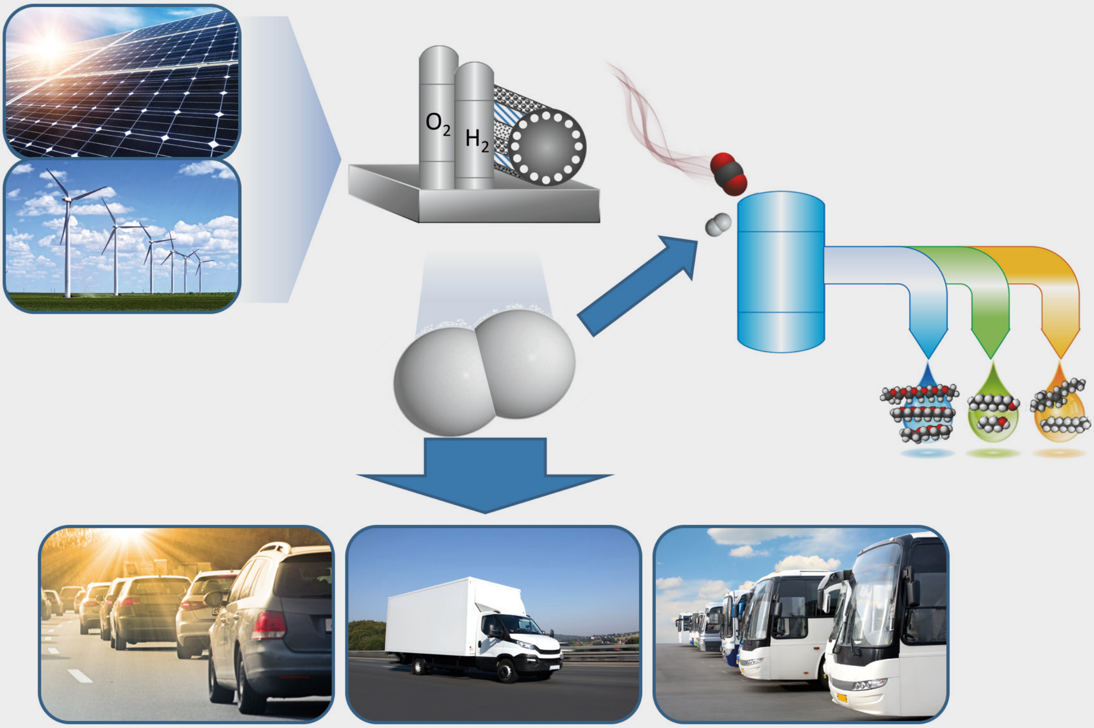

TRENDS 2017
Transition to Renewable Energy Devices and Systems

Detlef Stolten, Ralf Peters (Editors)

Energie & Umwelt / Energy & Environment
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Reihe Energie & Umwelt / Energy & Environment Band / Volume 447

Forschungszentrum Jülich GmbH
Institut für Energie- und Klimaforschung
Elektrochemische Verfahrenstechnik (IEK-3)

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Contents

Preface

The round table discussion, *TRENDS 2017: Transition to Renewable Energy Devices and Systems* took up relevant topics in the area of the transformation of the energy system. The objective of the conference was to highlight game changers and address missing links in order to achieve the G8 goals of reducing CO_2 emission by 80% by 2050 and realizing a major share of renewable power by 2030.

TRENDS 2017 focused on relevant topics in relation to the transformation of the energy system and highlighted the interconnection of the power and transport sectors against the backdrop of the COP21 goals. The conference proceedings provide useful data, facts and figures to share different insights from power generation, energy transport and the use of energy in the transportation sector.

There are various approaches to make use of the volatility of renewable power generation in today's energy system as efficiently as possible. Thus, it is necessary to determine appropriate storage technologies and/or to further develop the existing energy system with consideration to fluctuating power generation. The main topics of the conference were the status and prospects of hydrogen vehicles and batteries, Power-to-Fuel, DCDC grids, ideas for sector coupling and the connection of climate zones.

We have compiled most of the presentations of TRENDS 2017, together with a short abstract to a proceedings book. We would once again like to thank all participants for their valuable presentations and contributions to the discussion. With regard to a follow-up, we invite interested readers of this compilation to send their comments to the editors. We would be glad to implement new features in a future event.

Detlef Stolten, Ralf Peters,

Forschungszentrum Jülich GmbH
Institute of Energy and Climate Research
IEK-3: Electrochemical Process Engineering

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Sector Coupling for Germany until 2050 - An Energy Systems Perspective -

Detlef Stolten, Martin Robinius
d.stolten@fz-juelich.de

Institute of Electrochemical Process Engineering (IEK-3)

TRENDS2017 – Transition to Renewable Energy Devices and Systems
Interconnecting Power and Transport in View of COP21
Aachen
December 5 – 6, 2017

Interconnecting Power and Transport

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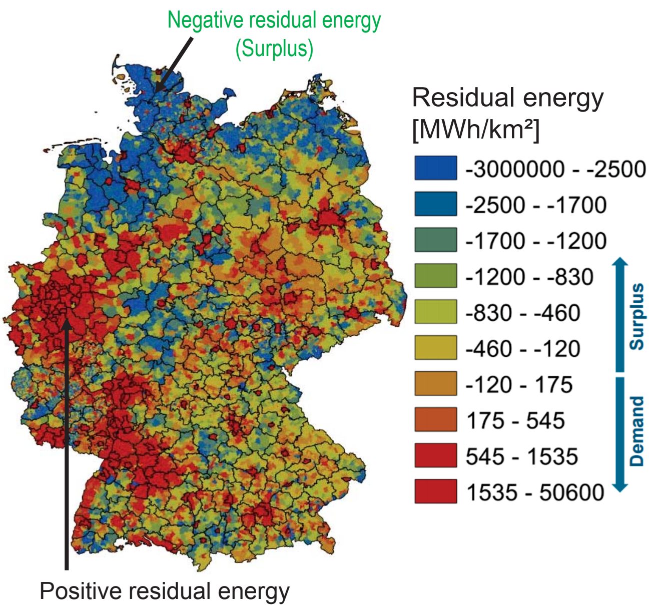

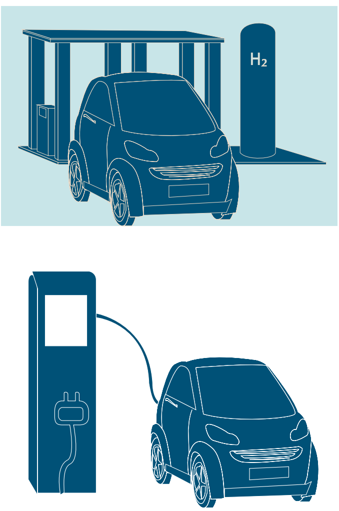

Setting the Scene

Basic Requirements for a Future Energy System

- In 2050 **CO_2 emissions** based on 1990 shall **be reduced** by **80-95 %**
- After the transition period energy should **not** be **more expensive** than today
- **Limited emissions** shall be reduced

- Electricity, fuels and heat must be available with **high reliability**
- **All energy sectors** need **to be addressed**
- Teratogenic, carcinogenic and poisonous substances shall be avoided

Paramount Topics

- Storage
  - Short term: **grid stabilization** (pumped hydro, batteries, gas storage etc)
  - Long term: **compensate for** sustainedly **low power generation** (only gas storage feasible)
- **Transportation** (from generation to consumption; connecting regions of different climate)
- Compensation of fluctuating renewable input
- **Spatial restrictions**
- Handling dichotomy between a **very distributed** (e.g. household PV) vs. **very centralized** system (off-shore wind farms and coastal on-shore wind power generation)
- Interconnecting the energy sectors

Timeline for CO_2-Reduction and the Implication of TRL Levels

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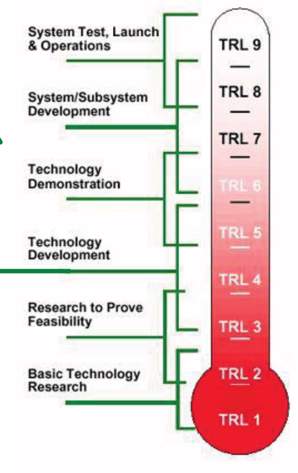
- **2050:** 80% reduction goal fully achieved
- **2040:** start of market penetration
- **2030:** research finalized for 1st generation technology

Development period: unil 2040

Research period: until 2030

⇒ 15 years left for research => TRL 5 and higher

TRL 4 at least



This is not to say research at lower TRL levels is not useful, it will just not contribute to the 2050 goal

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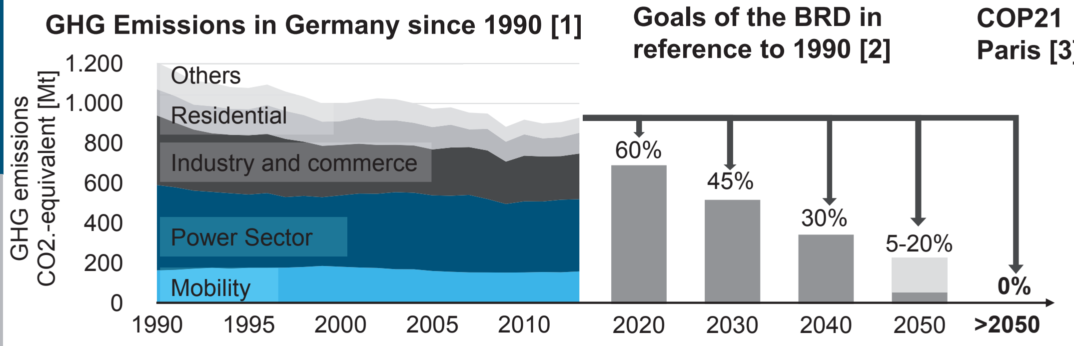
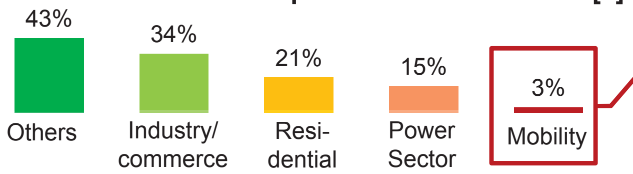
The Energy Systems Background

The overall GHG emission goals of Germany require a holistic transformation of all sectors

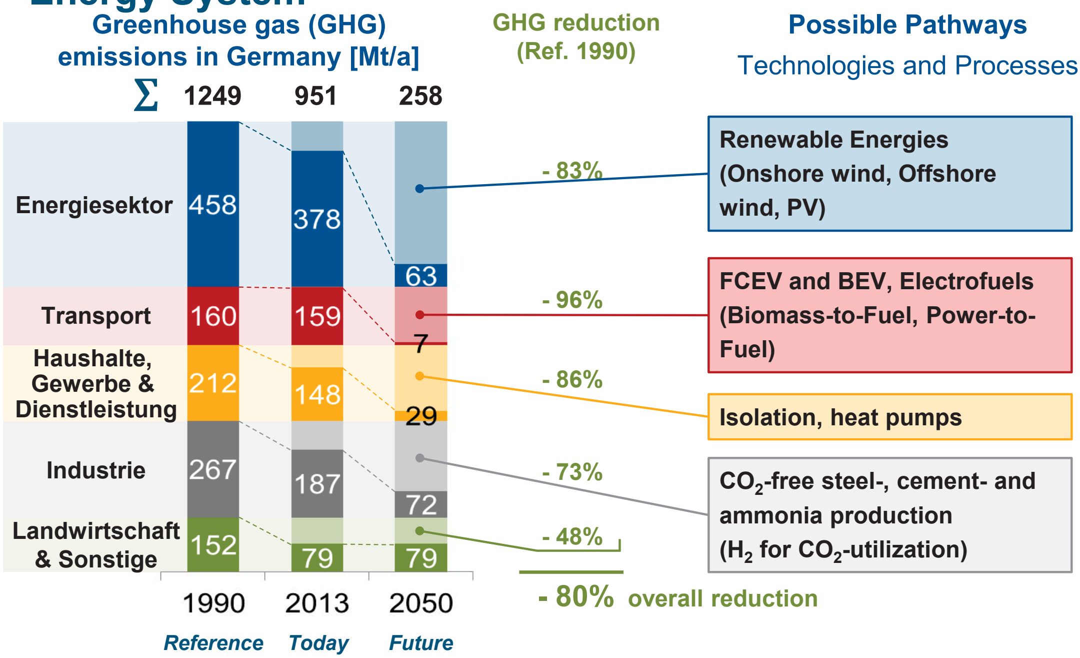




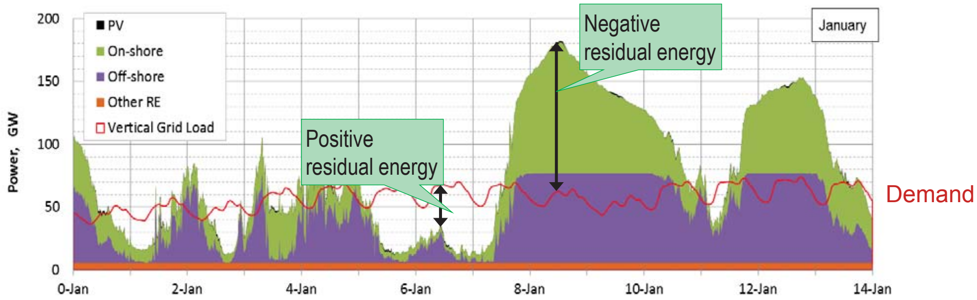
The mobility sector lags behind in comparison to the achieved emission reductions of the other sectors.

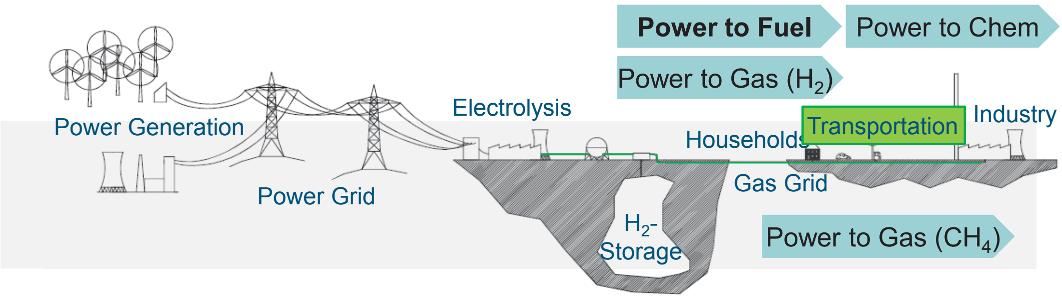
[1] BMWi, *Zahlen und Fakten Energiedaten - Nationale und Internationale Entwicklung*. 2016, Bundesministerium für Wirtschaft und Energie: Berlin.
[2] BRD, *Energiekonzept für eine umweltschonende, zuverlässige und bezahlbare Energieversorgung*, Bundeskabinett. 2010: Berlin.
[3] UN, *Paris Agreement - COP21*, United Nations Framework Convention on Climate Change 2015: Paris.

Sector Coupling for the Future Energy System



Excess Power is Inherent to Renewable Power Generation





Overcapacity in Power is Inherent for Full Renewable Energy Supply

$$\text{Capacity factor} = \frac{\textbf{energy harvested}}{\textbf{nameplate power} * 8670\ hrs}$$

Average power demand for Germany: ~ 60 GW (based on **528 TWh** grid electricity)

	Capacity factor	Necessary Power, if just one Technology is applied	Reasonable power mix DE 2050 (DE gov. Installation plans extrapolated)	Reasonable electricity mix DE 2050	Electricity to be converted to H_2 (serving 75% of passenger vehicles in DE)
Offshore wind	0.46	120 GW	59 GW	236 TWh	
Onshore wind	0.23	230 GW	132 GW	267 TWh	
PV	0.12	460 GW	120 GW	126 TWh	
Total	--------	----------	311 GW	**629 TWh**	101 TWh (**2,1 mt H_2**)
Untimely produced electricity				≈ 200 TWh (to be stored)	
CO_2 cut Ø 80%				90% (10% power by NG)	54% of passenger cars

Projection of Renewables According to Current German Policy

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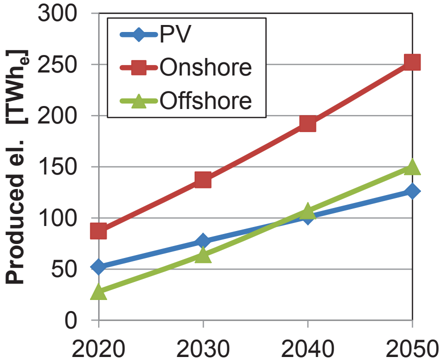

		2020	2030	2040	2050
Peak excess power*	GW_e	22	55	90	125
Excess energy*	TWh_e	2,5	30	100	200
Minimum storage size**	TWh	0,9	6	12	17

Simple Model to Illustrate the Impact of Cost Considerations

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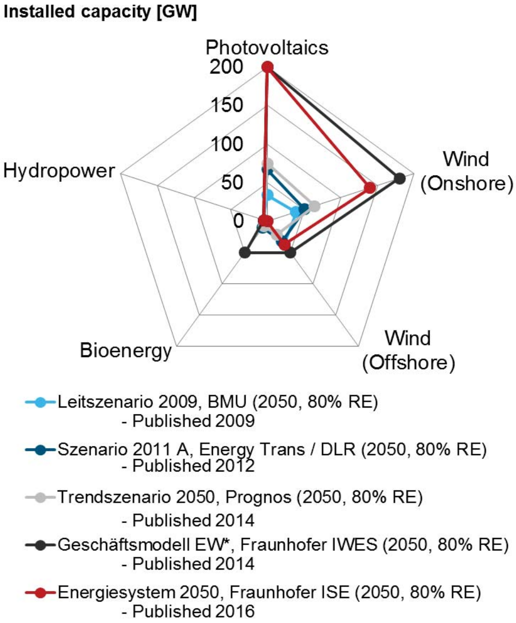
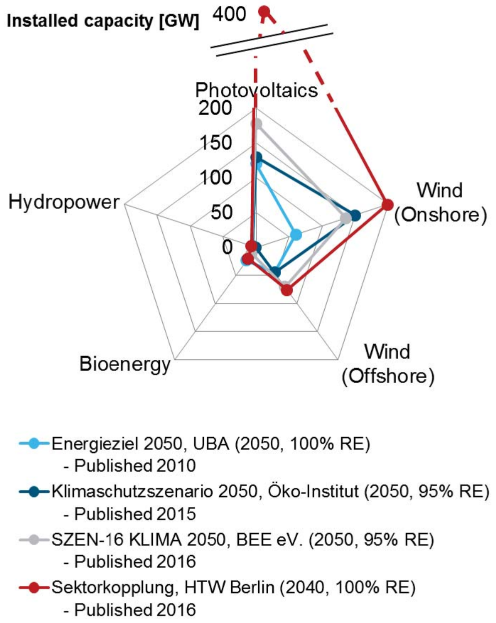
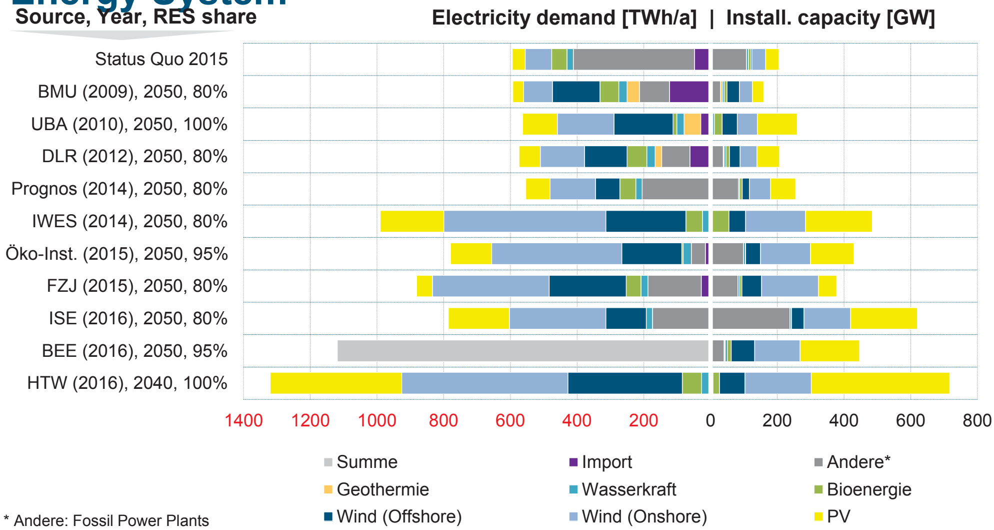
		Base Case	The Value of Transport
Energy transport		Pipeline	Not connected
North	Onshore wind	49.9 GW	8.1 GW
North	Inst. electrolyzers	40.8 GW	7.3 GW
North	Storage capacity (UGS)	8.8 TWh	1.6 TWh
South	Onshore wind	0 GW	75.8 GW
South	Inst. electrolyzers	0 GW	34.9 GW
South	Storage capacity (Large vessel)	0.3 TWh	12.3 TWh
Total annual cost (TAC)		**TAC_{bc}**	**199% of TAC_{bc}**

CO_2 Reduction from 80 to 95% is About as Challenging as from Today Down to 80%





Sector Coupling changes the Energy System

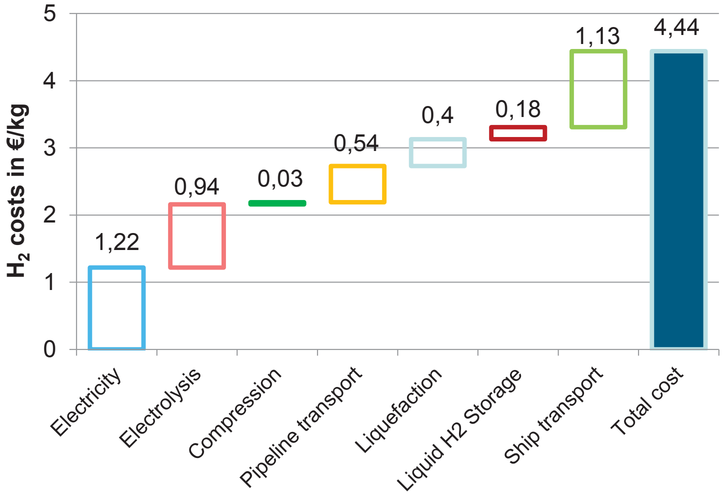


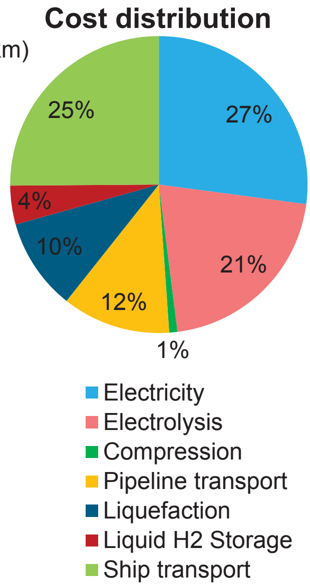
* Andere: Fossil Power Plants

- **Higher electricity demand due to P2X technologies which will be served throw Renewable Energy Sources**

Cost Results for H_2 provision – Patagonia to Japan

- H_2 Production of 8.8 Mt/a in Patagonia (use of wind energy)
- Domestic transport via Pipeline (4,500 km)
- Liquefaction and storage in domestic harbor (Cap.: 113,600 tons)
- International transport via ship (Punta Arenas to Yokohama: 17,712 km)





Transportation

Estimated Data for Passenger Car-based Transport in 2050

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Battery vehicle (renewable electricity)		Fuel cell vehicle (renewable electricity)	
Efficiency:	80 % x 85 % = **68 %** (WTT) (TTW)	Efficiency:	63 % x 60 % = **38 %** (WTT) (TTW)
Vehicle cost:	⊖⊖	Vehicle cost:	⊖⊖
Fuel production:	⊕	Fuel production:	⊖
Storage & distrib.:	⊖⊖⊖	Storage & distrib.:	⊕
Operating range:	low	Operating range:	medium - high
Resources:	sufficient	Resources:	sufficient
Soot/NOx emissions:	none	Soot/NOx emissions:	none
Combustion engine (CO_2-based fuels)		**Combustion engine (bio-fuels)**	
Efficiency:	70 % x 50 % x 25 % = **9 %** (H_2) (plant) (TTW)	Efficiency:	50 % x 25 % = **13 %** (WTT) (TTW)
Vehicle cost:	⊖	Vehicle cost:	⊖
Fuel production:	⊖⊖	Fuel production:	⊖⊖
Storage & distrib.:	⊕⊕	Storage & distrib.:	⊕⊕
Operating range:	high	Operating range:	high
Resources:	sufficient	Resources:	limited
Soot/NOx emissions:	medium	Soot/NOx emissions:	medium

TTW: Tank-to-wheel
WTT: Well-to-tank

First Fuel Cell Vehicles in Market Introduction Phase

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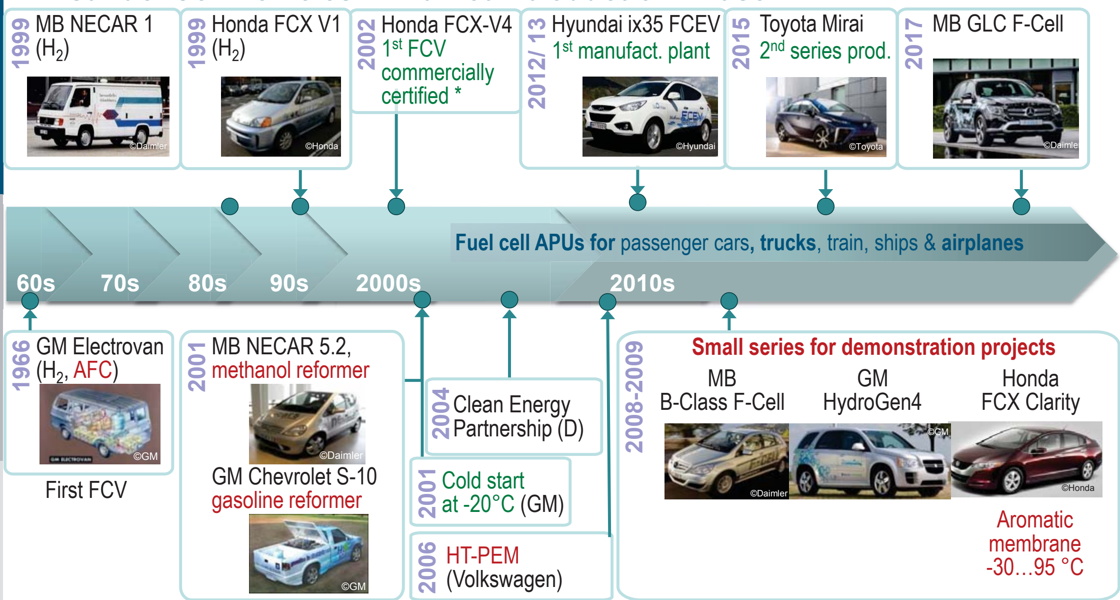
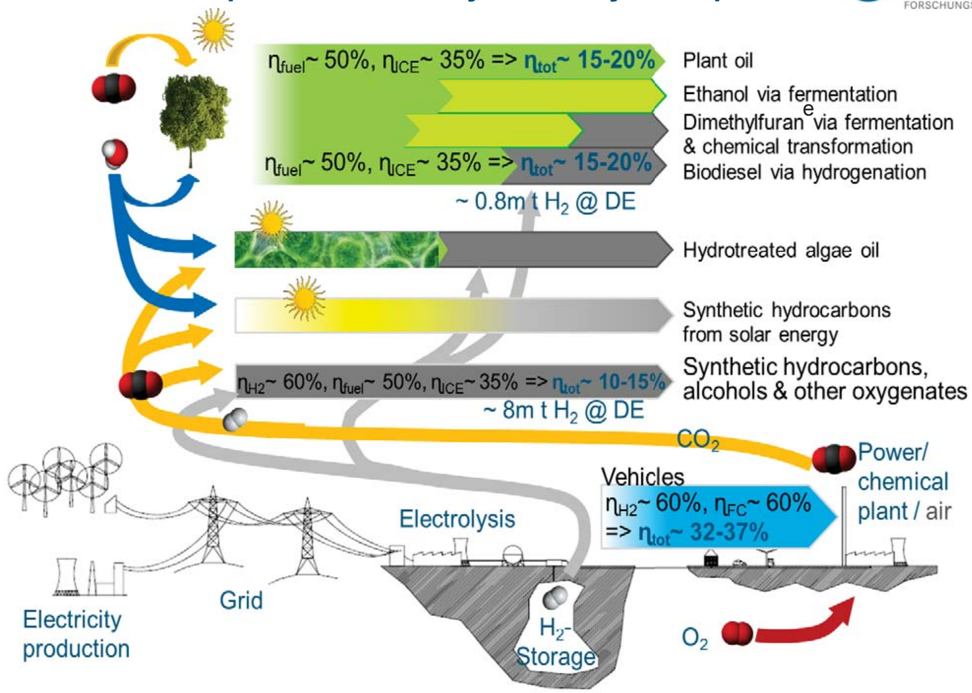


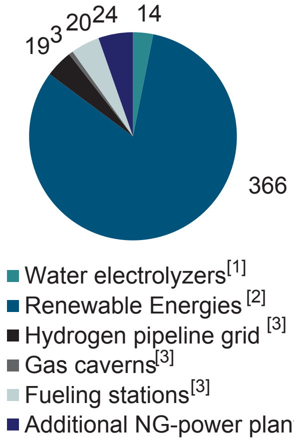
* First fuel-cell vehicle certified by the U.S. EPA and California Air Resources Board (CARB) for commercial use
MB: Mercedes-Benz; GM: General Motors
All cars with PEFC except GM Electrovan with AFC

Power to Fuel: Option or Necessity for Heavy Transportation?



Infrastructure Analysis (simplified)

Infrastructure of Energy Concept 2.0 Cost Aanalysis [Bn €]

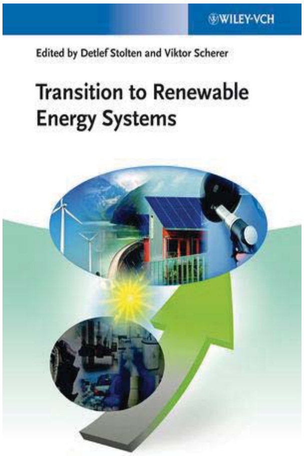


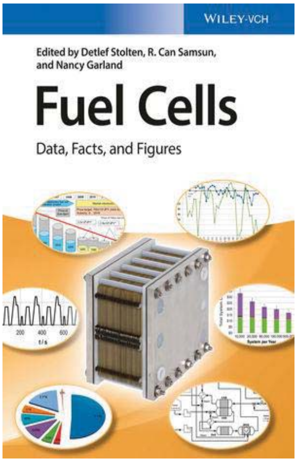
[1] Electrolyzer @ 500 €/kW
[2] PV @ 1000 €/kW; wind onshore @ 1400 €/kW; offshore @ 3000/kW; Installed capacities after **[3]** Robinius, M. (2016): Strom- und Gasmarktdesign zur Versorgung des deutschen Straßenverkehrs mit Wasserstoff. Dissertation RWTH Aachen **[4]** 42 GW GT + comb. Cycles, 23 GW already in place **[5]** Zeitreihen zur Entwicklung Erneuerbarer Energien, BMWi, August 2016 [6] Netzentwicklungsplan NEP 2025, BNA

The Systems Analysis Team

Thank You for Your Attention!

d.stolten@fz-juelich.de





Options and Challenges of Electrification of the Transport Sector from the Point of View of an Automotive OEM

Jörg Wind
Daimler AG

The presentation introduces the different options for alternative fuels and alternative drivetrains with a focus on electrified drivetrains. A well-to-wheel (WTW) comparison of energy consumption and green-house-gas (GHG) emissions clearly shows that electric vehicles, like battery electric vehicles (BEV) and fuel cell electric vehicles (FCEV), cause the lowest energy consumption and GHG-emissions, whereas biofuels and synthetic fuels have only the potential to reduce GHG emsissions, but leading to a significant increase in energy consumption compared to fossil fuels derived from crude oil. Both BEVs and FCEVs have significant advantages especially concerning environmental impact, but still face some challenges, especially the lack of a sufficient charging and refueling infrastructure. The choice of the specific electric drive train, e.g. the use of batteries and/or fuel cells depends on the size of the vehicle and the requested mileage: the larger the vehicle and the longer the trip, the more is a fuel cell system the adequate solution. For very large vehicles, like ships and airplanes and very long distances synthetic fuels come into play.

Electromobility with battery and/or fuel cell is already reality. Quite a number of electric vehicles are already available on the market. The EV sales numbers was more than 700,000 in 2016 (and exceeded one million in 2017). Daimler has a large experience with FCEVs and has shown the maturity of FCEVs while driving 10 million kilometers with the Mercedes B-Class F-Cell passenger car and more than 4 million kilometers with the Citaro FuelCell Hybrid bus in customers´ hands. Daimler´s next generation FCEV, the Mercedes GLC F-Cell has been presented at the international automobile exhibition in Frankfurt in September 2017. The vehicle is a big step forward in FCEV technology. It was possible to reduce the platinum content of the FC stack by 90%, while increasing the power by 40% and reducing the volume of the fuel cell system (FCS) by 30%. Additionally, with its 9 kWh Li-ion battery and an on-board charger, it is the first plug-in FCEV on the market.

The build-up of a suitable hydrogen infrastructure is key for a successful market introduction of FCEVs. All new hydrogen refueling stations (HRS) fulfil the necessary standards for a fast refueling of the full hydrogen tank in three minutes. To accelerate the build-up of a HRS network in Germany, six companies have founded the joint venture H2Mobility Deutschland GmbH, supported by five associated partners and the German government via the NOW-organization. Daimler is one of the founding members.

The build-up of charging infrastructure for BEVs and PHEVs is also promoted by many market players and governments. Contrary to HRS, at least four different standards have been established world-wide, which is a barrier for seamless electric mobility. The number of charging stations is growing worldwide, with a focus on the US, Europe, Japan and China.

In the truck segment, especially heavy duty trucks, the first electrified vehicles have just been presented in the last months. It is very likely that especially FCEV-trucks will be seen on the road in future.

DAIMLER

Options and Challenges of Electrification of the Transport Sector from the Point of View of an Automotive OEM

Dr. Jörg Wind, TRENDS 2017, Aachen 5th December 2017

Responsibility for our Blue Planet

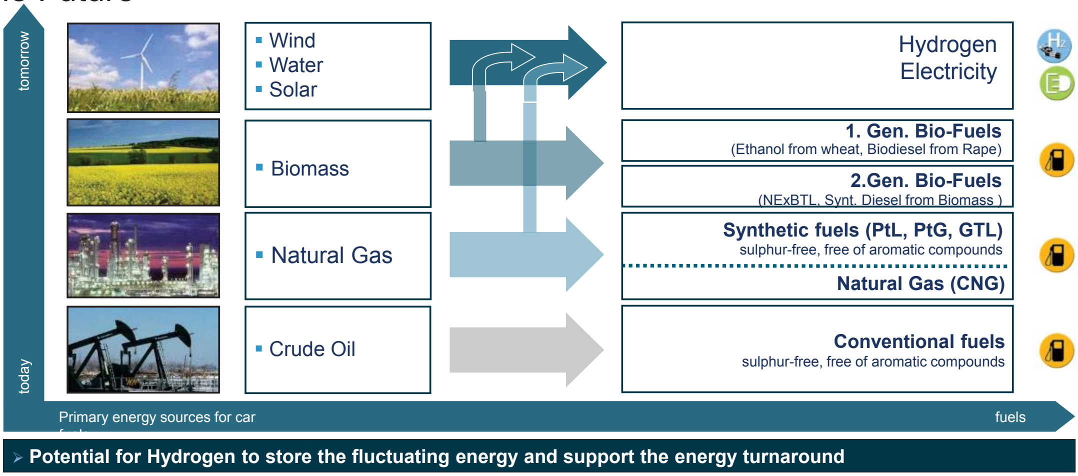
- Worldwide rising demand for mobility will increase CO_2 emissions
- Fossil resources are limited and will therefore become more expensive

Daimler is shaping the future of mobility in many aspects. We re-invent the car!

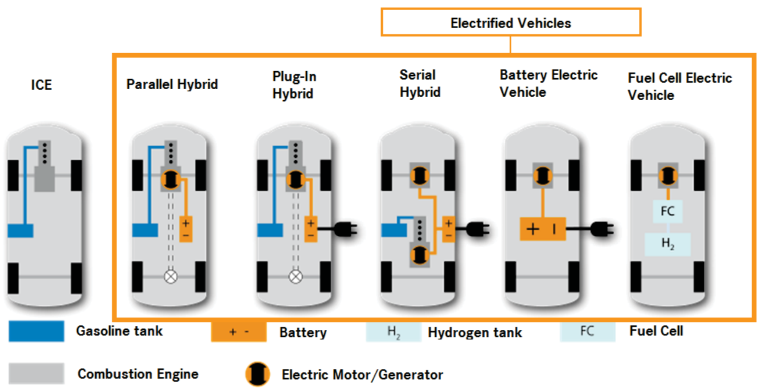
EV Technology (BEV & FCEV) is an Integral Part of Daimler‘s Powertrain Strategy

Highly efficient combustion engines	Full- and plug-in-hybrids	Electric vehicles with battery and fuel cell
		
A 180 CDI BlueEFFCIENCY 3,5 l/100 km, 89 g CO_2/km	S 500 e 2,8 l/100 km, 65 g CO_2/km	B-Class Electric Drive, smart electric drive, B-Class F-CELL 0 l/100 km, 0 g CO_2/km

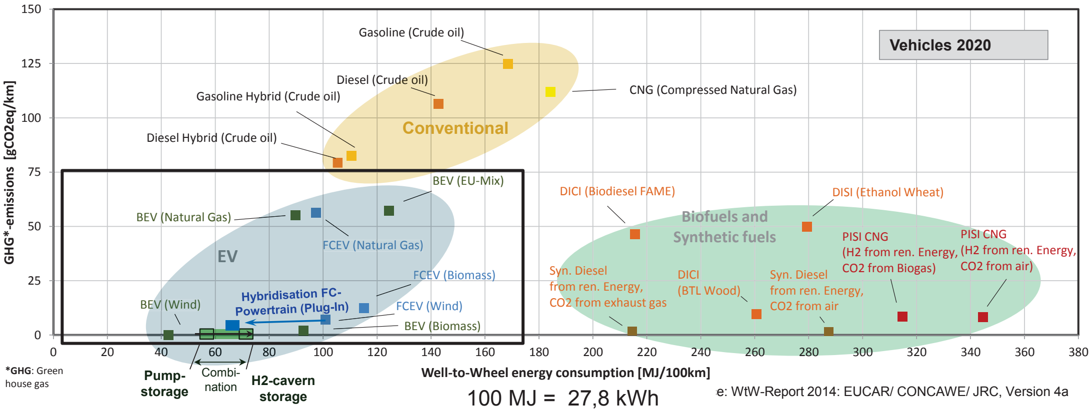
Revolution of the Mobile Drive vs. Evolution of the Alternative Fuels of the Future



Choice of electrified powertrains

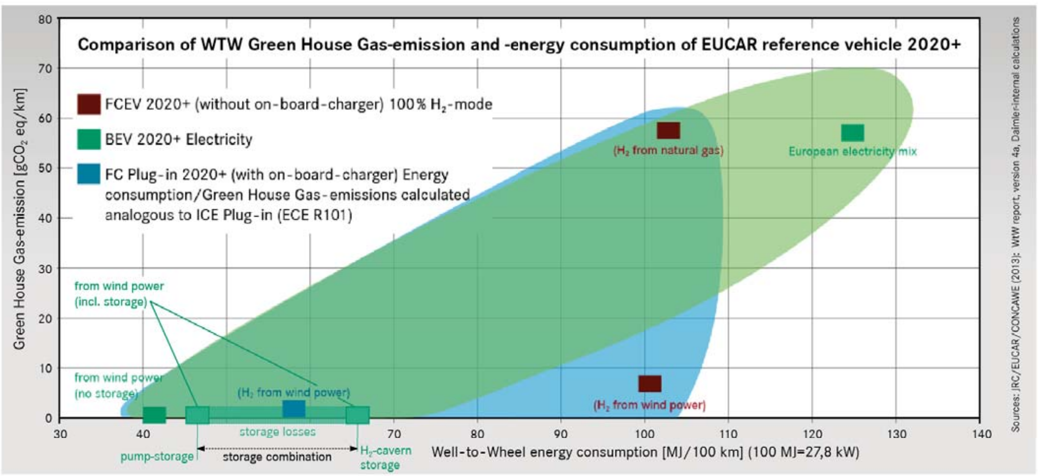


Well-to-Wheel Comparison of Greenhouse Gas Emissions and Energy Consumption of EUCAR Reference Vehicles (C-segment passenger car) 2020+



Daimler AG

Well-to-Wheel Consideration of Fuel Cell Plug-in-Hybrid

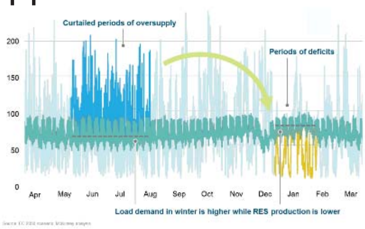


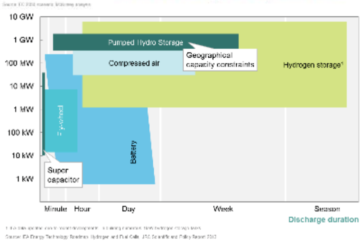
FCEV and BEV Characteristics

Electric Vehicles with Batteries		Electric Vehicles with Fuel Cells
	**Common Strengths** • Reduction of greenhouse gas with zero emission vehicles • Efficient energy usage • Independence of oil • Drive and comfort with electric drive • Low noise emissions	
• Highest energy efficiency and lowest greenhouse gas emissions of all drive trains	**Strengths**	• Short refueling time and thus unlimited range • Fuel cell drivetrain suitable for larger vehicles and long range
• High charging time • Inexpensive and long-lasting batteries • Supply of carbon-free electricity • **A nationwide charging system**	**Challenges**	• Component costs • Inexpensive and long-lasting fuel cells • Supply of carbon-free hydrogen • **A nationwide refueling system**

For future emission-free mobility, both drive train technologies will be needed!

