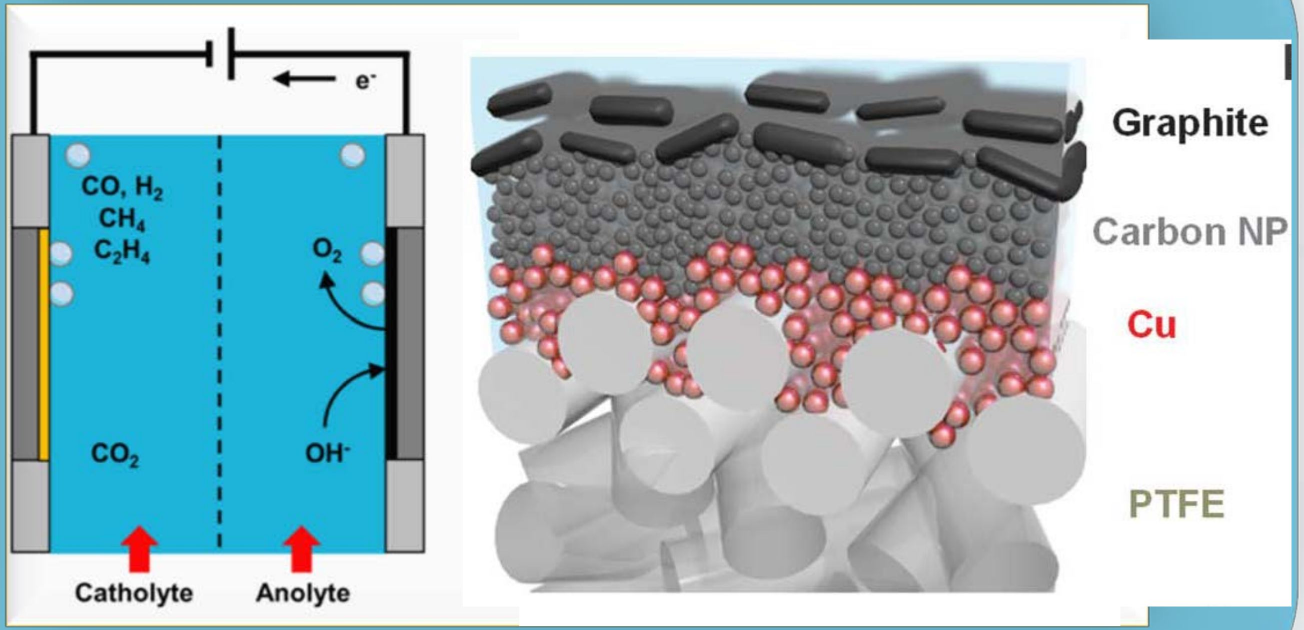
(Thermal neutral potential: $E = -\Delta H/nF = 1309kJ/\ (12*96485)\ -1.13\ V$)

TU Delft

Tom Burdyny

Science 360, 2018

What cell configuration



Limited CO_2 solubility in water

High OH^- concentration favours diffusion

Formation of Carbonates at high pH:

$CO_2 + OH^- \rightarrow HCO_3^-$

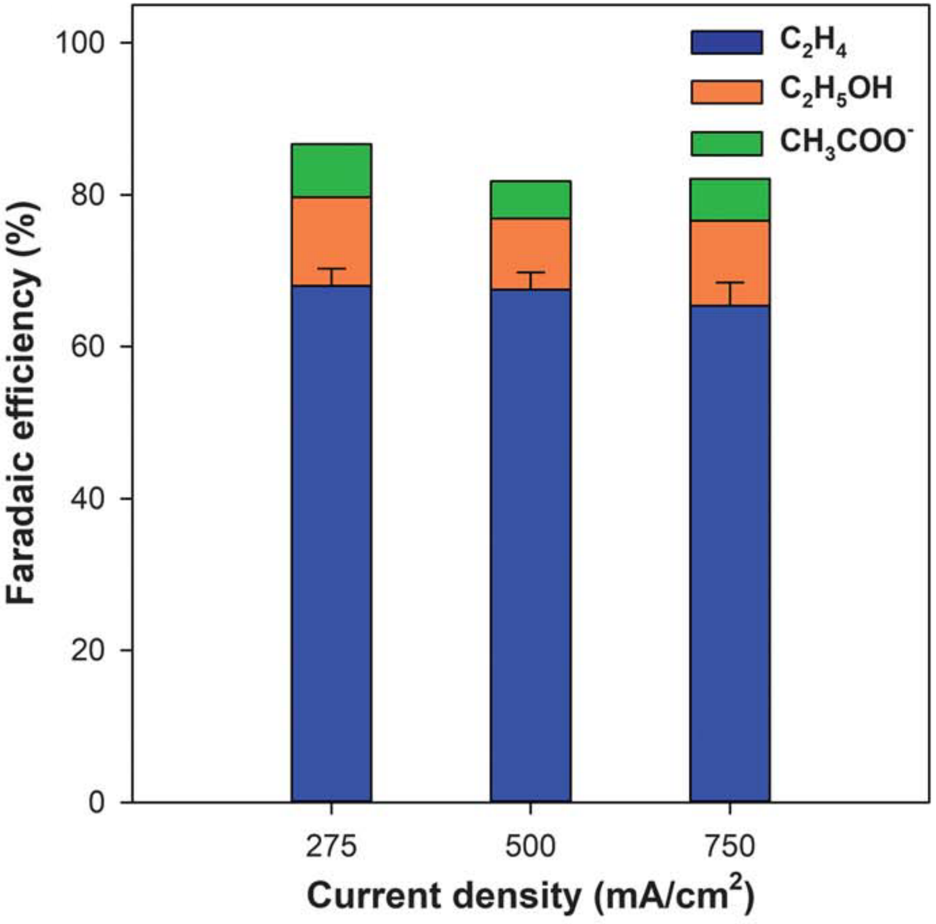
TU Delft

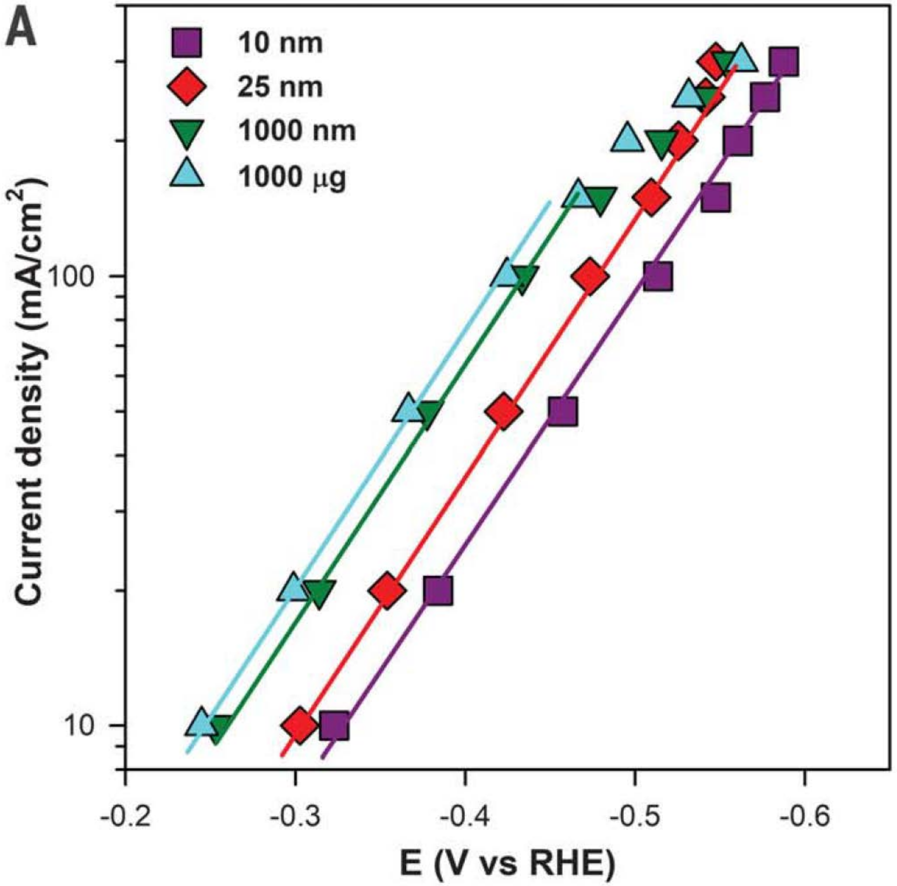
e-Refinery

High current densities, catalysis is not the problem

Tom Burdyny

Science 360, 2018



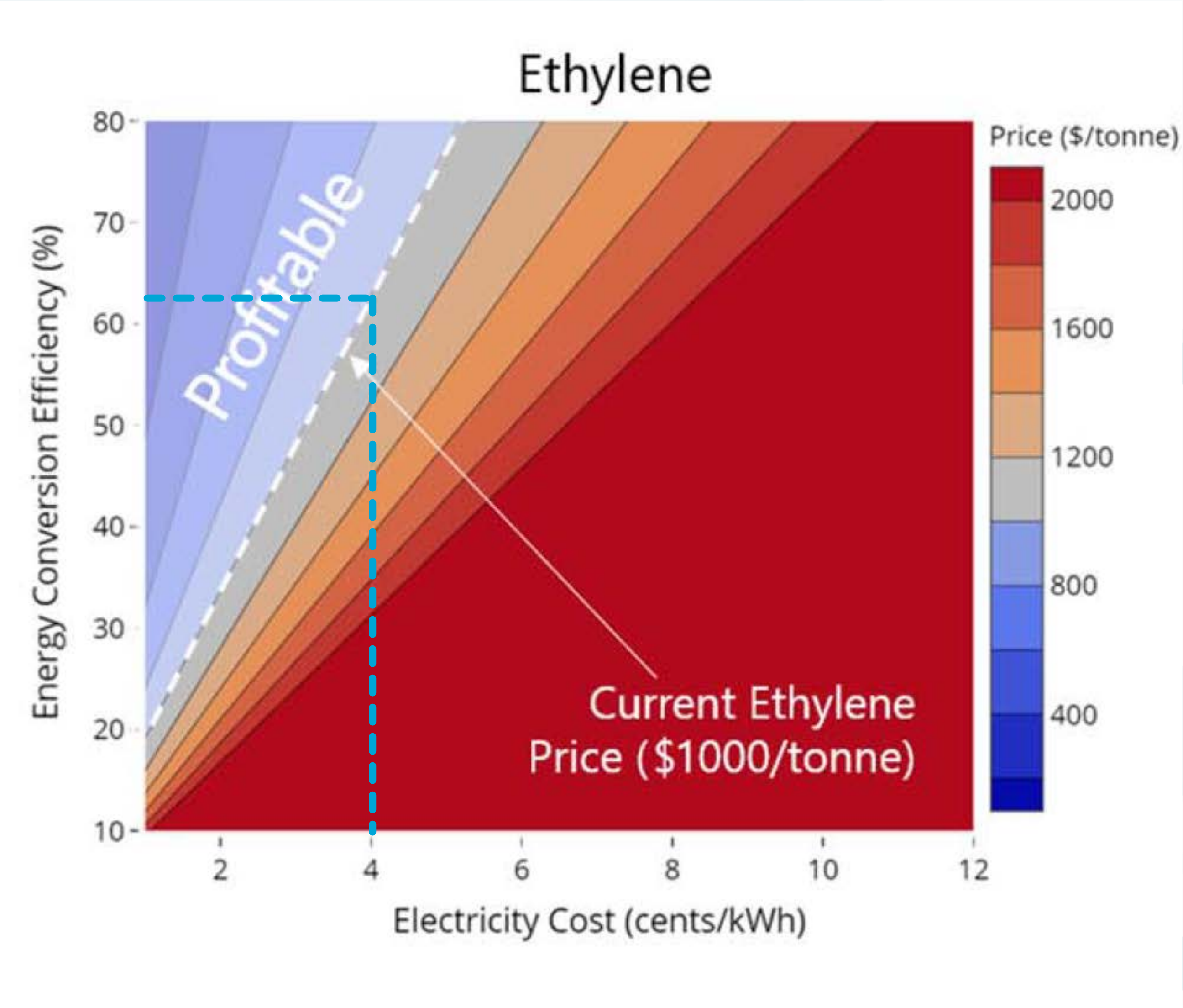


Faradaic efficiency 70%, Potential 3V, hence total energy efficiency 27%