Energy supply and infrastructure: Challenges and opportunities

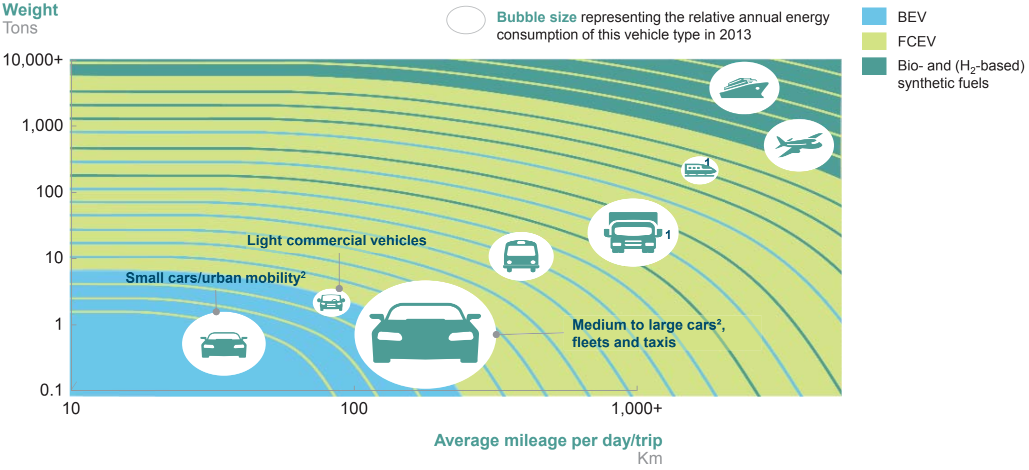




Hydrogen as fuel for transport:
- Long time storage of large quantities
- Viable option to balance intermittent supply of renewabel electricity
- Fast refuelling of vehicles (200km/minute)
- Worldwide standardized refueling protocols
- Positive business case for HRS operation possible
- Operation mode and fuel cost similar to conventional fueling stations

Electricity as fuel for transport:
- Lower invest in the starting phase
- Lower energy losses
- Large number of equipment suppliers
- Up to now no positive business case for public charging stations
- Large invests in electricity grid needed, especially for fast charging

Choice of electric vehicles type and electric fuels depends on vehicle segment and driving distance



1 Battery-hydrogen hybrid to ensure sufficient power
2 Split in A- and B-segment LDVs (small cars) and C+-segment LDVs (medium to large cars) based on a 30% market share of A/B-segment cars and a 50% less energy demand

Source: Toyota, Hyundai, Daimler

11

Electric Mobility is already real, innovative products coming soon

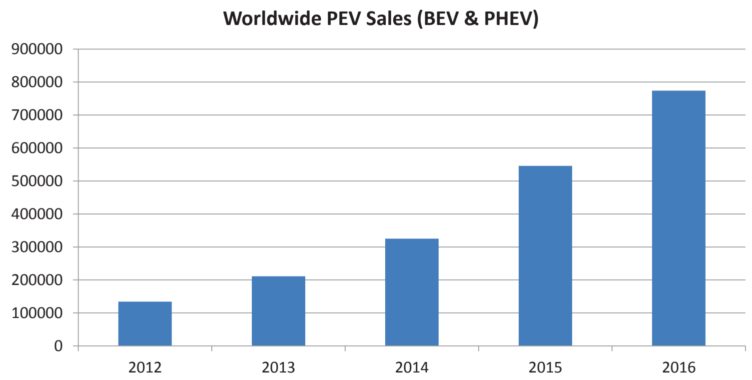
Mercedes-Benz B-Class electric drive (BEV)

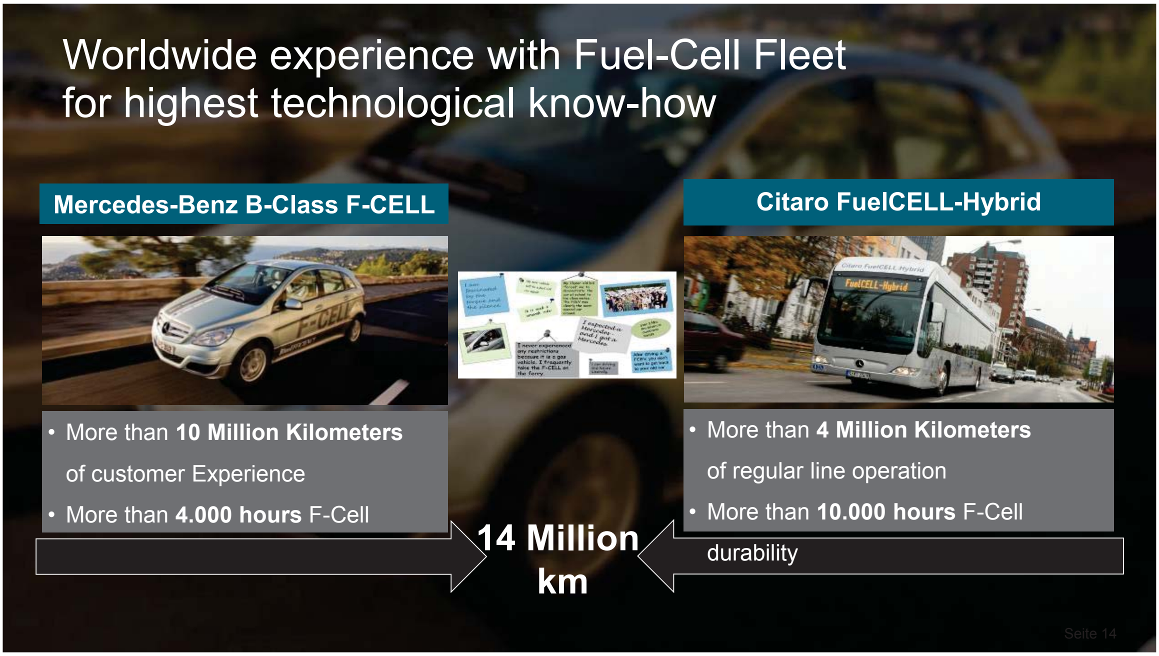
Mercedes-Benz EQ (BEV)

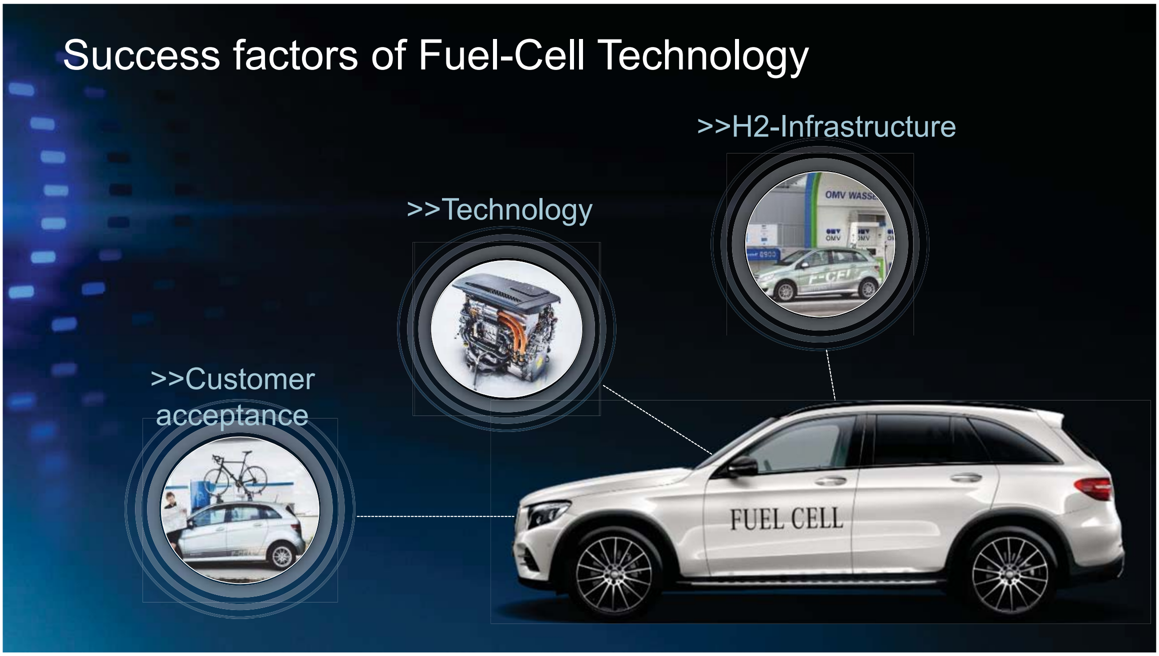
Mercedes-Benz GLC F-CELL (FCEV)

Mercedes-Benz Vision Van (BEV)

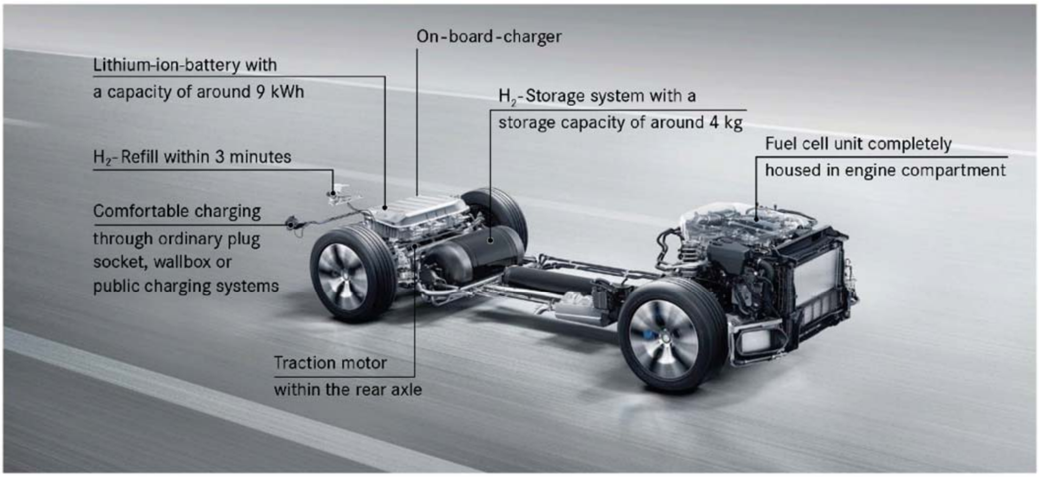
Worldwide PEV Sales are rising significantly







Next Generation Fuel Cell Powertrain



Next Generation Fuel Cell Vehicle: „The Fuel Cell gets a Plug!“

Daimler AG | Page 17

Technical Configuration of a Hydrogen Fueling Station

Status quo of hydrogen filling stations:

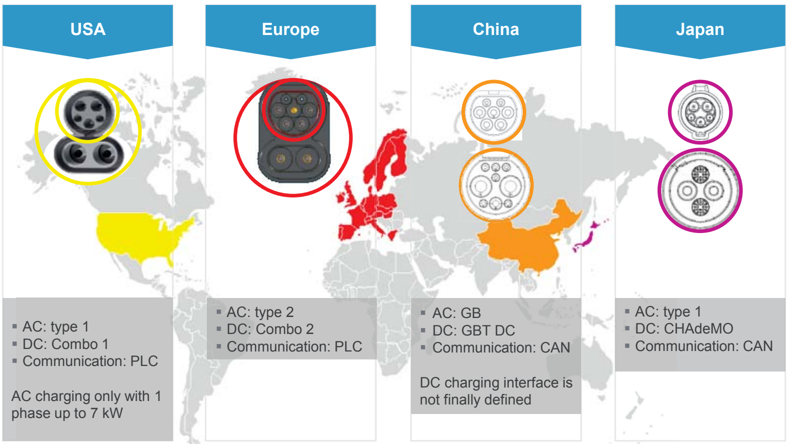
- Pre-cooling down to -40° Celsius
- Pressure of hydrogen: 350 and 700 bar
- Standardized refueling process (SAE TIR J2601, ISO/TS 20100) using infrared data interface for communication vehicle <> filling station (SAE J2799)
- Refueling time: approx. 3 minutes for the B-Class F-CELL (ca. 4 kg hydrogen)
- Standardized hydrogen filling connector (SAE J2600, ISO/FDIS 17268)
- Hydrogen fuel quality (SAE J2719, ISO/FDIS 14687)
- Unitized construction / scalable

Daimler AG | Dr. Jörg Wind

Infrastructure: H_2 Mobility Initiative in Germany
Built-up of Nationwide Hydrogen Station Network till 2023

Daimler AG Page 19

Overview of plugs and inlets



Development of public charging infrastructure Example: DC infrastructure in Europe

> 3000 Chademo DC charging stations in Europe

SLAM-project:
Up to 600 DC charging stations in Germany

Tesla
Superchargers in Europe

Heavy duty vehicles: BEVs and FCEVs enter the market

Mercedes-Benz Citaro Fuel Cell Bus

Mercedes-Benz Urban e-Truck (BEV)

FUSO Canter E-Cell (BEV)

Nikola One FC Truck (Prototype)

Toyota FC Truck (Prototype)

Alstom Coradio iLint FC-Train (Prototype)

Thank you for your attention

Power-to-Fuel – A Promising Future Fuel Alternative for the Transport Sector?

Ralf Peters, Maximilian Decker, Steffen Schemme, Stefan Weiske, Detlef Stolten
Forschungszentrum Jülich GmbH, Institute for Energy and Climate Research – Electrochemical Process Engineering (IEK-3)

Renewable energy from wind and solar sources is affected by fluctuations which do not correspond to the demand for electrical energy. Storage options are therefore required and also other possibilities of utilizing this power in a future energy system. An important first step is water electrolysis for the production of hydrogen. If this hydrogen cannot be used directly then it must also be stored by chemical storage. Fuel synthesis using CO2 from industrial waste gases and hydrogen from electrolysis is an attractive approach.

The following contribution outlines the role of the transport sector in the energy system and the resulting challenge for the transport sector in the context of the transition of the energy system (Energiewende). As an option to face the challenge, coupling the energy-generation and the transport sector using power-to-fuel (PTF) technologies is presented. The paper offers the fundamental approach as well as a basis for discussion concerning the implementation of this option. The focus is on the potential of non-fossil and non-biological diesel fuels produced from CO2 and hydrogen from renewable energy sources and CO2 regarding a possible implementation strategy.

The physical and chemical properties of synthetic diesel fuels are compared with those of conventional diesel. Methylal and higher oxymethylene ethers represent one fuel option due to the low-emission combustion of ethers with their characteristic C-O bonds. However, conventional synthesis is an elaborate process because of the large number of intermediate steps. The direct synthesis of methylal and higher oxymethylene ethers would considerably simplify the technical implementation. Here we present a method that considers Gibbs energy in order to analyze the possibilities of direct synthesis from CO2-H2. High operating pressures and influence of the critical states of educt and products on the thermodynamic state parameters of enthalpy and entropy mean that the real gas properties can be modeled by an equation of state. Methylal can therefore be formed with high conversion rates at pressures of 100 bar and temperatures below 373 K. The formation of dimethyl ether as a potential by-product must be suppressed by a suitable catalyst since it is thermodynamically favored. Higher oxymethylene ethers are difficult to directly synthesize by the following thermodynamic analysis. First of all, formaldehyde must be formed from methanol. Three formaldehyde molecules ultimately form cyclic trioxane, which reacts with methylal to form higher oxymethylene ethers.

This contribution creates a basis for discussion regarding the selection, production, and implementation strategies for promising future fuel alternatives for the transport sector. There are already techno-economic calculations – and in some cases pilot plants – for various pathways for synthesizing these fuels. However, in order to achieve a comparative evaluation of the various paths, standardized calculations are necessary. This evaluation creates the basis for an efficient implementation strategy for a future, ideally greenhouse-gas-neutral, transport sector, and thus to achieve the objectives of the Energiewende and the Energy Roadmap 2050 set by the European Commission. The detailed analysis is published by Schemme et al. in Fuel 205 (2017) 198–221.

Power-to-Fuel – A Promising Future Fuel Alternative for the Transport Sector?

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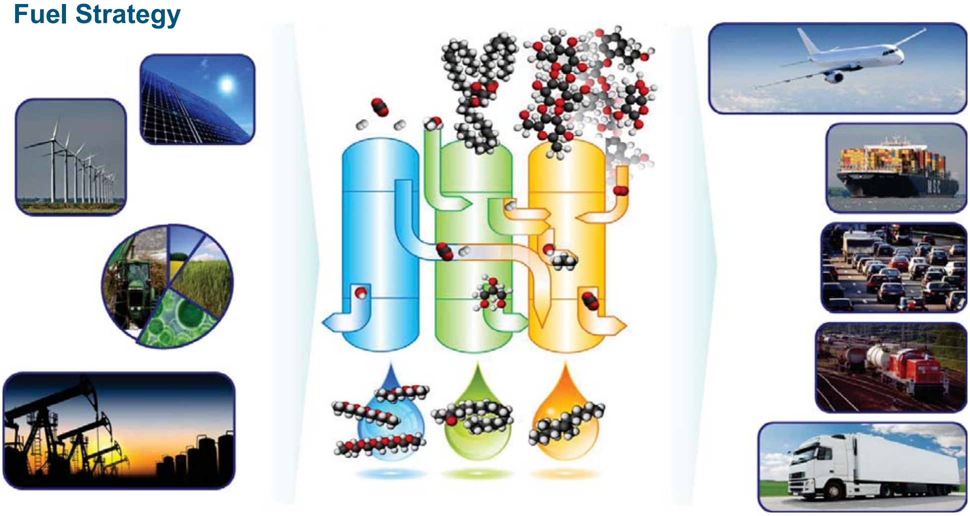
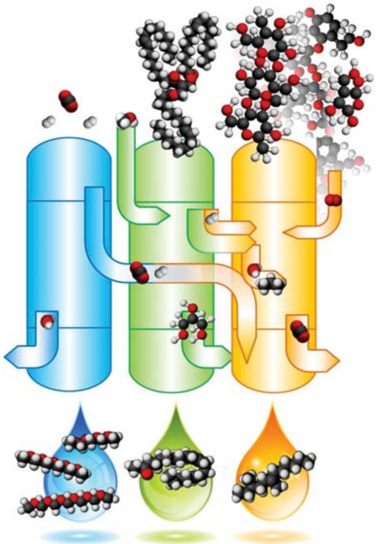
Forschungszentrum Jülich
Institute of Energy and Climate Research
IEK-3: Electrochemical Process Engineering

2. Topic Workshop „Fuel Cells, Electrolysis & Hydrogen“,
6. November 2017, Frankfurt Airport Center, Frankfurt a. Main

Electrofuels Connecting Power and Mobility Sector

- Motivation
- Process development
- Assessment of available quantities
- Connection to biofuels
- Fuel Strategy





Motivation

Process Development

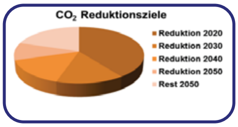
Fischer-Tropsch | OME_{3-5} | Comparison

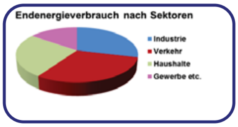
Assessment of Available Quantities

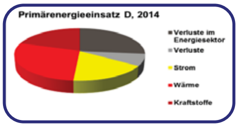
Connection to Biofuels

Fuel Strategy

Political Boundary Conditions and Conclusions







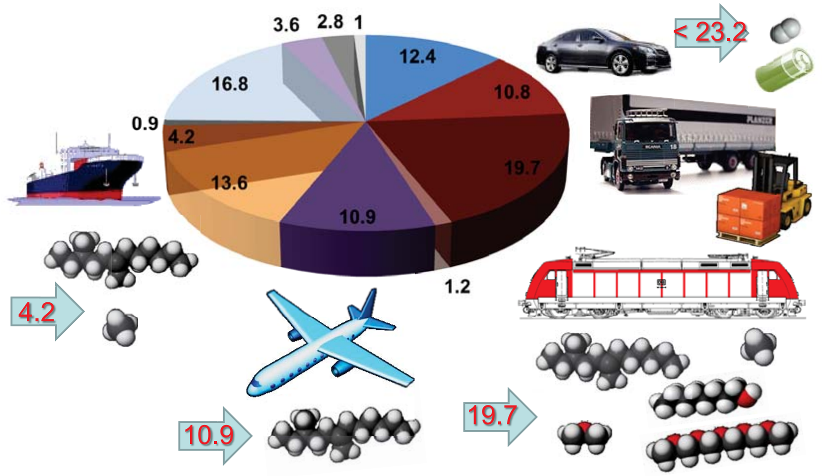
- Reduction of anthropogenic GHG emissions by $80\%_{1990}$ by 2050
- Reduction of primary energy demand in transport by $40\%_{2005}$ by 2050
- The energy transition must affect the transport sector with a share of 30%
- Interconnection of energy and fuel sectors
- Improvement of energy efficiency
- Security of supply
- Reduction of fossil feedstocks
- Reduction of emissions

Fuels from Perspective of Petroleum Industry

Prediction 2025

Data of *Mineralöl-Wirtschaftsverband* for Germany in **mio. tonnes**

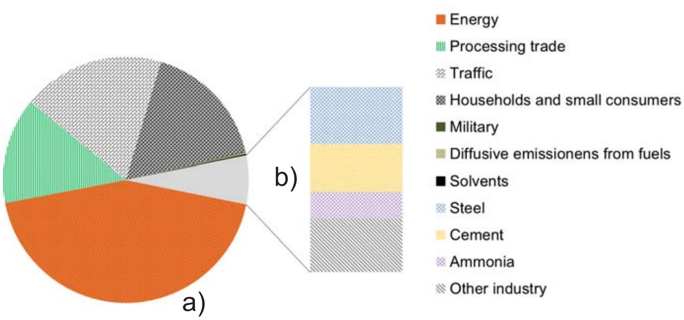
- Gasoline
- Diesel LDV
- Diesel HDV
- Diesel, Others
- Kerosene
- Heating oil, light
- Heating oil, heavy
- Lubricants
- Straight-run gasoline
- Liquid gas
- Bitumen
- Other products

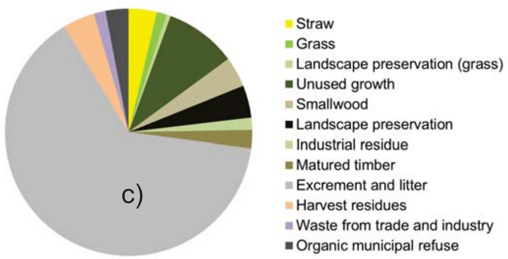


- Fuel for trucks, ships and aircraft with comparable power density
- Power to Fuel /w potential to improve engine effiency and limited emissions

„Drop-in“ quality → **Gradually integration in given infrastructure**

CO_2 Sources Today and in Future

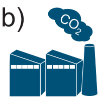




a)

Carbon Capture Utilization & Storage
15 % CO_2 in flue gas
Test facility
No option for 2050

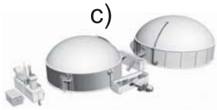
b)



German industry:
52.2 Mio. t CO_2 (6.3 %)
16 mio. t from steel
13.5 mio. t from cement
7.5 mio. t from ammonia

15 – 100 % CO_2

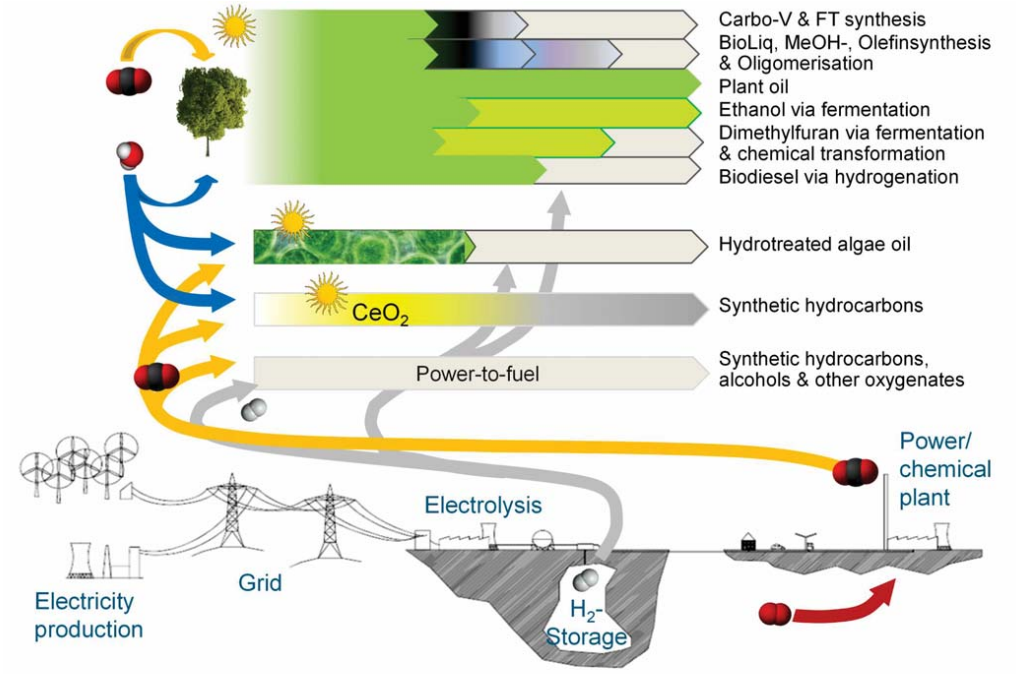
c)



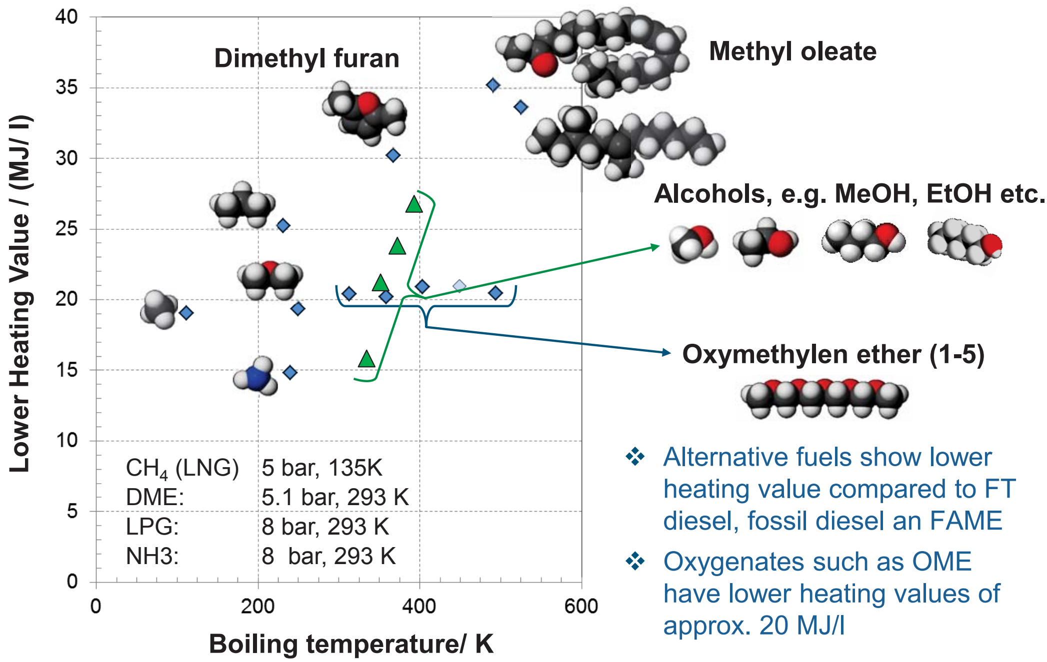
Bio gas plants in Germany:
9004 in 2016 with 500 kW_e,
4.17 GW_e installed
50 : 50
16 mio. t CO_2

CO_2 from air
0.04 % CO_2
High investment beyond 2050?

Different Synthesis Pathways for BTL & PTL Fuels



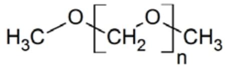
Lower Heating Value and Boiling Points of PTF und BTL

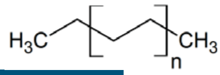


- Alternative fuels show lower heating value compared to FT diesel, fossil diesel an FAME
- Oxygenates such as OME have lower heating values of approx. 20 MJ/l

Motivation for Selecting these Electrofuels
$OME_{3\text{-}5}$ and n-Alkanes (for the analysis)

- same educt → $H_2 + CO_2$
- same field of application for product → fuel for diesel engine





	$OME_{3\text{-}5}$ (Power-to-Fuel)	n-Alkanes C_{15}-C_{20} (Power-to-Fuel)
Chain atom bonds	beneficial combustion C-O	high energy density C-C → closely related to fossil diesel
challenges due to **complex separation**	various vapor-liquid- and liquid-liquid-equilibriums (mixing gaps, azeotropes)	broad product distribution
TRL (technology readiness level)	no development on an industrial scale (low product demand)	state-of-the-art industrial processes (Fischer-Tropsch)
…	…	…

Comparison requires standardization and calculations with high level of accuracy
- **thermodynamic models** & **kinetics** must be considered

Each process route must be **optimized** with same target
- yield / efficiency / costs

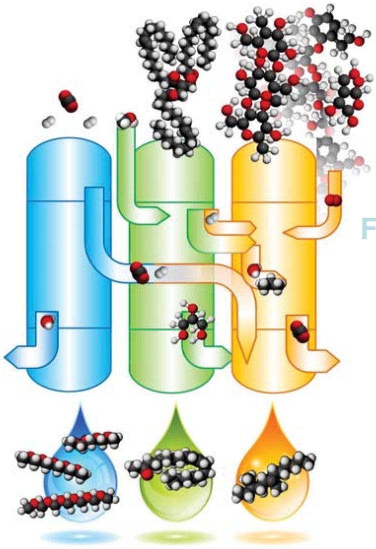
Well-to-wheel must be considered

Electrofuels vs. Standard (fossil) Diesel

	Diesel DIN EN 590	$OME_{3\text{-}5}$ (Power-to-Fuel)	n-Alkanes C_{15}-C_{20} (Power-to-Fuel)	
Density at 15 °C [kg/m³]	820 to 845	1073	779.6	
Cetane number	min. 51	72	< 85	**Benefit**
Viscosity at 40 °C [mm²/s]	2 to 4,5	1 to 3	≈ 4	
Sulphur [mg/kg]	max. 10	0	0	**Benefit**
Polyaromatics [wt.-%]	max. 11	0	0	
Melting point [°C]	- 20	- 43 to 28	N/A	
Distillation range [°C]	200 (T10 ASTM D86) 360 (T95 ASTM D86)	155 to 242	270 (T10 ASTM D86) 355 (T95 ASTM D86)	
Flash point[°C]	min. 55	69	N/A	
LHV [MJ/Liter]	36	20.9	34.2	
O_2 content [wt.-%]	-	49	0	**Benefit**

cetane number ↑ → η_{engine} ↑

$OME_{3\text{-}5}$	O_2-content ↑	→ better emission values (no NOx-soot-tradeoff)
n-Alkanes	energy density ↑	→ consumption per mile similar to fossil diesel



Motivation

Process Development

Fischer-Tropsch | $OME_{3\text{-}5}$ | Comparison

Assessment of Available Quantities

Connection to Biofuels

Fuel Strategy

State of the Art Regarding Fuel Synthesis

Matured industrial Process

Fischer-Tropsch synthesis:
$n\,CO + (n+m/2)\,H_2 \rightarrow C_nH_m + n\,H_2O$

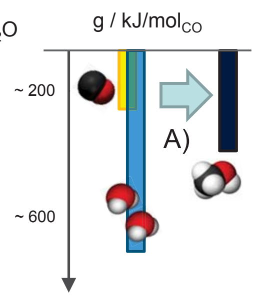
Methanol synthesis:
$CO + 2\,H_2 \rightarrow CH_3OH$

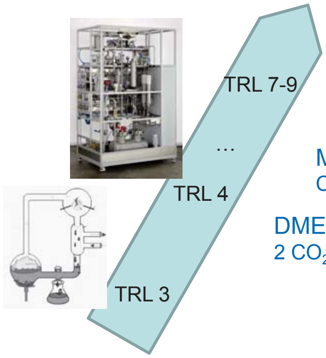
DME synthesis:
$2\,CH_3OH \rightarrow CH_3OCH_3 + H_2O$

Methanol to Gasoline

Methanation:
$CO + 3\,H_2 \rightarrow CH_4$

Reverse Water-Gas-Shift
$CO_2 + H_2 \rightarrow CO + H_2O$

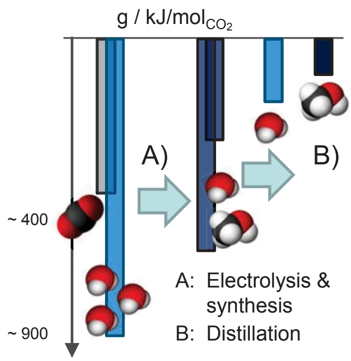




Methanation:
$CO_2 + 4\,H_2 \rightarrow CH_4 + 2\,H_2O$

Methanol synthesis:
$CO_2 + 3\,H_2 \rightarrow CH_3OH + H_2O$

DME synthesis:
$2\,CO_2 + 6\,H_2 \rightarrow CH_3OCH_3 + 3\,H_2O$



TRL 1-2: Idea, concept & techno economic analysis

Approach: Concept of Power-to-Fuel

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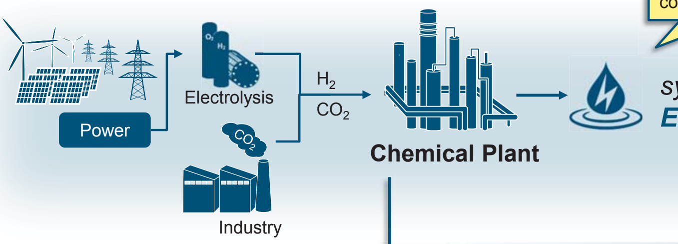
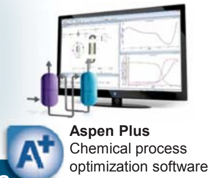
coupling of 3 sectors





Analysis

All calculations and recommendations from one hand

Input for Diss. M. Decker (Fuel Strategy)

Fischer-Tropsch	n-alkane
Alcohol synthesis	methanol, …, octanol
Ether synthesis	DME, OME_1, $OME_{3\text{-}5}$
Oligomerization (Methanol-to-Gasoline)	alkanes, aromatics

Process design of established and novel fuel pathways

Optimization → *η, yield*

CAPEX & OPEX → €

„Drop-in" quality

Conventional:
- Biofuels
- Fossil fuels

DIN EN 590 (diesel)
DIN EN 228 (gasoline)
Jet A-1 (kerosene)

Comparative Assessment

- Technical feasibility
- Economical potential
- Ecological impact
- Identify research gaps

Methodology – Efficiencies

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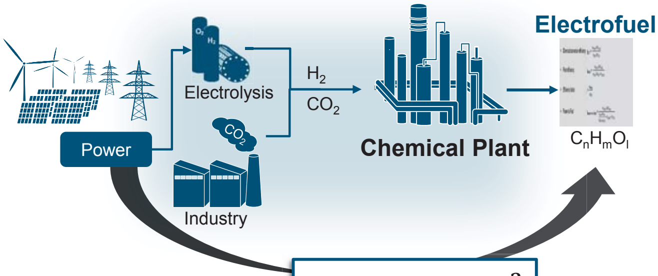


$$\underbrace{(m/2 + 2\,n\text{-}l)\ \mathbf{H_2} + n\ \mathbf{CO_2}}_{Input} \rightarrow \underbrace{\mathbf{C_nH_mO_l}}_{Fuel} + (2\,n\text{-}l)\ H_2O$$

(Output)

$$\eta = \frac{Output}{Input}$$

$$\eta_{Power-to-Fuel} = ?$$

Assumptions:

$\eta_{electrolysis} = 0{,}7$

$\eta_{H2-storage} = 1$

$P_{CO2,cement} = 1.2 - 1.5\ \mathrm{MJ_{el}}/kg_{CO2}$[1]

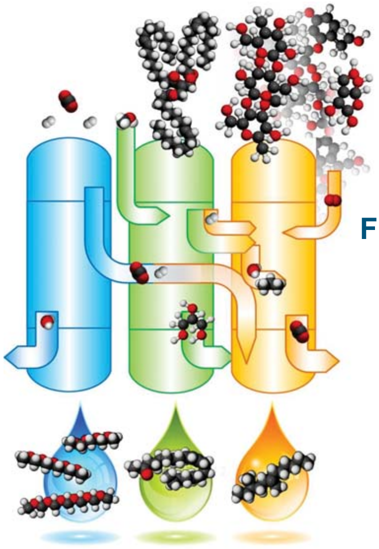
Sensitivity analysis needed

Definitions

- Chemical conversion efficiency $\eta_{CCE} = \frac{\dot{m}_{Fuel} \cdot LHV_{Fuel}}{\dot{m}_{H2} \cdot LHV_{H2}}$
- Plant efficiency $\eta_{Plant} = \frac{\dot{m}_{Fuel} \cdot LHV_{Fuel}}{\dot{m}_{H2} \cdot LHV_{H2} + P_{Plant}}$ LHV = lower heating value [MJ/kg]
- Efficiency factor $f = \frac{\eta_{Plant}}{\eta_{CCE}}$
- Power-to-Fuel $$\eta_{Power-to-Fuel} = \frac{\dot{m}_{Fuel} \cdot LHV_{Fuel}}{\frac{\dot{m}_{H2} \cdot LHV_{H2}}{\eta_{Electrolysis}} + P_{CO2} + P_{Plant}}$$

! Attention ! $\eta_{Well-to-wheel} \neq \eta_{Electrolysis} \cdot \eta_{Power-to-Fuel} \cdot \ldots \cdot \eta_{Car}$

1. Ho, M.T. and D.E. Wiley, 28 - Liquid absorbent-based post-combustion CO2 capture in industrial processes A2 - Feron, Paul H.M, in Absorption-Based Post-combustion Capture of Carbon Dioxide. 2016, Woodhead Publishing. p. 711-756.



Motivation

Process Development

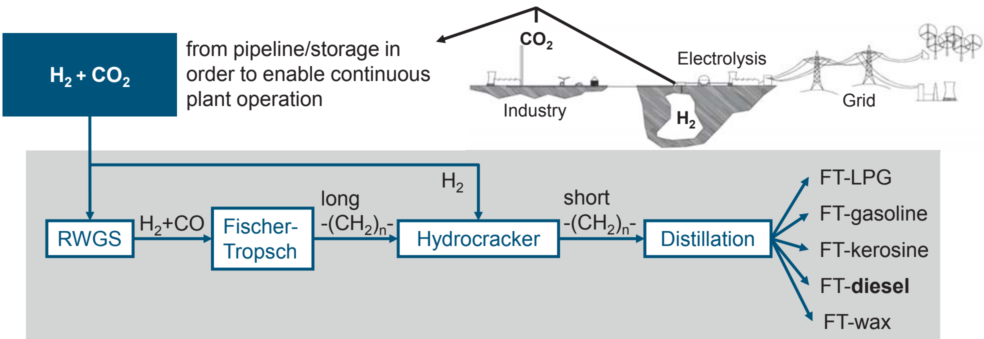
Fischer-Tropsch OME$_{3-5}$ Comparison

Assessment of Available Quantities

Connection to Biofuels

Fuel Strategy

Process Design and Assessment
Technically feasible production?

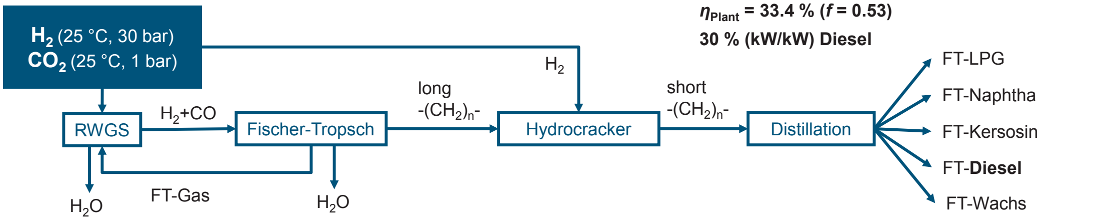


$\eta_{\text{Power-to-Liquid}}$ = ?

η_{Plant} = 33.4 % (f = 0.53)
30 % (kW/kW) Diesel

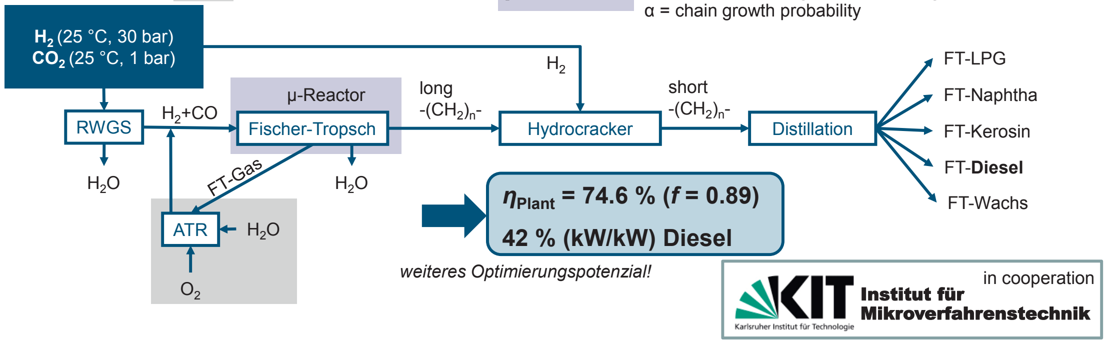
Process Efficiency: Fischer-Tropsch – Optimization

Base Case



Base Case + ATR (autothermal reformer) + µ-Reactor (α variable along reactor length) + heat int.

α = chain growth probability

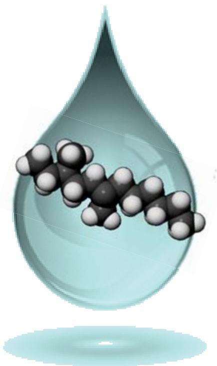


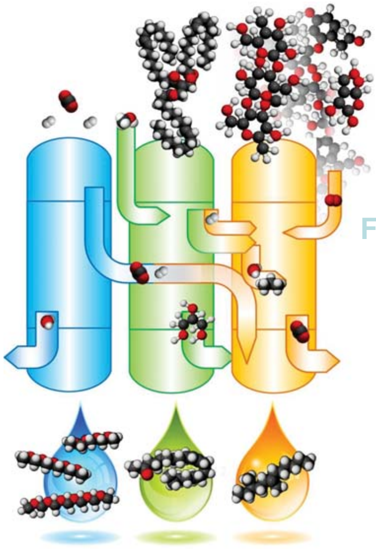
Opportunities and Challenges of Fischer-Tropsch synthesis

- Decreased limited emissions
- Higher engine efficiency
- „Drop-In“-feasibility & base fuel for future drop-in solutions

- No synthesis pathways from CO_2/ H_2
  ⇨ reverse water-gas shift reactor required
- Chain growth up to waxes
- Hydrocracking required
- Product spectrum from gases to waxes

Target: high share of kerosene or diesel





Motivation

Process Development

Fischer-Tropsch | $OME_{3\text{-}5}$ | Comparison

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Fuel Strategy

Process design for OME
Direct synthesis of methylal (OME-1)

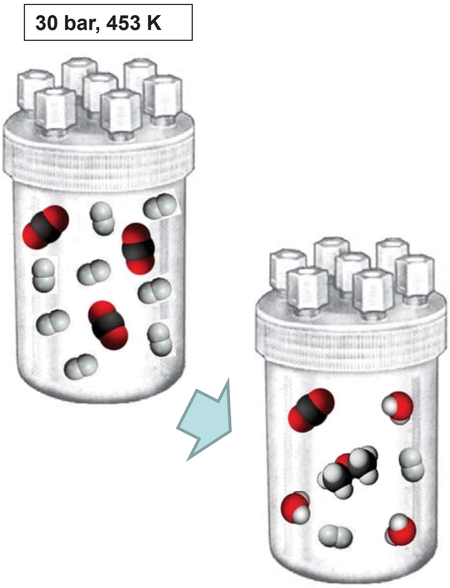
$3\ CO_2 + 8\ H_2 \rightleftharpoons C_3H_8O_2 + 4\ H_2O$

Feasibility of synthesis pathways

- Thermodynamic modeling in the gas phase
- Chemical equilibrium
- G^E-model for real mixtures in liquid phase

Design of ASPEN Plus flow sheet

- Reactor models: a) yield reactor; b) Gibbs reactor; c) reactor w/ reaction kinetic model
- Separation columns
- Pumps & compressors
- Recycle streams & valorization of side streams



Thermodynamic Modeling for Gas Phase Reactions

- Calculation of change in Gibbs energy for real gases by cubic equations of state from gaseous educt mixture (CO_2 - H_2) to gaseous product mixture (CO_2 - H_2 – H_2O – OME-1 – DME - MeOH etc.)

$$n\,\Delta \bar{G}^{RG}(T) = n_{Product}\ \bar{G}^{RG}_{Product}(p,T) - n_{Educt}\ \bar{G}^{RG}_{Educt}(p,T)$$

$$\Delta G|_{p,T} = n_{Product}\cdot \bar{G}_{Product}(y_{i,Product})|_{p,T} - n_{Educt}\cdot \bar{G}_{Educt}(y_{i,Educt})|_{p,T} \rightarrow min.$$

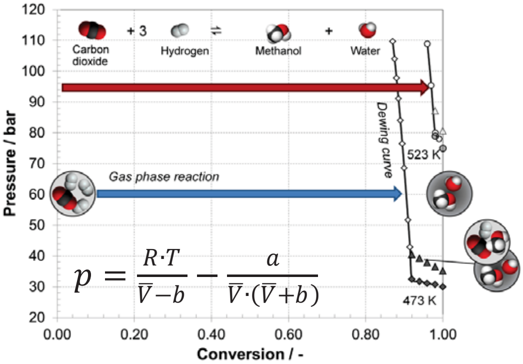
$$\varphi_i^v \cdot y_i = \varphi_i^l \cdot x_i$$

$$ln\varphi_i = ln\left(\frac{\bar V}{\bar V - b}\right) - lnZ + \left(\frac{b_i}{\bar V-b}\right) - \frac{2\sum_{j=1}^N x_i\, a_{ij}}{b\, R\, T}\cdot ln\left(\frac{\bar V+b}{\bar V}\right) + \frac{a\cdot b_i}{b^2\, R\, T}\cdot ln\left(\frac{\bar V+b}{\bar V} - \frac{b}{\bar V+b}\right)$$

$$\bar G^{RG}(p,T) = \bar H^{RG}(p,T) - T\cdot \bar S^{RG}(p,T)$$

$$\bar H_j^{RG}(p_o,T) = \bar H_j^{IG}(T) + (Z(p_o)-1)RT + \frac{\left(\frac{\partial a}{\partial T}\right)_p T - a}{b}\cdot ln\left(\frac{\bar V(p_o)+b}{\bar V(p_o)}\right)$$

$$\bar S_j^{RG}(p_o,T) = \bar S_j^{IG}(p_o,T) + R\cdot ln(\bar V(p_o)-b) + \frac{1}{b}\left(\frac{\partial a}{\partial T}\right)_p \cdot ln\left(\frac{\bar V(p_o)+b}{\bar V(p_o)}\right)$$



OME-1: $3\ CO_2 + 8\ H_2 \rightleftharpoons C_3H_8O_2 + 4\ H_2O$ **Vs.** $2\ CO_2 + 6\ H_2 \rightleftharpoons C_2H_6O + 3\ H_2O$ *: DME*

Selectivity: CH_4 > DME > CH_3OH > OME-1 >> OME-2 etc.

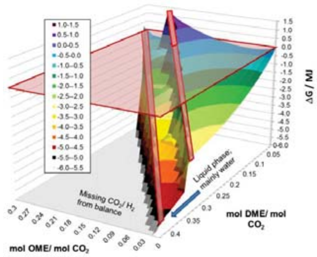
Challenge: thermodynamic restriction for **direct synthesis for methylal** (OME-1) and higher OMEs

Peters Energy 138 (2017) 1221-1246

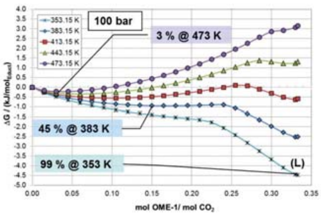
Process design for OME
Direct synthesis of methylal (OME-1)

$3\ CO_2 + 8\ H_2 \rightleftharpoons C_3H_8O_2 + 4\ H_2O$

30 bar, 453 K

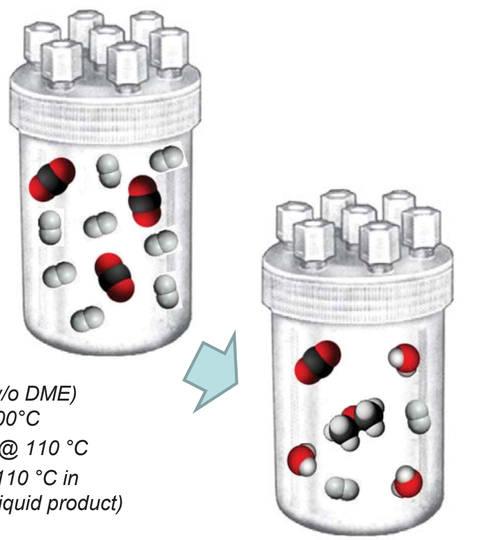


Formation of dimethylether (DME) surpress methylal (OME-1)

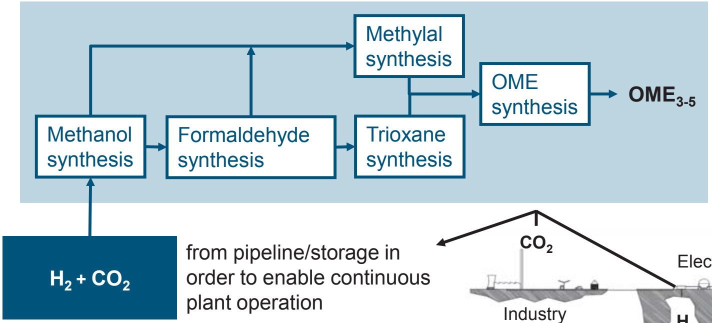


With selective catalyst (w/o DME)
a) low conversion @ 200°C
b) medium conversion @ 110 °C
c) High conversion @ 110 °C in loop reactor (within liquid product) or @ 80°C

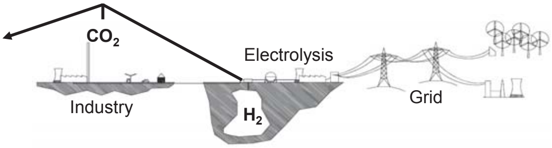
30 bar, 453 K



Process Design and Assessment
Technically feasible production?

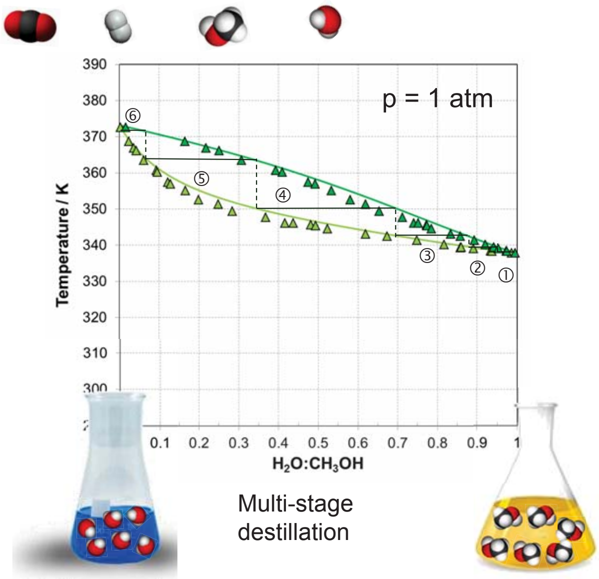


Advantages of the OME path via intermediate products
- high selectivity
- no unwanted by-products
- lower separation effort

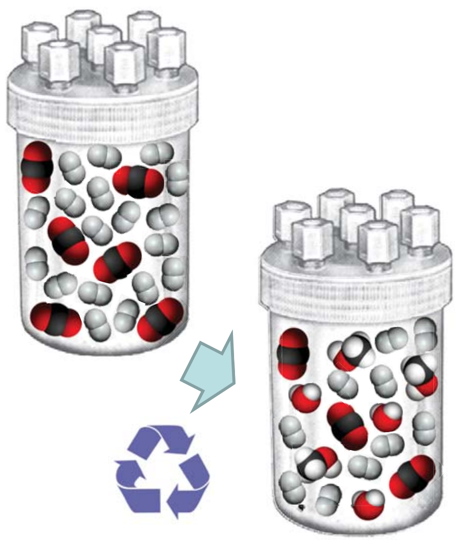


Process design for OME
Synthesis of methylal (OME-1): methanol synthesis

$CO_2 + 3\ H_2 \rightarrow CH_3OH + H_2O$



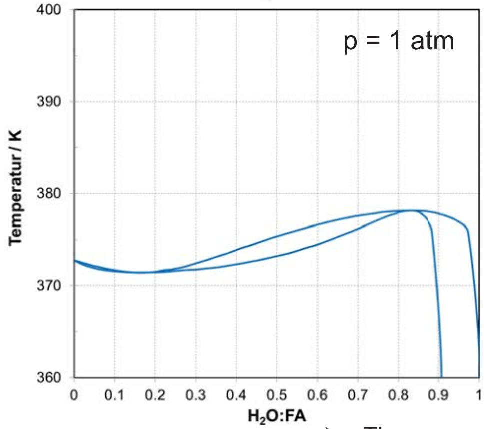
75 bar, 523 K

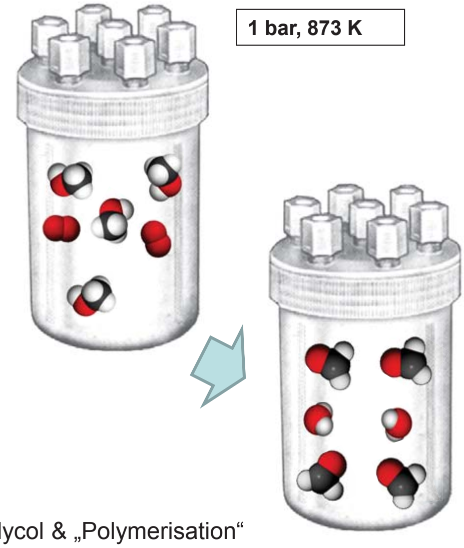


Chemical conversion~ 45 - 50 %
@ 200 – 250 °C & 75 bar

Process design for OME
Synthesis of methylal (OME-1): Formaldehyde synthesis

$CH_3OH + ½\,O_2 \rightarrow CH_2O + H_2O$



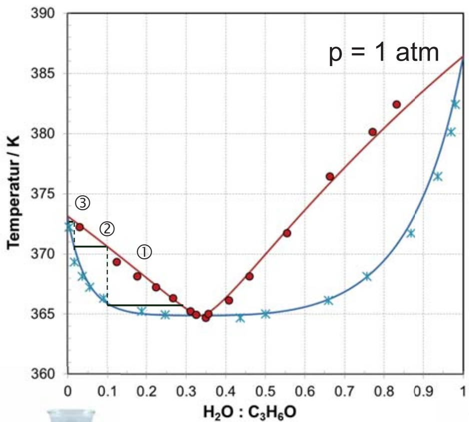


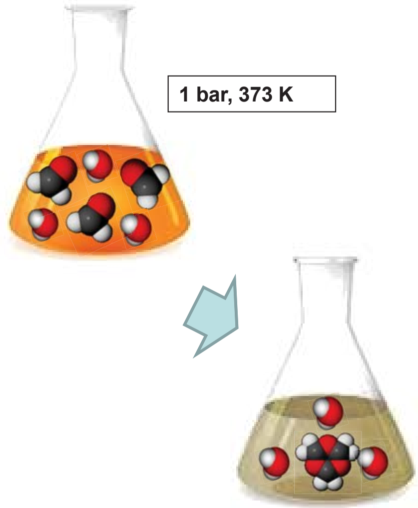
1 bar, 873 K

- Three azeotropes
- Formation of methylglycol & „Polymerisation“
- **<u>Use of an aqueous formaldehyde solution</u>**

Process design for OME
Synthesis of methylal (OME-1): trioxane synthesis

$3\,CH_2O \rightarrow C_3H_6O_3$



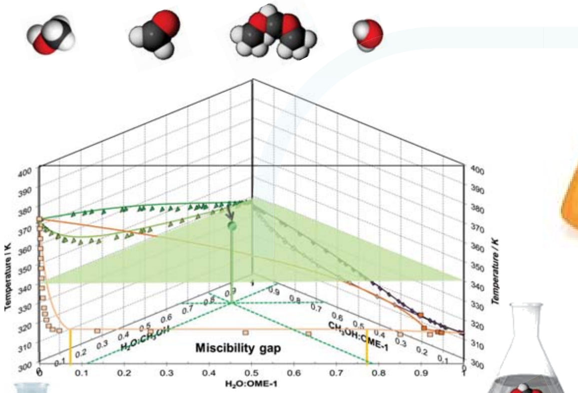


1 bar, 373 K

Pressure swing rectification (less energy intensive and less complex than extraction)

Process design for OME
Synthesis of methylal (OME-1): methylal synthesis

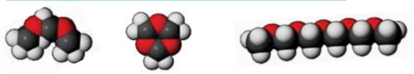
$2\ CH_3OH + CH_2O \rightarrow C_3H_8O_2 + H_2O$

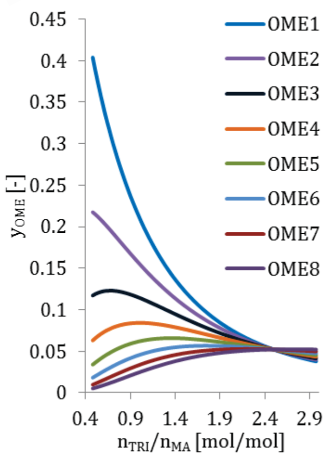


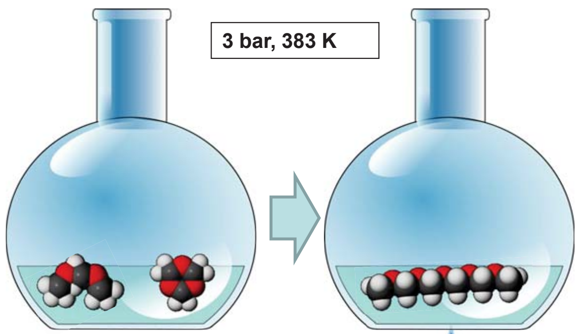
- *Surpressed side reactions*
- *Avoidance of the miscibility gap methylal - water*
- *Use of an aqueous formaldehyde solution*
- *Reactive distillation w/ pressure swing*

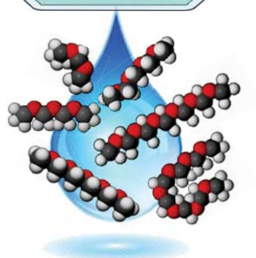
Process design for OME
Synthesis of methylal (OME-1): OME synthesis

$C_3H_8O_2 + C_3H_6O_3 \rightarrow C_6H_{14}O_5$



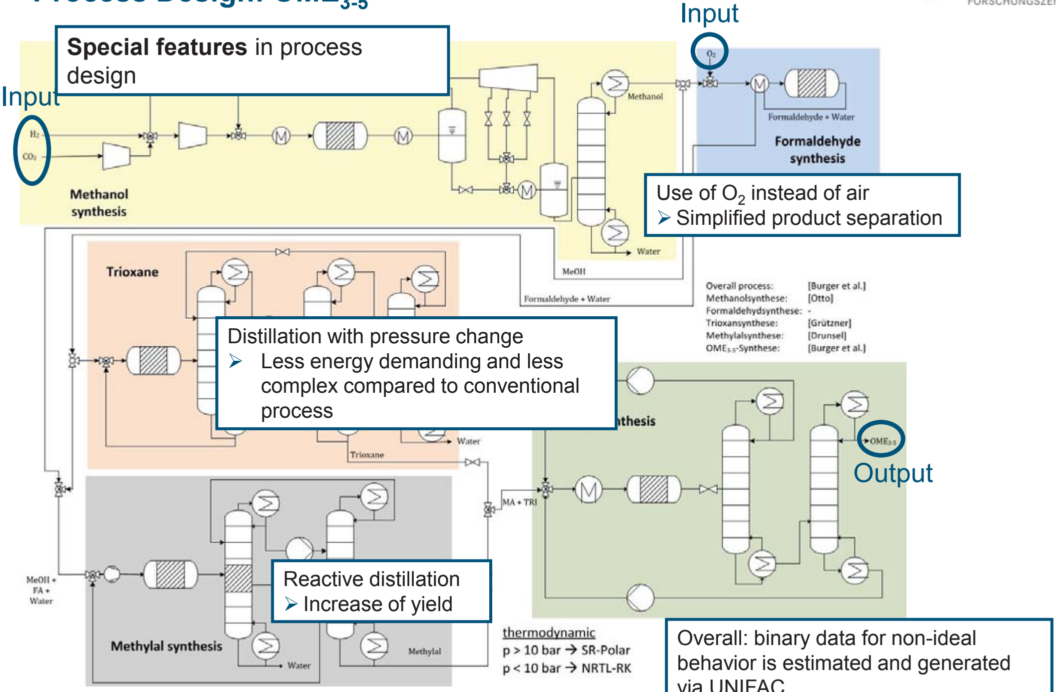






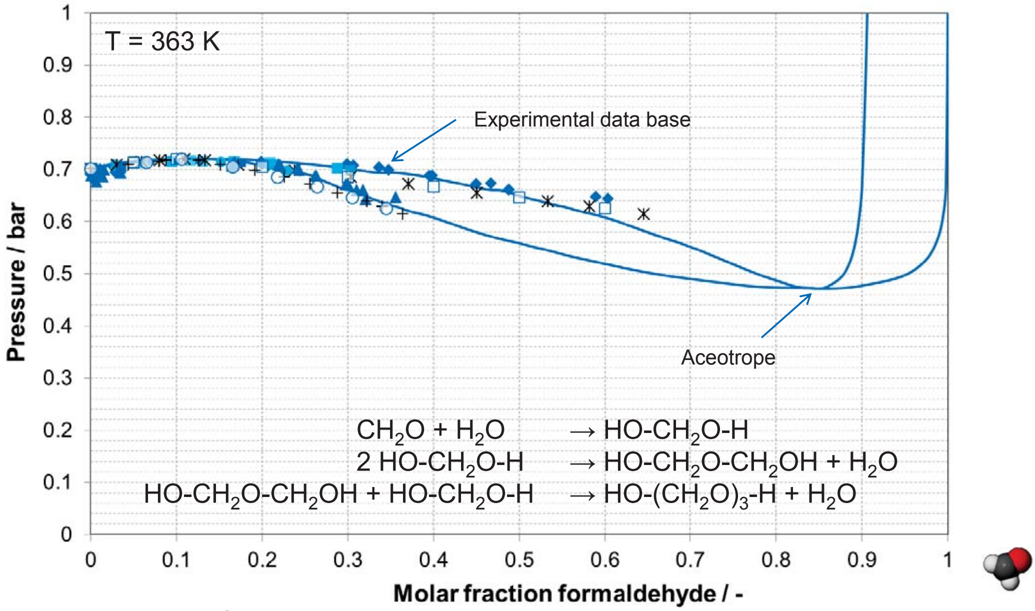
- *Mulit-stage distillation*
- *Recycling of OME 2 & OME 6+*

Process Design: $OME_{3\text{-}5}$



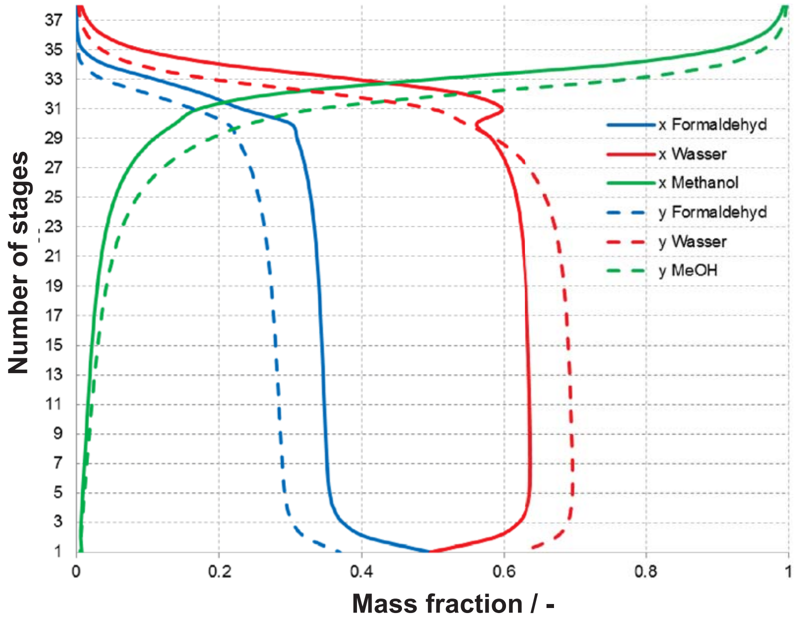
Vapor-Liquid Equilibria of the Water – Formaldehyde System

Liquid phase: UNIFAC + quasi-chemical reaction equilibrium forming methylen glycole etc.
Gas phase: EOS Redlich Kwong



$$CH_2O + H_2O \rightarrow HO\text{-}CH_2O\text{-}H$$
$$2\ HO\text{-}CH_2O\text{-}H \rightarrow HO\text{-}CH_2O\text{-}CH_2OH + H_2O$$
$$HO\text{-}CH_2O\text{-}CH_2OH + HO\text{-}CH_2O\text{-}H \rightarrow HO\text{-}(CH_2O)_3\text{-}H + H_2O$$

Vapor-Liquid Equilibria of Ternary Systems



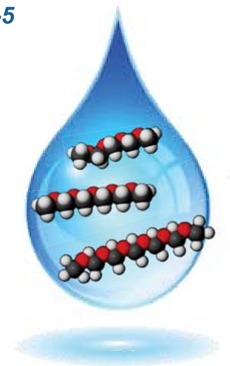
Design of destillation column by ASPEN Plus

- Optimization of:
  Number of stages;
  Feed stage;
  Reflux;
  Reboiling.
- Bottom product:
  formaldehyde – water:
  50:50 (Molar fraction)
- Top product:
  methanol

Opportunities and Challenges for OME-Synthesis

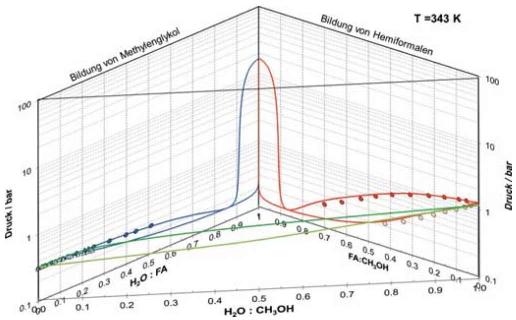
- Decreased particle/ NO_x-emissions in diesel engine
- Higher motor efficiency
- „Drop-In"-feasibility within borders

Target: OME 3-5

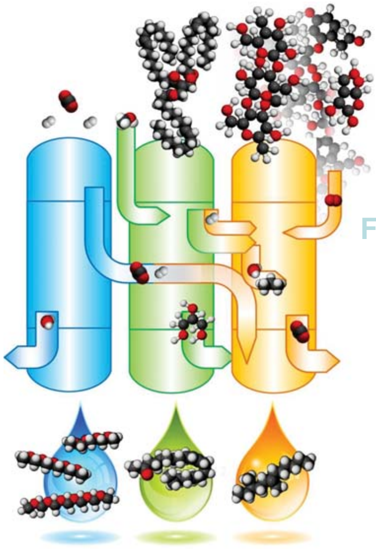


Starting from OME-1 and Trioxan
in the liquid phase @ 3 bar & 383 K
under formation of OME-2 – OME-8

- Lower energy density of diesel
  ⇨ halved range
- No direct synthesis from CO_2/ H_2
- Complex multistage synthesis process
- Non-ideal thermodynamic properties of multicomponent mixtures out of intermediate and final products
- Complex separation in each step



JÜLICH FORSCHUNGSZENTRUM



Motivation

Process Development

Fischer-Tropsch | $OME_{3\text{-}5}$ | **Comparison**

Assessment of Available Quantities

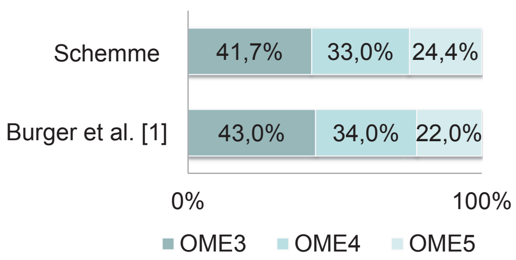
Connection to Biofuels

Fuel Strategy

JÜLICH FORSCHUNGSZENTRUM

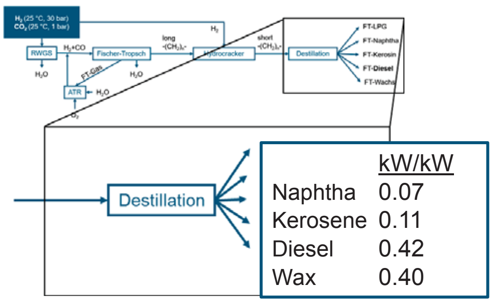
Product distribution $OME_{3\text{-}5}$ & FT products

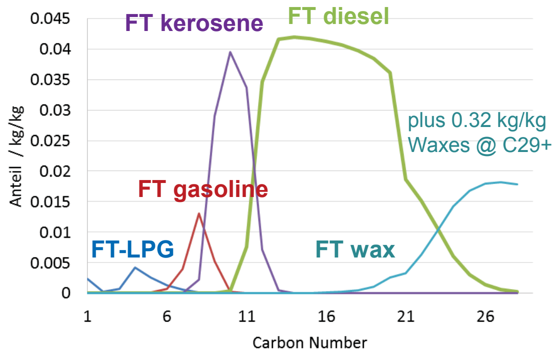
[kg/kg]



	kW/kW
OME_3	0.43
OME_4	0.33
OME_5	0.24

✓ Product distribution in agreement w/ literature data

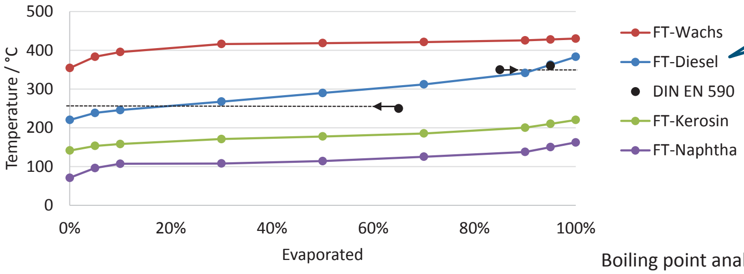




1. Burger et al., Chemical Engineering Research and Design, 2013. **91**(12): p. 2648-2662.
2. Liu, H., et al., Energy, 2015. **88**: p. 793-800
3. Lautenschütz, L., et al., Fuel, 2016. **173**: p. 129-137

Boiling Curves of Electrofuels

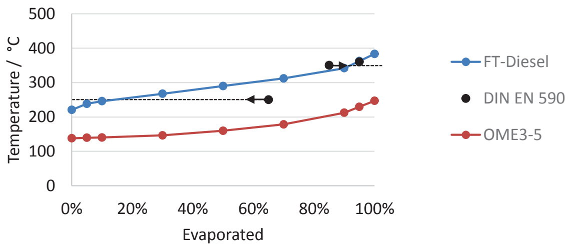
Boiling point analysis EN ISO 3405 / ASTM D86



✓ FT diesel fulfills DIN EN 590 in regard to distillation

AspenPlus method
ASTM D86 distillation curve for a petroleum mixture, on a liquid volume basis

Boiling point analysis EN ISO 3405 / ASTM D86



DIN EN 590, 2014	
250 °C	< 65 %
350 °C	> 85 %
360 °C	95 %

Fossil diesel
[1] 180-370 °C
[2] 170-390 °C

Boilung points[3]	
OME_3	156 °C
OME_4	202 °C
OME_5	242 °C

1. Gruden, D., *Umweltschutz in der Automobilindustrie: Motor, Kraftstoffe, Recycling*. ATZ / MTZ-Fachbuch. 2008, Wiesbaden: Vieweg +Teubner / GWV Fachverlage GmbH Wiesbaden.
2. Iannuzzi, S.E., et al., Fuel, 2016. 167: p. 49-59.
3. Liu, H., et al., Energy, 2015. 88: p. 793-800.

Comparison of Efficiencies

OME_3

$5\ CO_2 + 15\ H_2 + 1{,}5\ O_2 \rightarrow C_5H_{12}O_4 + 9\ H_2O$

LHV_{H2} = 120.21 MJ/kg

LHV_{OME3} = 19.14 MJ/kg

$\eta_{CCE,theoretical}$ = 68.8 %

P_{ein} [kW]	
Electrolysis	69 %
Utilities	25 %
Pumping	2.2 %
CO_2	3.5 %

$OME_{3\text{-}5}$

η_{CCE} = 66.8 % (64.8 %)

η_{Plant} = 42.6 % (41.4 %)

f = 0.64 (0.64) $LHV_{Lautenschütz\ et\ al.}$ ($LHV_{Lui\ et\ al.}$)

η_{PTL} = 32.3 % (31.3 %)

n-Hexadecane

$16\ CO_2 + 49\ H_2 \rightarrow C_{16}H_{34} + 32\ H_2O$

LHV_{H2} = 120.21 MJ/kg

LHV_{C16H34} = 44.32 MJ/kg

With a value of 100, hexadecan is the reference for cetane numbers

$\eta_{CCE,theoretical}$ = 83.8 %

P_{ein} [kW]	
Electrolysis	88 %
Utilities	5.6 %
Pumping	1.9 %
CO_2	4.6 %

Fischer-Tropsch

η_{CCE} = 83.7 %

η_{Plant} = 74.6 %

f = 0.89

η_{PTL} = 51.5 %

Literature[1]

η_{CCE} = 83.4 %

η_{Plant} = 69.3-75.1 %

f = 0.83-0.9

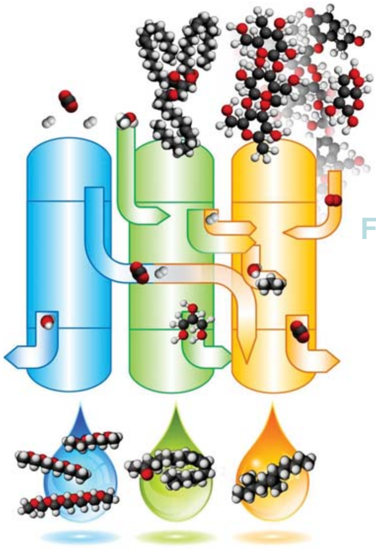
Chemical conversion efficiency $\eta_{CCE} = \frac{\dot{m}_{Fuel} \cdot LHV_{Fuel}}{\dot{m}_{H2} \cdot LHV_{H2}}$

Plant efficiency $\eta_{Plant} = \frac{\dot{m}_{Fuel} \cdot LHV_{Fuel}}{\dot{m}_{H2} \cdot LHV_{H2} + P_{Plant}}$

Efficiency factor $f = \frac{\eta_{Plant}}{\eta_{CCE}}$

Power-to-Liquid $\eta_{Power-to-Liquid} = \frac{\dot{m}_{Fuel} \cdot LHV_{Fuel}}{\frac{\dot{m}_{H2} \cdot LHV_{H2}}{\eta_{Electrolysis}} + P_{Plant} + P_{CO2}}$

1. A. Tremel et al., International Journal of Hydrogen Energy, 40 (2015) 11457–11464.



Motivation

Process Development

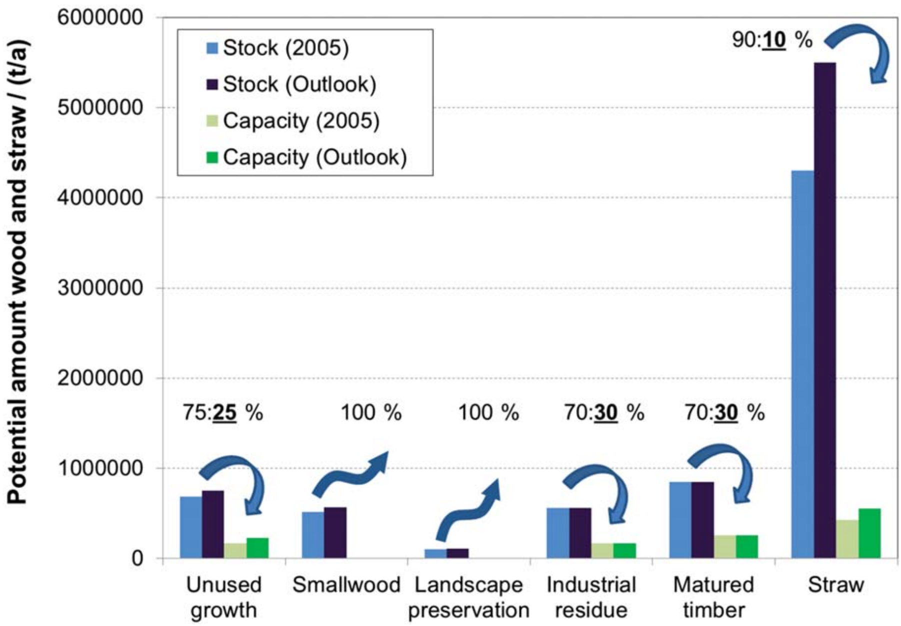
Fischer-Tropsch OME$_{3\text{-}5}$ Comparison

Assessment of Available Quantities

Connection to Biofuels

Fuel Strategy

Competition for Residual Wood



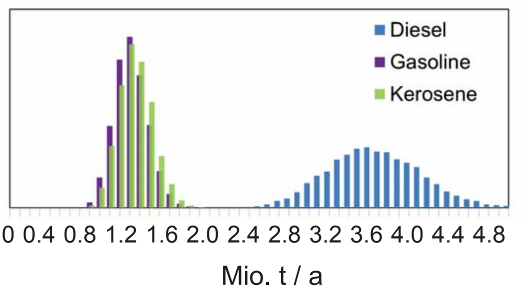
T. Grube, R. Menzer, R. Peters, K. Arnold, S. Ramesohl - VDI BERICHTE, 2006 - VDI

Fuels from Biomass

2. Generation Biofuels

- Whole plant use
- No direct competition to food product used for consumable oils and grains
- No indirect competition to food production due to use of fertile soil
- Biomass: residual wood and straw, grasses (Miscanthus), vegetable oil from algae or jatropha, salt tolerant plants etc.
- Process technologies:
  Hydrogenation of vegetable oil (commercial)
  Fischer-Tropsch synthesis (SoA, high investment)
  Bioliq (R&D, medium TRL, bridge to chemistry)
  Fermentation & biochemical pathways (low TRL)

Estimation for Germany



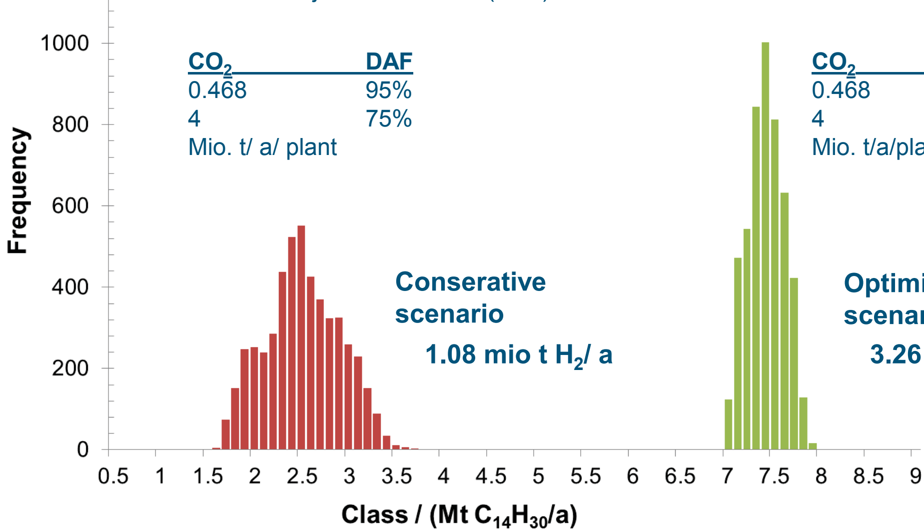
18% truck diesel
11% gasoline
11.5% kerosene

Basis: Forecast 2025 of MWV
19.7 Mio. t / a truck diesel
11.7 Mio. t/ a gasoline
10.9 Mio. t/ a kerosene

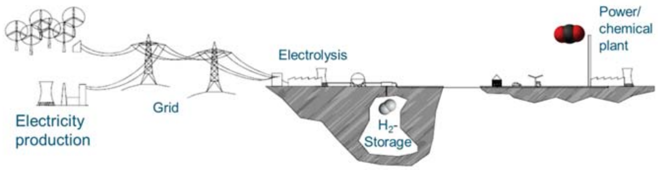
CO_2 Emissions from Industry for Fuel Production

<u>Assessment</u>:

- CHOREN planned to start with ***150,000***-200,000 kt/a ⇨ ***0.468*** Mio. t CO_2/ a/ scource
- Commercial FT plants have capacities of 0.36 – 7.5 Mio. t FT product/a
- Downward adjustment factors (DAF) between min. **0.48** und max. **4** Mio. t CO_2/ a/ plant

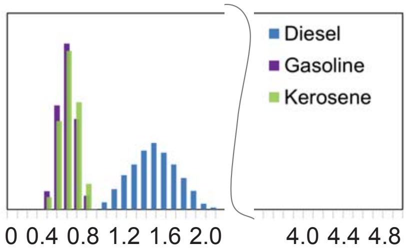


Power-to-Fuel concept: Fuels from CO_2 and H_2



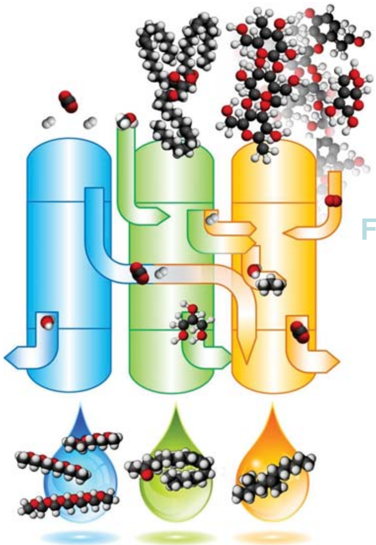
- **Interconnecting energy and transport sector**
- Storage of fluctuating renewable energy
- Fuels in analysis:
  - **Fischer-Tropsch (FT)** products (SoA, high investment)
  - Methanol & DME (SoA for *syngas*, bridge to chemistry, R&D for direct use of CO_2)
  - Higher alcohols & ethers (R&D, TRL 2-4)
- **Industrial CO_2** source with 0.4 – 4 Mio t CO_2/a/source reasonable link to FT synthesis
- **CO_2 from coal fired power plants is not an option; with regard to the COP21 goals**
  Demand: **1.2 Mio. t H_2 /a** & 8.3 Mio. t CO_2 /a

Estimation for Germany



Available quantities
7.5 % truck diesel
5 % gasoline
5.5 % kerosene

Assumend demand 2025
19.7 Mio. t / a truck diesel
11.7 Mio. t/ a gasoline
10.9 Mio. t/ a kerosene
Source: MWV



Motivation

Process Development

Fischer-Tropsch OME$_{3-5}$ Comparison

Assessment of Available Quantities

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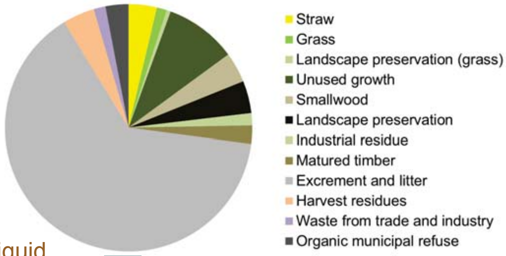
Fuel Strategy

Usage of Biomass for Fuels

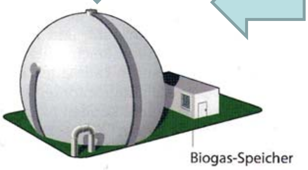


Residual wood & straw

a) Fischer-Tropsch synthesis:
$n\,CO + (n+m/2)\,H_2 \rightarrow C_nH_m + n\,H_2O$

b) BioLiq-process, gasification & MTG-process

Liquid manure

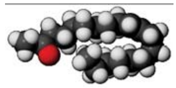


2 mio. ha energy crops
w/ 12 t short rotation coppice / ha
+
1.3 – 1.5 mio. ha for rape harvest

⇨ 0.65 – 0.95 mio. tons rape oil

a) Fermentation: CH_4/CO_2 = 1:1
& combined heat & power plant

b) Connecting H_2 from wind via electrolysis
for methanation CH_4 as PTG



Distributed Biomass for Fuel Synthesis at Farms

Concept:

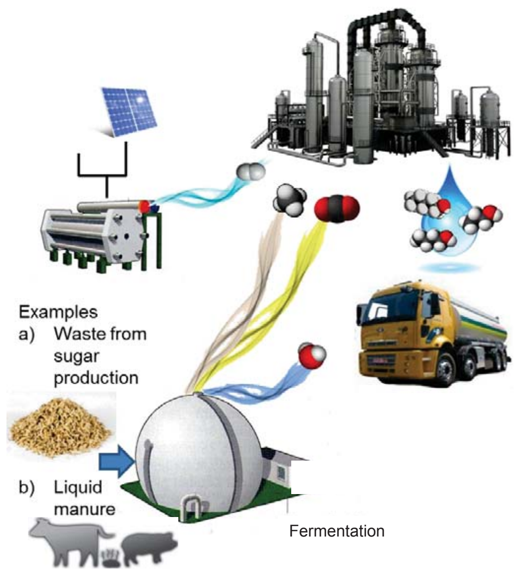
- Distributed **production of fuel intermediates** in liquid state for suitable transport at farms
- **Reduction of eutrophication** by increased usage of liquid manure
- Liquid fuels economically advantageous over gaseous fuels

Facts & figures:

- Liquid manure: 309.5 bn l/a (82% cattle) ≈ 320 Mt/a*
- 9004 biogas facilities in Germany w/ 4166 MW_e installed power & an average size of 500 kW_e w/ 30% feedstock manure (rest: silage) [2016]
- CO_2:CH_4 ≈ 50:50 ⇨ 5.7 mt CH_4 & 16 mt CO_2

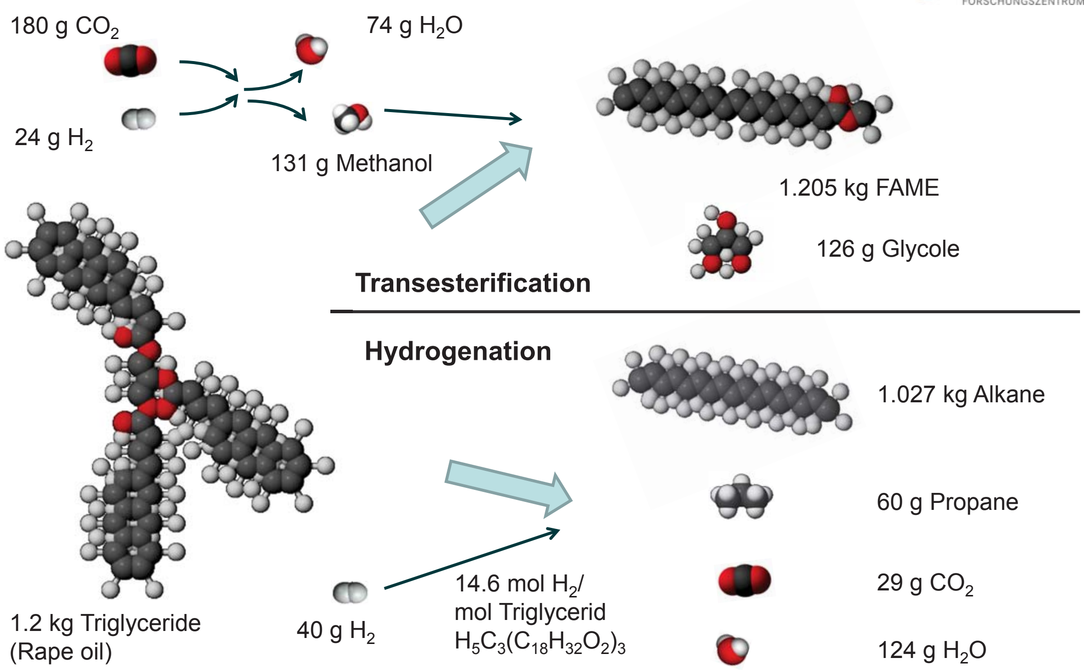
Outlook:

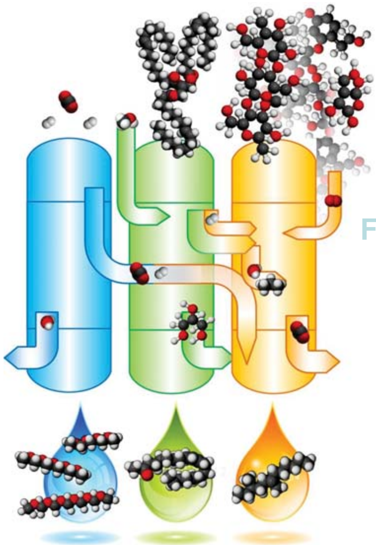
- Design of butanol synthesis plant from CO_2 (1750 t/a) combined w/ 75 kW_e electrolysis producing 750 t/ a



Source: http://www.riskagua.de/index.php?id=110 funded by BmBF

Connecting Biomass and Renewable Energy





Motivation

Process Development

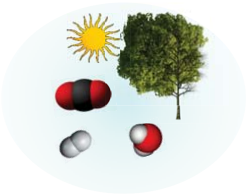
Fischer-Tropsch | OME_{3-5} | Comparison

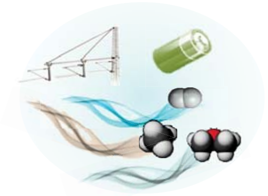
Assessment of Available Quantities

Connection to Biofuels

Fuel Strategy

Development of a Fuel Strategy: Production & Logistics





- Limited amounts: hydrogen, carbon dioxide, water, solar energy and cultivated area or bio mass production
- Process and techno-economic analysis of complete process chains inclusive separation of components and refinement
- Consideration of competing or supporting system solutions, i.e. electrical driving (batteries, catenary supply) or gaseous fuels such as hydrogen, methane or dimethyl ether
- Socio economic studies especially for cultivation of energy plants or for double-use of fossil carbon
- Logistics: storage and transport systems, local und centralized process untis in the production chain

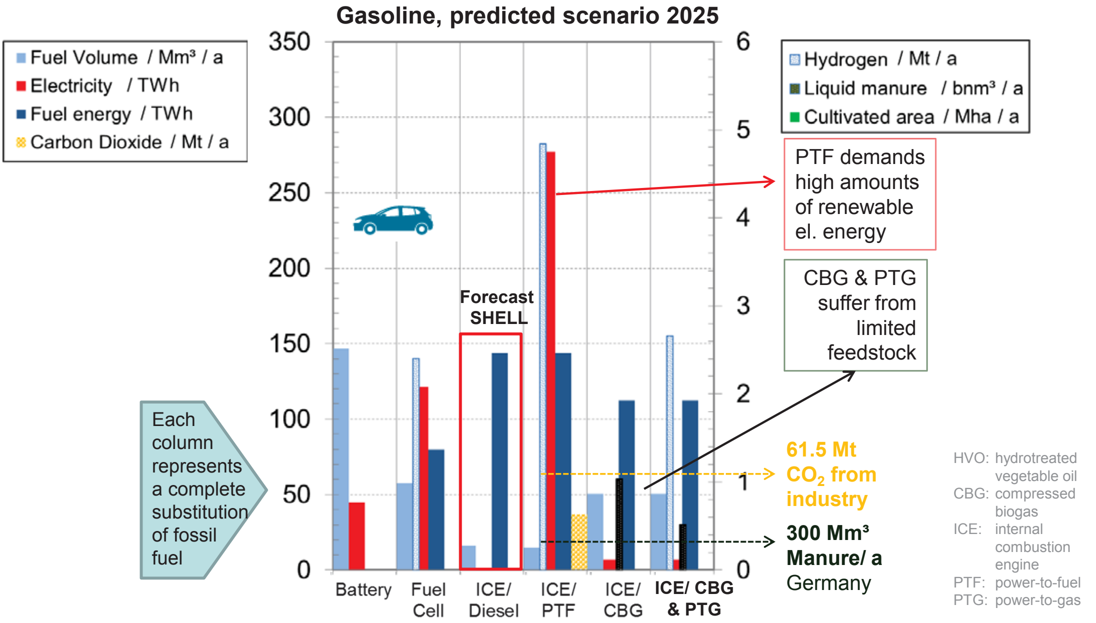
Overcapacity in Power is Inherent for Full Renewable Energy Supply

$$\text{Capacity factor} = \frac{\text{energy harvested}}{\text{nameplate harvest}}$$

Average power demand for Germany: ~ 60 GW (based on **528 TWh** grid electricity)

	Capacity factor	Necessary Power, if just one Technology is applied	Reasonable power mix DE 2050 (DE gov. Installation plans extrapolated)	Reasonable electricity mix DE 2050	Electricity to be converted to H_2 (serving 75% of passenger vehicles in DE)
Offshore wind	0.46	120 GW	59 GW	236 TWh	
Onshore wind	0.23	230 GW	132 GW	267 TWh	
PV	0.12	460 GW	120 GW	126 TWh	
Total	--------	----------	311 GW	**629 TWh**	101 TWh (**2,1 mt H_2**)
Untimely produced electricity				≈ 200 TWh (to be stored)	
CO_2 cut Ø 80%				90% (10% power by NG)	54% of passenger cars

Future fuels for light duty vehicles & passenger cars



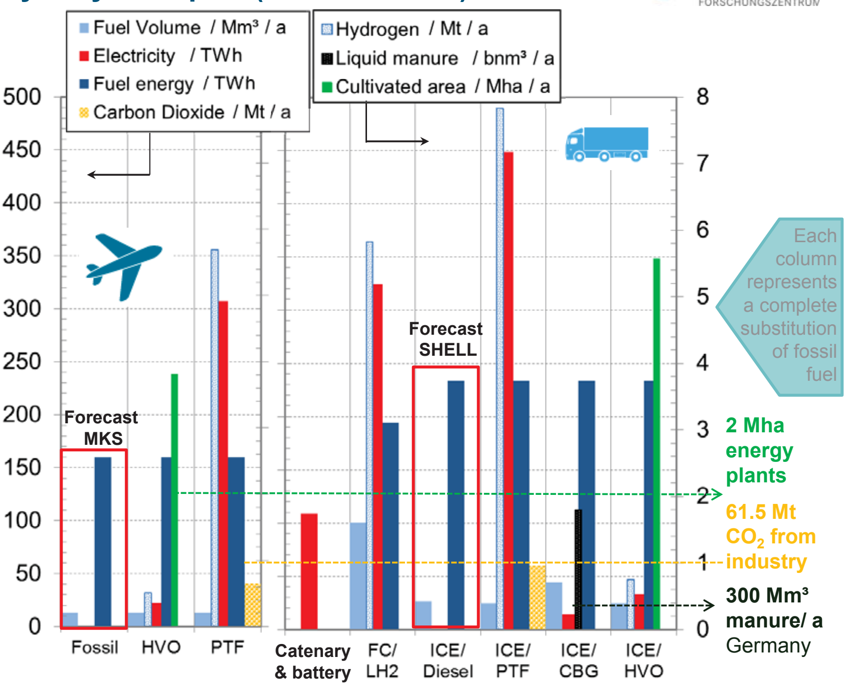
- Electrification of LDV w/ 120 – 260 TWh_e ⇨ mix of battery & fuel cell cars (short to long distances)

IEK-3: Elektrochemische Verfahrenstechnik 49

Future fuels in heavy duty transport (scenario 2025)

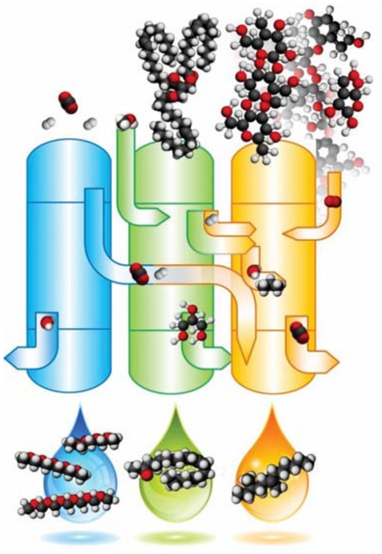
- Airplanes will use a HVO/PTF mix
- CBG can't fulfill high quotes for truck diesel
- H_2 best option for fleet operation of trucks
- H_2 w/ limited operation range and large tank
- H_2/ FC & PTF w/ high demand for electrolysis 275 – 450 TWh (trucks)
- Catenary systems only in combination w/ diesel & hybridization

- Heavy duty transport w/ high diversification of fuels to reach CO_2 reduction



IEK-3: Elektrochemische Verfahrenstechnik 50

Summary



- Linking energy production and mobility by hydrogen production via electrolysis
- Direct hydrogen usage for fuel cell drive systems
- Carbon capture from industrial flue gas in combination with other sources
- Synthesis of energy carriers for later electricity production (storage)
- Fuel synthesis *(link to mobility)*
  - Techno economic analysis
  - Development of fuel strategies
  - Catalyst characterization
  - Reactor development & testing
  - Component testing

Teilweise Förderung durch:

JARA|ENERGY

P2F Competence Center Power to Fuel | RWTH AACHEN UNIVERSITY

Projekthaus TESYS
Technikbasierte
Energiesystemanalyse | RWTH AACHEN UNIVERSITY

Energie System 2050
Ein Beitrag des
Forschungsbereichs Energie | HELMHOLTZ GEMEINSCHAFT

Kooperationspartner

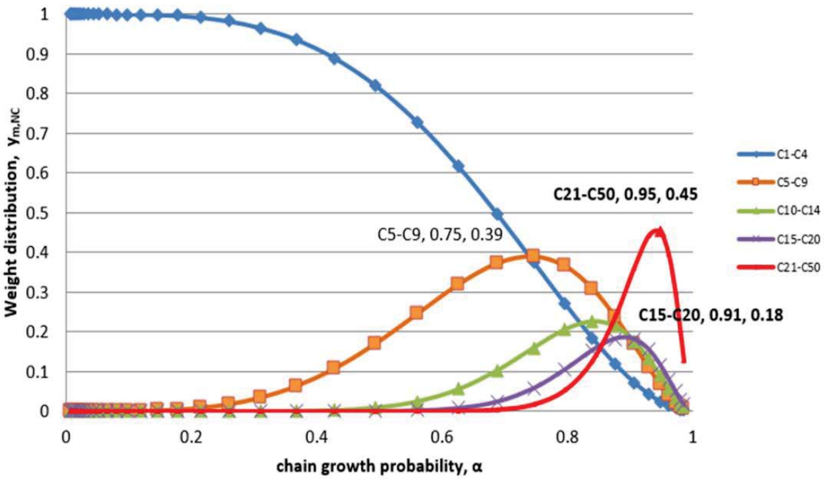
KIT Karlsruher Institut für Technologie — **Institut für Mikroverfahrenstechnik**

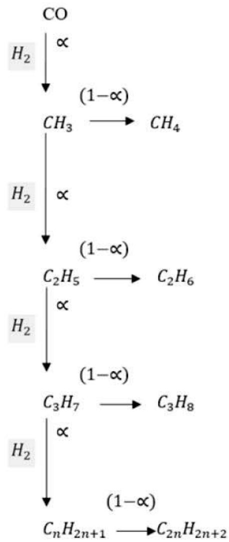
TECHNISCHE UNIVERSITÄT DRESDEN — **Institut für Verfahrens- und Umwelttechnik**

FINDING TOMORROW TODAY

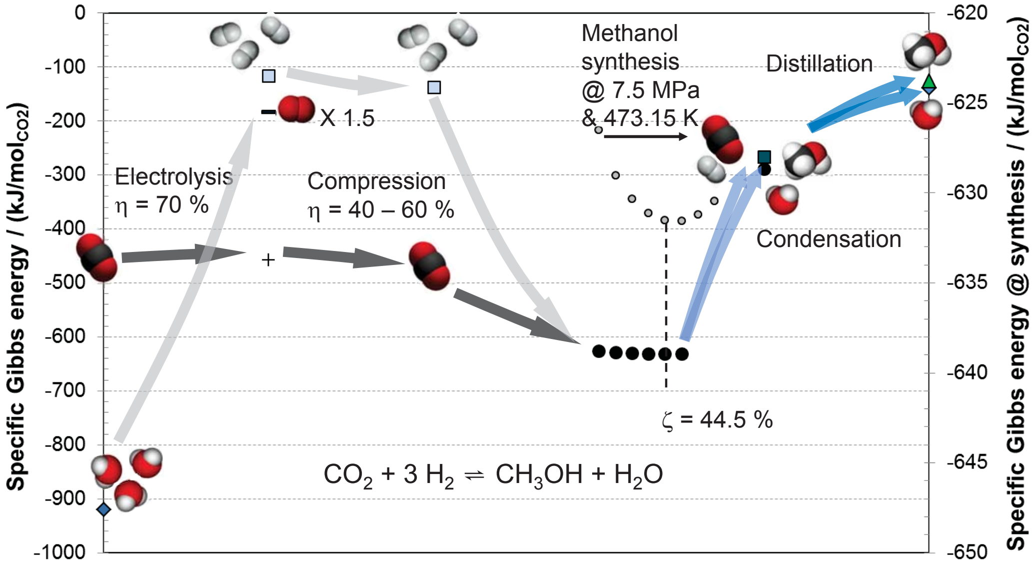
Polymerization by ASF-model

$$y_{m,NC} = \mathrm{NC} \propto^{NC-1} (1-\propto)^2$$



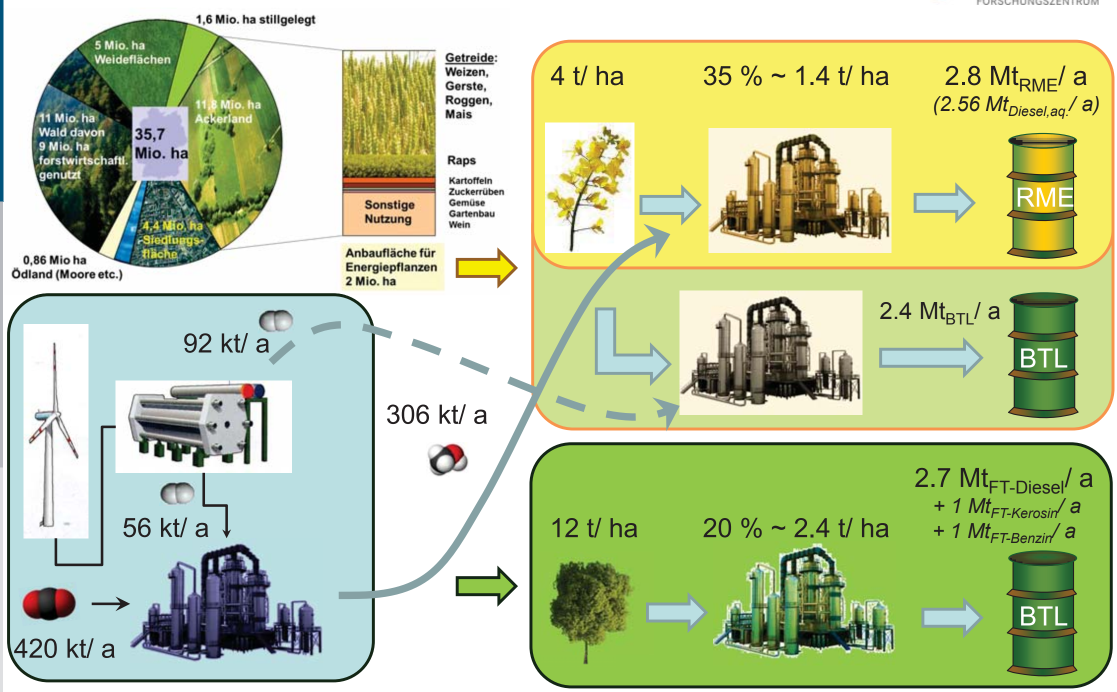


Gibbs Energy analysis for CH_3OH synthesis from CO_2



- Methanol synthesis from CO_2 suffers from low Gibbs Energy of CO_2
- Additional separation effort for product mixture CH_3OH / H_2O

Land Use for Energy Crops



The Separation of CO_2 from Ambient Air – a Techno-Economic Assessment

Ralf Peters, Daniel Krekel, Remzi Can Samsun, Detlef Stolten
Forschungszentrum Jülich GmbH, Institute for Energy and Climate Research – Electrochemical Process Engineering (IEK-3)

The following cotribution assesses the separation of CO2 from ambient air from a technical and economic viewpoint. The reduction of CO2 emissions and its separation from the atmosphere is indispensable to counteract ongoing climate change. The most promising technology for CO2 separation is first identified by reviewing the literature and comparing the most important technical and economic parameters. The results point to amines/imines as adsorbing agent to separate CO2 from ambient air. A system layout is then designed and a technical analysis is conducted by solving mass and energy balances for each component. An economic analysis is performed by applying a specific model. The energy demand of our system is calculated as 3.65 GJ/tCO2. This high energy demand mainly results from the system specific implementation of two compressors that compress air/CO2 and overcome the pressure losses. The second law efficiency calculated ranges of 7.52-11.83 %, depending on the option of heat integration. The costs of avoiding CO2 emissions vary between $ 824-1,333/tCO2 depending on the energy source applied. The analysis results from our contribution basically present higher values for energy demand and costs compared to other values stated in literature. Reasons for this deviation are often insufficient and overoptimistic assumptions in other literature on the one hand side, but also related to the specific system design investigated in this paper on the other hand side. Further case studies reveal that enormous land requirements and investments would be needed to reduce prospective CO2 amounts in the atmosphere down to contemporary levels. A comparison between CO2 removal from the atmosphere and carbon capture and storage technology for coal power plants shows that this technology is not yet able to economically compete with carbon capture and storage. Furthermore, the impact of CO2 separation on the production costs of industrial commodities like cement and steel clearly shows that CO2 removal from the atmosphere is not yet a strong alternative to solving our climate change problem. In the long-term, CO2 separation from ambient air may still play a vital role in the sequestration of CO2 from dilute and dispersed sources since the technology has the potential for optimization. The detailed analysis is published by Krekel et al. in Applied Energy 218 (2018) 361–381.