TUDelft

e:Refinery

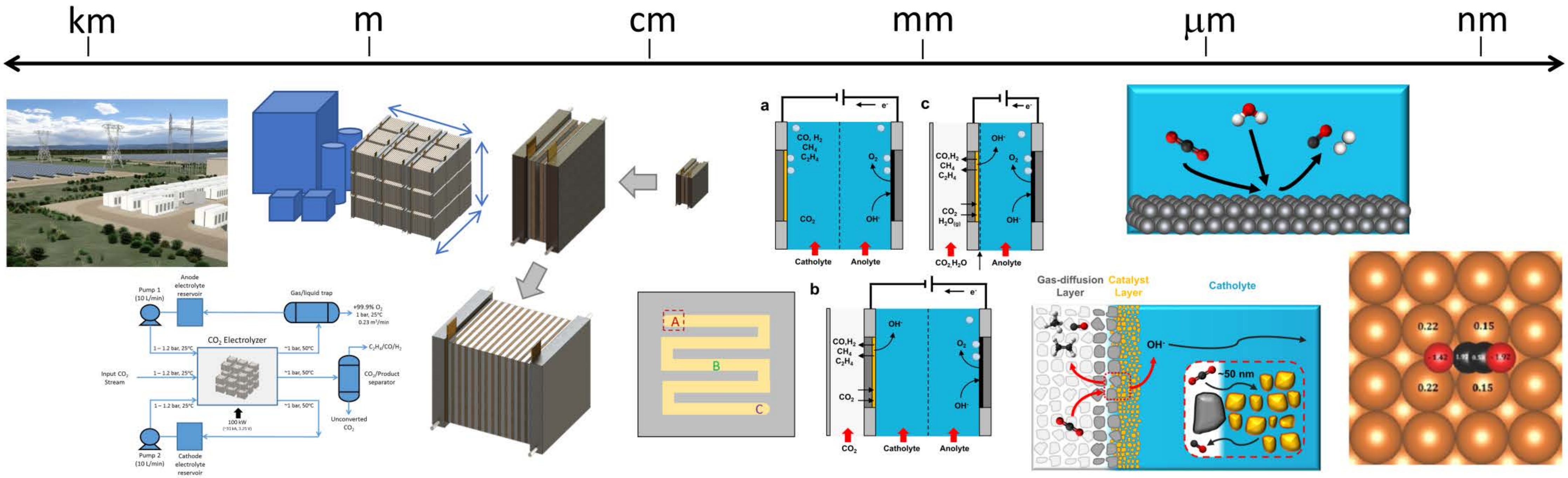
When is the electrochemical production profitable



- DAC of CO_2 cost = $30/tonne
- Faradaic efficiency 90%
- Current density 500 mA/cm^2
- Electrolyser $300/kW

De Luna *et al.*, *Science* **364**, eaav3506 (2019)   26 April 2019

Electro-conversion: from atoms to factories



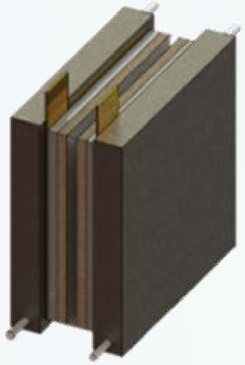
Large scale means: high current density + abundant materials

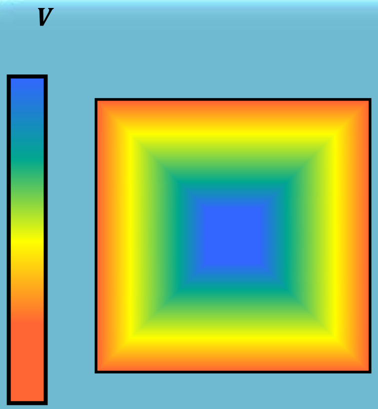
Ramirez De Jong Zeman Paddingv Ommen Mulder Burdyny Smith Vermaas Gonzalez Kortlever Straathof