Mitglied der Helmholtz-Gemeinschaft

JÜLICH FORSCHUNGSZENTRUM

The Separation of CO_2 from Ambient Air – a Techno-Economic Assessment

TRENDS 2017

5.- 6. December 2017

D. Krekel, R. C. Samsun, R. Peters, D. Stolten

Institute of Energy and Climate Research IEK-3: Electrochemical Process Engineering

JÜLICH FORSCHUNGSZENTRUM

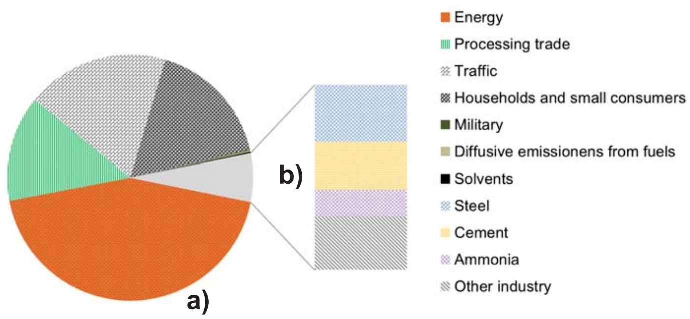
Motivation

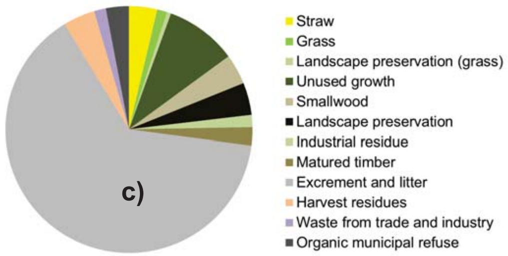
Global sectoral CO_2 emissions (2013)

- ~ 60 % of global CO_2 emissions could be captured if CCS technology is applied extensively in the industry and electricity and heat sectors
- In other sectors, the application of CCS is questionable, because of the numerous emitters, which all would need to be equipped with a CO_2 capturing device

→ **Direct capture of carbon dioxide from ambient air offers the advantage of directly capturing 100% of CO_2 emissions, which are "stored in the air"**

CO_2 Sources Today and in Future



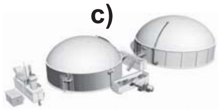


a) Carbon Capture Utilization & Storage
15 % CO_2 in flue gas
Test facility
No option for 2050

b) German industry:
52.2 Mio. t CO_2 (6.3 %)
16 mio. t from steel
13.5 mio. t from cement
7.5 mio. t from ammonia

15 – 100 % CO_2

c)

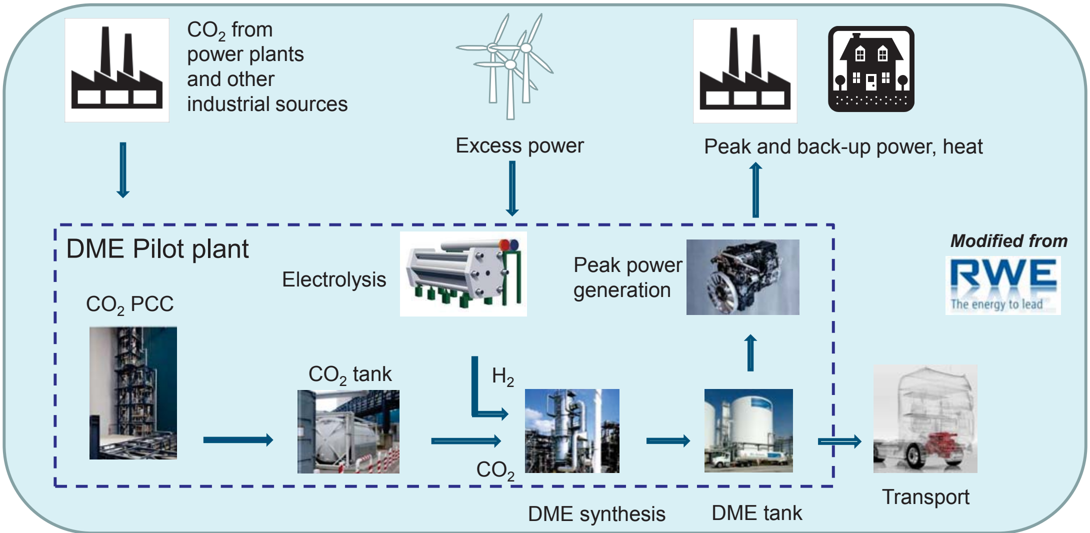


Bio gas plants in Germany
9004 in 2016 with 500 kW_e,
4.17 GW_e installed
50 : 50
16 mio. t CO_2

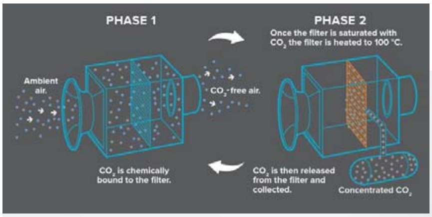
CO_2 from air
0.04 % CO_2
High investment
beyond 2050?

WP 4 RE-USE: DME as Chemical Long-term Energy Storage & Link to Mobility

- Chemical long-term energy storage
- Fuel for peak power generation & transport sector
- /w co-benefit: DME offers lowers emissions of Diesel engines



CO_2 Sources in Future: Capturing from Air

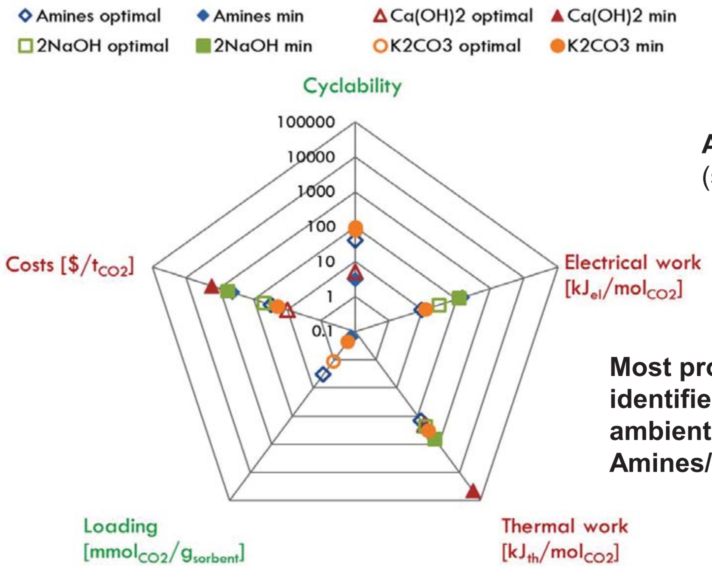


Source: http://www.climeworks.com/our-products/

Necessary free Gibbs energy to separate carbon dioxide from a diluted gas stream

Separation of carbon dioxide from air just consumes about <u>four times</u> as much energy that is needed to extract CO_2 from a flue gas stream in a post-combustion capture system in terms of thermodynamics, although the concentration differs by a factor of about <u>≥ 250</u>.

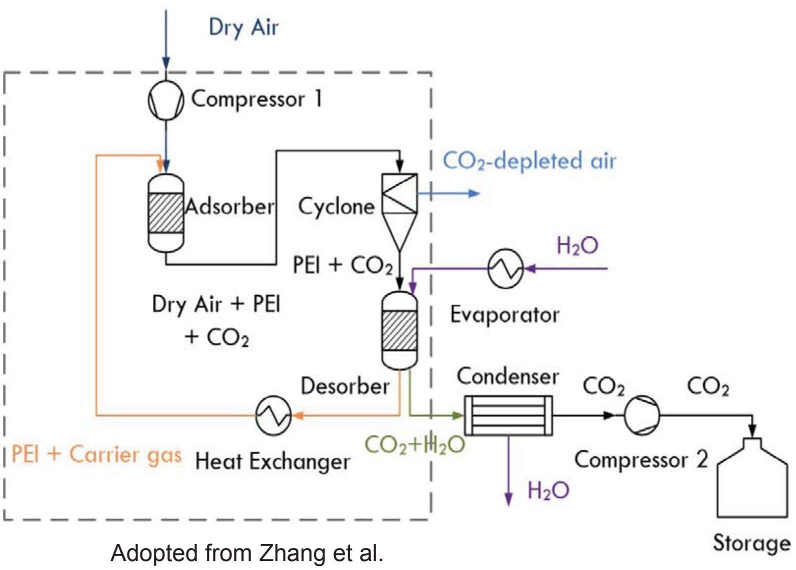
Comparison of processes for CO_2 separation from air in terms of different process parameters



Analysis based on 35 sources
(sources see next slide)

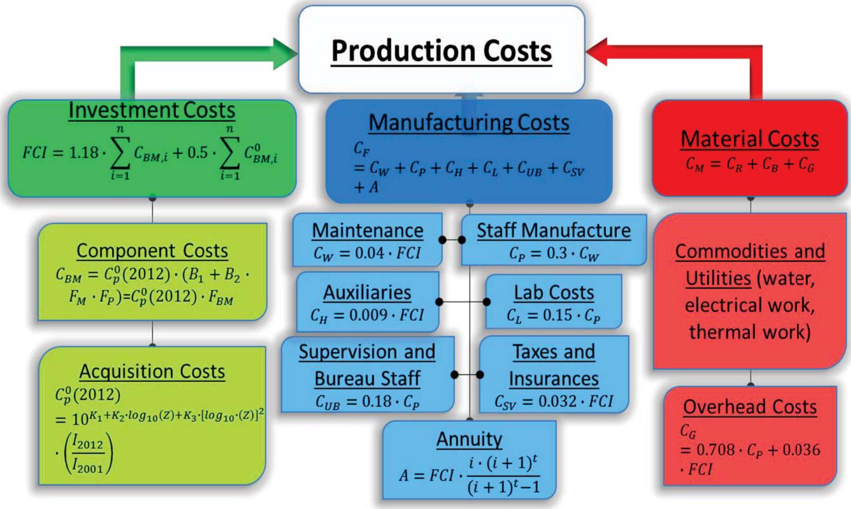
Most promising technology identified for CO_2 separation from ambient air:
Amines/imines

System flow chart of the analyzed CO_2 separation plant



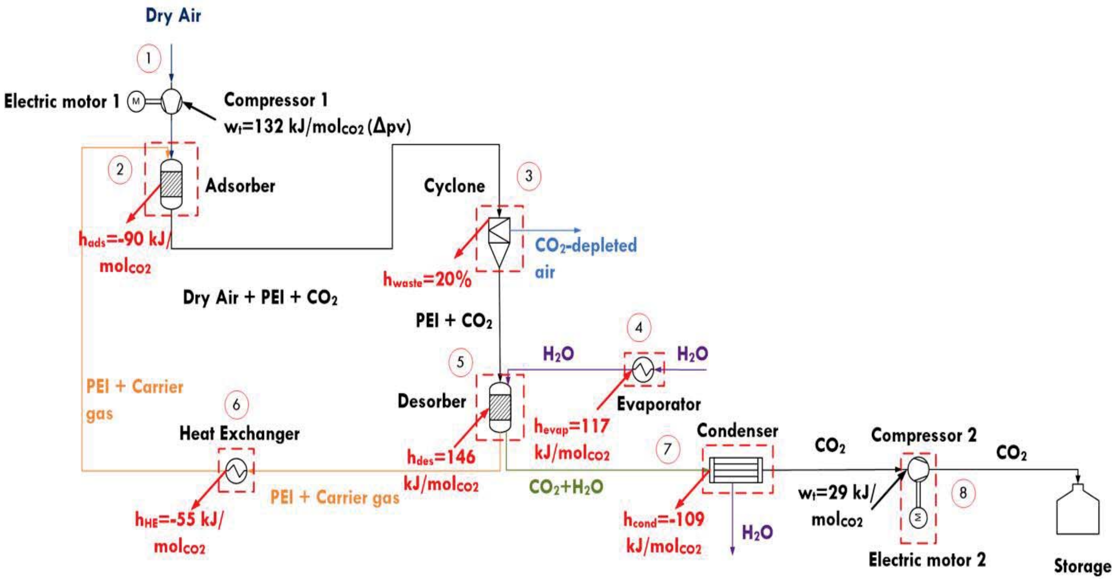
Adopted from Zhang et al.
(Chem Eng Sci, 116 (2014) 306-316)

Model for the economic analysis of the CO_2 separation plant



after:
R. Socolow et al., in, APS Physics, 2011, pp. 100.
A.R. Kulkarni et al., Industrial & Engineering Chemistry Research, 51 (2012) 8631-8645.
A. Otto, Forschungszentrum Jülich GmbH, Zentralbibliothek, Verlag, Jülich, Germany, 2015.

Detailed system flow chart of the analyzed CO_2 separation plant including thermal and electrical sources and sinks

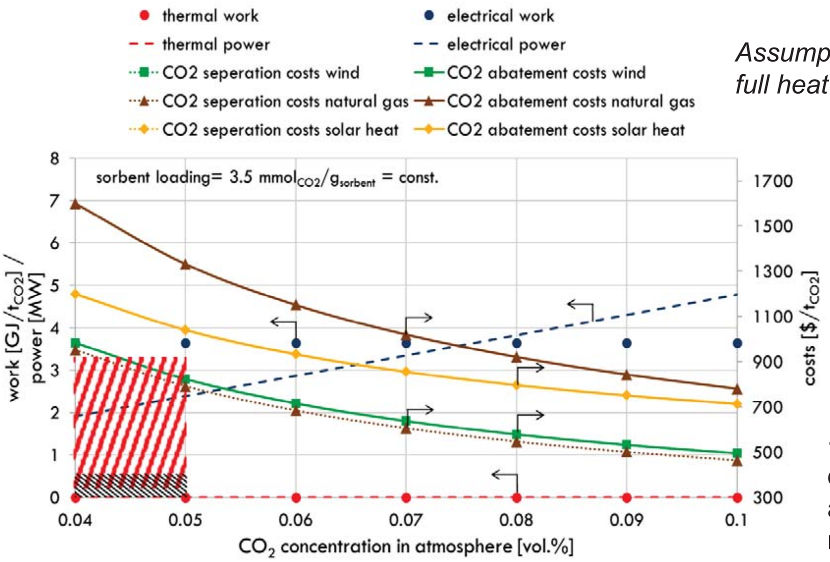


Economic Analysis - Results

Investment Costs								
Component	Adsorber	Desorber	Evaporator	Heat exchanger	Condenser	Cyclone	Compres-sor 1/ 2	E-motor 1/ 2
$C_P^0\ [10^6\$]$	1.89	0.07	0.24	0.03	0.27	3.04	0.67/ 0.21	0.2/ 0.12
$C_{BM}\ [10^6\$]$	7.57	0.26	0.7	0.09	0.79	12.39	2.55/ 0.81	0.3/ 0.18
$FCI\ [10^6\$]$	43.08							
Manufacturing Costs								
Cost Center	C_W	C_P	C_{UB}	C_H	C_L	C_{SV}	A	Σ
$C_F\ [10^6\$/a]$	1.72	0.52	0.09	0.39	0.08	1.38	4.13	8.31
Material Costs								
Cost Center	Water		Electrical work (natural gas)		Overhead costs		Σ	
$C_M\ [10^6\$/a]$	0.04		0.95		1.92		2.91	
Production Costs								
$C_{PC}\ [10^6\$/a]$	11.21				Specific production costs (separation costs) [$/$t_{CO2}$]		792 (@14,250 t_{CO2}/a)	

System sensitivity analysis

Energy demand and costs for CO_2 separation from ambient air in dependence on the CO_2 concentration



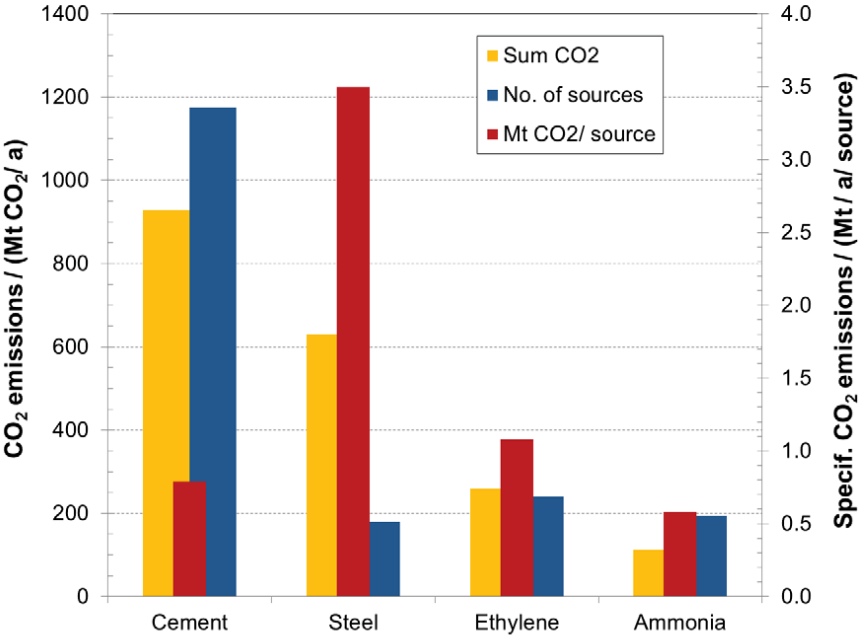
Assumption:
full heat integration

→ In this work, a detailed model was applied which resulted in costs in the upper range.

Considered Scenarios

- Compensating CO_2 emissions from industrial sources
- Reduction of CO_2 emissions worldwide

Sources for CO_2 from Industry Worldwide

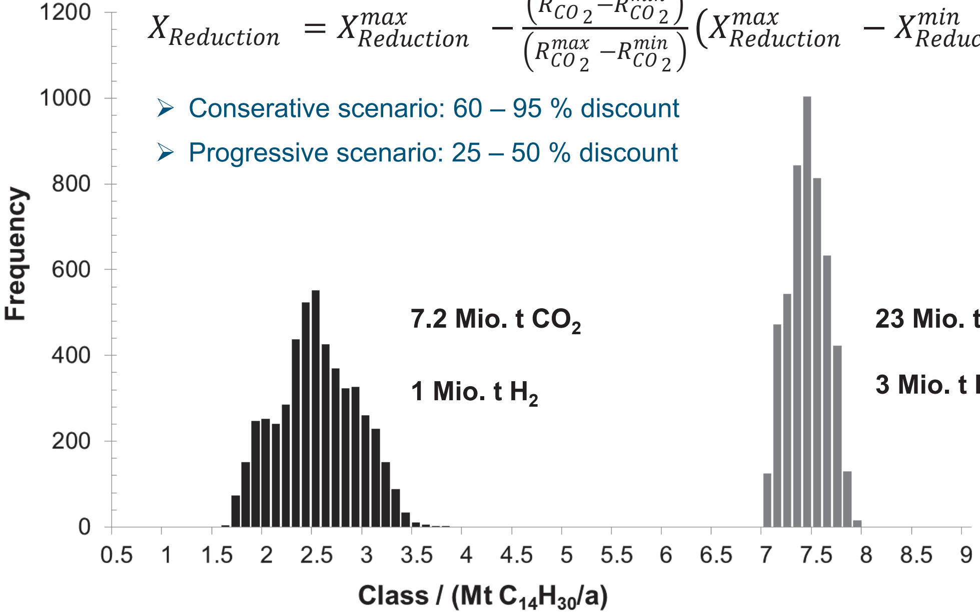


Fuel synthesis & CO_2 source must fit to eachother

Mass balances for Power-to-Fuel

$$X_{Reduction} = X_{Reduction}^{max} - \frac{\left(R_{CO_2} - R_{CO_2}^{min}\right)}{\left(R_{CO_2}^{max} - R_{CO_2}^{min}\right)} \left(X_{Reduction}^{max} - X_{Reduction}^{min}\right)$$

- Conservative scenario: 60 – 95 % discount
- Progressive scenario: 25 – 50 % discount

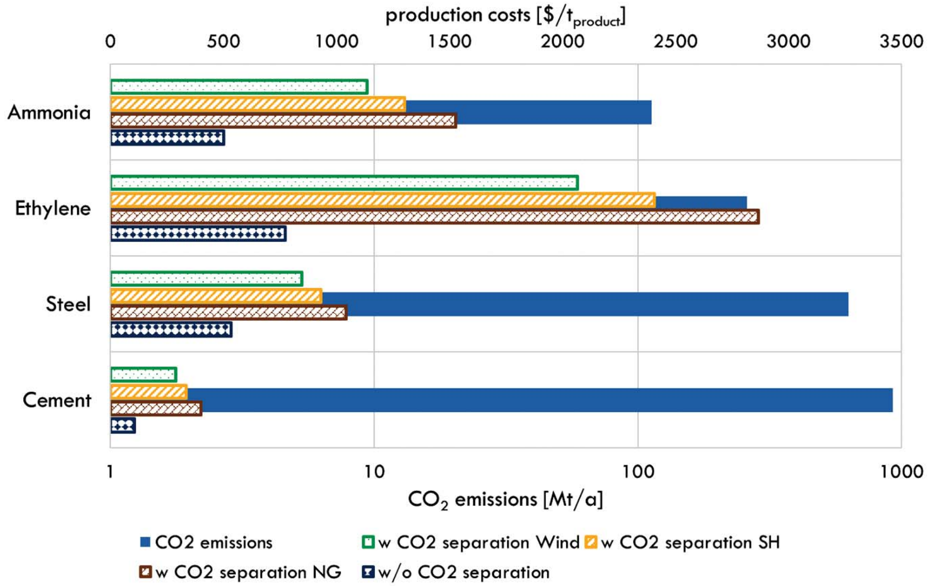


CO_2 emissions, production rates and plant sizes for global steel, cement, ethylene and ammonia production

		Product			
Category	Unit	Cement	Steel	Ethylene	Ammonia
CO_2 emissions [12] (2002)	Mt/a	928.3	630.0	259.2	112.5
No. of sources [12] (2002)	-	1,175	180	240	134
Specific CO_2 emissions	Mt/a/source	0.79	3.5	1.08	0.58
Production rate (2002)	Mt/a	1,946 [6]	905 [7]	75 [3]	107 [5]
Number of separation plants/ source	-	56	246	76	41
Investment costs	Bill. $	2.4	10.6	3.3	1.8
Footprint (Solar)	km²	2.47	10.93	3.37	1.81
Average Production rate (2013-2015)	Mt/a	4,200 [6]	1,650 [7]	165 [2]	146 [5]
Price (2002)	$/t	91.9 [8]	402 [6]	400 [4]	70 [11]
Average price (2013-2015)	$/t	105.5 [6]	533 [1]	772 [9]	500 [10]

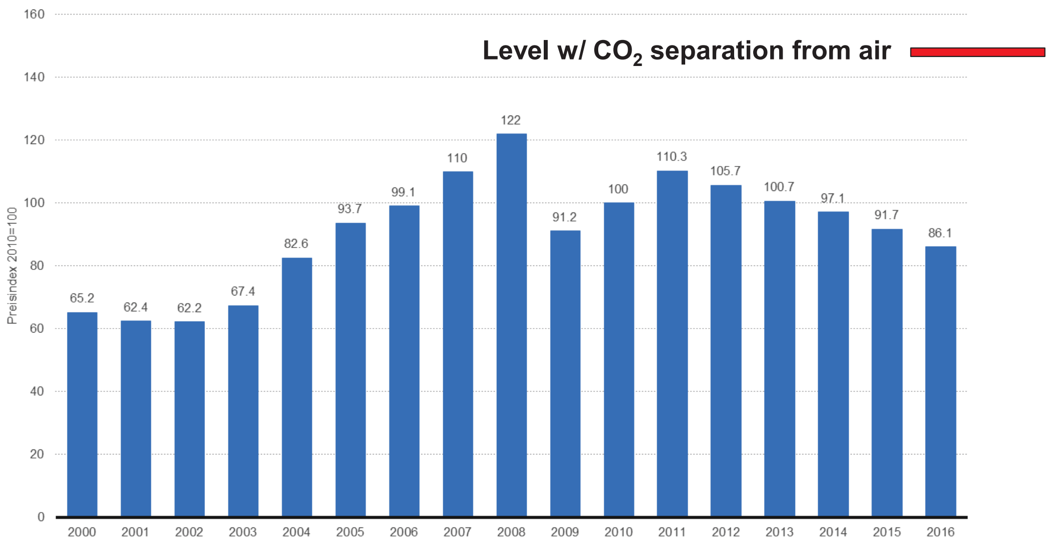
Sources: see next slide

Influence of the CO_2 separation from ambient air on the production costs of exemplary industry sectors



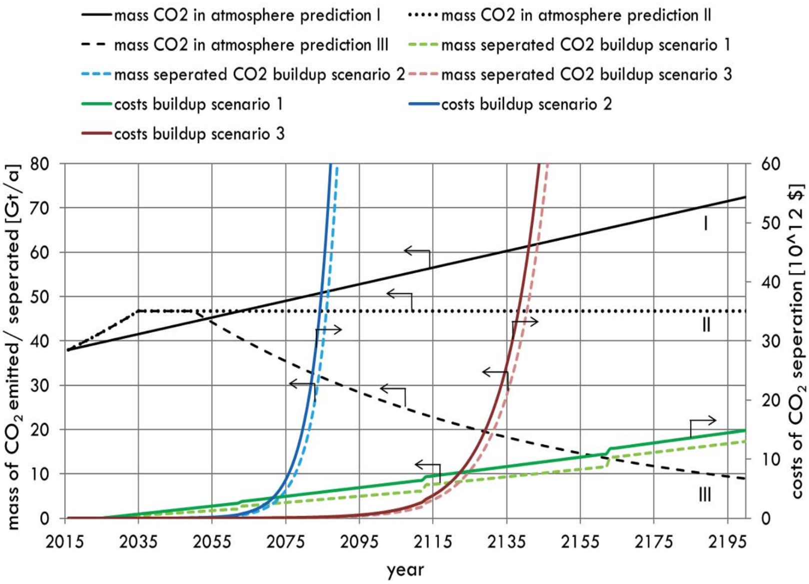
Sources: see next slide

Influence of the CO_2 separation from ambient air on the production costs of steel (related to steel price index)



Sources: statista

Case study 1:
Scenarios for the separation of global CO_2 emissions

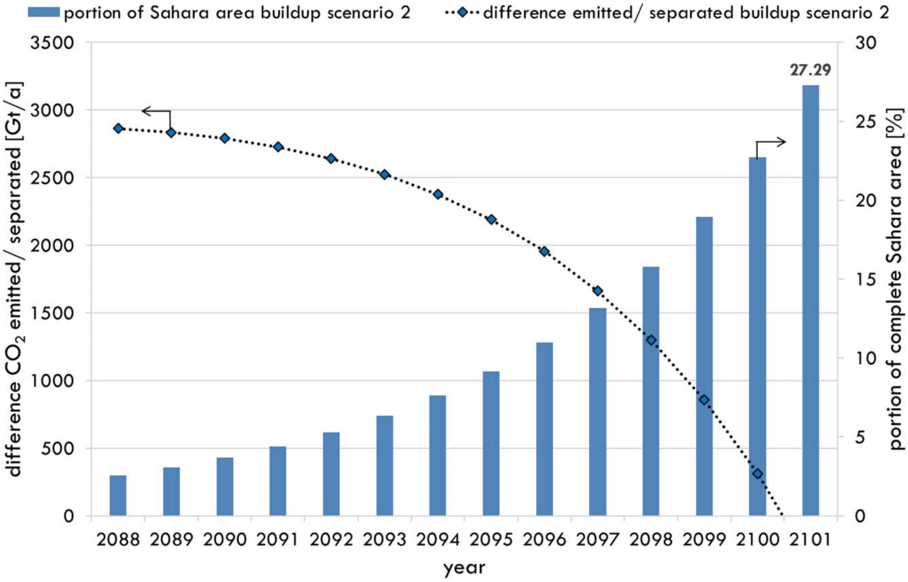


Results from Case Study 1

Overview buildup scenarios in dependence on CO_2 development predictions

Buildup Scenario 1 (+ 5,000 plants/a)	CO_2 development prediction		
	I (increase)	II (constant)	III (decrease)
Break-even year [-]	-	-	2163
Separation plants [10^6]	-	-	0.7
Costs [10^12 $]	-	-	12
Sahara area [%]	-	-	0.4
Buildup Scenario 2 (+ 20 % plants/a)	I (increase)	II (constant)	III (decrease)
Break-even year [-]	2087	2086	2084
Separation plants [10^6]	3.9	3.3	2.3
Costs [10^12 $]	58	48	34
Sahara area [%]	2.1	1.8	1.2
Buildup Scenario 3 (+10 % plants/a)	I (increase)	II (constant)	III (decrease)
Break-even year [-]	2144	2141	2131
Separation plants [10^6]	3.9	2.9	1.1
Costs [10^12 $]	61	46	18
Sahara area [%]	2.1	1.6	0.6

Case study 2: Results of buildup scenario 2 to reduce the amount of CO_2 to 2016 level



Results from Case Study 2

Overview buildup scenarios in dependence on CO_2 development predictions for the reduction of global CO_2 emissions to the level in 2016 (Deadline: 2300)

Buildup Scenario 1 (+ 5,000 plants/a)	CO_2 development prediction		
	I (increase)	II (constant)	III (decrease)
Break-even year [-]	-	-	-
Separation plants [10^6]	-	-	-
Costs [10^12 $]	-	-	-
Sahara area [%]	-	-	-
Buildup Scenario 2 (+ 20 % plants/a)	I (increase)	II (constant)	III (decrease)
Break-even year [-]	2101	2101	2100
Separation plants [10^6]	51	51	42
Costs [10^12 $]	747	747	623
Sahara area [%]	27.29	27.29	22.74
Buildup Scenario 3 (+10 % plants/a)	I (increase)	II (constant)	III (decrease)
Break-even year [-]	2169	2168	2164
Separation plants [10^6]	42	38	26
Costs [10^12 $]	710	645	441
Sahara area [%]	22.52	20.48	13.99

Comparison of carbon capture and storage (CCS) and CO_2 separation from ambient air

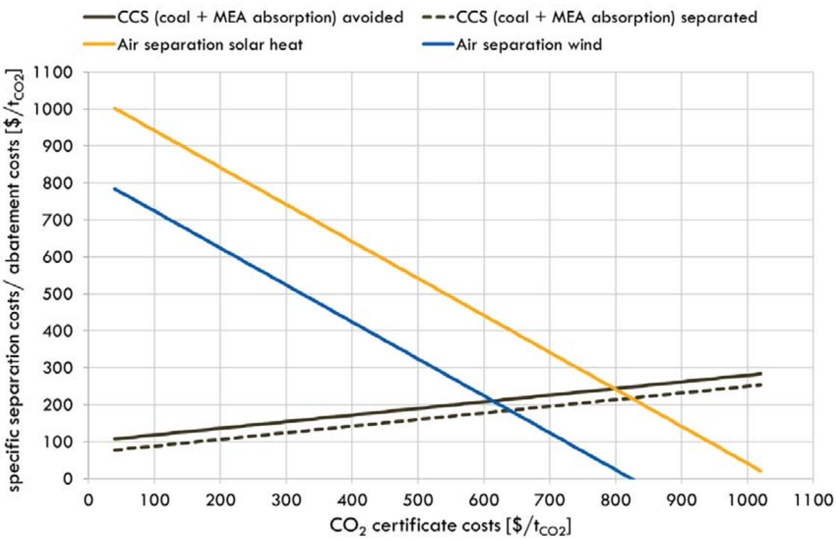
	Carbon capture and storage technology		
	Post-Combustion	Oxyfuel	Pre-Combustion
Efficiency decrease[1] [%]	9-14	7-11	6-11
Energy demand [kJ_{el}/mol_{CO2}]	42		
Status of development	+	-	-
Complexity	+	+	-
Possibility to change setup	+	(+)	-
CO_2 abatement costs [$\$/t_{CO2}$]	Coal: 34	Coal: 36	Coal: 23
	Natural gas: 58	Natural gas: 102	Natural gas: 112
	Range literature: 20-260		
CO_2 transport and storage [$\$/t_{CO2}$]	4.5-10		
	CO_2 separation from ambient air		
Energy demand [kJ_{el}/mol_{CO2}]	161		
CO_2 abatement costs [$\$/t_{CO2}$]	Coal: -	Natural gas: 1,333	Wind: 824
	Solar heat: 1,041		

[1]net efficiency loss incl. CO_2 compression for a coal-fired steam power plant

Sources: see next slide

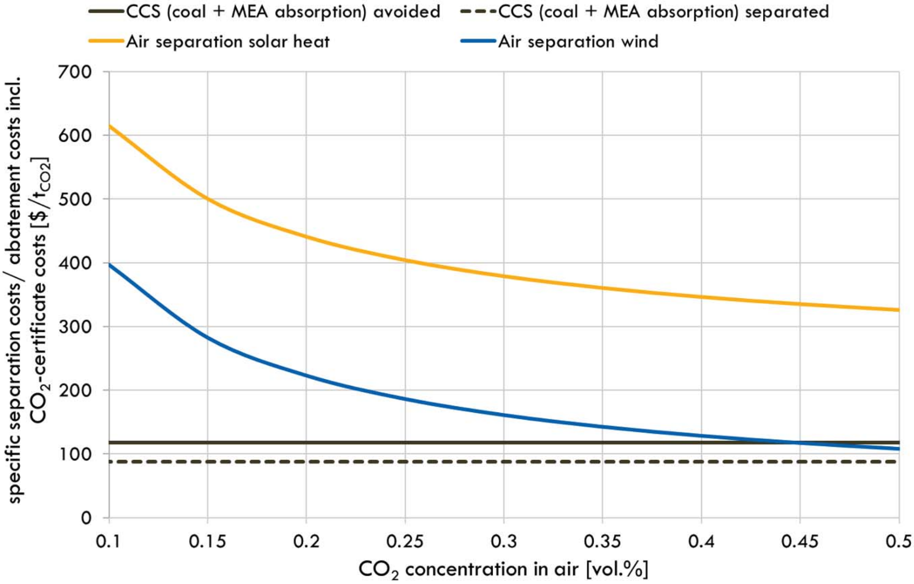
CO_2 separation costs/ abatement costs

for CCS and CO_2 separation from ambient air in dependence on the CO_2 certificate cost



CO_2 separation costs/ abatement costs

including CO_2 certificate costs for CCS and CO_2 separation from ambient air in dependence on the CO_2 concentration in the air



Summary 1/2

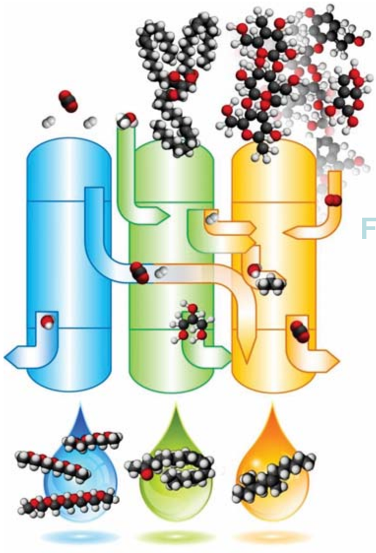
- In terms of costs, cyclability, loading and necessary electrical and thermal work, amines/imines were analyzed to have the highest potential for directly separating carbon dioxide from ambient air
- The technical analysis of the system design showed that second law efficiencies of 7.52-11.83 % are feasible, depending on the heat integration of the system
- Higher CO_2 concentrations in the ambient air increase the efficiency of the separation process
- Coupling CO_2 separation from ambient air with renewable energy has the potential to lower the CO_2 abatement costs compared to systems powered by fossil fuels.
- In two case studies, the separation of the global carbon dioxide amount was investigated by coupling the separation plants with solar thermal power plants.
- The results revealed that an exponential construction of separation plants is mandatory to reduce the carbon dioxide amount to the level of 2016 by 2300.

Summary 2/2

- Different CO_2 separation plant buildup scenarios in combination with diverse CO_2 development predictions showed that costs of up to $ 747 trillion might be needed to erect up to 51 million CO_2 separation plants. This amount of money corresponds approximately to a tenth of the global gross domestic product in 2014. In addition, up to 27.3 % of the total Sahara area would be occupied if plants were built in this region.
- Compared to carbon capture and storage (CCS) technology, which can be applied to big point emitters, CO_2 separation from ambient air consumes up to a factor of 4 more energy and has much higher abatement costs with increases of up to a factor of 8-13
- A further comparison of both technologies shows that CO_2 separation from ambient air cannot feasibly compete with CCS economically. Unconceivably high CO_2 certificate costs of $ 620-830/tCO_2 or hygienically harmful CO_2 air concentrations of 0.45 vol.% and higher would be necessary to reach a cost parity between both technologies.
- With regards to the influence of subsequent CO_2 separation from ambient air on the production costs of industrial commodities like cement, steel, ethylene and ammonia, calculations show a dramatic increase. Depending on the power source of the CO_2 separation plant, production costs are likely to increase by a factor of 1.6-3.8, which makes the production of these products economically unfavorable.

Conclusion

- The results of this contribution show that CO_2 separation from ambient air will not be able to play a vital role in the abatement of the CO_2 climate problem until 2050 due to the fact that the technology has strong technological and economic drawbacks.
- To efficiently counteract climate change, a distributed system consisting of technologies to increase the efficiency of the state-of-the-art technology, substitution of conventional technologies by e.g. renewable energy, and the separation and utilization of carbon dioxide in e.g. power-to-x (PtX) processes will be mandatory.
- CO_2 separation from ambient air still has the potential for optimization, e.g. by constructing separation plants which use the natural air draft to lower the necessary electrical work or by applying improved materials and efficient system designs.



Motivation

Process Development

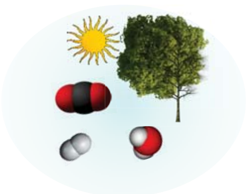
Fischer-Tropsch | OME_{3-5} | Comparison

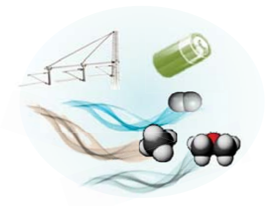
Assessment of Available Quantities

Connection to Biofuels

Fuel Strategy

Development of a Fuel Strategy: Production & Logistics





- Limited amounts: hydrogen, carbon dioxide, water, solar energy and cultivated area or bio mass production
- Process and techno-economic analysis of complete process chains inclusive separation of components and refinement
- Consideration of competing or supporting system solutions,
  i.e. electrical driving (batteries, catenary supply) or gaseous fuels such as hydrogen, methane or dimethyl ether
- Socio economic studies especially for cultivation of energy plants or for double-use of fossil carbon
- Logistics: storage and transport systems, local und

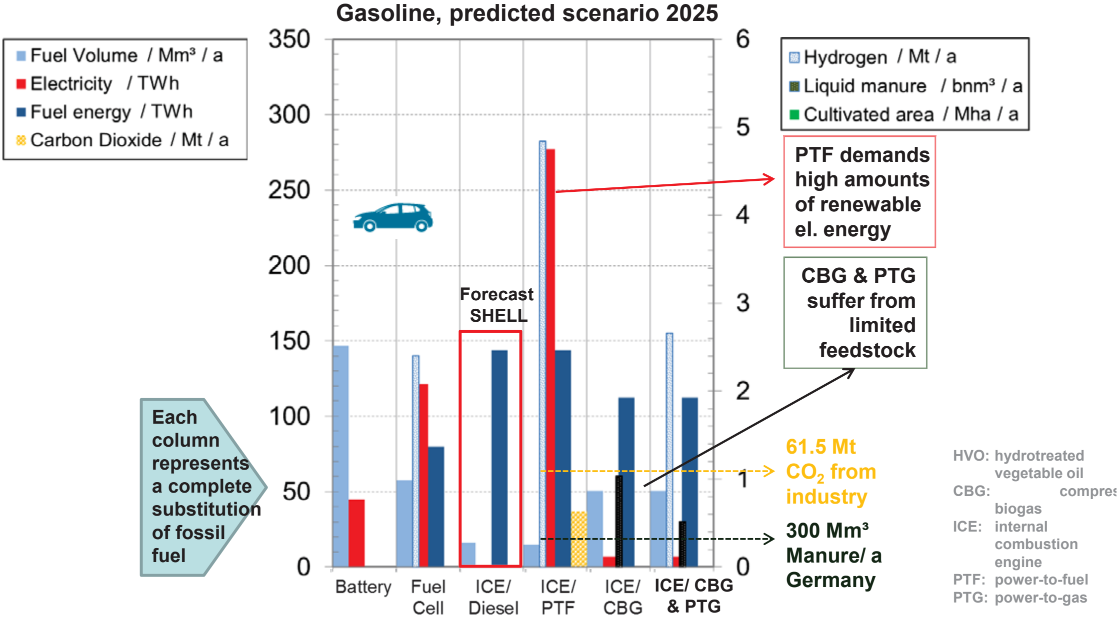
Overcapacity in Power is Inherent for Full Renewable Energy Supply

$$\text{Capacity factor} = \frac{\text{energy harvested}}{\text{nameplate harvest}}$$

Average power demand for Germany: ~ 60 GW (based on 528 TWh grid electricity)

	Capacity factor	Necessary Power, if just one Technology is applied	Reasonable power mix DE 2050 (DE gov. Installation plans extrapolated)	Reasonable electricity mix DE 2050	Electricity to be converted to H_2 (serving 75% of passenger vehicles in DE)
Offshore wind	0.46	120 GW	59 GW	236 TWh	
Onshore wind	0.23	230 GW	132 GW	267 TWh	
PV	0.12	460 GW	120 GW	126 TWh	
Total	--------	----------	311 GW	**629 TWh**	101 TWh (**2,1 mt H_2**)
Untimely produced electricity				≈ 200 TWh (to be stored)	
CO_2 cut Ø 80%				90% (10% power by NG)	54% of passenger cars

Future fuels for light duty vehicles & passenger cars



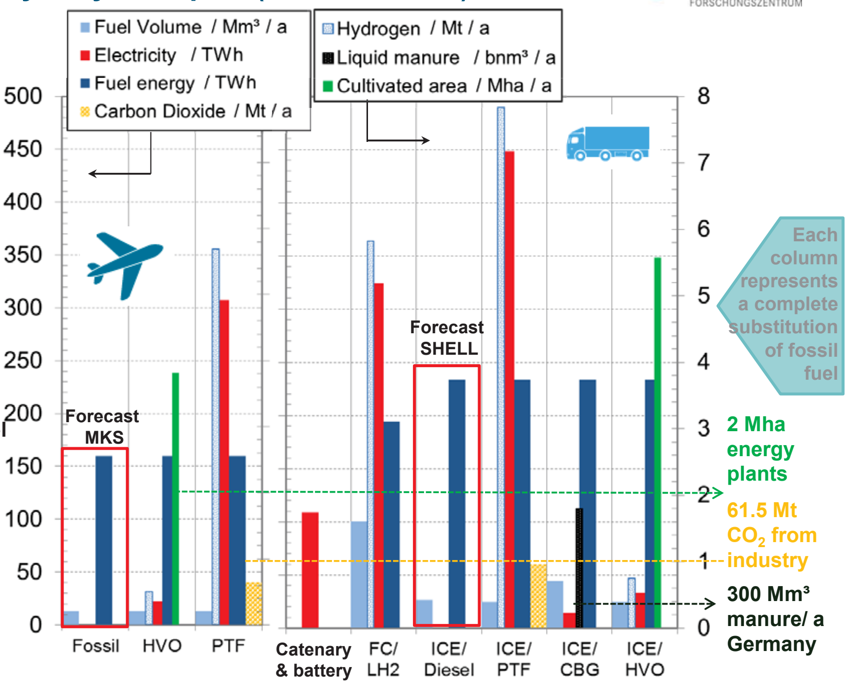
- **Electrification of LDV w/ 120 – 260 TWh$_e$ ⇨ mix of battery & fuel cell cars (short to long distances)**

Future fuels in heavy duty transport (scenario 2025)

JÜLICH FORSCHUNGSZENTRUM

- Airplanes will use a HVO/PTF mix
- CBG can't fulfill high quotes for truck diesel
- H_2 best option for fleet operation of trucks
- H_2 w/ limited operation range and large tank
- H_2/ FC & PTF w/ high demand for electrolysis 275 – 450 TWh (trucks)
- Catenary systems only in combination w/ diesel & hybridization

- **Heavy duty transport w/ high diversification of fuels to reach CO_2 reduction**



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Future and mobility – perspectives and needs

Konstantin Kersten, Martin Lohrmann
Volkswagen Aktiengesellschaft, Group Research

The Two-Degree Goal confirmed in the Paris Agreement in 2015 and currently having 194 participating nations is the worldwide attempt to finally stop further anthropogenic climate change and the disastrous effects which are generally accepted to be connected to it. In order to reduce emissions it is first important to understand where these emissions stem from and how they can be reduced efficiently from a system-wide point-of-view, while also considering ecological and economical side-effects. CO2 is undoubtedly a greenhouse gas that has played and still plays a major role with respect to climate change and for which a reduction in emissions is technologically feasible. However, to effectively reduce CO2 emissions a reduction in all sectors (automobile, transport, energy, industry, etc.) is of paramount importance. With respect to powertrains, the question which technology is most suitable to reach the climate target and will prevail in the long run, is driving research and development at Volkswagen Group Research.

The presentation gives a brief overview on challenges the automotive industry is facing in terms of sustainability and business environment. Hereinafter the group activities regarding electrified powertrains – battery electric vehicles and fuel cell electric vehicles – and their challenges are illustrated. It is followed by an overview on alternative commercial vehicle powertrains.

Besides electrified powertrains, renewable fuels can contribute to the target of greenhouse gas reduction as well and might even bring benefit to the present global vehicle fleet. Some possible pathways on CO2 neutral fuel production are depicted, followed by a close-up on e-Gas plant of the brand Audi in Werlte, producing methane from renewable electricity and CO2 from a biogas plant. The presentation concludes with a possible timeline for the development of sustainable energy carriers in the automotive sector until 2050.

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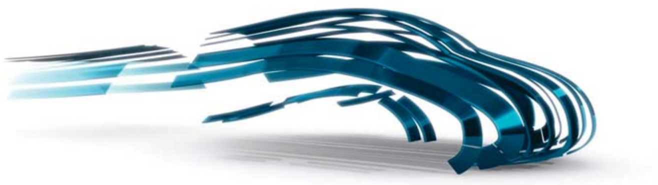

FUTURE AND MOBILITY – PERSPECTIVES AND NEEDS

VOLKSWAGEN AG | KONZERNFORSCHUNG ANTRIEBS- UND ENERGIESYSTEME | DR. MARTIN LOHRMANN
Konstantin Kersten

TRENDS 2017 | AACHEN | DECEMBER 6TH 2017

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VOLKSWAGEN GROUP RESEARCH

THE BRANDS – OUR CUSTOMERS

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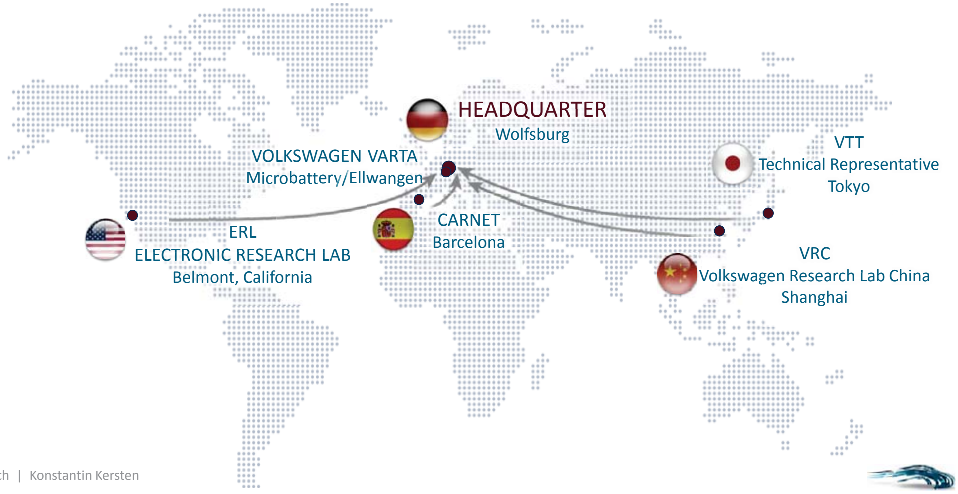
RESEARCH AND DEVELOPMENT LOCATIONS



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VALUE CREATION IN THE AUTOMOTIVE INDUSTRY IS UNDERGOING CHANGE

Digitalization

Hydrogen

Downsizing

CO_2-emissions

Plug-In-Hybrid

Urbanization

Climate change

Sustainability

Car-Sharing

E-mobility

Connected Car

Battery technology

Autonomous Driving

Lithium-ion

Peak Oil

Major cities

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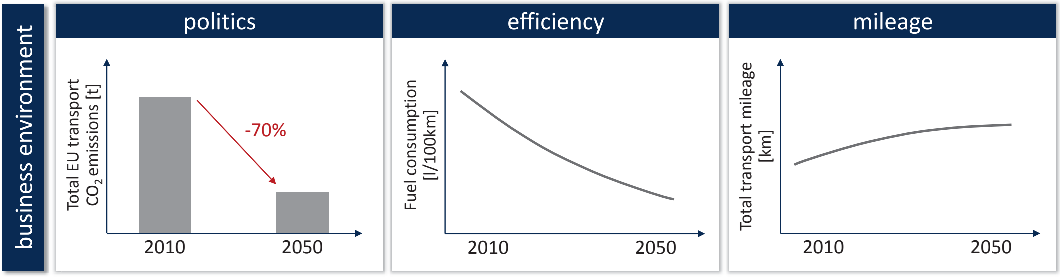
FUEL TRENDS FOR TRANSPORT



fuel trends

(1) Electrification of transport

(2) CO_2-reduced fuels for transport

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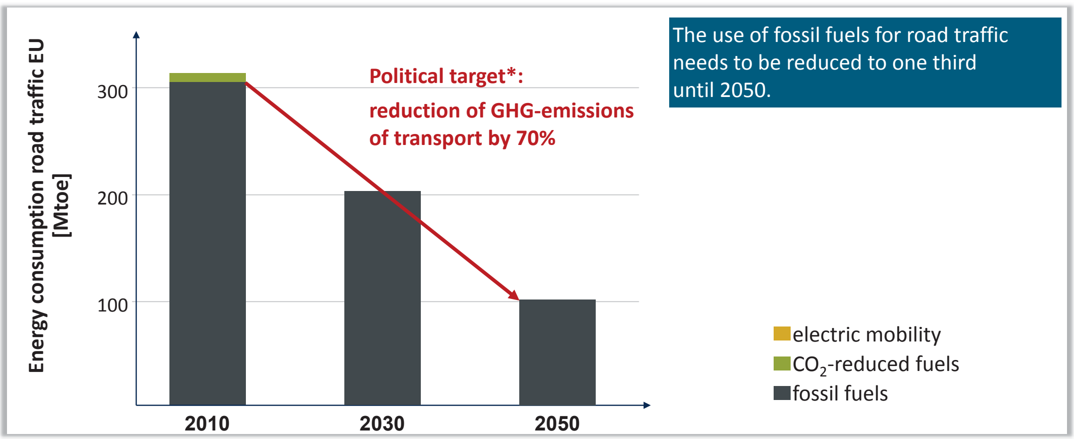
FUEL TRENDS FOR PRIVATE AND COMMERCIAL TRANSPORT

CASE STUDY: ENERGY CONSUMPTION FOR ROAD TRAFFIC IN THE EU*



* 2011 EU WHITE PAPER: Roadmap to a Single European Transport Area – Towards a competitive and resource efficient transport system

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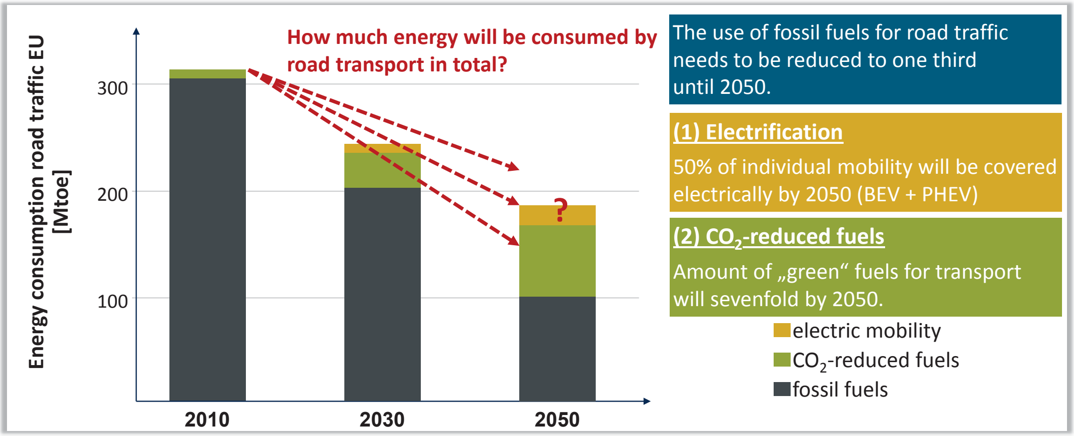
FUEL TRENDS FOR PRIVATE AND COMMERCIAL TRANSPORT

CASE STUDY: ENERGY CONSUMPTION FOR ROAD TRAFFIC IN THE EU*



*based on data of IEA Mobility Modell, progtrans, World Transport reports 2012/2013, own consumptions

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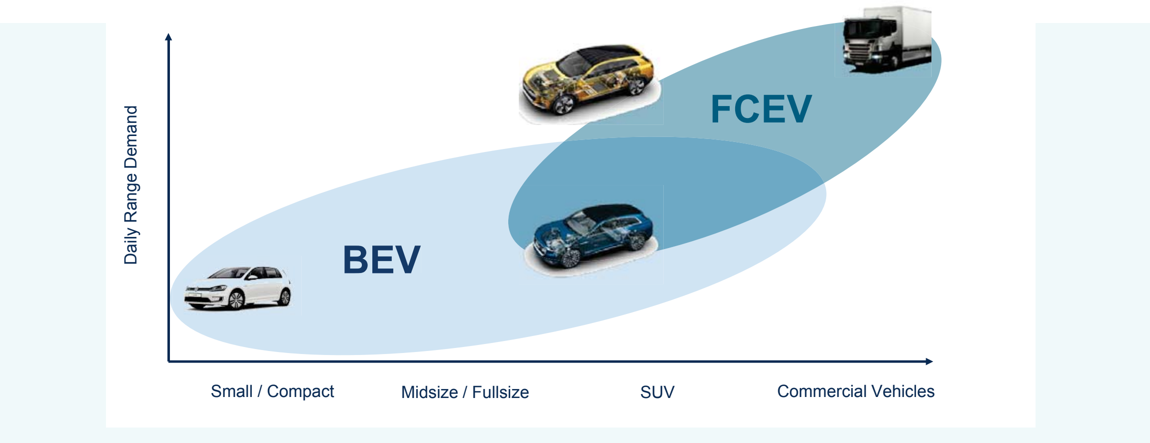
COMPARISON BEV – FCEV



Quelle: AUDI AG N/EA-H4

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BEV - E-GOLF TODAY

Technical Data

Maximum speed:	**140 km/h**
Electric motor:	85 kW
Torque:	270 Nm
Consumption, NEFZ:	12.7 kWh/100 km
Electrical range (NEFZ):	**300 km**
Energy content battery	35.8 kWh

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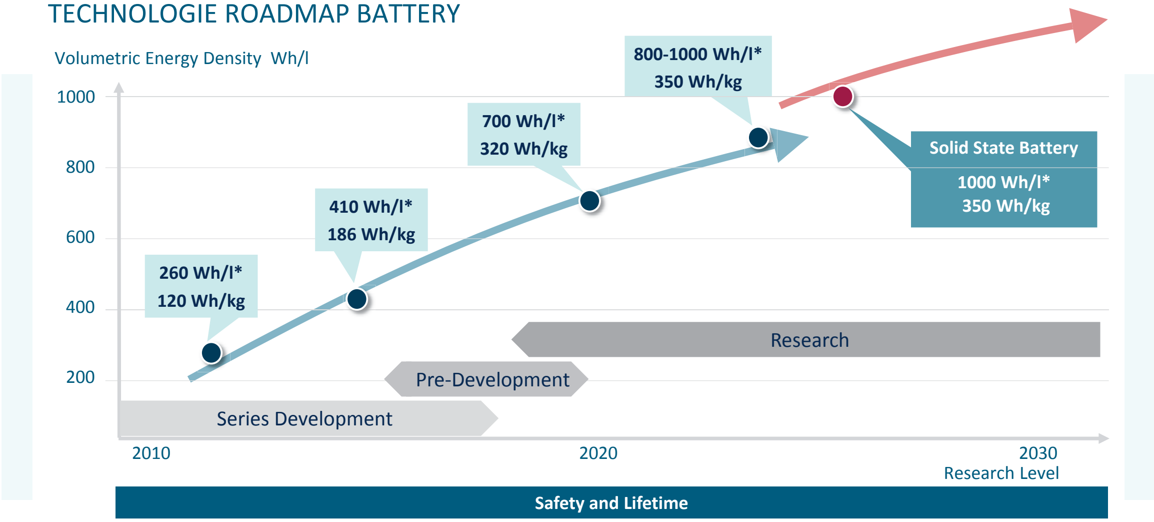
TECHNOLOGIE ROADMAP BATTERY



* Energy density based on cell level

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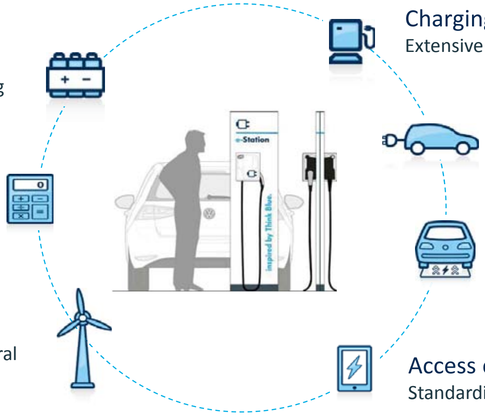
CHALLENGES OF CHARGING



Charging capacity
HV-batteries with high energy content require higher charging capacities.

Operation
Economic efficiency of operation of charging stations

Regenerative energy
Further expansion of CO_2-neutral mobility

Charging infrastructure
Extensive provision of charging stations

Charging interface
Worldwide standardization of the charging plug

Charging comfort
Automatic charging via induction

Access charging station
Standardized authentication and billing

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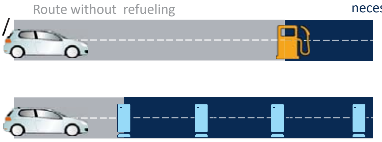
HIGHWAY INFRASTRUCTURE FOR BEV*

ASSUMPTION: 5 % OR 30 % BEV IN 2030

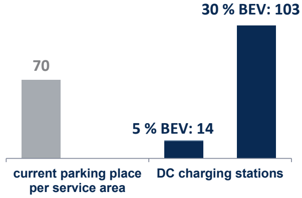
Influence of vehicle range

Example: highway trip



Number of refueling operations is increasing

Fast-charging stations (200kW)



- ⊕ Individual demand adaption
- ⊖ charging time ~15 minutes for 80% state-of-charge
- ⊖ Stressing of the battery

Connecting power from the grid for service areas of 2.5 MW for 5 % BEV and 20 MW for 30 % BEV in 2030 is required!

* assuming 500km NEFZ-range in 2030

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FUEL CELL

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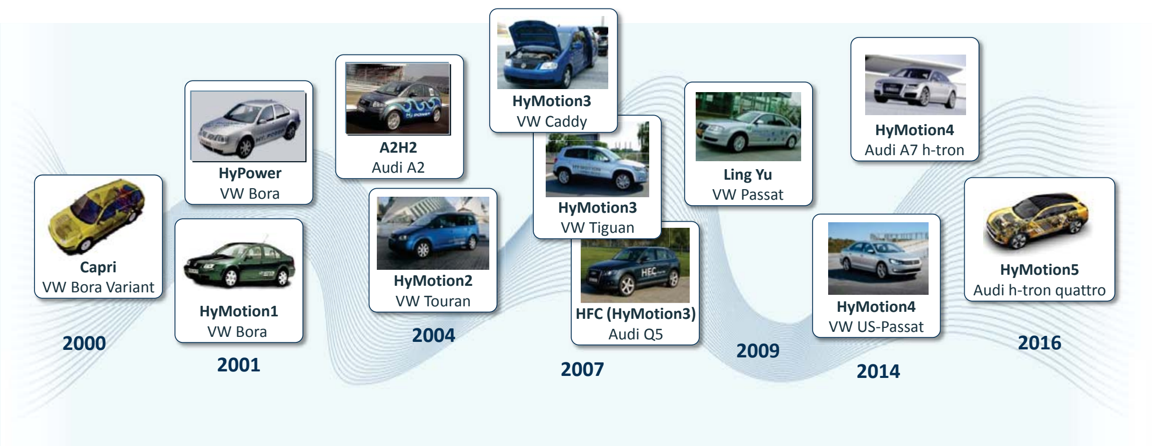
HISTORY OF FC-TECHNOLOGY IN VOLKSWAGEN-GROUP



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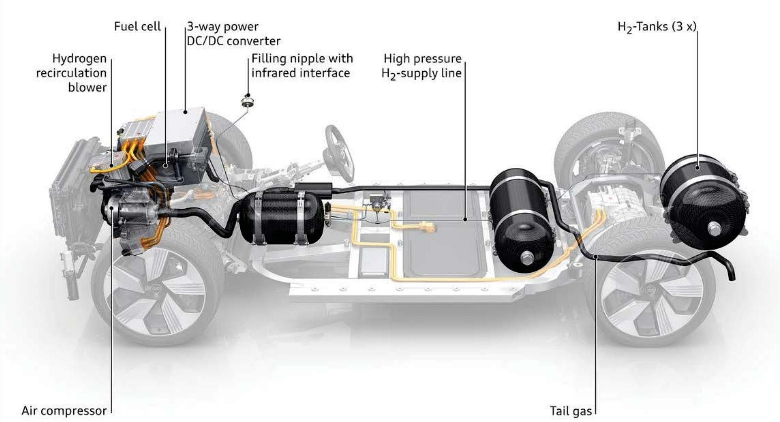
FUEL CELL DEVELOPMENT
SET UP FUEL CELL VEHICLE- H_2 COMPONENTS



- Electrified **quattro** layout: Electric machine at front and back axle
- Power fuel cell: up to **110 kW**
- Range up to **600 kilometers** with one tank (~4 min)
- Maximum speed electrically limited at **200 km/h**

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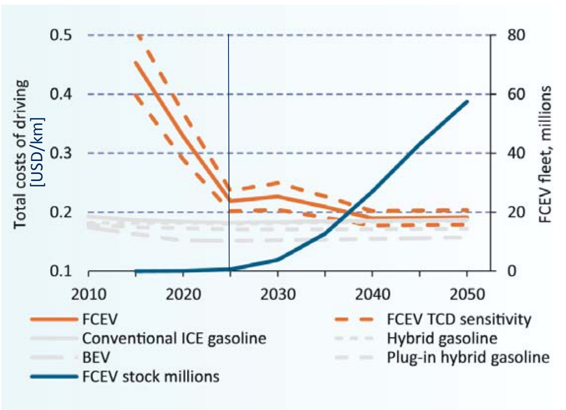
HYDROGEN TECHNOLOGY ROADMAP (INTERNATIONAL ENERGY AGENCY – IEA)

“Based on the scenario results […], the market for passenger FCEVs could be fully sustainable 15 years after introduction of the first 10 000 FCEVs.“

Requirements

- Fuel/energy tax exemption
- No car and registration taxes
- Rapid market penetration supported by subsidies for customer, OEM and infrastructure



Source: IEA 2015, Technology Roadmap, Hydrogen and Fuel Cells

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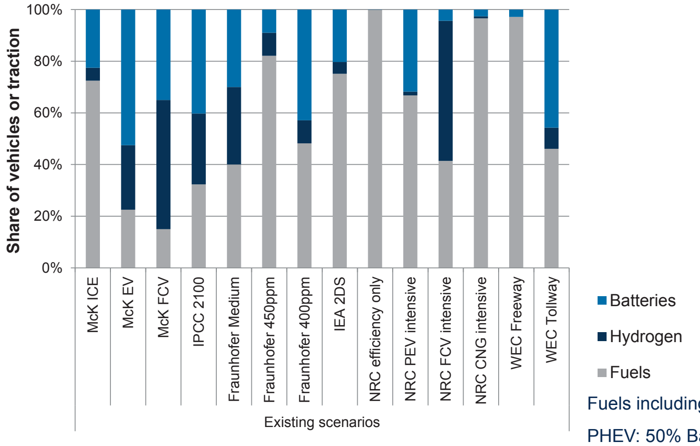
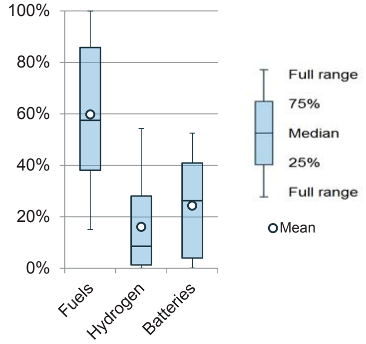
MOBILITY SCENARIOS 2050





Fuels including hybridisation

PHEV: 50% Battery, 50% Fuel

Source: McKinsey & Company (2010), Palzer & Henning (2014), IPCC (2014), Schade et. Al. (2010), IEA (2012), NRC (2013), WEC (2011)

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ENERGY CARRIER TRENDS IN CARGO AND PASSENGER TRANSPORTATION

Catenary Truck

Diesel Hybrid Truck

Battery / Fuel Cell City Bus

CNG City Bus

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EXAMPLE FOR ELECTRIFICATION OF LONG HAUL SEGMENT

BMUB FUNDED PROJECT ERS FOR LONG HAUL TRUCKS

SCANIA Hybrid ERS long haul truck on public test route in Sweden

Source: SCANIA

- Public test route in Sweden
- Set up of 3 German test routes (Hessen, Schleswig-Holstein, Baden-Württemberg) in 2018-2019
- Set up of vehicle fleet for realistic tests of operation starting in 2019

Planned test route in Schleswig-Holstein on the A1 near Lübeck

Source: BMUB

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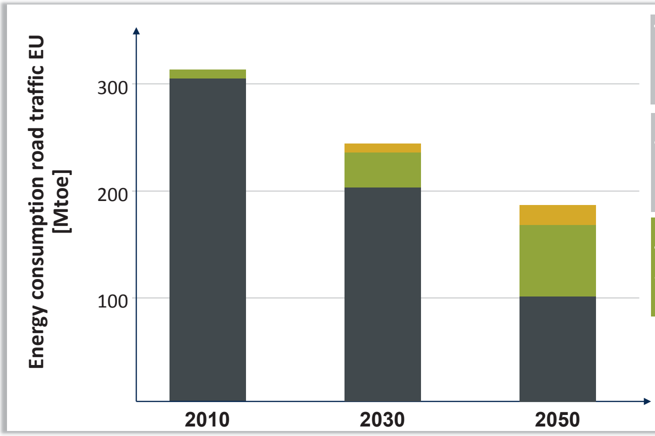
FUEL TRENDS FOR PRIVATE AND COMMERCIAL TRANSPORT

CASE STUDY: ENERGY CONSUMPTION FOR ROAD TRAFFIC IN THE EU*



The use of fossil fuels for road traffic needs to be reduced to one third until 2050.

(1) Electrification

50% of individual mobility will be covered electrically by 2050 (BEV + PHEV)

(2) CO_2-reduced fuels

Amount of „green“ fuels for transport will sevenfold by 2050.

- electric mobility
- CO_2-reduced fuels
- fossil fuels

*based on data of IEA Mobility Modell, progtrans, World Transport reports 2012/2013, own consumptions

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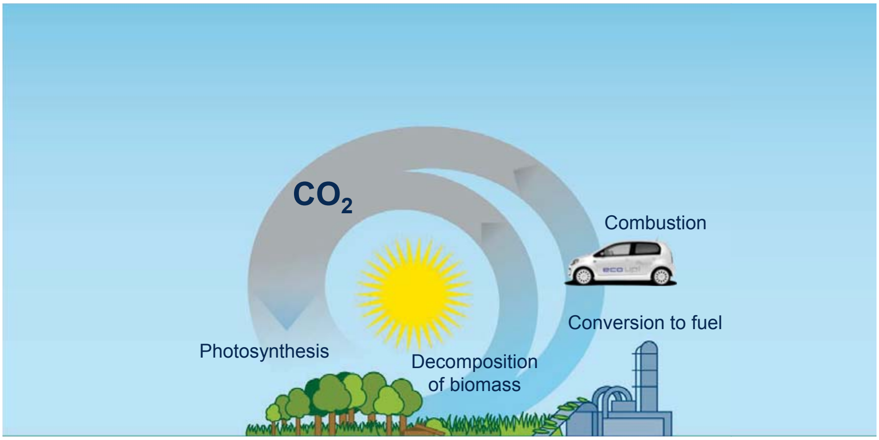
CO_2-REDUCED FUELS



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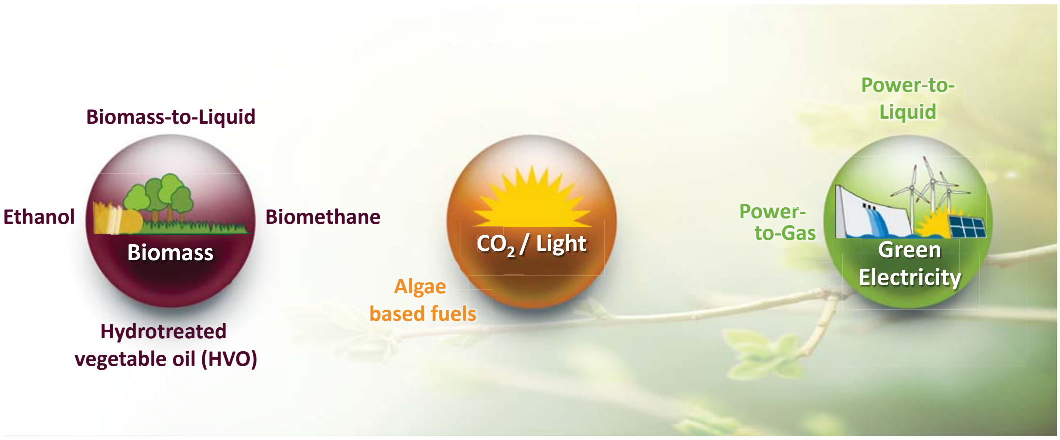
CO_2-REDUCED FUELS



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CLASSIFICATION OF BIOFUELS AND THEIR COMPETITION

Evolution pathway of biofuels

Type	Example	No competition with: food	land use*	biomass
• Conversion/use of sugar, starch and oil	• Ethanol from sugar beets, wheat • HVO** from rape seed	✗	✗	✗
• Conversion of cellulose	• Biomethane from grass silage • Diesel from wood	✓	✗	✗
• Conversion of cellulose from residues via algae/bacteria/yeast	• Ethanol from straw • Biomethane from straw • Diesel from residual wood	✓	✓	✗
• „Green" electricity as basis • Modified photosynthesis with algae or bacteria	• Power-to-Fuel / E-Gas • Ethanol	✓	✓	✓

* Agricultural land
** HVO Hydrotreated Vegetable Oil

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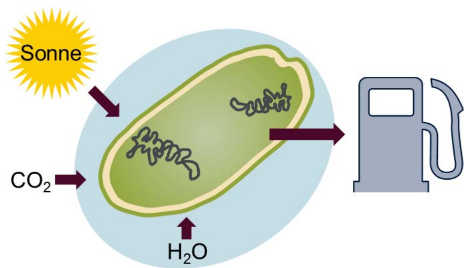
MODIFIED PHOTOSYNTHESIS WITH ALGAE OR BACTERIA



Cyanobacteria as miniaturised plant for direct fuel production

Challenges biotechnology:

- Fuel production with limited cell growth
- Optimized metabolism for fuel
- Tolerance of the cells (e.g. salt, temperature)
- Secretion of the fuel

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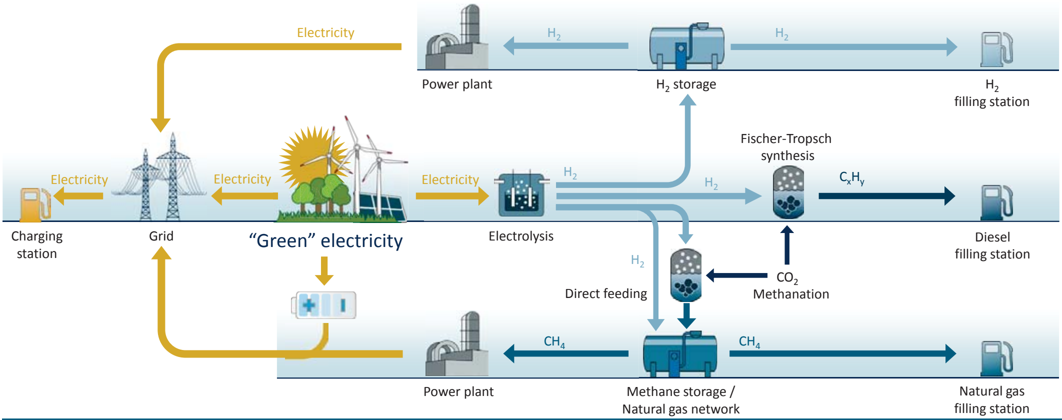
OPTIONS FOR STORING AND USING „GREEN“ ELECTRICITY



The question of future vehicle concepts can only be answered in context with future energy solutions of the energy sector.

Power-to-Gas: Audi e-gas plant | Werlte (Germany)

Quelle: EWE Netz

Audi
Vorsprung durch Technik

Electrolysis & Methanisation Unit

Technological highlights of the Audi e-gas plant

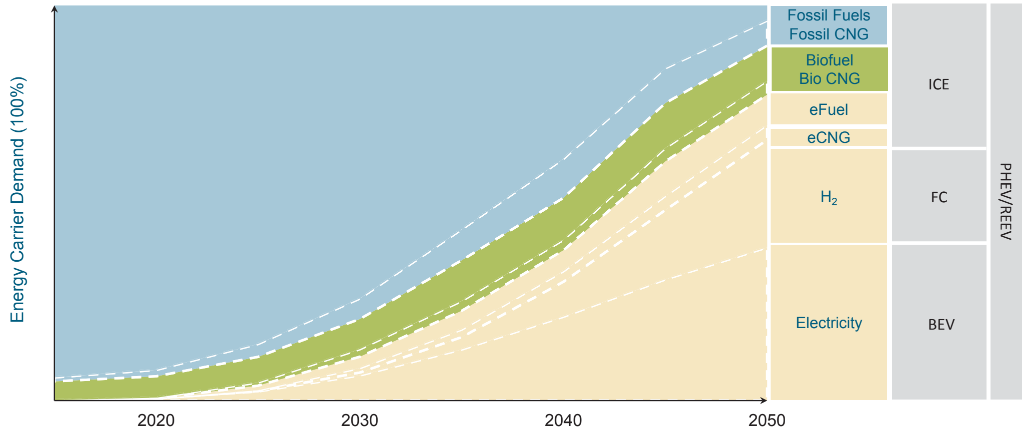
- World's first industrial power-to-gas plant
- Rated output of electrolysis: 6 MW
- Target: Intermittent operation, use of surplus renewable electricity

- World's largest methanation reactor (manufactured by MAN)
- e-gas production: max. approx. 1000 t p.a.

- Complex heat management with biogas plant
- Target: Overall efficiency ratio >70%

Possible Development of Sustainable Energy in the Automotive Sector

ENERGY CARRIER DEMAND BY PASSENGER CARS IN THE EU



VOLKSWAGEN
AKTIENGESELLSCHAFT

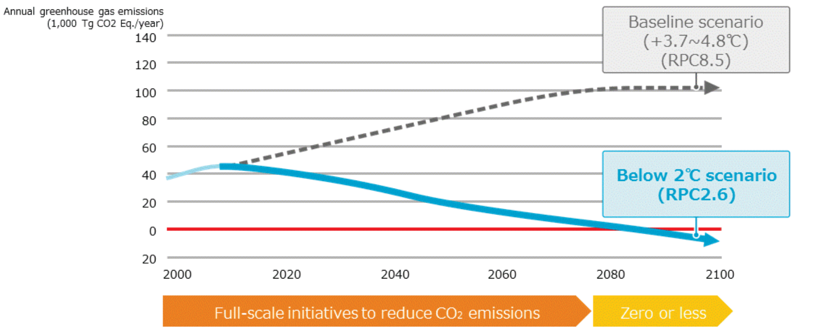
THANK YOU FOR YOUR ATTENTION!

Toyota’s aspirations on Hydrogen and Fuel Cells

Muriel Desaeger
Toyota Motor Europe

Aachen, 6 Dec 2017

Forecast international climate change



Source: From the IPCC Working Group III 5th Assessment Report (2014)

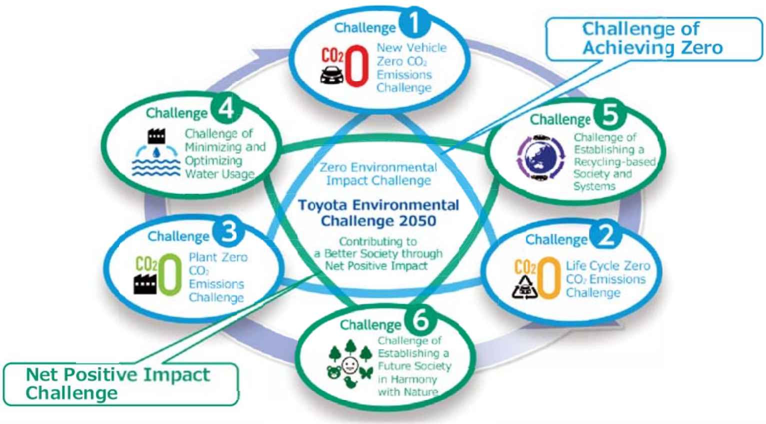
Regarding GHG emissions, there is no time to lose

TOYOTA

TOYOTA ENVIRONMENTAL CHALLENGE 2050

To go beyond zero environmental impact and achieve a net positive impact, Toyota has set itself six challenges. All these challenges, whether in climate change or resource and water recycling, are beset with difficulties, however we are committed to continuing toward the year 2050 with steady initiatives in order to realize sustainable development together with society.

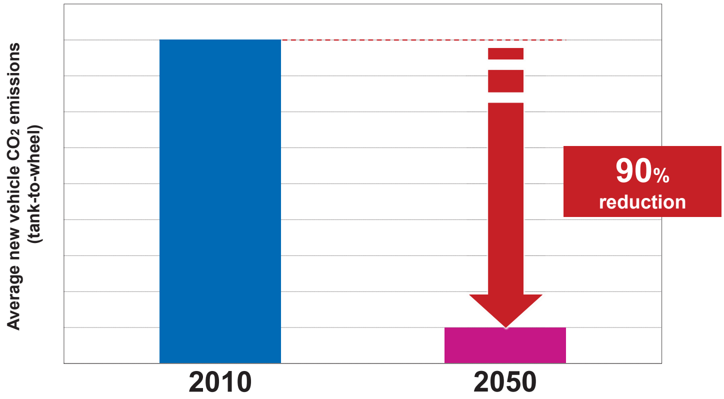
Toyota Environmental Challenge 2050



Achieving zero CO_2 impact for new vehicles, prod. plants, life cycle;
Net positive impact through recycling, optimal water usage, acting in harmony with nature;

Toyota Environmental Challenge 2050

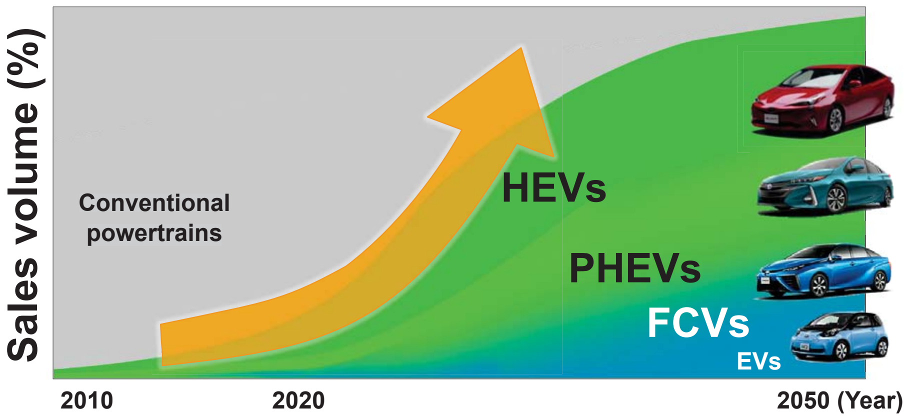
New Vehicle Zero CO_2 Emissions Challenge



90% reduction in new vehicle CO2 emissions by 2050 compared to 2010.

TOYOTA

Toyota's future powertrain image



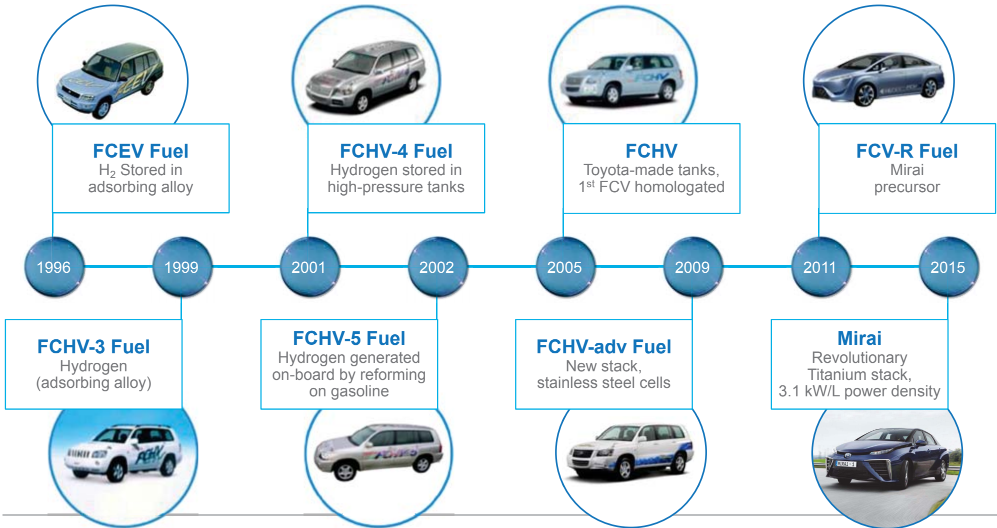
Next generation vehicles to accelerate technological development

TOYOTA

New "Hydrogen Council"

TOYOTA

Developing Hydrogen FCV for 20 years

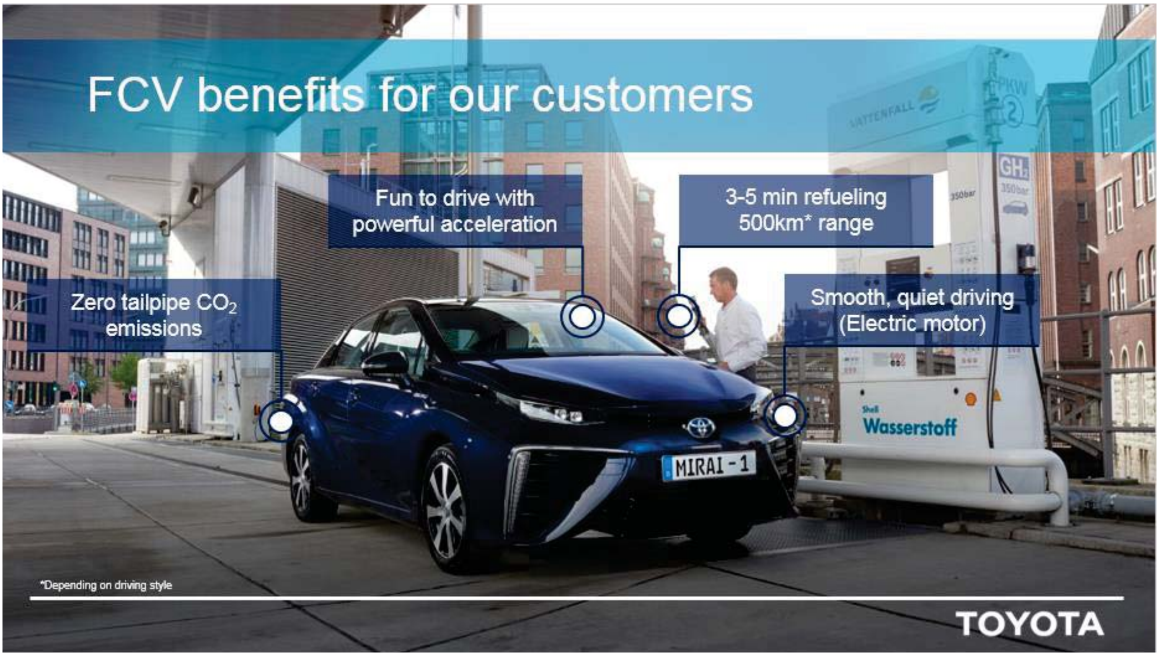


TOYOTA

Toyota Mirai

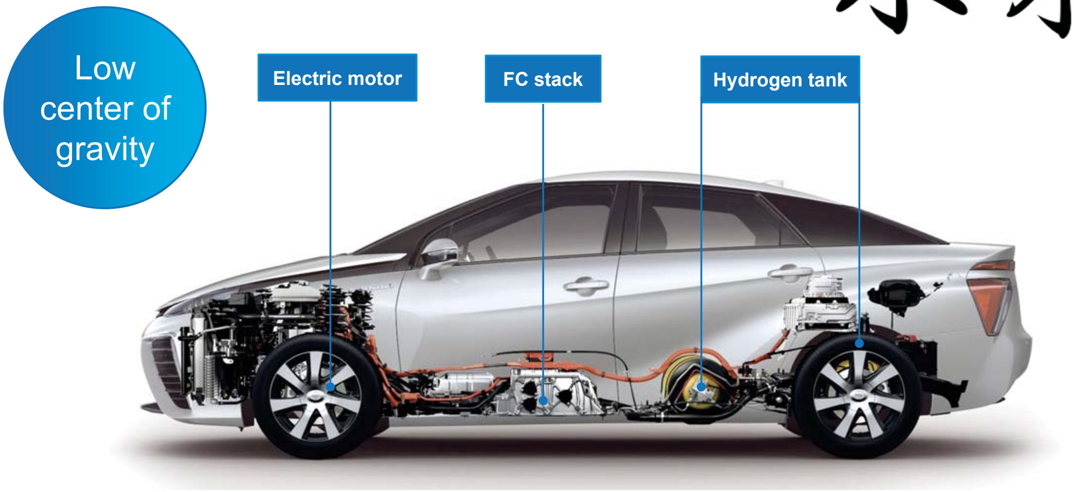
Mirai
= “Future” in Japanese

未来

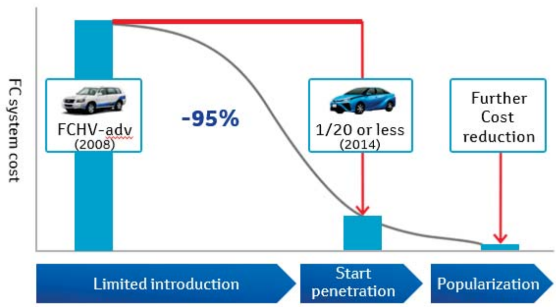


Toyota Mirai

Mirai
= “Future” in Japanese 未来

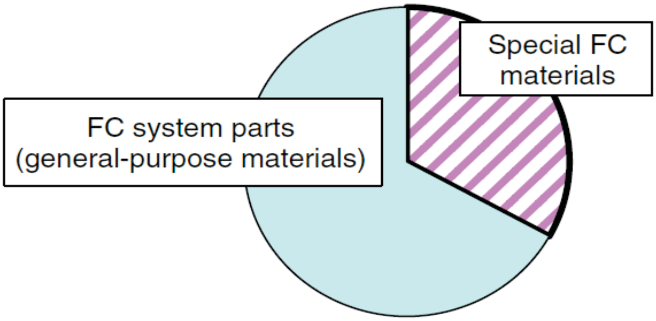


Cost



Apply HV technology to accelerate cost reduction

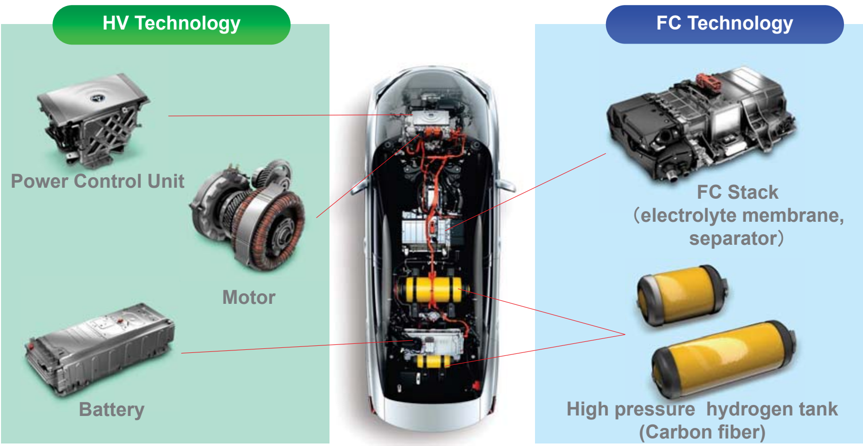
Cost structure of FCHV-adv system (2008)



Focus on cost reduction of general FC system and FC specific materials

TOYOTA

General system cost reduction

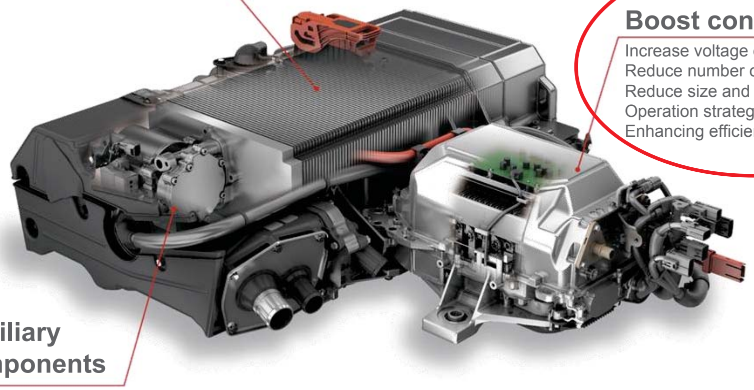


Use of high volume mass production components and technology from hybrid

TOYOTA

Toyota FC stack

Type: Polymer electrolyte fuel cell
Maximum output: 114 kW (155PS)
Volume power density: 3.1 kW/L
Humidification system: Internal circulation



Boost converter

Increase voltage of motor (max.650V)
Reduce number of fuel cell stack cells
Reduce size and weight of system.
Operation strategy at cold start
Enhancing efficiency of system

Auxiliary components

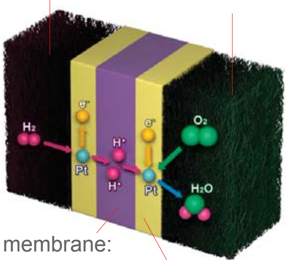
Application of mass production technology to reduce fuel cell specific cost

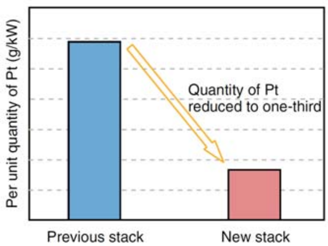
TOYOTA

High performance cell

Electrode

Gas diffusion layer: Lower density and thinner base material
⇒Gas diffusion performance more than doubled





Electrolyte membrane: Thinner by one-third
⇒Proton conductivity increased by 3 times

Catalyst layer: Highly reactive Pt/Co alloy catalyst
⇒Activity increased by 1.8 times

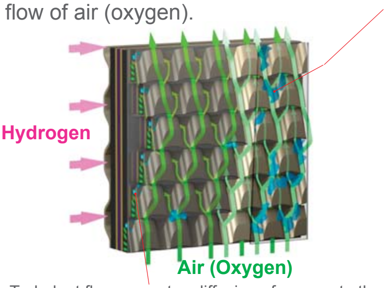
Performance and cost improvement by innovative electrode

TOYOTA

High performance cell

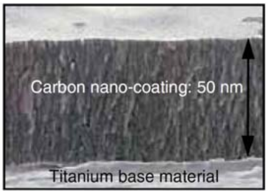
Optimised cell flow channels (Cathode) using 3D fine-mesh flow field improve water exclusion and air (oxygen) diffusion, achieving uniform generation in cell surfaces.