Management of internal gradients

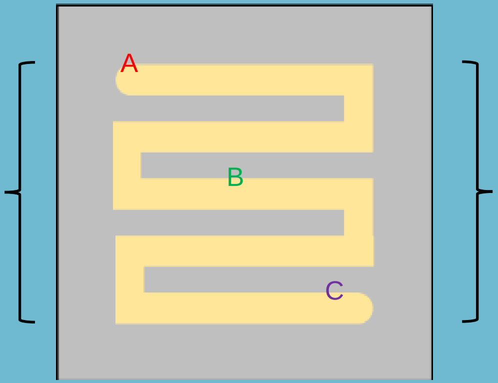
Tom Burdyny

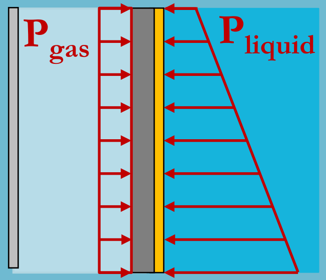
10-400 cm^2 Area





Voltage





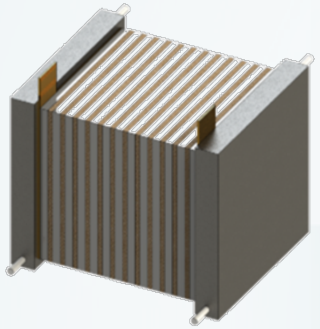
Pressure

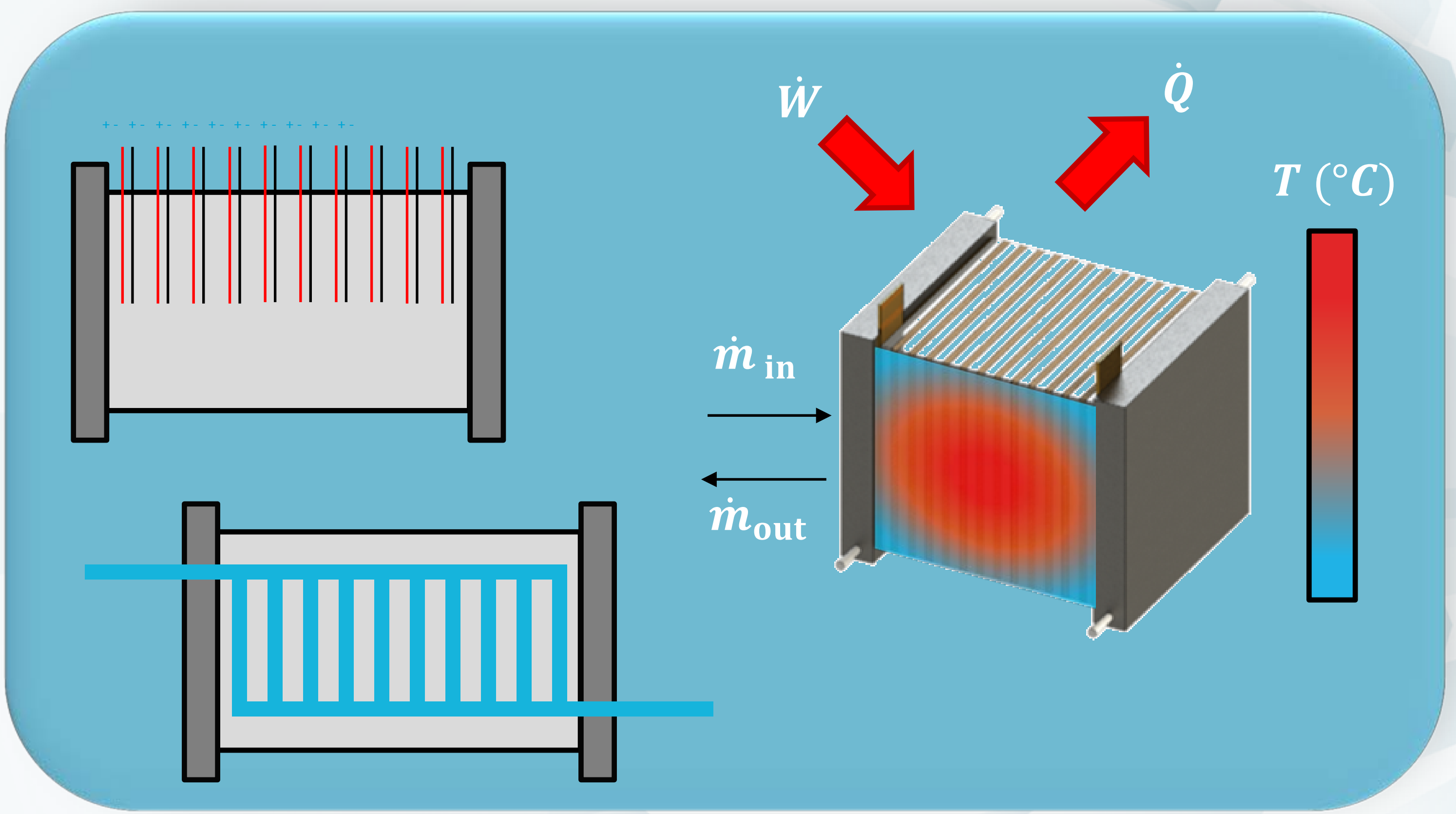
How to maintain uniform potential and pressure, to ensure that the same conversion takes place everywhere

Design of Stack:
Management of electrical potential and overall heat and mass balance