Generated water is quickly drawn out through 3D fine-mesh flow field, preventing obstruction flow of air (oxygen).



Turbulent flow promotes diffusion of oxygen to the catalyst layer.

Material of separator flow field:
Corrosion-resistant Titanium
with carbon nano-coating
(FCHV-adv: stainless steel + Au plating)



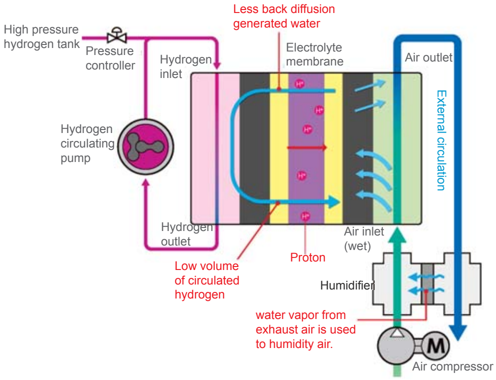
Innovative flow channels and materials for performance, cost reduction

TOYOTA

Internal circulation system – Humidifier-less

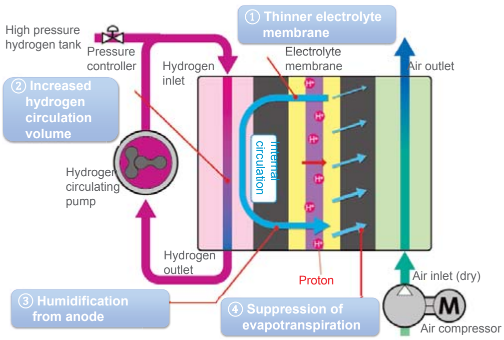
FCHV-adv External circulating humidifier

System humidifies supplied air (oxygen) using a humidifier to maintain proton conductivity of the electrolyte membrane.



Mirai Internal circulation system – Humidifier-less

System self humidifies by circulating water (water vapor) produced from power generation within cells to maintain proton conductivity performance of electrolyte membrane.

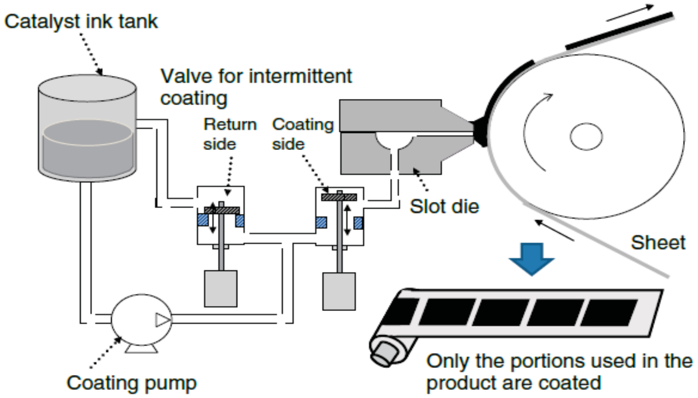


System simplification by eliminating humidifier (-15kg, -15L)

TOYOTA

Production technology

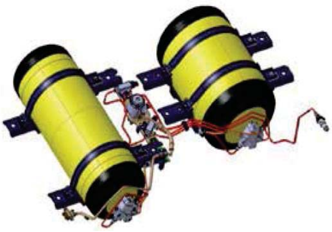
Intermittent slot die coating technology for catalytic layers reduces amount of Pt used

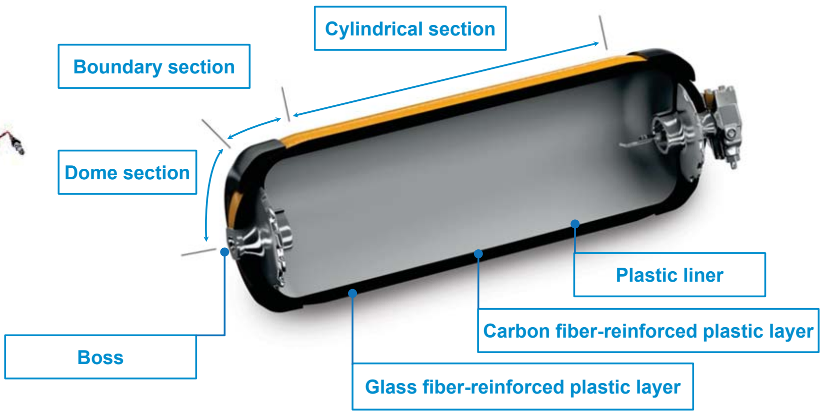


Production technologies significantly influence cost

TOYOTA

H_2 tank technology

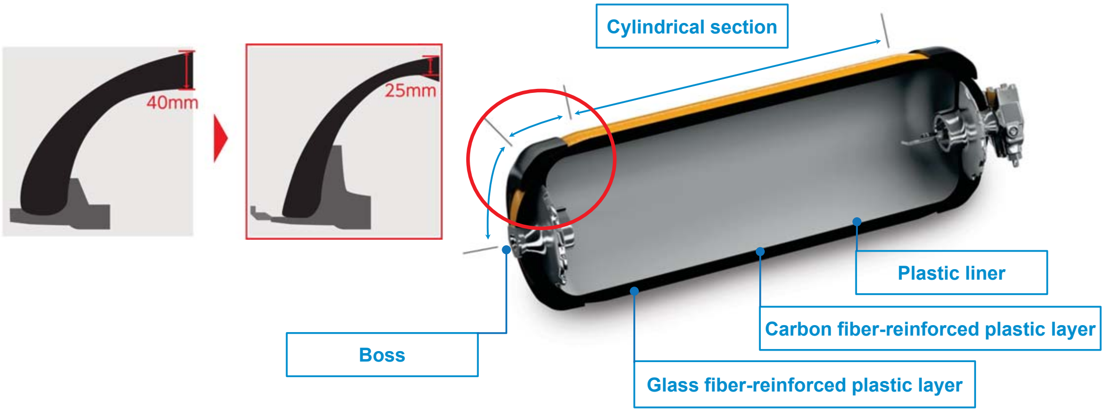




CFRP tank developed for Mirai

TOYOTA

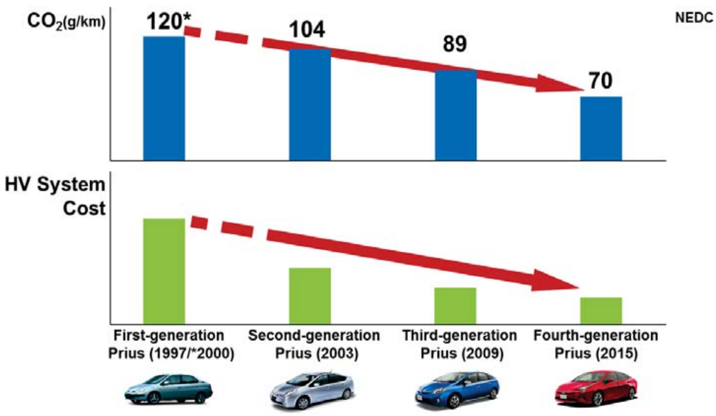
H_2 tank technology



Lamination method reduces required CFRP by about 20%

TOYOTA

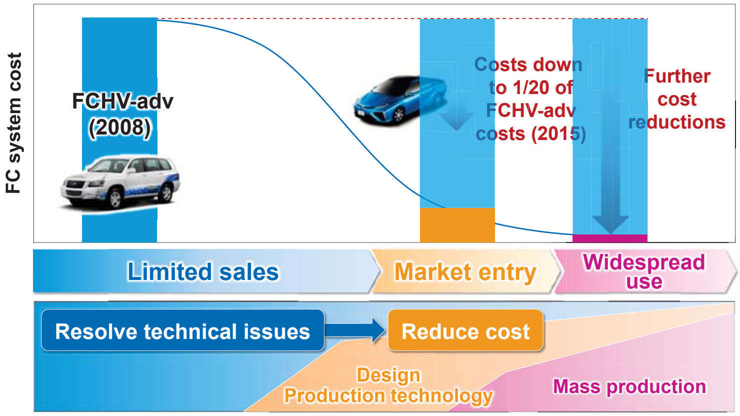
Evolution of the Toyota Hybrid System



Substantial reduction of fuel consumption and costs have been achieved

TOYOTA

Challenge for cost reduction



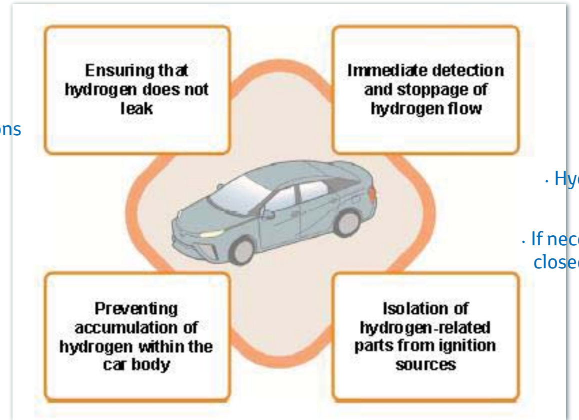
Fuel cell system costs have been reduced significantly. Efforts for cost reduction will be continued towards widespread use of FC technology.

TOYOTA

Safety

· No Hydrogen permeation
· Robust Carbon-fiber body
· Certification to stringent regulations
· Collision-safe body

· All hydrogen-related parts (FC stack, hydrogen pipes, tanks located outside of the cabin.



· Hydrogen detectors located in strategic spots

· If necessary, the valve on the tank is closed to automatically shut off the fuel line.

Comprehensive approach to handle Hydrogen safety

Source: Toyota's Safety Guidance manual 2015.

TOYOTA

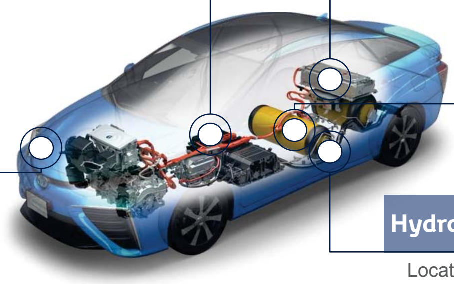
We ensure safety on board

Toyota FC stack

Steel frame and aircraft grade fibre-reinforced plastic used in protect the FC Stack

Impact safety structure

Protects the FC Stack and Hydrogen tanks in the event of an accident



Hydrogen sensors

Provide warnings and can shut off tank main stop valves

High pressure Hydrogen tank

Made from reinforced carbon of the highest quality

Hydrogen related parts

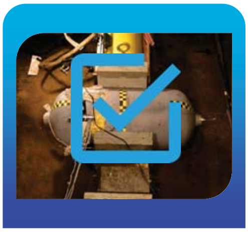
Located outside the cabin.

H2 tanks pass extremely demanding testing

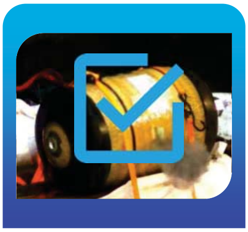
Tank designers and inspectors run a multitude of tests in laboratories to ensure safety

Burst test

Bonfire tests



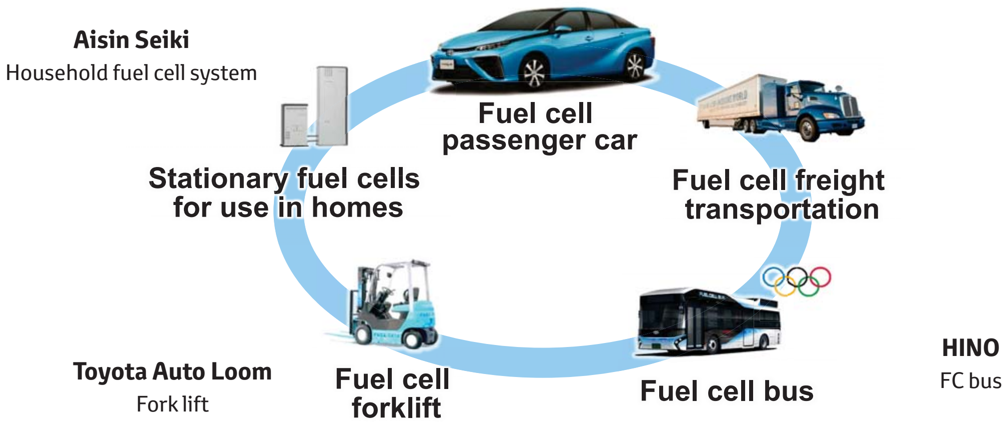
Crush test



Gunshot test

[1]Armour-piercing 7mm test according to UN Technical Regulation

Fuel cell technology



Applying Fuel Cell technology on broader scale

TOYOTA

FCV market penetration initiatives

- FCV sales volume
  Global : More than 30,000/year around 2020 and later
  Japan : Approx. 1,000/month around 2020
  1X,000/year @2020 and later

- FC bus introduction
  to start from February 2017 for Tokyo
  100 or more by 2020
  for Tokyo Olympics/Paralympics

TOYOTA

FC Bus

Toyota to start sales of FC buses under the Toyota brand from early 2017
The Tokyo Metropolitan Government plans to utilize as fixed-route buses.

Toyota aims to engage continuously in the diligent development targeted at the expansion of the introduction of the new FC buses from 2018

Vehicle	Length/width/height	10,525/2,490/3,340（mm）
	Capacity（seated+standing+driver）	77（26＋50＋1）
FC stack*（Fuel Cell）	Name	Toyota FC stack
	Type	Solid polymer electrolyte
	Maximum output	114 kw x 2units
Motor*	Type	AC synchronous
	Maximum output	113kw x 2units
	Maximum torque	335N・m x 2units
High-pressure hydrogen tank*	Type	Compression hydrogen
	Nominal working pressure	70MPa
	Tank internal volume	600L
	Number of tanks	10
Drive battery*	Type	Nickel-metal hydride
V2H system	Maximum output/voltage	9kW/DC300V

*Existing component

Use unit of MIRAI & Cruising range approximately 200km

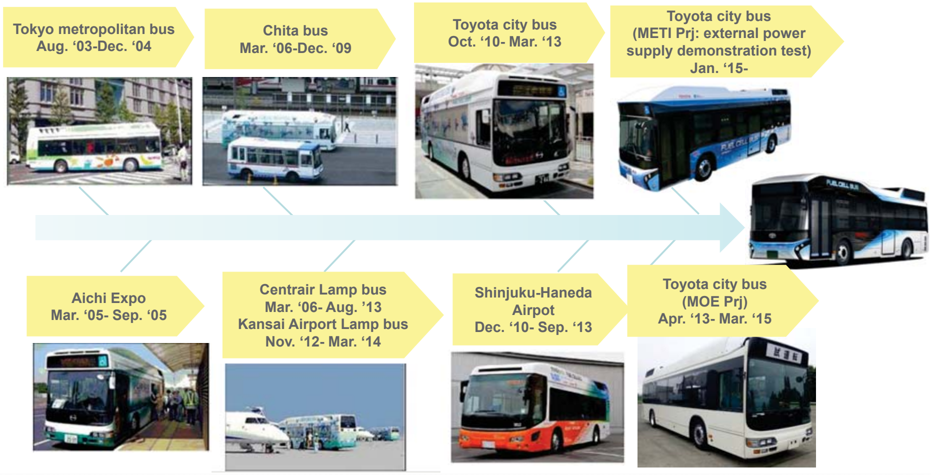
Advantage and Significance of the FC Bus

	scene	mileage (km/day)	Maximum speed (km/h)	Infra cooperation	Task	Introduction time
Large route bus 	The city and the suburban area	160	60	◎	Price Durability	FY 2016
Commuter bus 	Narrow road width, small route	100	60	◎	Market size	Undecided
Limousine 	City and airport interval	300	100	○	Power performance	Undecided
Large sightseeing bus 	From the city to the mountains Various areas	400～1000	100	△	Power Range	Undecided

◎：Very Good　○：Good　△：Fair

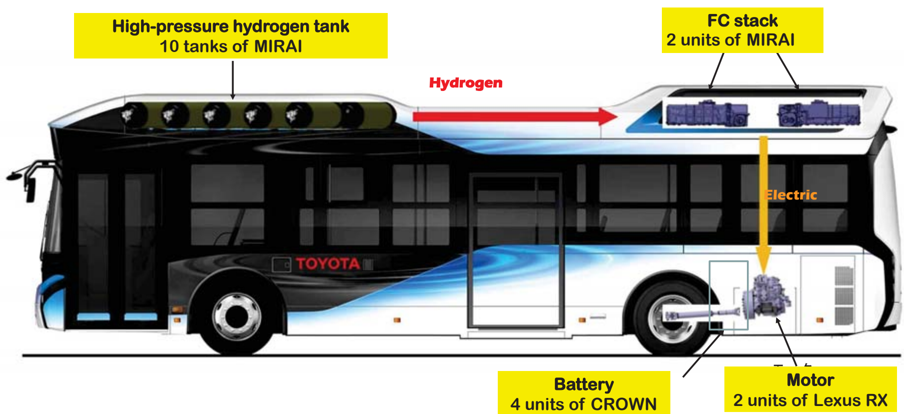
Route bus is the most suitable for hydrogen society realization

History of fuel cell bus



Continuous proof of examination for fuel cell bus introduction.
Development is supported as a national project.

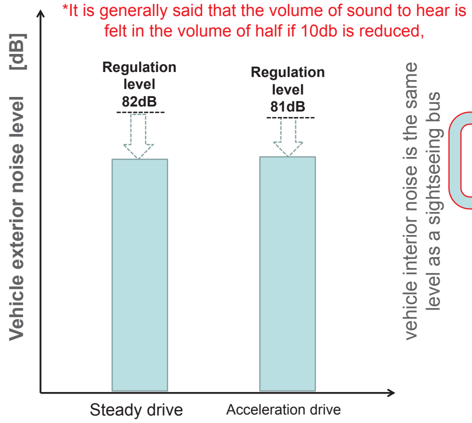
Structure of Toyota FC Bus



Upgrade of Technologies developed for passenger cars

Advantage of Toyota FC Bus

■Noise reduction effect



Source：http://ozami.jp/sound-living/

No engine noise to contribute to quiet environment

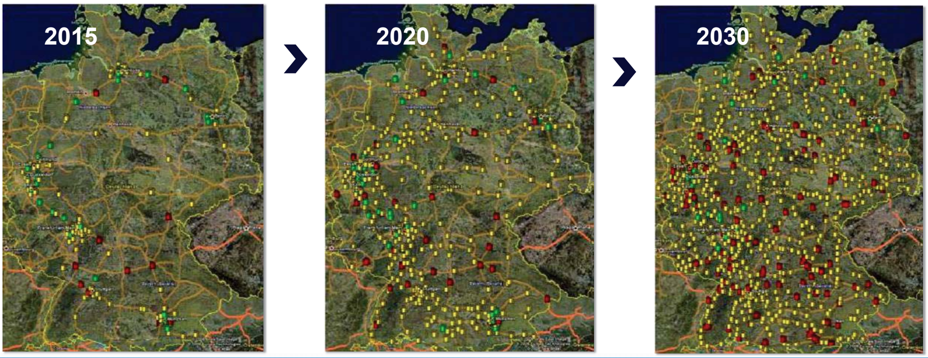
TOYOTA

Future of Zero Emission Trucking in US

TOYOTA

Clean Energy Partnership〈Germany〉

- **Initiative gathering the German government and industrial companies and focusing on technology**
- **400 hydrogen refuelling stations by 2023, distributed all over the country**



Fuel cell infrastructure is expected

TOYOTA

Significance of Toyota FC Bus

■ **Base of the local hydrogen infrastructure**

FCV H_2 demand*1	Annual mileage Fuel consumption rate annual H_2 consumption	: 9000km/year : 105km/kg : 86kg/year
FC Bus H_2 demand*2	Quantity of day filling Annual business drive annual H_2 consumption	: 11kg/day : 350 days/year : 3850kg/year

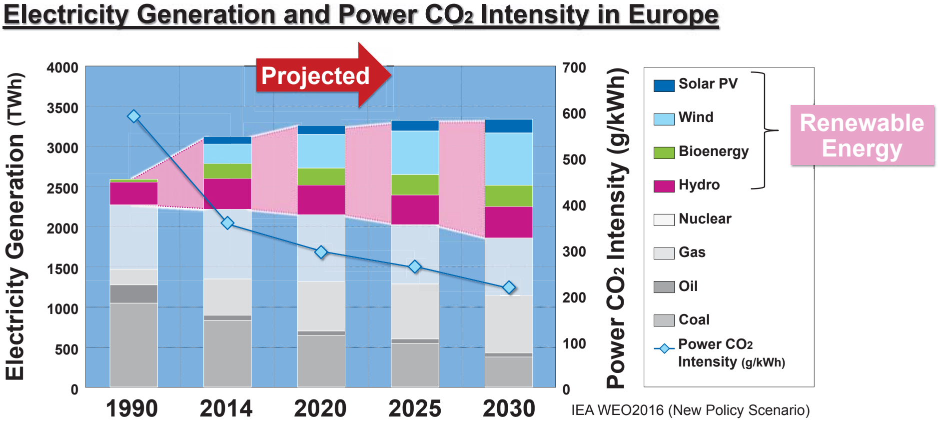
*1 : Council for a Strategy for Hydrogen and Fuel Cells
*2 : Toyota estimated

- H2 consumption of One FC Bus = 45 FCVs
- Stable consumption for a hydrogen station

FC Bus hydrogen consumption is equivalent to 45 FCVs.
FC Bus could contribute hydrogen station business.

TOYOTA

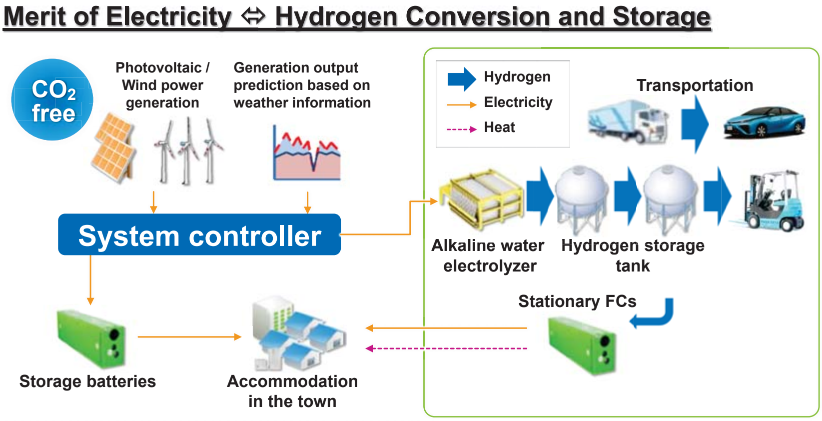
Electricity generation



The increasing share of renewable energy requires an effective energy storage system for stable power supply.

TOYOTA

Energy storage

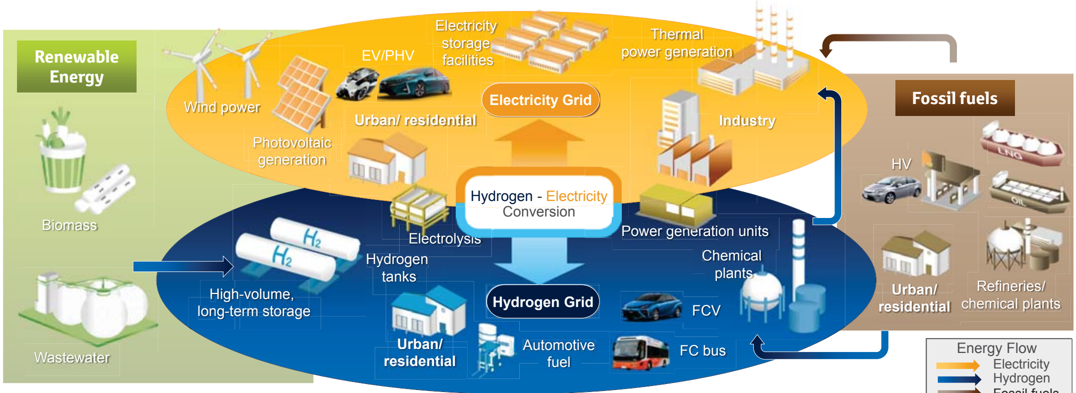


Compensating for fluctuations in renewable energy production and enabling renewable energy utilization in many applications

TOYOTA

Future vision: HyGrid ⟨Hybrid Grid⟩

Minimum use of fossil energy and maximum use of renewables



Source: HyGrid Study Group HP

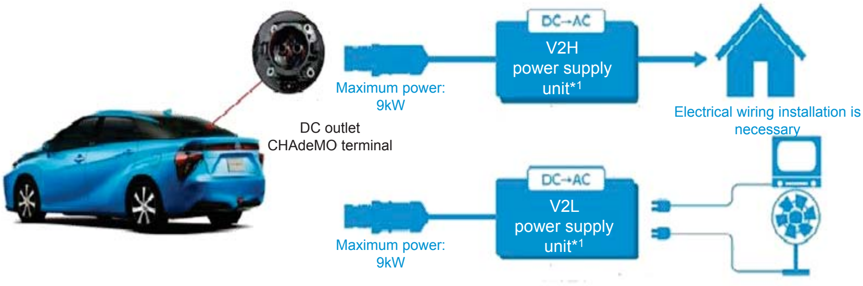
Creation of a future with coexistence RE & CO2-free hydrogen

TOYOTA

High-capacity external power supply system

Power can be supplied to homes or electrical products by connecting a power supply unit

Household lighting, TV, air-conditioning, and other electrical products can be used, maintaining nearly normal living conditions even during power outage.



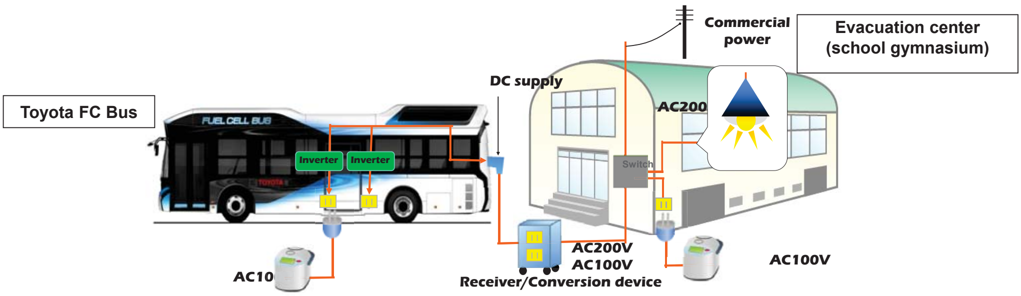
*1 V2H: power supply from Vehicle to Home, V2L: power supply from Vehicle to Load (electrical products)

TOYOTA

High-capacity external power supply system

Power supply image by FC Bus

The FC bus equipped with a high-capacity external power supply, could be useful in care of disaster.
(9kW output: 235kWh capacity = approximately 4.5 days at evacuation center)



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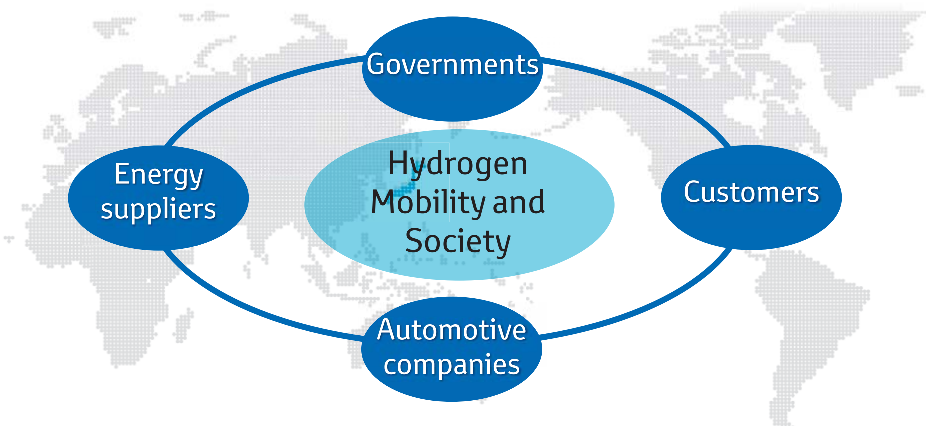
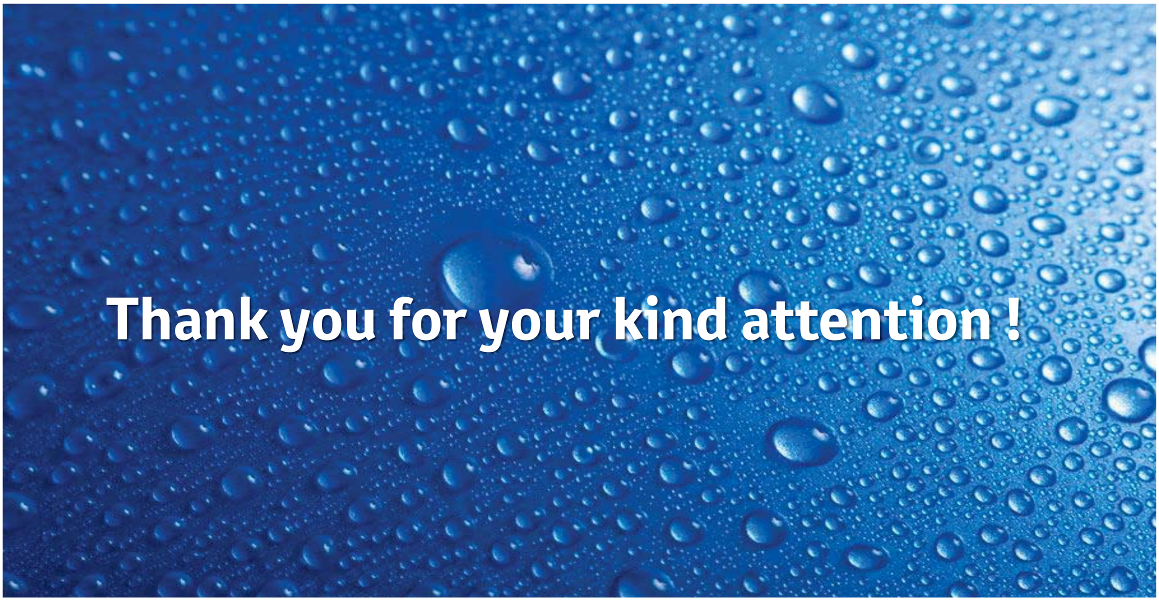
Cooperation of all stakeholders



New Vehicle Zero CO_2 Challenge in cooperation with stakeholders

TOYOTA



TOYOTA

Sector coupling – Needs and selected concepts

Manfred Waidhas
Siemens AG, Hydrogen Solutions

The forced extension of renewable energies (RE) is mandatory if worldwide targets for CO2-reduction are seriously followed. The price decay of renewable power generation facilitates related efforts. However, due to the volatile character of its power generation there will be an increasing mismatch between generation and demand. In that context the storage of excess production will become more and more essential in the future in order to enable viable business cases. The estimated storage demand for many countries with related CO2 reduction plans will be in the TWh range.

There are many concepts and technologies to store electrical energy. Here, hydrogen plays a unique role: among the three options for large-scale storage – pumped hydro, compressed air and hydrogen - hydrogen is the only viable option to address storage capacities >10 GWh. In addition, hydrogen is a multifunctional chemical energy carrier. It provides the option to be re-electrified without CO2 emissions by fuel cells, gas motors or gas turbines. But it is also a valuable raw material in chemical industry with an existing market volume of more than 100 billion USD. The production of ammonia, methanol, aniline and even gasoline require huge volume of hydrogen, which – at least in parts – can be provided by green electricity without any CO2-footprint. Even the coal in steel production could be replaced to a certain degree. Calculations - the most sensitive parameter are ‘electricity price’ and ‘operational hours’ - indicate that positive business cases are close or even already exist in certain niches.

Enabling component of the hydrogen storage concept is the electrolyzer system. It must – among a number of other features – be reliable under industrial working conditions and its efficiency must be optimized for intermittent operation. With the intention to provide solutions for future energy grids Siemens developed the PEM system called “SILYZER”. The first corresponding systems are successfully in operation since the year 2015 in the lighthouse project ‘Energiepark Mainz’ (funded by BMWi). In ‘H2Future’, funded by FCHJU a new Siemens electrolyzer line will be evaluated which is designed to cover the power range from 10 to 100 MW.

In particular, the mobility sector is far behind Germany´s CO2 reduction targets. A specific example for Siemens engagement in CO2 free mobility is the eHighway project. Basic idea is to combine the advantages of road traffic with the efficiency advantage of electric drives. Conventional trucks are additionally equipped with an electric drive drain while the electric power is provided by a catenary. This concept eliminates the capacity limitation of batteries and is expected to be beneficial in particular for heavy duty transport along established and highly utilized roads. In Germany a project is supported by the BMUB. There are equivalent tests running in US and Sweden.

In a nutshell: CO2 reduction targets can only be achieved by a rapid and significant (over-) installation of renewables. The consequent use of the produced green electricity in ALL sectors is mandatory !

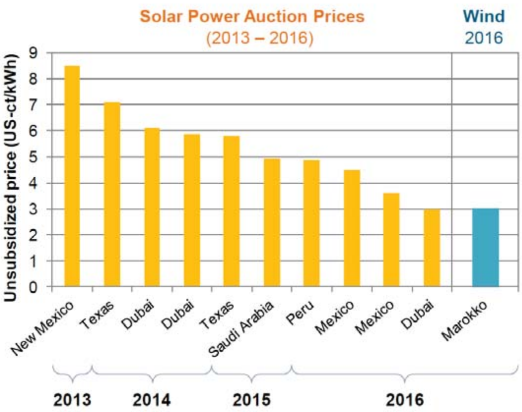
Sector coupling
Needs and selected concepts

Manfred Waidhas, Siemens AG, Hydrogen Solutions, **91058 Erlangen, Germany**

Trends2017, Aachen, Dec 06, 2017.

SIEMENS

Renewable power generation technologies
becomes cost competitive



source:http://cleantechnica.com,16.04.2016

- Most recent electricity contracts in Middle East are below 24 USD/MWh (e.g. Saudi-Arabia: 17.8 USD/MWh)
- Countries with low electricity costs are highly interested to invest in green P2X technologies
- In Germany / Europe hurdles have to be removed regarding regulatory framework (e.g. Renewable Energy Directive, sector coupling, „EEG-Umlage", etc.)

Renewable power generation
Extension and smart storage concepts essential

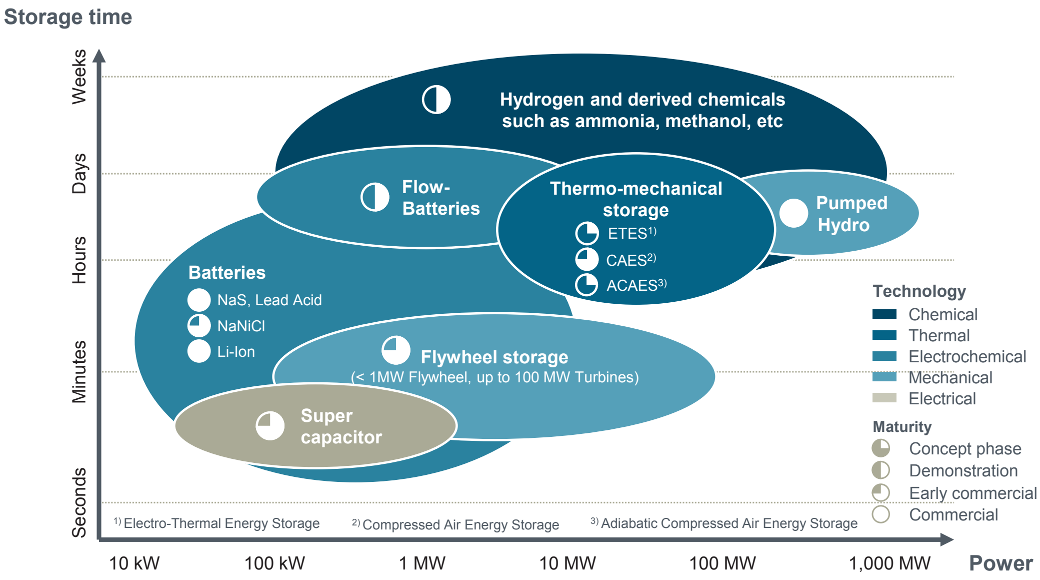
SIEMENS

1. CO_2-reduction is clearly linked with renewables.
2. Enforced extension of renewables is mandatory to reach defined CO_2 reduction targets

Energy storage capacities in the TWh-range will be needed

Hydrogen as energy storage concept –
the only option to address capacities > 10 GWh

SIEMENS



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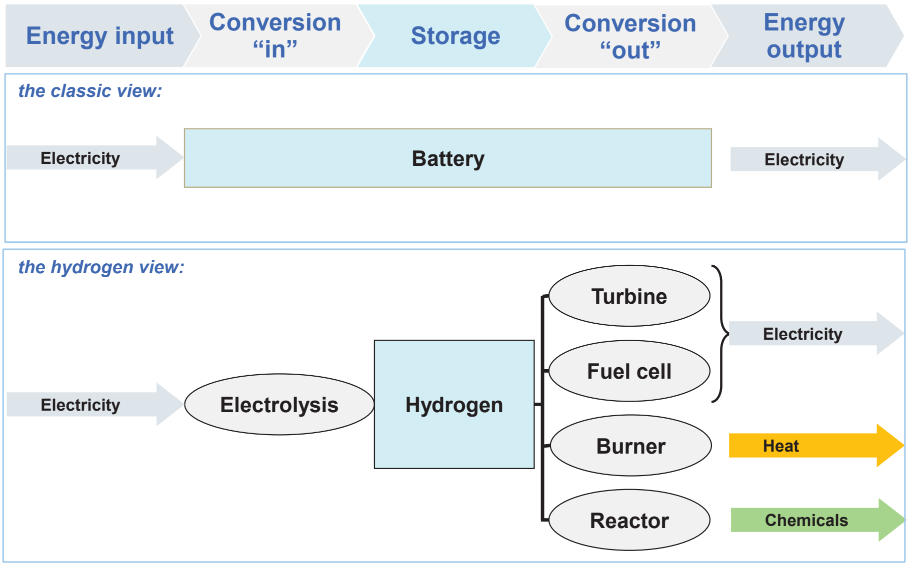
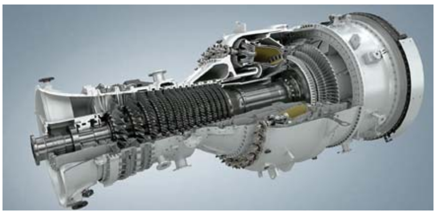
Electrical Energy Storage
The common understanding has to be re-defined

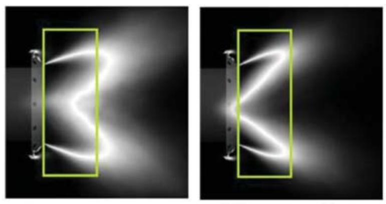


Page 5

SIEMENS

Hydrogen combustion @ Siemens
From fundamentals to real engines





0 % hydrogen 80 % hydrogen

SGT-800 (54 MW)

- 30 DLE burners of so-called 3rd generation
- air enters combustor with ≈ 20 bar and 700 K

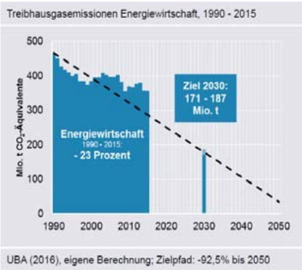
- Re-electrification of H2 in gas turbines technically feasible: most of existing NG gas turbines will allow an admixing of H2 to a certain extent
- Projects @ Siemens with H2 gas turbines were successfully performed
- Mid- to long-term: high demand in gas turbines estimated (≥ 100 GW in Germany by 2050) Products will be available as soon as energy market and customers ask for related solutions

Page 6

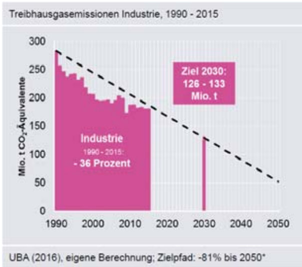
Becoming serious – CO_2-emission reduction targets DE

ludwig

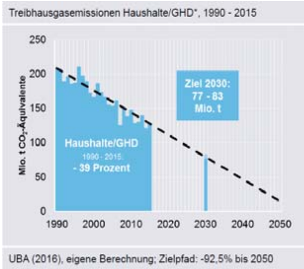
Electricity sector (target: -92.5%)



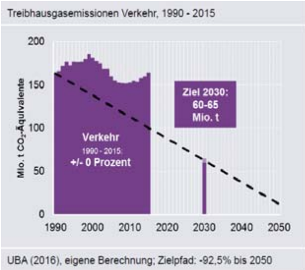
Industry (target: -81%)



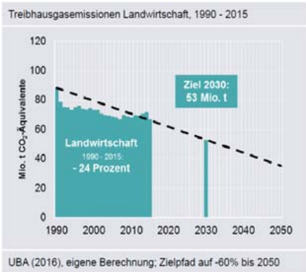
Households/SMEs (target: -92.5%)



Mobility (target: -92.5%)



Agriculture (target: -60%)



Source: Agora Energiewende, 20.09.2016

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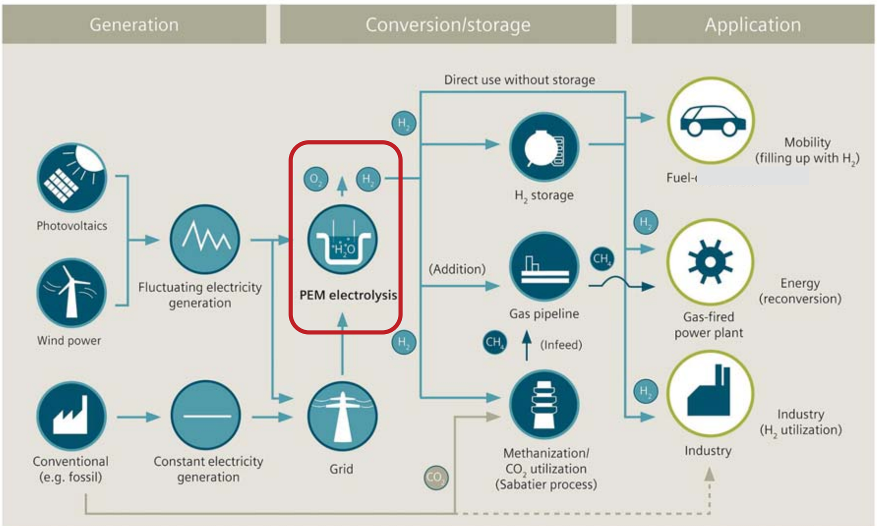
Hydrogen is multi-functional: shifts CO_2-savings in power generation to mobility and industry



H_2 enables the coupling between energy, mobility & industry markets

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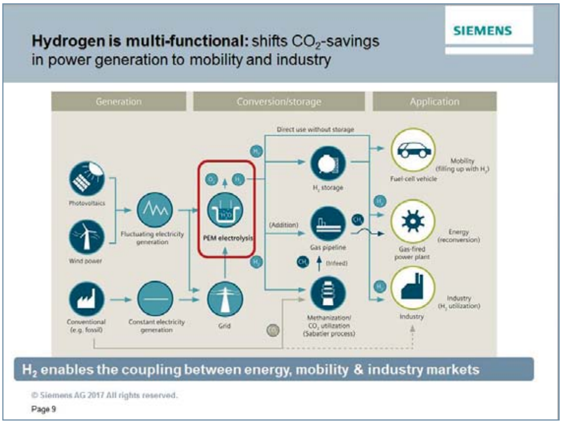
The different use cases for green hydrogen…
….follow a `merit order´ principle



current H_2 market prices

mobility	~ 4 – 10 USD/kg
industry	~ 1,4 – 5 USD/kg
energy	~ 0,7 – 1 USD/kg

- Compared to re-electrification ("power to power") the use of hydrogen in industry or mobility leads more easily to a positive business case.
- The three use cases have different maturity, market potential and market starting points.

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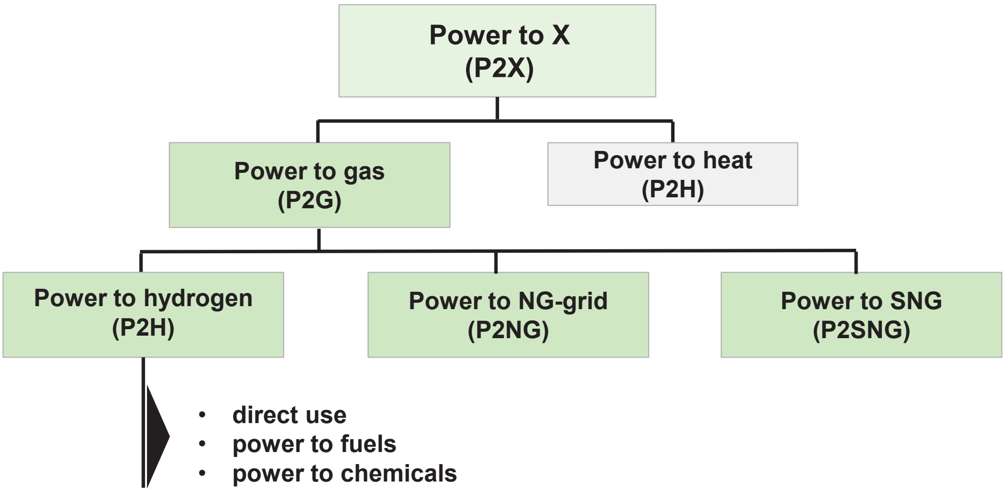
Power-to-X-concepts
Most of them base on hydrogen as intermediate step



The business cases of the individual P2G(X) approaches differ notably.

Green (CO_2-free) hydrogen:
a broad variety of potential applications

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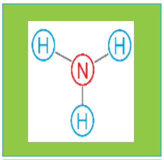
Industry *

• Refineries



• Ammonia plant

• Steel production

Mobility

• H_2 as fuel for public transport

• Substitute of bio-ethanol admixing

Energy

• Re-electrification in H2-turbines

• Admixing to conventional gas turbines

• Generator cooling

* Besides these: glass, semiconductor, food&beverage

H_2 production via electrolysis
Economy of operation

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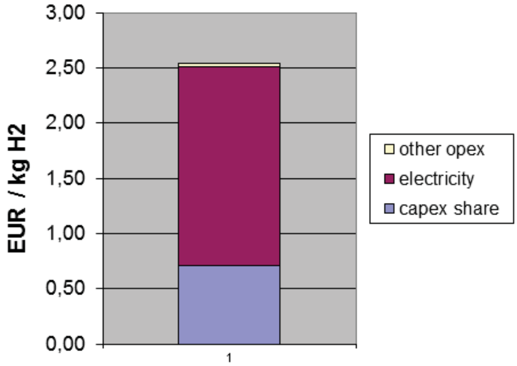
input parameter:	
electricity costs [ct/kWh]:	**3,2**
capex electrolyzer [€/kW]:	**1.000**
utilization rate [hours per year]:	**4000**
product life [y]:	20
system efficiency [% HHV]:	70
additional capex [€/kW]:	0
additional opex [%] * :	5
interest rate [%]:	0
depreciation period [a]:	10

* service, maintenance, operation (without electricity)

H2 production costs



Important: above choosen parameter are arbitrary values and do not reflect data of Siemens electrolyzers !

ENERGIE PARK MAINZ

Project scope and key facts

Development of an decentralized hydrogen energy storage plant

- Location: Mainz (Germany)
- Partners Stadtwerke Mainz, Linde, Siemens, RheinMain University
- Connected to a wind-farm (8 MW)
- 6 MW peak electrolyzer (3 stacks, each 2 MW)
- 1000 kg H_2 storage (33 MWh)
- 200 tons H_2 target annual output
  - Injection in local gas grid
  - Multi-use trailer-filling
- Funding: ~50% (BMWi)
- Timeline: 10/2012 – 12/2016

Source: Wikipedia Source: Energiepark Mainz

Ein Forschungsprojekt von STADTWERKE MAINZ AG Hochschule RheinMain University of Applied Sciences Wiesbaden Rüsselsheim Linde SIEMENS Gefördert durch Bundesministerium für Wirtschaft und Energie aufgrund eines Beschlusses des Deutschen Bundestages ENERGIESPEICHER Forschungsinitiative der Bundesregierung

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H2FUTURE

Hydrogen from electrolysis for low carbon steelmaking

Blast Furnace in Linz; Source: Voestalpine

Project Consortium:

- **Verbund** (*utility/grid operator in AT = Electricity provider*)
- **VoestAlpine** (*steel manufacturer = Hydrogen consumer)*
- ***ECN (****Energy Research Centre of the NLD*)
- **Siemens Hydrogen Solutions** (*Technology provider)*

Project description:

EU funded project to show viability of a PEM electrolyzer as flexible load for grid services. Hydrogen used within the steel making/processing to reduce CO_2 foot-print.

Time line:

Jan. 2017 – Jun. 2021

Electrolyzer:

- 6 MW rated power
- new cell and stack design
- designed for power range of ≈ 10 - 100 Megawatt

More details:

http://www.h2future-project.eu

Funded by FCH FUEL CELLS AND HYDROGEN JOINT UNDERTAKING

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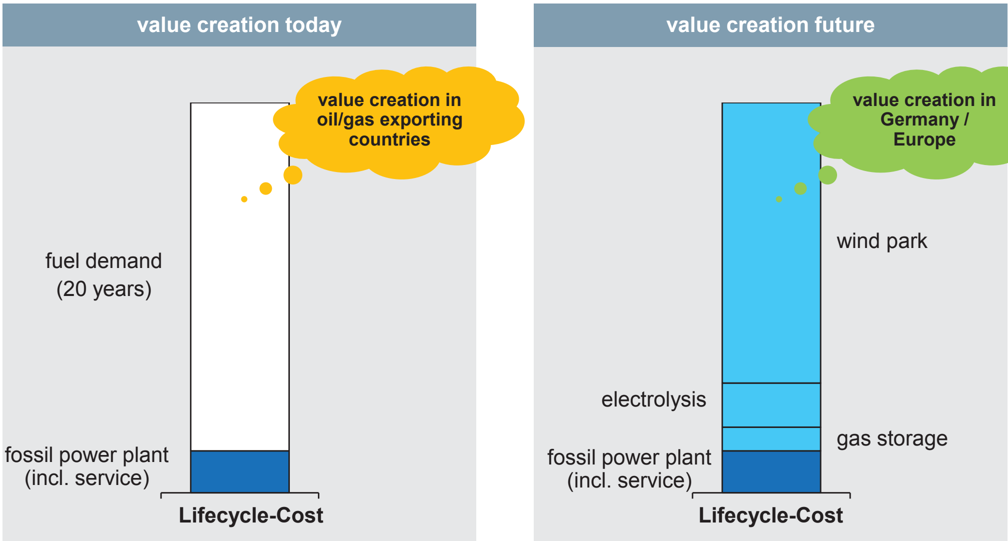
Power to X is more than only CO2 reduction
Opportunity to create added value in Germany



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eHighway -
An energy-efficient concept for CO2-free transportation

source: H. Grünjes, Siemens MO TI EH

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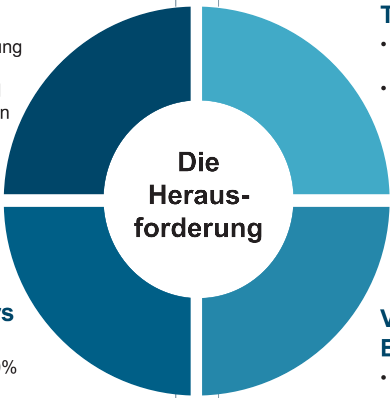
Die THG-Emissionen des Straßengüterverkehrs -
zunehmende Herausforderung für die Dekarbonisierung

Prognostiziertes Wachstum im Güterverkehr

- Verdreifachung der Güterverkehrsleistung von 2015 bis 2050
- Straßengüterverkehr ist in Deutschland von 2015 auf 2016 um 2,8% gewachsen

Reduktionsziele hinsichtlich THG-Emissionen bis 2050

- Sektorübergreifendes Ziel der Bundesregierung: 80% bis 95% (Basis 1990)
- Notwendiger Beitrag des Verkehrssektor ist eine Reduktion um 98%



Modal Split des Güterverkehrs in 2050

- Anteil des Straßengüterverkehrs ca. 60%
- Schienengüterverkehr wächst bei maximaler Ausschöpfung des Verlagerungspotenzials auf 30%

Verkehrssektor als THG-Emittent

- 20% der THG-Emissionen fallen im Verkehrssektor an
- Anstieg um 5,4 Mio. t Emissionen im deutschen Verkehrssektor in 2016

Quellen: Klimaschutzbeitrag des Verkehrs bis 2050, Umweltbundesamt, Texte 56/2016, Juni 2016;
Erarbeitung einer fachlichen Strategie zur Energieversorgung des Verkehrs bis zum Jahr 2050, Umweltbundesamt, Texte 72/2016, November 2016
TF Transport Outlook 2017, Januar 2017
Umweltbundesamt, Pressemitteilung Nr. 09 vom 20.03.2017

source: H. Grünjes, Siemens MO TI EH

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eHighway –
current demonstrations in Germany, Sweden and US

Forschungsprojekte

- **ENUBA (Deutschland)**
  - Erstes Forschungsprojekt mit BMUB (05/2010 – 09/2011)
- **ENUBA 2 (Deutschland)**
  - Zweites Forschungsprojekt mit BMUB (05/2012 – 12/2015)
- **ELANO (Deutschland)**
  - Drittes Forschungsprojekt mit BMUB (01/2016 – 09/2019)

Projekte auf öffentlichen Straßen

- **Los Angeles – Hafenanwendung**

- Demonstrationsprojekt über eine Strecke von einer Meile der Verbindung zum Schienenterminal
- Kooperation mit Volvo und lokalen LKW-Herstellern

- **Schweden – Autobahnanwendung**

- Teststrecke auf einer öffentlichen Straße zwischen einem Industriegebiet und Hafen
- Benchmark verschiedener Elektrifizierungsmöglichkeiten für Langstrecke
- Kooperation mit Scania

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Summary

- CO_2-reduction targets are clearly linked with renewables. They will require storage capacities in the TWh-range.
- Hydrogen via Power-to-Gas is the only viable approach to store electrical energy >10 GWh.
- Hydrogen is multifunctional: it can be re-electrified, but also shifted to the industry or mobility sector (“sector coupling“).
- Sector coupling will be essential to reach CO_2 reduction targets.
- Transportation is the sector with highest need for pushing forward CO_2 reduction.
- eHighway is an energy efficient concept for heavy duty road transport based on proven technologies.

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Contact page

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Hydrogen Solutions

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Sector Coupling as a Chance for the Power Sector

Klaus Görner
University of Duisburg-Essen
LUAT: Chair of Environmental Process Engineering and Plant Design Essen, Germany

The presentation covers the sector coupling technology as a substantial contribution for the energy transition (Energiewende) in Germany.

The energy system transformation in Germany will generate to some amount surplus renewable power coming from wind and sun in a very volatile manner. This leads to the problem of storing power for a longer time, which is not economic currently, or to use existing power plants in combination with P2X technologies to realize sector coupling. On the other hand dispatchable power generation is needed to stabilize the electrical grid. To some extend Power-to-Products (P2X) technologies like Power-to-Gas (P2G), -Fuels (P2F), -Chemicals (P2C) or-Heat (P2H) can be used in combination with a modified power plant operation.

To integrate these new technologies in the existing energy system, a complex variety of pathways are possible and have to be analysed for the energy system integration.

Possible pathways are investigated by the Virtual Institute "Power to Gas and Heat" in North Rhine Westphalia (NRW). In this context the pathways: "industrial demand side management", "Power-to-Heat", "renewable hydrogen in the mobility sector", "H2 based synthetic products for mobility and industry", "H2 injection into the natural gas grids and decentralized power generation", "large scale H2 storage and centralized power generation" and "decentralized direct use of renewable hydrogen" had been in the focus.

Sector coupling technologies are analyzed with respect to their significance in relation to the power generation in Germany.

The energy sector and the industrial sector (specially the chemical industry in North Rhine Westphalia) show a very high potential for the sector coupling. Both the technical and the economic conditions are very attractive.

In more detail a EU funded H2020 project "MefCO2" was presented. It focuses on the production of methanol as a platform chemical for the chemical industry or as a fuel for the mobility sector. The integration of the CO2 capture plant, the electrolyzer and the methanol synthesis plant in the power plant itself ends up with an efficiency of about 61 % (electrically resp. thermally without an O2 usage), which is a good basis for an economic production. In this context the main idea is to increase the operational time of the plant by producing fuels in periods of low power prices on the market and to generate additional marginal incomes. In addition to this effect the plant is for a longer time in operation condition to participate in the primary control regime, also producing marginal returns.

This contribution gives an overview over the technologies and some possible applications in the context of a future power plant operation.

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Univ.-Prof. Dr.-Ing. habil.
Klaus Görner

Sector Coupling as a Chance for the Power Generation

Klaus Görner
Univ.-Prof. Dr.-Ing. habil.
LUAT - Lehrstuhl für Umweltverfahrenstechnik und Anlagentechnik | Universität Duisburg-Essen
Rhein Ruhr Power e.V. | Düsseldorf
GWI - Gas- und Wärme-Institut e.V. | Essen
Virtuelles Institut Strom zu Gas und Wärme | NRW

UNIVERSITÄT DUISBURG ESSEN | Rhein Ruhr Power | gwi | VIRTUELLES INSTITUT NRW STROM ZU GAS UND WÄRME

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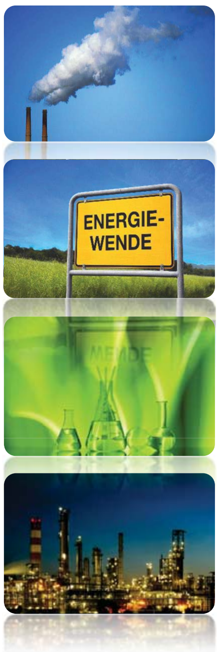
Klaus Görner

Content

- **The Energiewende**
  - energy transition
- **Flexible and dispatchable power generation**
  - Rhein Ruhr Power e.V.
- **Storage**
  - Capacities and periodes
- **Sector coupling**
  - Classification and potentials
- **Virtual institutes**
  - Combined Heat and Power
  - Power to Gas and Heat
- **Infrastructure**
  - Power plants and chemical sites in NRW
- **Sector coupling in the chemical industry**
- **Projects**
  - EU Horizon 2010 project $MefCO_2$
- **Conclusions**



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Energiewende

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Challenges and potentials of the Energiewende

The main challenge of the Energiewende is:
- **The Carbon-Footprint must be reduced significantly**.

In the moment the energy sector carries the main burden:
- **Reduction of CO_2 emissions related to power generation**.

In other sectors additional contribution can be made:
- **Combined heat and power generation**
- **Closing of carbon cycles (chemistry, iron and steel, …)**
- **Reduction of CO_2 emissions in the mobility sector**
- …

By means of
sector coupling
a much bigger effect can be generated.

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The Energiewende

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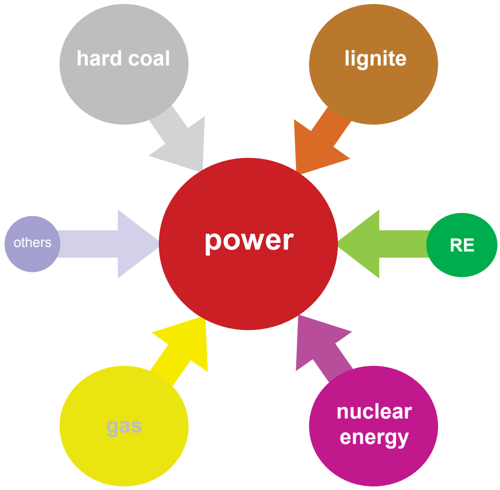
Change of shares by the energy transition („Energiewende")



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Energiewende and its consequences

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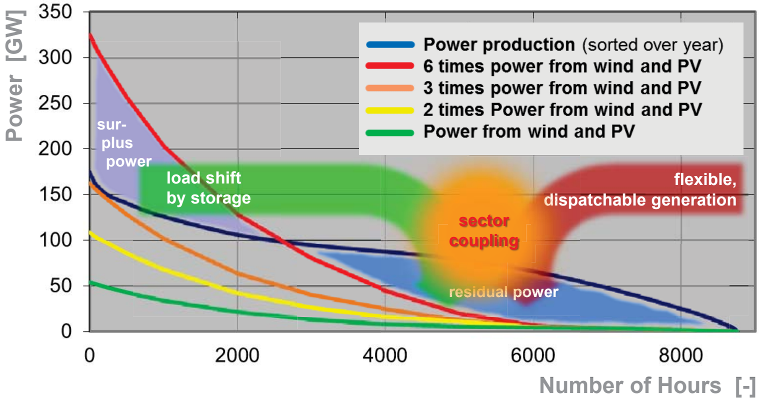
Problem of power production at the „wrong" time



generation | storage | sector coupling

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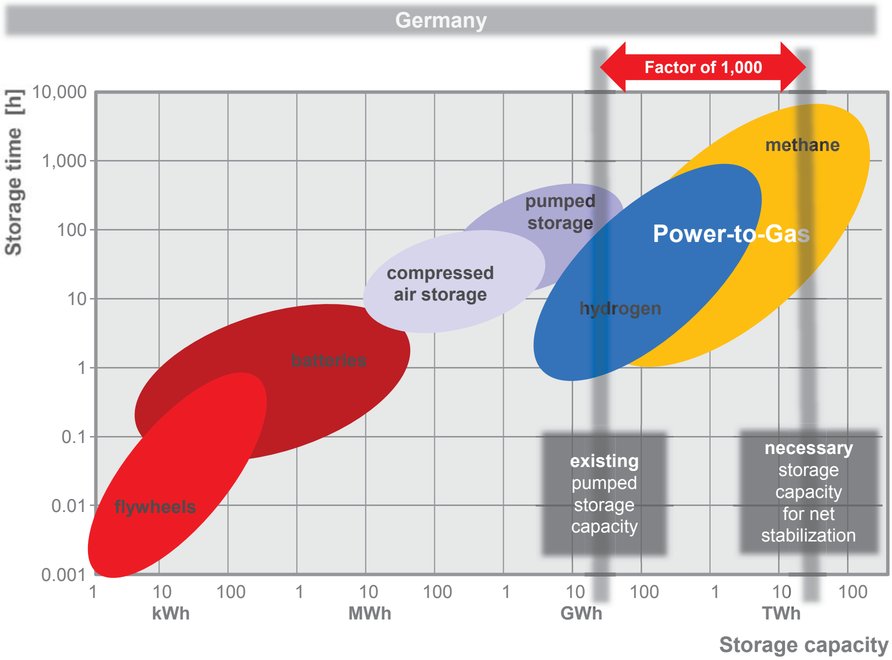
Storage – capacities and periodes

storage

Suitable technologies for the situation in Germany



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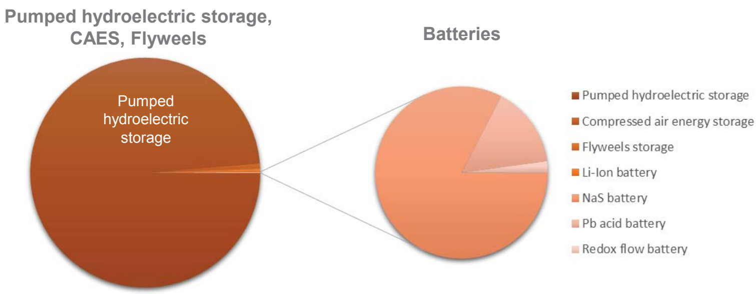
Storage – capacities and periodes

Existing capacities in Europe

Europe EU28 plus Norway plus Switzerland

Pumped hydroelectric storage	48,325	MW
Compressed air energy storage	322	MW
Flyweels storage	77	MW
Li-Ion battery	186	MW
NaS battery	38	MW
Pb acid battery	7	MW
Redox flow battery	1	MW



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Quelle: Valuing dedicated storage in electricity grids. Leopoldina, 2017

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sector coupling

Sector Coupling

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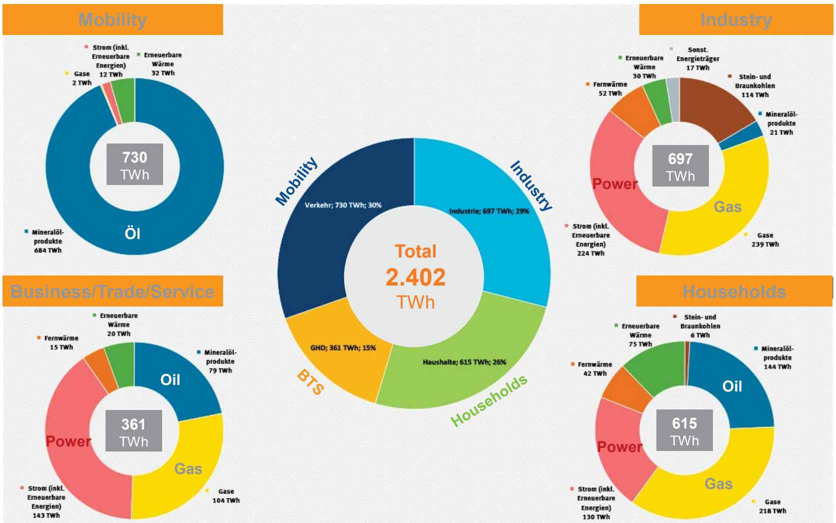
Sector classification

Significance of the different sectors

- **Energy sector**
  - Power
  - Heating / Cooling
  - Fuels (Gas / Oil / Coal)



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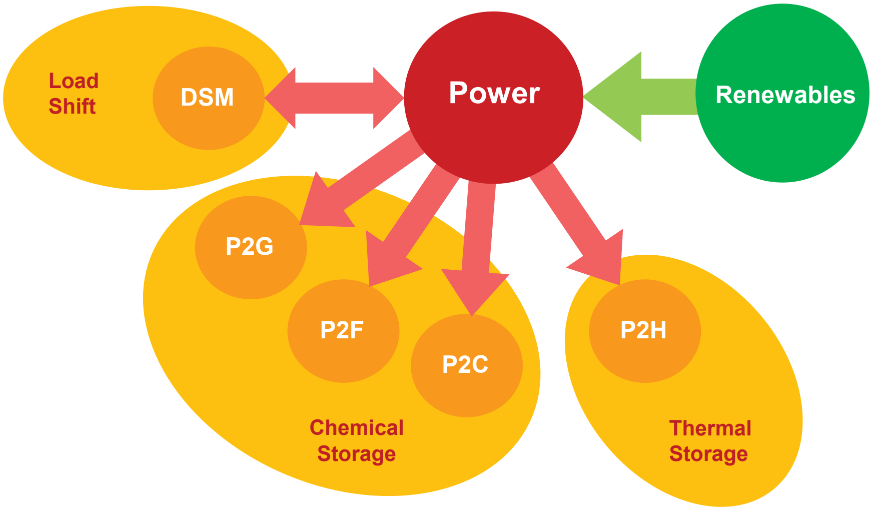
Sector coupling

P2X and DSM as flexibility options



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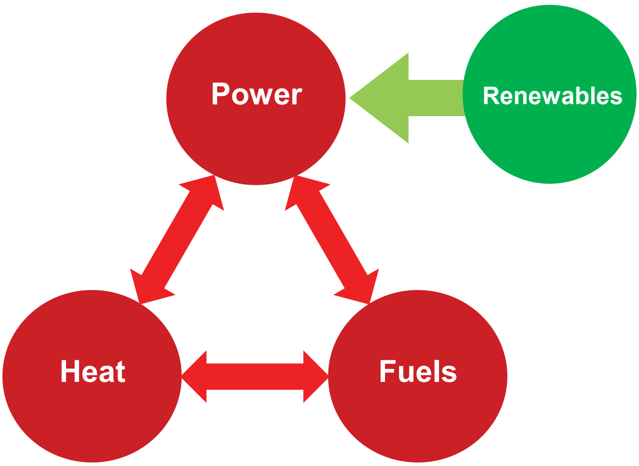
Sector coupling

Linkage between the sectors power, heat and fuels (mobility)



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Sector coupling technologies

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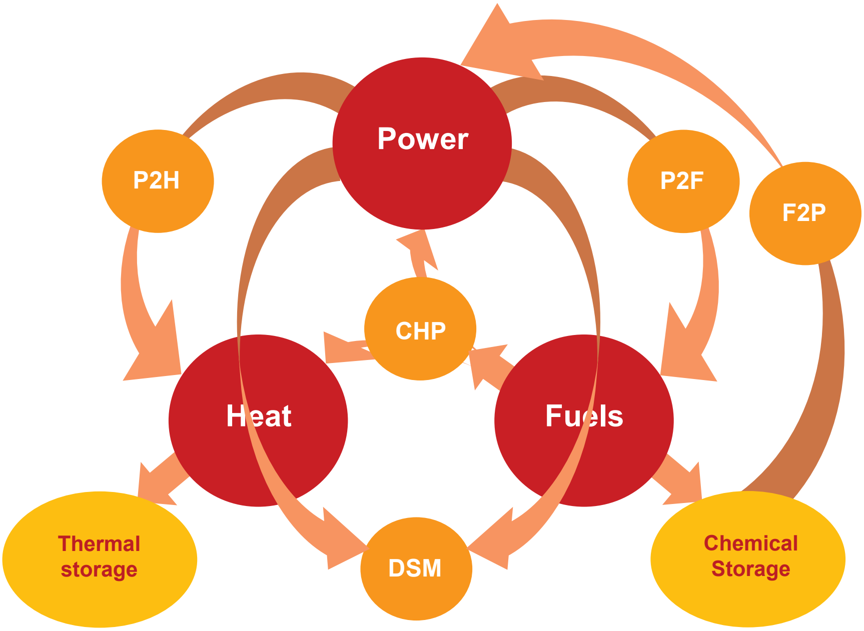
Enabler for all flexibility options and contribution to storage and production



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Chemical Industry

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Infrastructure and nearness of energy and chemistry in NRW

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Locations of chemical sites in NRW (selection)

Oberhausen - Oxea

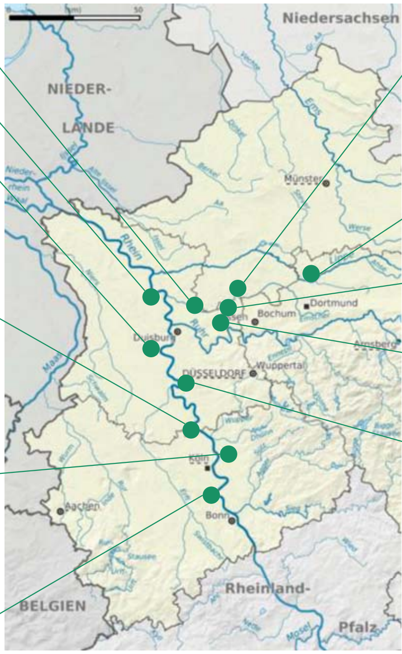
Rheinberg - Solvey

Krefeld - Covestro

Dormagen - Lanxess

Leverkusen - Bayer

Wesseling - Shell



Marl - Evonik

Hamm – DuPont de N.

Gelsenkirchen – Ruhr Oel

Essen – Evonik (Golds.)

Düsseldorf - Henkel

Source for the map: Liste der Flüsse in NRW. Wikipedia, aufgerufen am 25.07.2016

VGB Summer School POWER PLANT 2017:

Sector Coupling

Electricity, Heat and Transport - Challenges and Potentials -

31.08.2017

VGB, Essen

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Infrastructure and nearness of energy and chemistry in NRW

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Locations of power plants in NRW (selection)

Voerde - RWE/STEAG

Walsum - STEAG

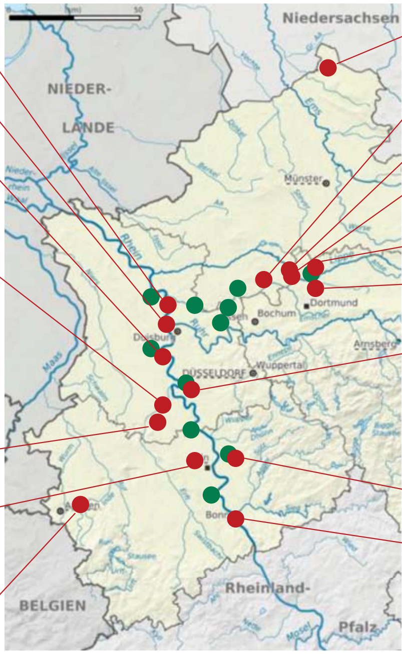
Huckingen - RWE

Neurath - RWE

Frimmersdorf - RWE

Hürth - Statkraft

Weisweiler - RWE



Ibbenbüren - RWE

Datteln – E.ON

Lünen - Trianel

Lünen - STEAG

Marl - Evonik

Westfalen - Hamm - RWE

Düsseldorf - Stadtwerke

Köln - Rheinenergie

Bonn - Stadtwerke

Source for the map: Liste der Flüsse in NRW. Wikipedia, aufgerufen am 25.07.2016

VGB Summer School POWER PLANT 2017:

Sector Coupling

Electricity, Heat and Transport - Challenges and Potentials -

31.08.2017

VGB, Essen

Folie 16

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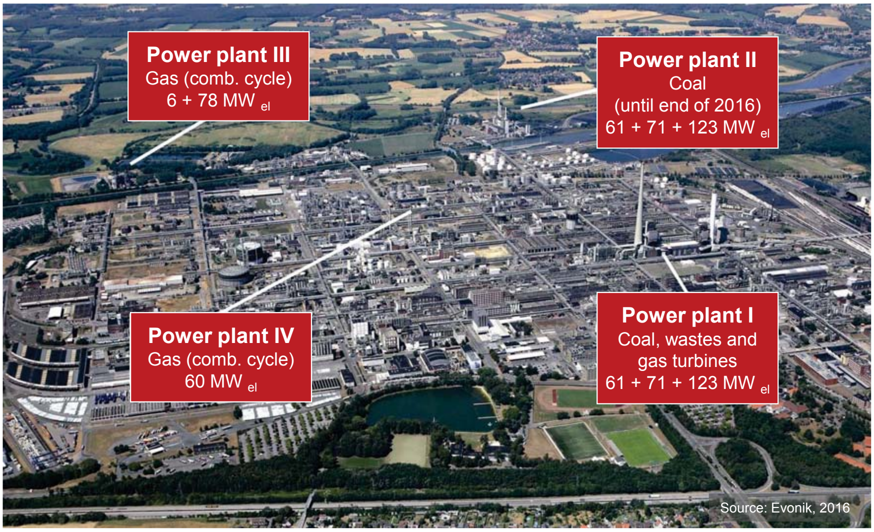
Folie 17

Sector coupling between energy and chemistry

Chemical site from Evonik in Marl

4 power plants with a total capacity of 457 MW_{el}



About 100 production plants for different intermediate and final products

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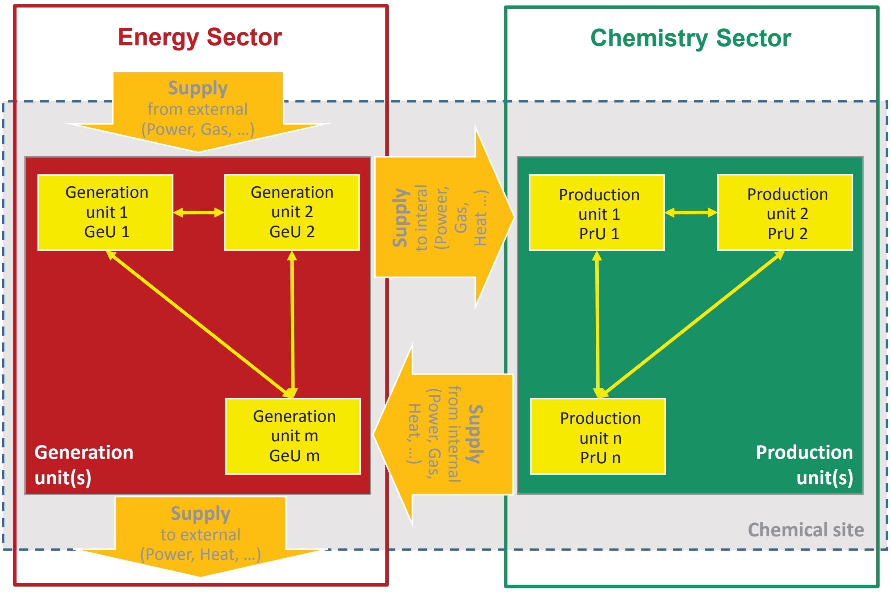
Sector coupling between energy and chemistry

Cooperation of different units



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Virtual Institute

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Folie 19

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Virtual Institute – Power to Gas and Heat

Flexibilisation of the Energy System

by Means of Power-to-X
as a Sector Coupling Technology
in North Rhine-Westphalia

Representation of the Energy System

Flexibility options in the power, gas and heat systems

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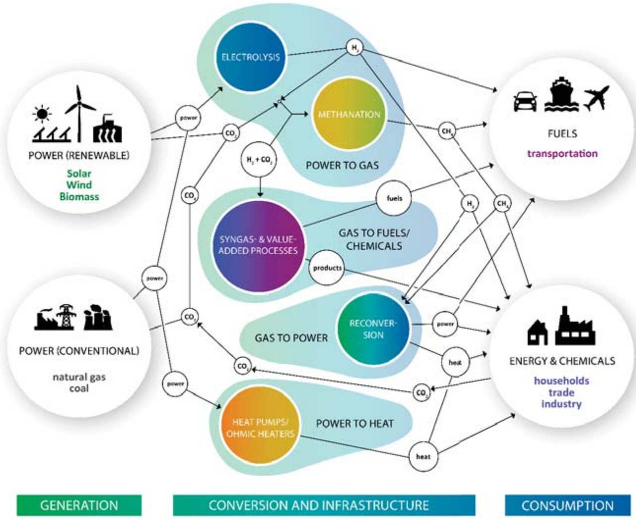
From the network diagram system pathways are identified

1) Industrial demand side management
2) Power-to-Heat
3) Renewable hydrogen in the mobility sector
4) H_2 based synthetic products for mobility and industry
5) H_2 injection into the natural gas grids and decentralised power generation
6) Large scale H_2 storage and centralised power generation
7) Decentralised direct use of renewable hydrogen



CEF.NRW ewi gwi Fraunhofer UMSICHT JÜLICH RUB Wuppertal Institut für Klima, Umwelt, Energie GmbH ZBT

Klaus Görner, Flexibilisation of the Energy System, IST2016 Conference - International Sustainability Transitions Conference, Wuppertal, 09.09.2016

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Projects

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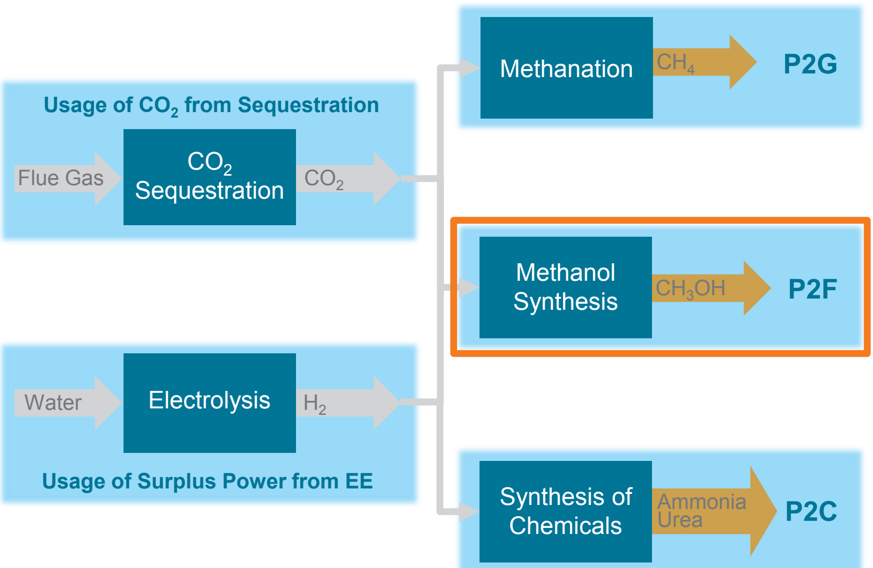
MefCO$_2$ - Methanol fuel from CO$_2$

Synthesis of methanol from captured carbon dioxide using surplus electricity

P2X Technologies



Project Approach

Project Approach

$MefCO_2$ (Methanol fuel from CO_2) - Synthesis of methanol from captured carbon dioxide using surplus electricity.

Aim

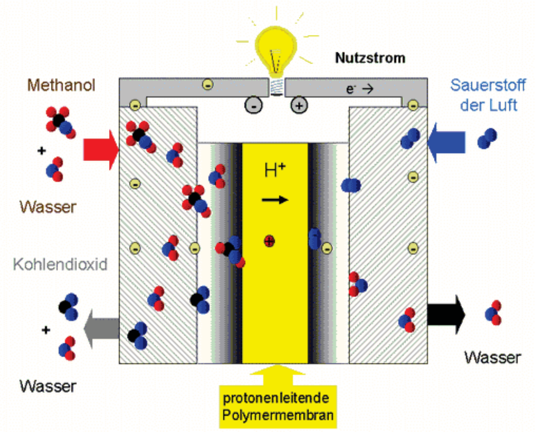
To develop an innovative green chemical production technology which contributes significantly to the European objectives of decreasing CO_2 emissions and increasing renewable energy usage, thereby improving Europe's competitiveness in the field.

Concept

The overall concept underpinning the project lies in the utilisation of ordinarily emitted greenhouse gas carbon dioxide and hydrogen, produced from redundant electrical energy into a widely-useable platform chemical, methanol. The technology is being designed in a modular intermediate-scale, with the aim of being able to adapt it to varying plant sizes and gas composition.

Methanol as Fuel for the Mobility Sector

Usage in Direct Methanol Fuel Cell



Anode:
$$CH_3OH + H_2O \longrightarrow CO_2 + 6\,H^+ + 6\,e^-$$

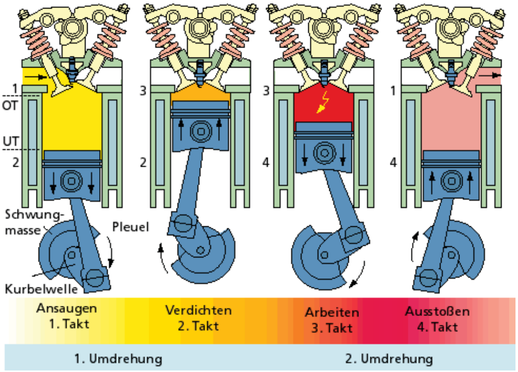
Kathode:
$$O_2 + 4\,H^+ + 4\,e^- \longrightarrow 2\,H_2O$$

Gesamtreaktion:
$$CH_3OH + 1.5\,O_2 \longrightarrow CO_2 + 2\,H_2O$$

Dyck, A.; Polymerverfahrenstechnik, 2005, Universität Paderbron

Methanol as Fuel for the Mobility Sector

Combustion in Internal Combustion Engine (Otto Engine)



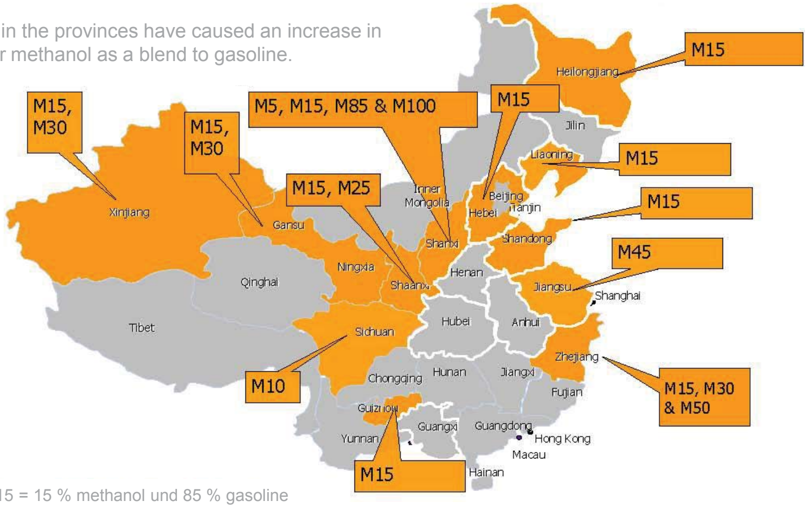
$CH_3OH + 3/2\ O_2 \rightarrow CO_2 + 2\ H_2O$

$\Delta H = -725$ kJ/mol

Advantages of Methanol versus gasoline (petrol)
•no fossil basis
•30 % higher efficiencies
•Environmental behaviour better

Methanol as Fuel for the Mobility Sector in China

Standards in the provinces have caused an increase in demand for methanol as a blend to gasoline.



Example: M15 = 15 % methanol und 85 % gasoline

Quelle: G. Dolan, Methanol Institute, 2014

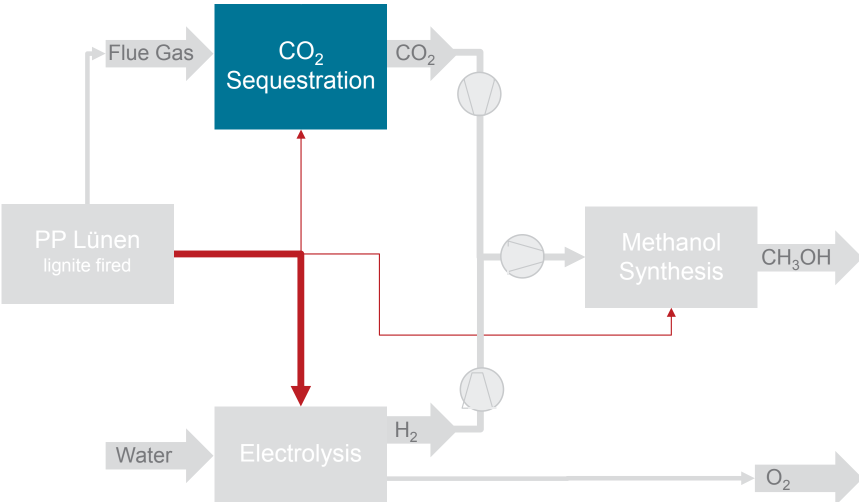
Power Plant - CO_2 Source and Power Generation

Hard Coal Fired Power Plant
507 MW_{el} with power production for railways

Historie

1938-42	Inbetriebnahme und Betrieb des Kraftwerks, 4 x 45 MW
1954-93	Inbetriebnahme und Betrieb des 50-MW-Blocks
1962	Inbetriebnahme des 150-MW-Blocks
1968	Erste Versuche zur Rauchgasentschwefelung nach dem Aktivkoksverfahren
1969	Inbetriebnahme des 350-MW-Blocks
1973-93	Inbetriebnahme mit Betrieb des 170-MW-Kombi-Blocks mit Kohledruckvergasung
1974	Erste Versuchsanlage zur Rauchgasentschwefelung nach dem Kalkwaschverfahren
1984/88	Inbetriebnahme des 110-MW-Bahnstrom-Turbosatzes (Teil des 150-MW-Blocks) / Rauchgasentschwefelungsanlage nach dem Kalkwaschverfahren
1989/96	Inbetriebnahme einer Stickstoffoxidminderungsanlage / Kessel 10 am 150-MW-Block
2003	Inbetriebnahme Fernwärmeversorgung für Stadtwerke Lünen

CO_2 Sequestration by Chemical Scubbing



CO_2 Sequestration by Chemical Scubbing

Semi-technical plant
in the STEAG power
plant in Lünen

Product:
very clean CO_2

Amount:
120 kg/h

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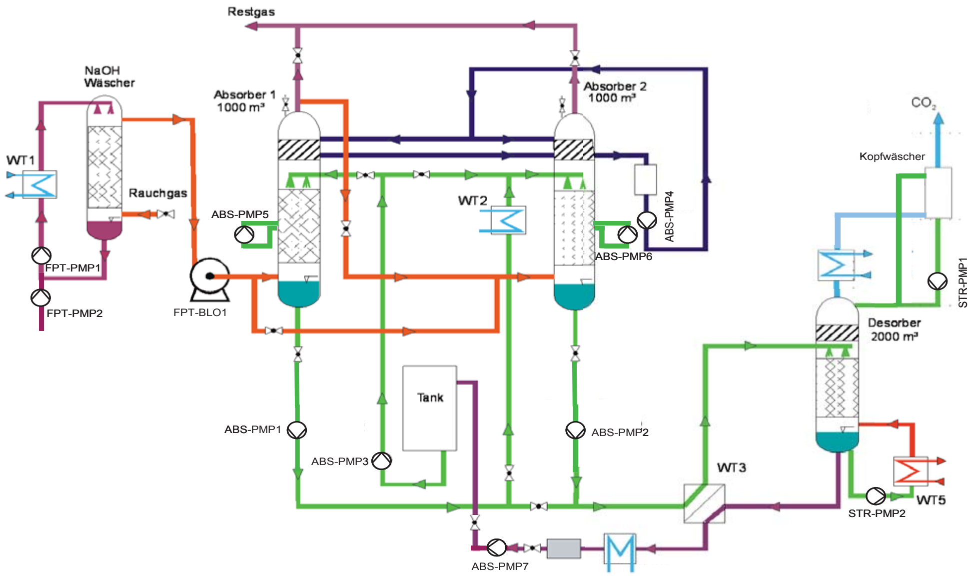
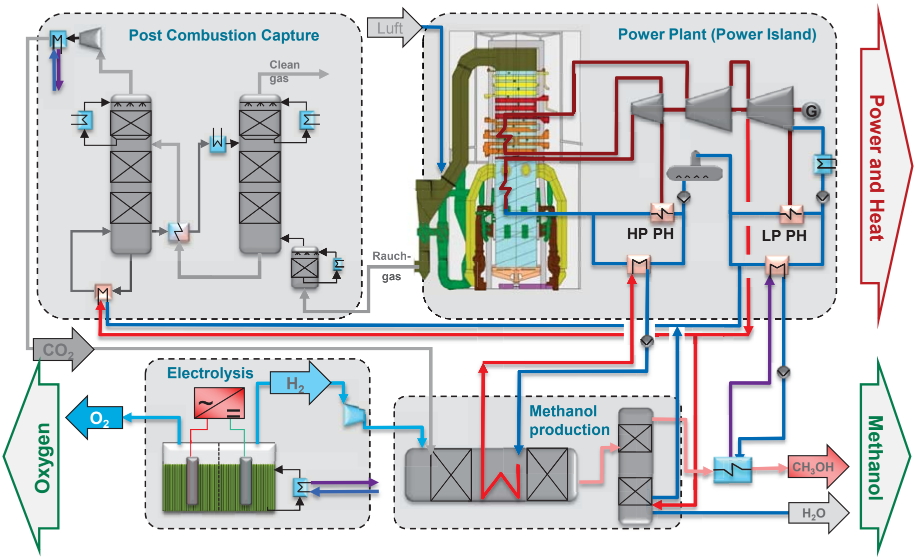
Technology: Chemical Scubbing with Amines, Amino Acid Salts or Alcalies

CO_2 Sequestration by Chemical Scubbing



System Integration

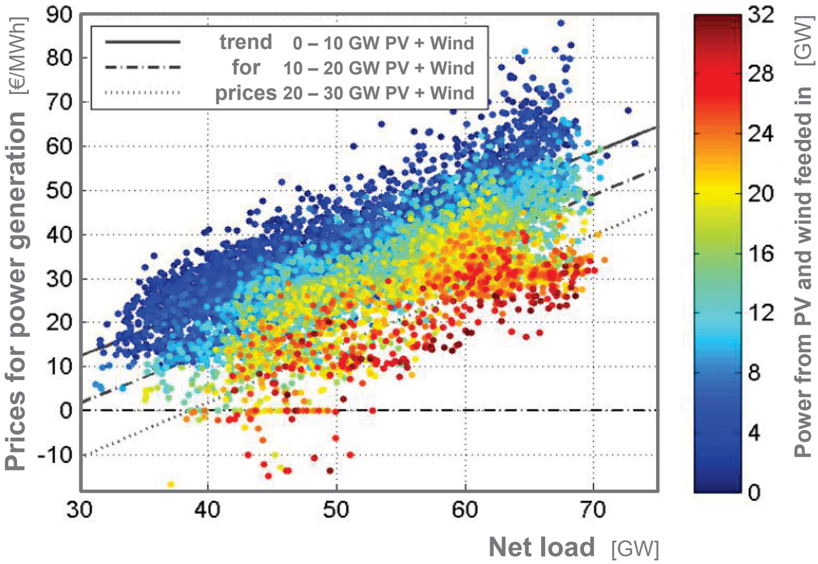


Conversion efficiency: $\eta_{el/th} = 61\ \%$ (without O_2 usage)

Source: Mitsubishi Hitachi Power Systems Europe

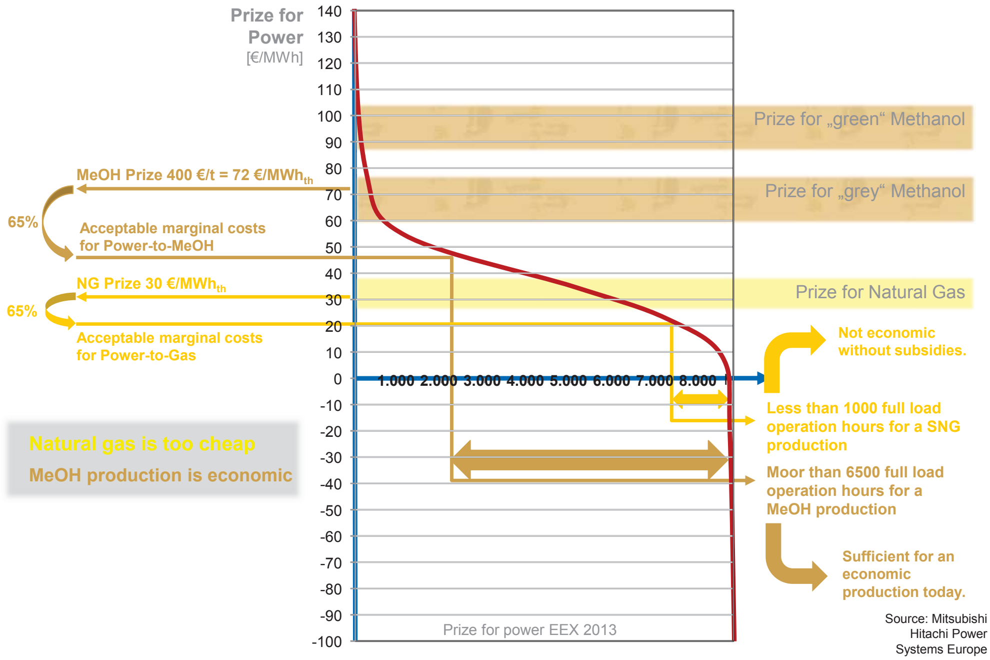
Economy – EEX prices for power

EEX prices for power as a function of the net load and the feed in by wind and PV (2014)



Sourcee: ETOGAS, EEX (public EPEX SPOT und Transparency data)

Economy – Situation for Gas and Methanol Production



Source: Mitsubishi Hitachi Power Systems Europe

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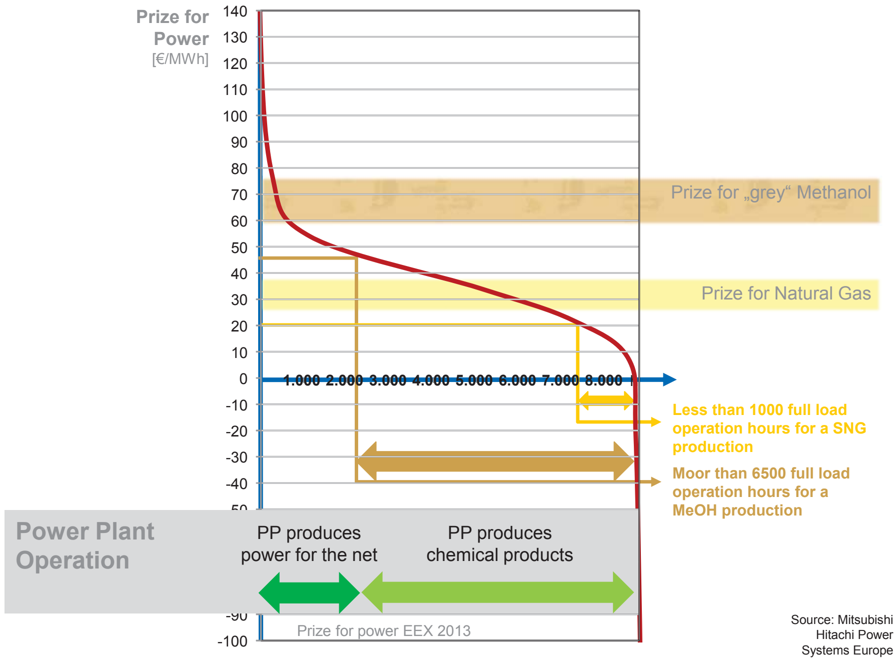
Economy – Situation for future Power Plant Operation



Source: Mitsubishi Hitachi Power Systems Europe

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Conclusions

Challenges of the Energiewende

- Carbon footprint must be reduced dramatically in all sectors.
- There is a big demand in power storage and flexible power generation.
- Surplus power should be used sensible (economy, flexibility).