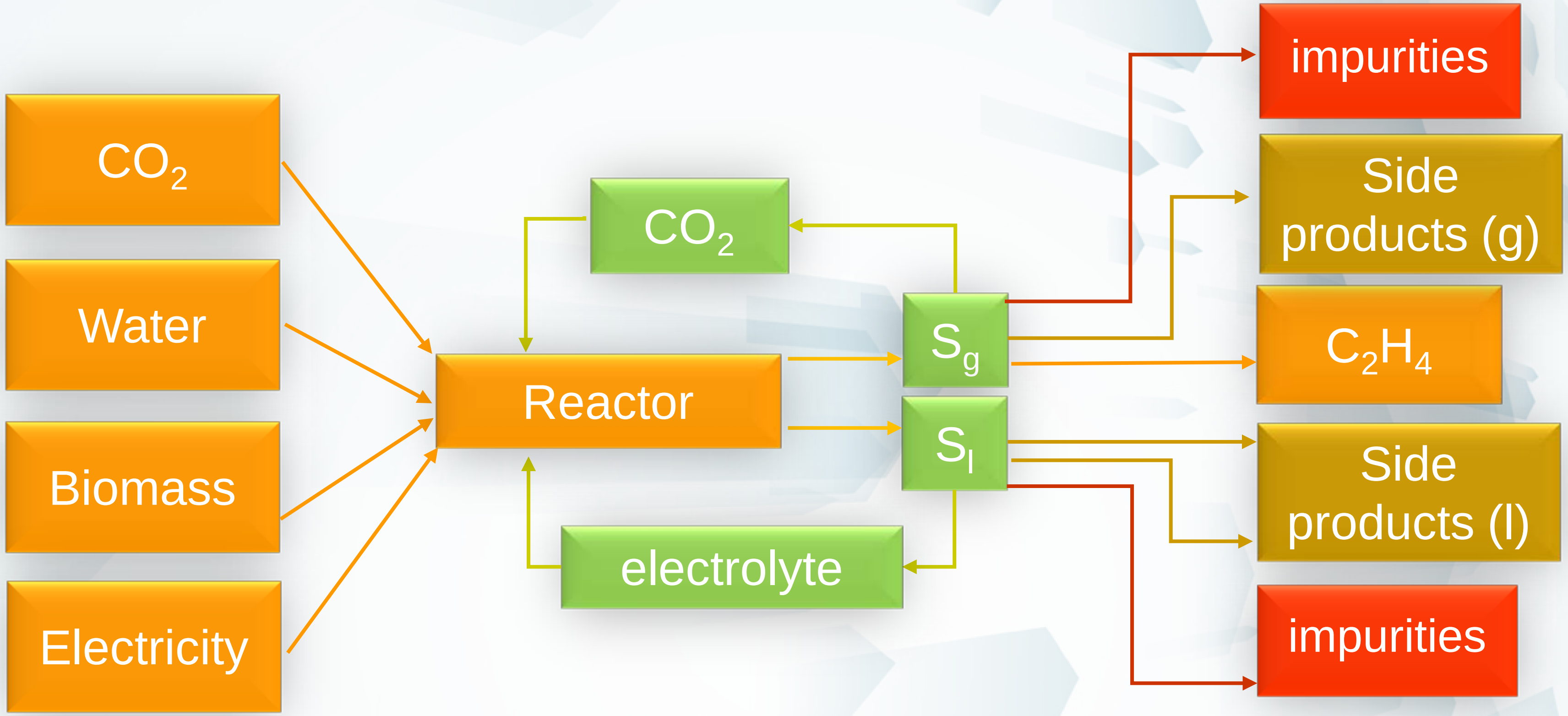
Tom Burdyny

'Stack'





System configuration



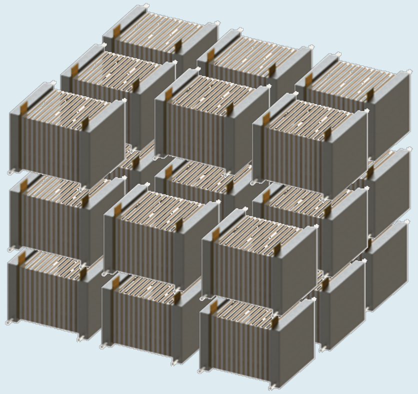
We need low temperature separation procedures!!

TUDelft

What does it take to make C_2H_4 from CO_2 and H_2O

System design

Total amperage:	~31 kA
Assumed potential	**~3 V**
C_2H_4 Produced:	~38 kg C_2H_4/day
Energy per tonne:	**~210 GJ/tonne**



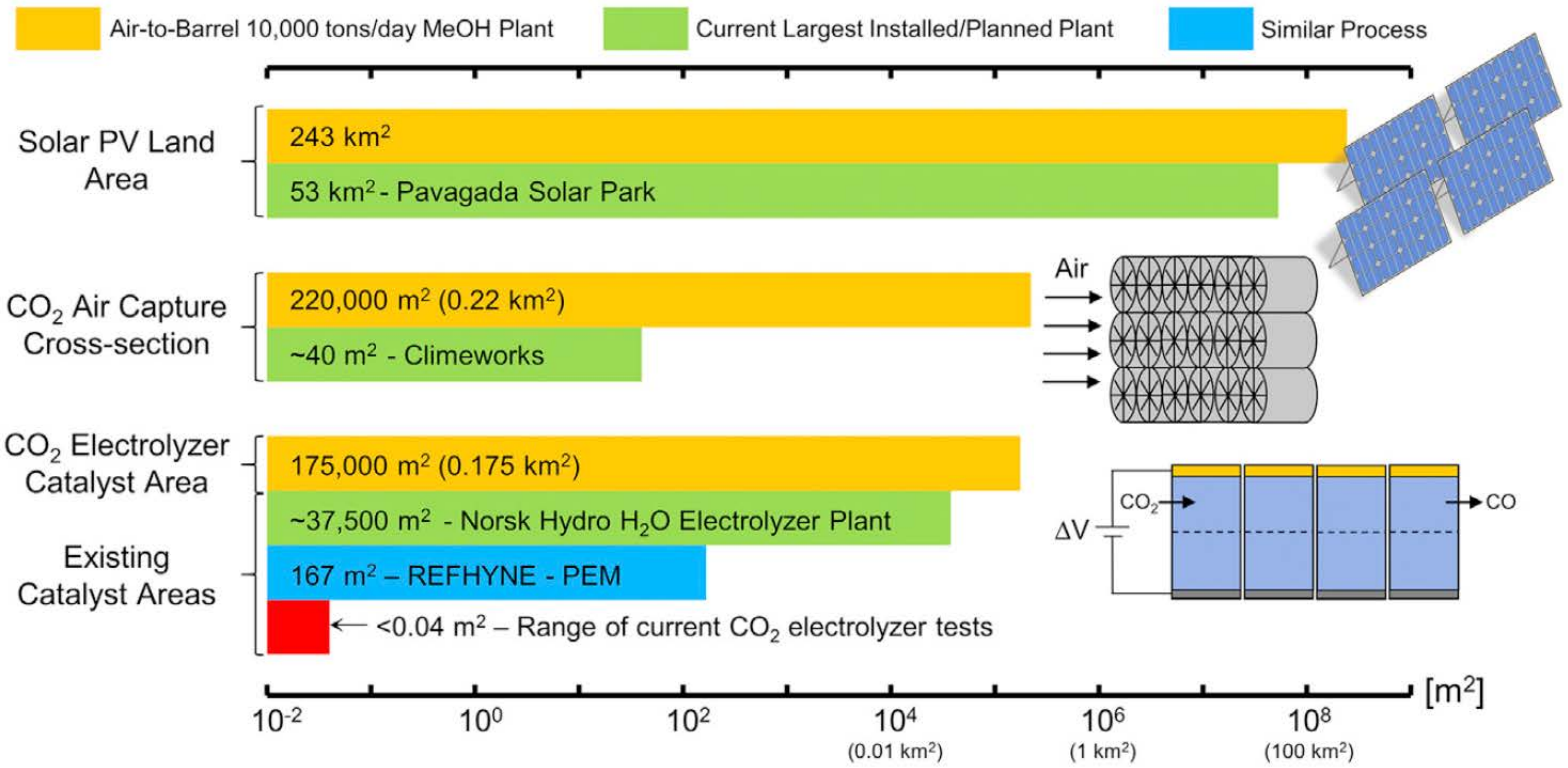
DOW Chemical plant in Terneuzen:

C_2H_4 from Naphta:	**1.5 Mton/year**
Energy cost:	**35,5 +20 = 55 GJ/ton***
	equivalent to 2.5 GW_e

This implies 10 GW_e electrochemically

*Energy 32 (2007) 1104–1123

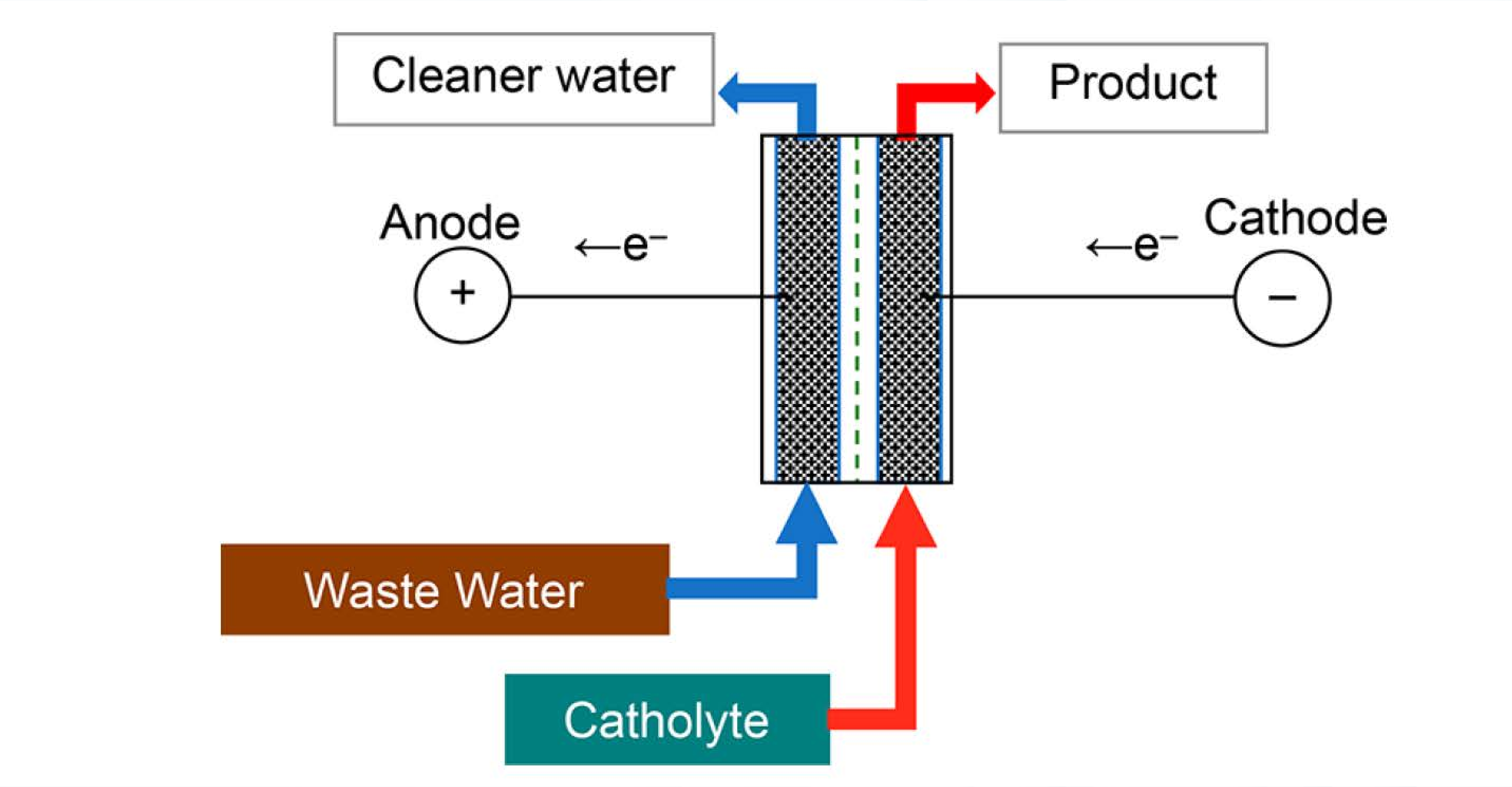
The scale of a 3.5 Mtonne/yr ‘air to barrel’ MeOH plant



The space needed for CO_2 capture <0.1 % of that of the PV panel space needed to generate the electricity

Smith et al. Joule 3, 1822–1834, August 21, 2019

System integration: a useful product at the anode?!



Weber ACS Catal. 2019, 9, 946–950

Conclusion

- CO_2 conversion to hydrocarbons is certainly possible
- Catalysis is not the only problem
- Many scientific and engineering challenges to be solved
- The scale of the technology needed for the energy transition is mind boggling
- The use of cheap and abundant materials is essential

Acknowledgements

Dr T Burdyny

Ir. John Nijenhuis

Dr. Wim Haije

Dr. Wilson Smith

Prof. Dr. Hans Geerlings

NWO Applied and Engineering Sciences

NWO Netherlands Organisation for Scientific Research

+ the whole e-Refinery community