Potentials of the sector coupling

- Sector coupling opens a big variety of flexibility options.
- Combined heat and power - as a proofen technology - should be extended.
- P2H can increase the flexibility and economy of existing power plants.
- Power-to-X technologies - P2G, P2F, P2H - should be further improved and optimized (increase of technology readiness level, reliability, investment and operational costs).
- DSM is able to reduce the demand on storage capacities and can use surplus power directly.

Needs for further developments

- The different sectors (chemistry, iron and steel, cement, pulp and paper, …) must be analysed for further potentials.

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Folie 37

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Folie 38

Transition of Public Transport to Emission Free Buses in Hamburg

Heinrich Klingenberg
hySOLUTIONS GmbH

As all metropolitan regions, the city of Hamburg is challenged by the increasing amount of traffic and its emissions caused by its growing population. This is why Hamburg is pursuing an ambitious program to increase electric and hydrogen mobility. Hamburg's city government has decided that from 2020 onwards only emission free buses will be purchased. Currently, there are various projects to increase the number of electric vehicles and charging infrastructure and prepare the timely transition to innovative systems for fast and more effective charging systems.

Regarding buses, a so called innovation line has been introduced: On this particular line, only buses with innovative electric drive trains are employed in order to compare different innovative drive trains under the same conditions. Currently, serial electric hybrid buses, parallel diesel-electric hybrid buses, battery buses with fuel cells as range extender and plug in buses are tested. The results are collected and compared and will show which systems is the most viable in the future.

Transition of Public Transport to Emission Free Buses in Hamburg

Heinrich Klingenberg, hySOLUTIONS GmbH

TRENDS 2017 Aachen – December 6, 2017

HOCHBAHN

About us

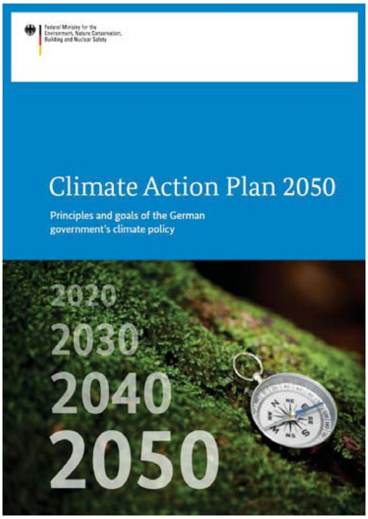
hy SOLUTIONS
Driving Innovation for Hamburg

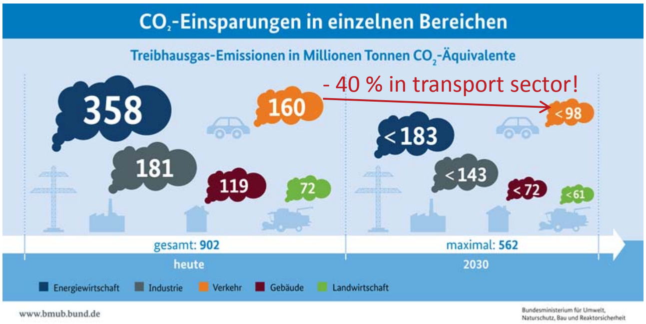
- hySOLUTIONS is a public private partnership organisation founded in 2005
- Shareholders: HOCHBAHN VATTENFALL Stromnetz Hamburg DNV·GL VHH Verkehrsbetriebe Hamburg-Holstein AG

  HK Handelskammer Hamburg Handwerkskammer Hamburg

- Project development and management in the field of hydrogen and fuel cell technology as well as in electric mobility
- Coordination agency for Hamburg, formally mandated by Hamburg Senate
- Portfolio: Some 30 projects (predominantly R&D) both national and international still running or successfully completed
- Networks: Regional, National and European organizations, working groups and expert committees

German climate protection targets





- Development of concepts for target achievement 2030 and long term agenda setting for 2050
- Submittal of concepts in 2018

Why do we act now.
Main drivers and actions.

- **Driver for City of Hamburg:** Realisation of the climate protection aims
- **Selected actions of City of Hamburg:**
  - Reissue of Clean Air Plan in 2017
  - Political mandate of senate for public transport companies: Procurement of emission free buses only from 2020 onwards, public fleets emission-free
- **Our driver – our mission:**
  „We organise the sustainable mobility in the Smart City Hamburg“
- **Our short-term actions to support the climate protection targets:**
  - Development of a **masterplan** for electrification of the bus fleet
  - Construction of a new **e-depot** for 250 electric buses
  - On-demand service with FC cars
  - Growing number of emission-free vehicles in city logistics

NDR.de Das Beste am Norden
Nachrichten Sport Ratgeber Unterhaltung Kultur
Niedersachsen Schleswig-Holstein Mecklenburg-Vorpom

Stand: 21.07.2016 17:46 Uhr - Lesezeit: ca.2 Min.

Hamburg braucht schnelleren Plan gegen dicke Luft

Das Hamburger Verwaltungsgericht zwingt den Senat zu einem schnelleren Luftreinhalteplan: Es forderte die Stadt am Donnerstag auf, spätestens in einem Jahr vorzulegen, wie man die Grenzwerte der Europäischen Union einhalten kann.

Hamburg verstößt bei den Stickstoffdioxidwerten in der Stadt gegen EU-Grenzwerte.

5.000 Euro Zwangsgeld angedroht

Der Umweltschutzverband BUND hatte ein Zwangsgeld gegen den Senat beantragt. Das Verwaltungsgericht folgt dem teilweise in seiner Entscheidung: Es droht dem Senat 5.000 Euro Strafe an, wenn er das Maßnahmepaket zur Luftsauberkeit später als Juni 2017 vorlegt. Der Senat wollte sich ursprünglich sieben Monate mehr Zeit nehmen.

Das Gericht begründete seine Entscheidung damit, dass es den Senat schon 2014 aufgefordert habe, die gesetzlichen EU-Grenzwerte für Stickoxide einzuhalten, die in Hamburg an Straßen-Messstationen überschritten werden.

BUND verlangt Fahrverbote wegen Stickoxid-Belastung

200.000 Anwohner großer Straßen in Hamburg litten unter den gefährlichen Stickoxiden, sagte Manfred Braasch vom BUND. Nun müssten schnell Fahrverbote für Dieselfahrzeuge in der Innenstadt und eine flächendeckende Geschwindigkeitsbegrenzung auf Tempo 30 her. "Bürgermeister Scholz kann sich nicht weiter vor Maßnahmen drücken", so Braasch. Aber auch die Umweltbehörde

Electric Buses

hy SOLUTIONS
Driving Innovation for Hamburg

Clear political commitment

- From 2020: Only emission-free buses to be purchased by HOCHBAHN

Long term strategy

- Early preparation to ensure attractiveness and performance capability of buses in the future
- Use of buses up to 14 years: safe energy supply needed
- Introduction of new technology (workshops, refuelling) only doable step by step
- Sufficient time for education and on-the-job training
- Functional view: different powertrains for different types of operation
- CAPEX and OPEX but also productivity and flexibility to be considered

Innovative Buses in Hamburg

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Driving Innovation for Hamburg

Fuel cell buses

- Since 2003: HyFLEET:CUTE with up to 9 fuel cell buses
- Since 2011: New generation of fuel cell hybrid buses, consumption: 8 kg hydrogen/100 km; range: 350 km
- Since end of 2014: 2 battery buses with a fuel cell as range extender

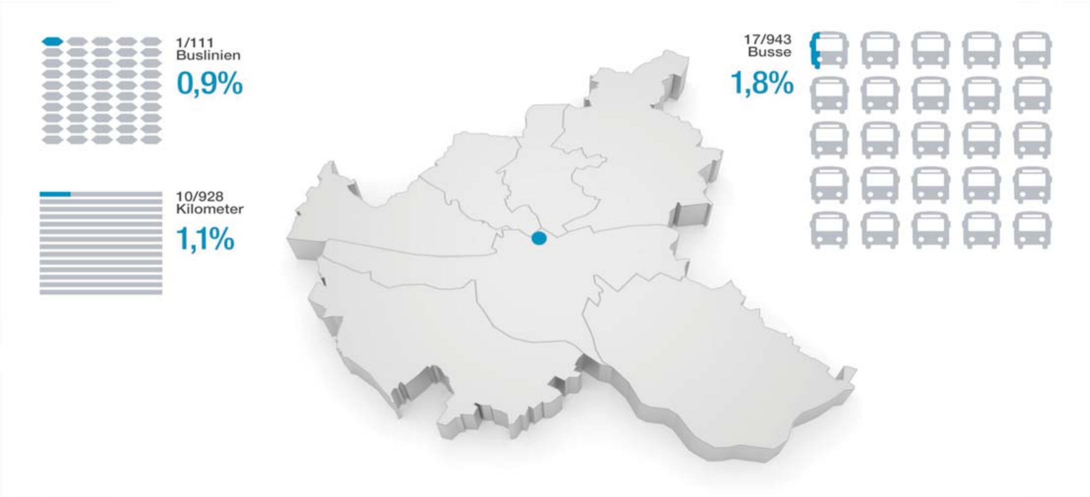
Hybrid buses

- Since 2010: Diesel-electrical hybrid buses
- Ongoing tests with hybrid buses

Battery buses

- Line operation with plug-in since end 2014
- Deployment of electric buses since 2016

From test site (Innovation Line 109) …



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… to Masterplan Electric Bus System (entire net)

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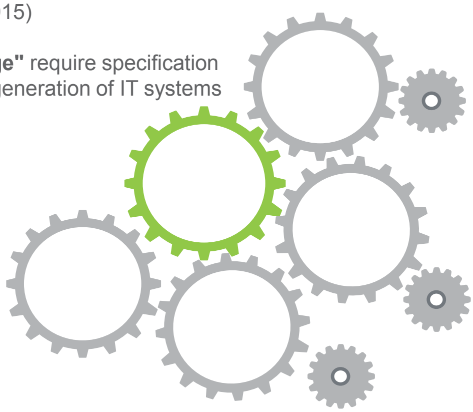
It‘s more than the electrification of a bus line.
It‘s the change of a complete system.

- **Complete electrification of the bus fleet from 2020 onwards within approx. 10-15 years**
- Predicted total energy demand of the depots with complete electrification of the bus fleet: approx. 132 GWh p.a.
  (compared to underground traction: approx. 112 GWh in 2015)
- New decisive influencing factors **"Technology"** and **"Range"** require specification and integration of new processes, interfaces and the next generation of IT systems in the topics
  - planning
  - operation/disposition
  - infrastructure/technology
  - depot management



Masterplan: the relevant targets

Lessons Learned.
Our main results: Innovation line 109.

- **Target:** Evaluation of performance of technology and optimization
- **The following innovative buses are evaluated:**
  - 3 battery buses (Solaris)
  - 3 plug-in buses (Volvo)
  - 2 battery buses with fuel cell as range extender (Solaris)
  - 4 fuel cell hybrid buses (Evobus)
  - 27 parallel diesel hybrid buses (Volvo)
  - 4 reference vehicles (Euro VI)
- **Selected results:**
  - High reliability of charging infrastructure and hydrogen station
  - Technical availability and reliability of the prototypes / customer field test not satisfactory yet
  - Seasonal variation of energy supply

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Lessons Learned.
Our main results: Depot Charger.

- **Battery bus (depot charger)**
  - Prognosis from market dialogue:
    - 1st level of development 2018/2020: 150 – 250 km range
    - 2nd level of development 2025: 200 – 300 km range
  - **Heating and air conditioning are critical factors**
  - Charging via **Combo 2 / CCS plug** with a charging capacity of 150 KW
  - **But:** Only part of today's tours **(planning)** with the currently projected ranges is possible through pure depot charging

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Lessons Learned.
Our main results: Opportunity Charging I.

- **Battery bus (opportunity charger)**
  - Current electric ranges of our opportunity charger:
    - Battery bus (Solaris): about 20 - 50 km (depending on outside temperature)
    - Plug-in hybrid (Volvo): about 6-8 km
  - Pantographs:
    - Charging capacity: 300 kW (2 per final stops on innovation line 109)
    - Daily charging of different brands successful (200 succesful charging processes per month, about 98%)
  - **Positioning assistance critical to success**: Combination of dynamic (driver assistance) and static information (lane marking) useful
  - Strong coordination need for charging infrastructure in public areas

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Lessons Learned.
Our main results: Opportunity Charging II.

- **Research project: „Evaluation of the operation of electric buses with local charging infrastructure in large cities using the example of HOCHBAHN“**
  - Scenario A (2016): chemical heating, 150 kWh (solo bus), 225 kWh (articulated bus)
  - Scenario B (2020): electric heating, 165 kWh (solo bus), 248 kWh (articulated bus)
- **Selected research objectives:**
  - Detailed energetic consideration of sub networks based on measured routes
  - Determination of the optimal location of charging infrastructure
- **Selected research results:**
  - Electrification of a sub network (about 23 % operating performance of HOCHBAHN bus network) requires either 26 (scenario A) or 40 pantographs (scenario B)

Bundesministerium für Verkehr und digitale Infrastruktur

Fraunhofer IVI

Hochschule für Angewandte Wissenschaften Hamburg
Hamburg University of Applied Sciences

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Lessons Learned.

Our main results: H$_2$/fuel cell buses.

- **General information on H$_2$/fuel cell technology:**
  - Basic advantage:
    - High (sufficient) **range,** therefore **flexible** deployment of buses
    - Productivity like diesel
  - Basic disadvantages:
    - Framework conditions concerning the handling with hydrogen

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Lessons Learned.

Our main results: H$_2$/fuel cell buses.

- **Fuel cell hybrid bus**
  - Imminent series production offered by established bus manufacturers not predictable today
- **Range extender battery bus with fuel cells (REX)**
  - Hydrogen demand (REX) is approx. only 1/3 of hydrogen demand of pure fuel cell buses
  - New depot for innovative drivetrains:
    - Considerable reduction of hydrogen demand (compared to 100% fuel cell bus fleet): about 1.5 t instead of 4-5 t H$_2$ per day (winter)
- **Hydrogen supply at depots**
  - Options: production or delivery (gaseous, liquid)
  - High security requirements, including:
    - Approval procedure depending on H2 quantities
    - Explosion protection concepts for plants necessary
    - Distances to protective goods

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Lessons Learned.
Our main results: Depots I.

- **Hydrogen supply at the depots**
  - Options: production or delivery (gaseous, liquid)
  - High security requirements, including:
    - Approval procedure depending on H2 quantities
    - Explosion protection concepts for plants necessary
    - Distances to protective goods
  - Storage and delivery of large H_2 volumes not possible at all locations without change in bus numbers

Lessons Learned.
Our main results: Depots II.

- **Stromnetz Hamburg:** Survey by Helmut Schmidt University:

  For all existing HOCHBAHN depots a **comprehensive energy supply at medium voltage level until 2030** can be guaranteed.

- For the **new depot for innovative drives** (HOCHBAHN) applies:
  - Charging of up to 250 e-buses (battery, REX) possible
  - **110 kV connection with own substation** required
  - Launch: 2019

Lessons Learned.
Our main results: Depots III.

- **Area requirements on HOCHBAHN depots:**
  - Substation (110kV connection): about 400m²
  - Charging technology (for about 50 e-buses each): about 420m² (incl. substation and transformers)
  - H_2-production or delivery: about 1,400m² (base area for plant engineering)

- **Realization periods for energy supply of buses with new drive technologies at HOCHBAHN depots:**
  - 110kV-substation : about 3 - 4 years
  - Charging technology: about 2 - 3 years
  - H_2 plant engineering: about 2 - 4 years depending of technology / volumes

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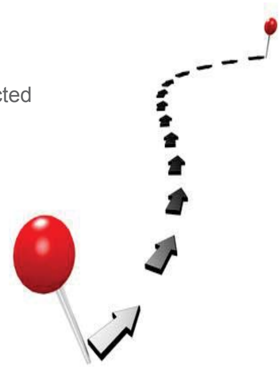
How to achieve the Masterplan.
How to achieve a system decision.

- **Strategic approach (preferred solution): battery buses, depot charger**
- **But:** Only part of today's bus cycles can be realized with the currently predicted ranges through pure depot charging
- **For longer cycles the following alternatives are under examination:**
  - Operational new conception of cycle (depot charger) with temporary increased demand for vehicles
  - Opportunity charger
  - Deployment of range extender buses



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How to achieve the Masterplan.
How to achieve a system decision.

- **Holistic evaluation of alternatives based on the following criteria:**
  - Feasibility
  - Sustainability
  - Productivity / efficiency
  - Opportunities / risks

- **But:** Currently a final decision is not possible due to still existing uncertainties about market maturity of new battery technologies

Therefore here HOCHBAHN will „run on sight“!

HOCHBAHN

2017 Coming soon.
Our next milestones.

- **Completion of masterplan**
- **Tender and order of 60 e-buses and appropriate charging infrastructure:**
  - 12m city buses as **depot charger** with a target minimum range of **200km** incl. air conditioning and **fossil auxiliary heating**
  - **CCS Combo 2 plugs as standard with 150 KW charging performance**
  - Tender of **close-to-standard** buses with appropriate contractual safeguarding (e.g. reliability, availability and range)
  - Division in 2 or 3 batches to test different buses
  - Planned delivery: until end of 2018

HOCHBAHN

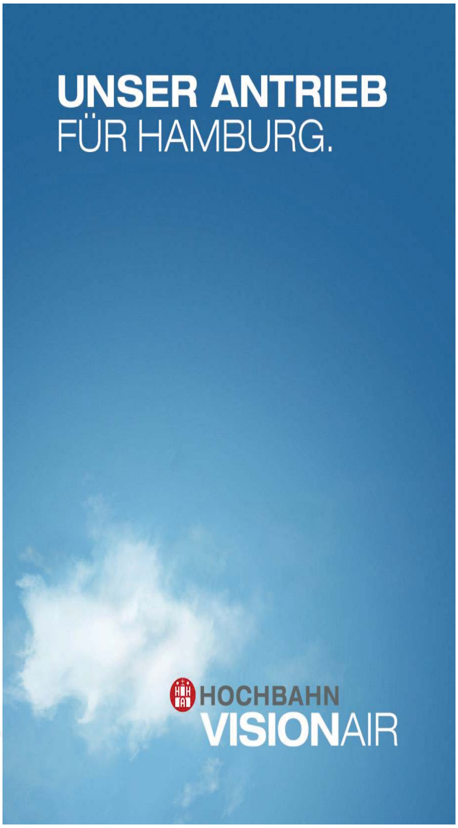
2018 Coming soon.
Our next milestones.

- Current bus fleet with EURO V and better
- Completion of new bus depot for innovative drivetrains

HOCHBAHN

from 2019 Coming soon.
Our next milestones.

- Actions according to Masterplan
- Tender and order of emission free buses only



HOCHBAHN e-bus strategy

Battery buses with depot charging
(gradual equipment of depots with charging infrastructure)

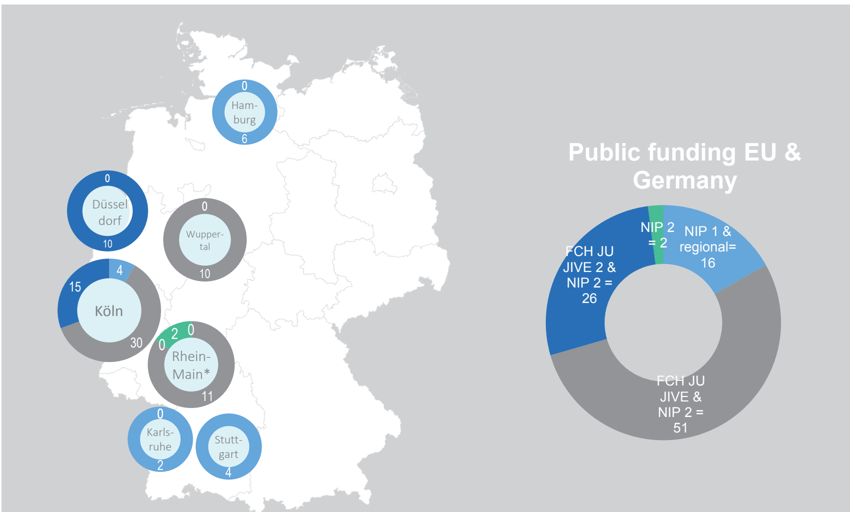
Basis

Option | Option | Option

Conversion of operational processes	Opportunity Charging	Battery bus with REX

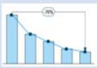

HOCHBAHN

Fuel Cell Buses in Germany – 16 in operation, 79 planned

*Frankfurt, Mainz & Wiesbaden

European Joint Projects - Buses

	JIVE	JIVE 2	Post 2020
Order volume 	Total of **230 buses** deployed in Europe by 2020	Total of **382 buses** deployed in Europe by 2020	Buses deployed in the **thousands** across Europe
Cost 	Business case possible with c. **200k** of EU subsidy	Business case possible with c. **150k** of EU subsidy	Fuel cell buses deployed through **local regulations and incentives** only
Locations 	Buses deployed in **nine cities** across five countries to validate the technology	Buses deployed in **fourteen cities** across Europe, including demo activities in Sweden and France	Technology validated and in widespread use **all across Europe**
Awareness 	Raise awareness of FC buses amongst **most environmentally aware / proactive** cities	FC buses considered **alongside alternative powertrains** by growing number of cities and operators	Fuel cell buses an **established mainstream choice**

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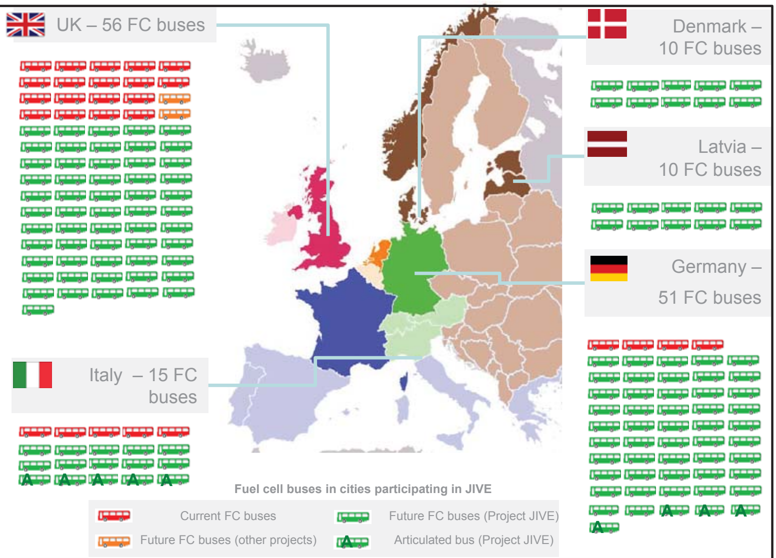
JIVE
Joint Initiative for Vehicles across Europe

Objectives

- Deploy 142 FC buses across nine cities
- Achieve 30% cost reduction versus state of the art
- Operate 50% of the vehicles for at least 36 months
- Deploy the largest capacity HRS in Europe
- Achieve near 100% reliability of HRS
- Demonstrate technological readiness of FC buses and HRS
- Encourage further uptake



Fuel cell buses in cities participating in JIVE

The National Strategic Framework – German targets on hydrogen Infrastructure

	2006-2016	until 2020	until 2025	until 2030
TASKS	Secure technological basis, meet conditions for ramp up	Basic coverage for Germany	Support market roll-out	Commercial roll-out
GOAL	**50 stations**	**100 stations**	**400 stations**	**1000 stations**
	INDEPENDENT OF VEHICLES		DEPENDENT OF VEHICLES	

29

Nationales Forum Diesel („Diesel Summit“)

Driving Innovation for Hamburg

August 2, 2017

- Meeting of Federal Ministers, Prime Ministers and representatives of the German car industry (no environmental associations) because of exhaust gas scandal (VW)

Results

- 1 billion euro fund announced to support municipalities improve air quality (major percentage provided by the federal government, approx. 25% by car industry).
- Federal Government intends to expand funding of low-emission and emission-free public transport
- Hamburg is an important partner in driving the implementation, Masterplan is in preparation
- Next steps: Additional acceleration of replacement of diesel buses
- Systematical realization of infrastructure

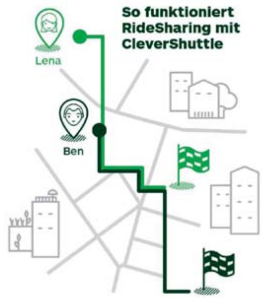
Ride Sharing – Clever Shuttle

hy SOLUTIONS Driving Innovation for Hamburg

Launch in Hamburg: September 8, 2017

- First Ride Sharing provider in Hamburg
- Start: 5 Toyota Mirais
- End of 2017: 20 Toyota Mirais
- Operation planned until end of 2019

How it works



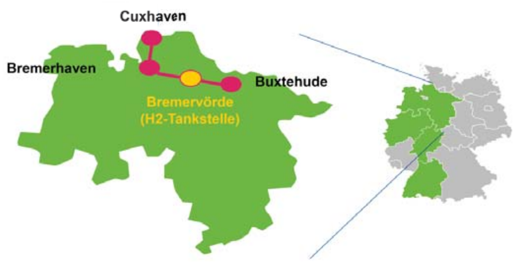
Alstom
Regional trains with hydrogen

hy SOLUTIONS Driving Innovation for Hamburg

CO_2 emission per vehicle-km (in gramme)

Emission free railway transport possible without overhead wires
> Coradia iLint

- Real passenger service
- Operated by EVB
- Service period: 2 years
- Service also in Northrhine-Westphalia, Hesse and Baden-Württemberg



Sustainable mobility in the Smart City Hamburg. Organised by HOCHBAHN.

HOCHBAHN

Comparative Analysis of Infrastructures: Hydrogen Fueling and Electric Charging of Vehicles

Thomas Grube
Forschungszentrum Jülich GmbH, Institute for Energy and Climate Research – Electrochemical Process Engineering (IEK-3)

Electric drivetrains are the key elements for low carbon, energy-efficient transport based on renewable energy. Furthermore, a transportation system with zero local emissions will substantially improve quality of life. This is particularly the case for metropolitan areas. Battery-electric vehicles, as well as hydrogen fueled fuel cell electric vehicles, feature these important characteristics. However, the construction of new infrastructures is necessary for both vehicle technologies.

The objective of this investigation is a detailed design study for the required infrastructures for battery, as well as hydrogen fuel cell, electric vehicles for Germany. Based on this, a comparative techno-economic assessment of the infrastructures is conducted. The starting point of the study is a meta-analysis of published studies containing assessments of the infrastructure roll-out costs for electric charging and hydrogen fueling. Particularly for high market penetration, the literature review reveals only aggregated and in part non-transparent information. As a consequence, detailed models for infrastructure development are applied and own scenario calculations carried out. In order to deliver transparent and comparative results, the analyses use the same scenario assumptions with regard to electricity generation and passenger car transport for both infrastructures.

The results of the scenario analyses point out for high market penetrations of the respective electric vehicles (higher than 25%) lower cumulative investments for a hydrogen fueling infrastructure. For low vehicle penetration scenarios, the electric charging infrastructure has advantages with regard to the needed investments. For the construction of both infrastructures, investment for the roll-out is low in comparison to other infrastructures, like electricity generation or transportation routes. A parallel development of both infrastructures allows for the maximization of energy efficiency and the optimized use of renewable energy resources, as well as the minimization of CO2 emissions over a broad range of transportation modes.

With the transformation of the entire energy system in mind, the electricity-based production of hydrogen, including the development of transport and distribution infrastructures, creates the important option of using surplus electricity in a temporally- and spatially-variable manner. The construction of a hydrogen infrastructure for transportation can thus be enhanced to become an essential key element of a renewable-dominated energy system.

Mitglied der Helmholtz-Gemeinschaft

Funded by:

H₂ MOBILITY WASSERSTOFF TANKEN

Comparative Analysis of Infrastructures: Hydrogen Fueling and Electric Charging of Vehicles

Project Team:

Martin Robinius, Jochen Linßen, Thomas Grube, Markus Reuß,
Peter Stenzel, Konstantinos Syranidis, Patrick Kuckertz and Detlef Stolten

Transition to Renewable Energy Devices & Systems
December 05-06, 2017, Aachen/Germany

Contents

- Introduction and meta analysis of scenario studies
- Approach, assumptions and scenario settings
- FCV refueling infrastructure
- BEV charging infrastructure
- Comparison of results
- Conclusion

Introduction and Meta Analysis of Relevant Studies

Introduction

Objectives of the Energiewende

- Transforming the national energy system to a sustainable system according to the Paris COP21 agreement with significant reduction of CO_2 emissions **achieved by renewable energy, energy efficiency and coupling of energy sectors**

Mobility sector as a key element

- **Measures in the transportation sector are essential** for reaching the ambitious climate protection goals and corresponding renewable energy goals for the entire energy system; important political objectives regarding transportation already installed

Approach

- Changing the current transportation fuel system from a fossil fuel dominated system to a renewable energy dominated system by **fuel switch and electrification of drivetrains**.

Obstacle

- The supply infrastructure for renewable fuels must meet further requirements, such as being **economically reasonable and societally accepted**.

Focus here

- Cost of fuel supply infrastructures: hydrogen for FCV and electricity for BEV

Status Quo of Infrastructure

Hydrogen Fueling

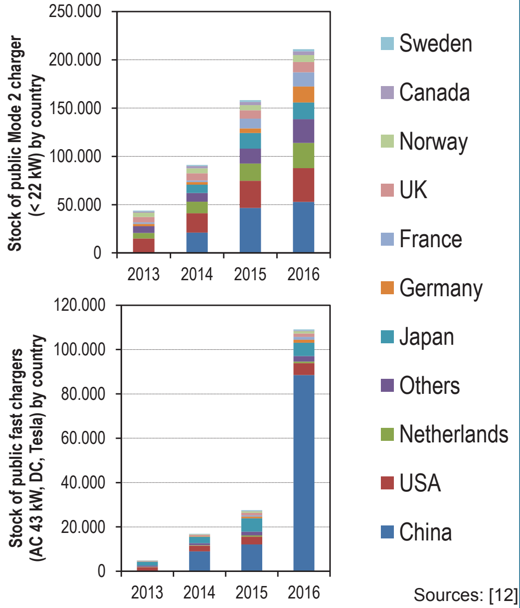
- **Worldwide:** End of 2016, 204 public Hydrogen Fueling Station (HRS) in operation worldwide: Japan (44%), the USA (17%) and Germany (13%)
- **Germany:** HRS network reached 30 stations by mid June 2017. At present, 27 HRS are under construction or being planned in Germany, with a goal to build up to **400 HRS before 2023**
- pipeline systems exist for the transportation and distribution of hydrogen concentrated for the chemical uses of hydrogen

Existing Hydrogen Pipelines (by 2017-05)

The USA	2,608 km
Europe	1,598 km
of which in Germany	340 km
Rest of world	337 km
World total	4,542 km

Sources: [6], [8], [10], [11]

Electric Charging



Sources: [12]

Meta Analysis of Scenario Studies

Selection criteria of scenario studies

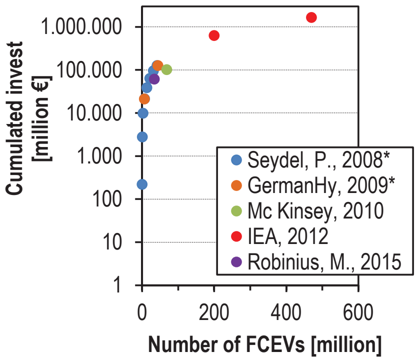
- Focus on Germany (broader context studies for EU, worldwide) and quantitative results; parameters: number of hydrogen fueling stations and charging points, cumulative investment for infrastructure set-up
- Total number of scanned literature sources: 79
- Selected studies for meta analysis: 25 (12 hydrogen and 13 electric charging)

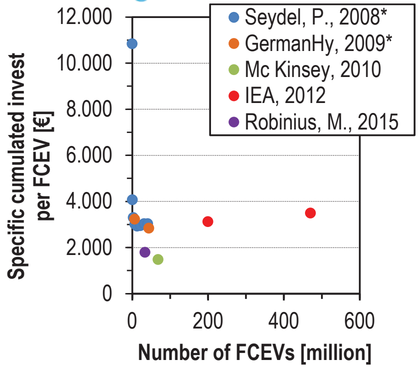
Lessons learned of the meta analysis

- Mostly **aggregated results** and, in many cases **without provision of techno-economic assumptions**
- Lack of information in literature of important **infrastructure parameters**, e.g., hydrogen pipeline length, number of trucks for hydrogen transport => no meta-analysis possible
- Regarding electric charging studies: **lack of studies considering high xEV penetration** scenarios, investment for infrastructure build-up, demand for fast-charging and impacts on the distribution grid

Meta Analysis:
H_2 Infrastructure – Cumulative Invest

H₂ MOBILITY WASSERSTOFF TANKEN JÜLICH FORSCHUNGSZENTRUM



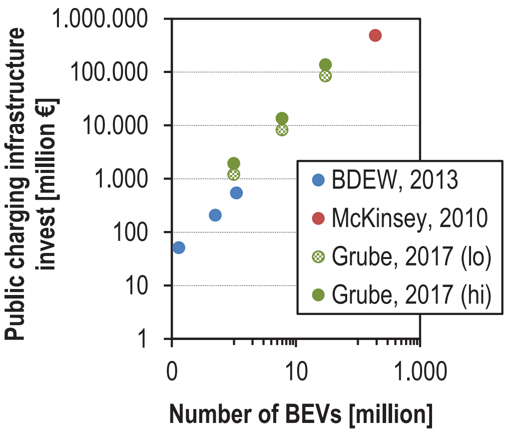


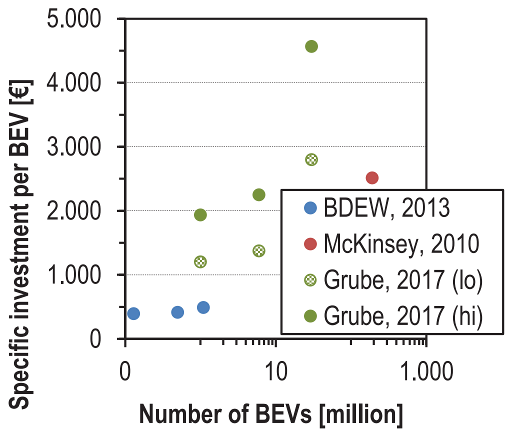
*: Including investment for power plants for upstream electricity production McKinsey – EU&CH&NO, IEA - worldwide

- *cumulative investments differ significantly → different assumptions: power plant investment, number of public hydrogen fueling stations for low market penetration*
- *Specific cumulative investment per FCEV: 1,500-1,800 €/FCEV in McKinsey/ Robinius; 3,000 €/FCEV in other scenarios*
- *In general, a decreasing specific cumulative investment per FCEV with increasing FCEV stock could be expected due to learning and economy of scale effects.*

Meta Analysis:
Charging Infrastructure – Cumulative Invest

H₂ MOBILITY WASSERSTOFF TANKEN JÜLICH FORSCHUNGSZENTRUM





Remarks:

- cumulative investment for public/semipublic normal & fast charging
- investment for private charging points not included.

Approach, Assumptions and Scenario Settings

Infrastructure Modelling
General Approach and Assumptions

Challenge of the comparison:

- Calculate **cumulative investment for charging and hydrogen infrastructure** for the same assumed market penetration scenario of BEVs and FCEVs as well as the same electricity generation scenario (no cost-optimized electricity supply scenario for each BEV and each FCEV penetration scenario; yet 60 day storage capacity for H_2)

General Methodical Approach

- **Spatial resolution of demand and production**, including sizing of the infrastructure for FCEV and BEV
- **Specific costs**, including all energy related and annualized infrastructure costs (no margins, taxes, fees or vehicle costs)

Assumptions

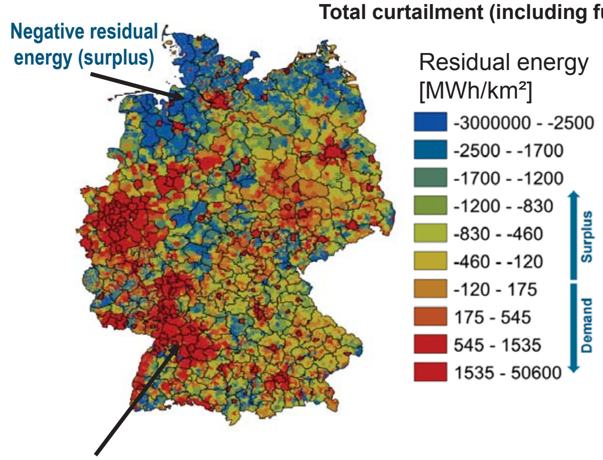
- market penetration scenarios for BEV or FCV (only passenger cars, PHEV not considered):
  - ***100,000 cars***
  - ***1,000,000 cars***
  - ***20,000,000 cars***

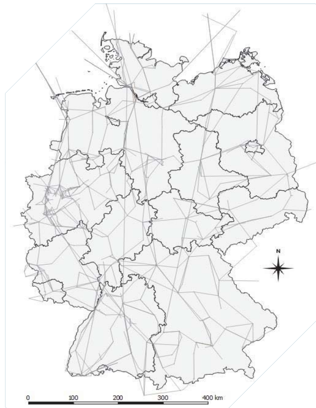
Assumed Electricity Scenario

Assessment based on municipal level and an hourly resolution of grid load and RES feed-in

Power-Sector		
	RES power [GW | **TWh**]:	onshore: 170 | **350**; offshore: 59 | **231**; PV: 55 | **47**; hydro: 6 | **21**; bio: 7 | **44**; fossil: 63 | **118**
	Further assumptions:	grid electricity: **528 TWh**; imports: 28 TWh; exports: 45 TWh; pos. residual: natural gas

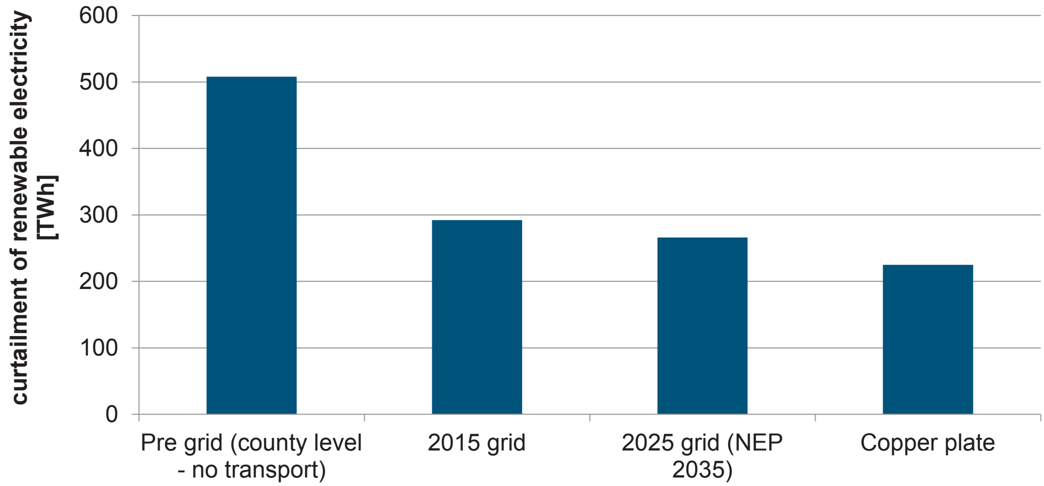
Share of RES electricity generation: 78 %
Total curtailment (including future grid): 266 TWh





Power flow analysis based on 523 nodes and 802 edges

Analysis of Curtailment Constrains of Transmission Grid



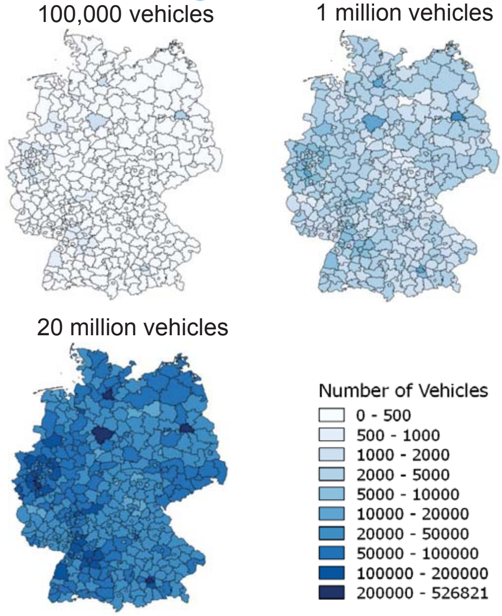
Transportation Scenario

	FCEV	BEV
Scenario	Hydrogen consumption [1000 t/year]*	Electricity Consumption [TWh/year]*
100,000	9.1	0.154
1,000,000	91	1.54
20,000,000	1820	30.8

*based on an annual mileage of 14,000 km [1] and 0.65 kg H2/(100 km), respective 11 kWh/(100 km) [2]

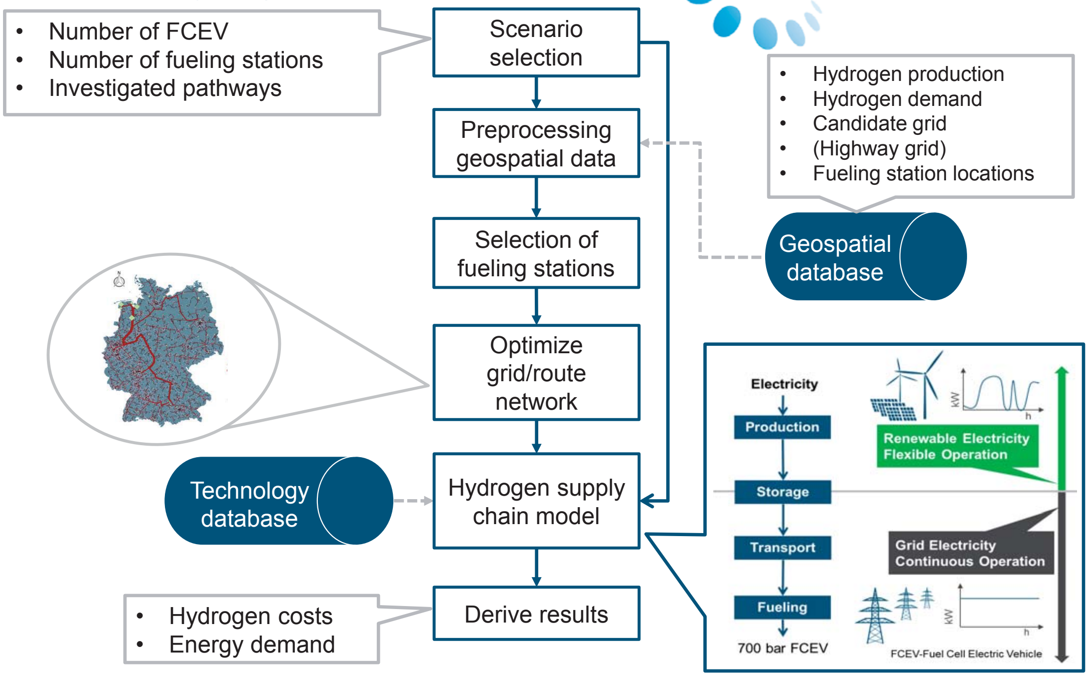
Vehicle distribution methodology:
1. Startup in metropolitan region first
2. Delayed start-up in neighbouring counties
3. Latest start-up in urban areas

[1] Bundesministerium für Verkehr und digitale Infrastruktur (2015). "Verkehr in Zahlen 2014/2015."
[2] Grube, T. (2014). Potentiale des Strommanagements zur Reduzierung des spezifischen Energiebedarfs von Pkw, Jülich, TU Berlin. **216:** IX, 255 pp.



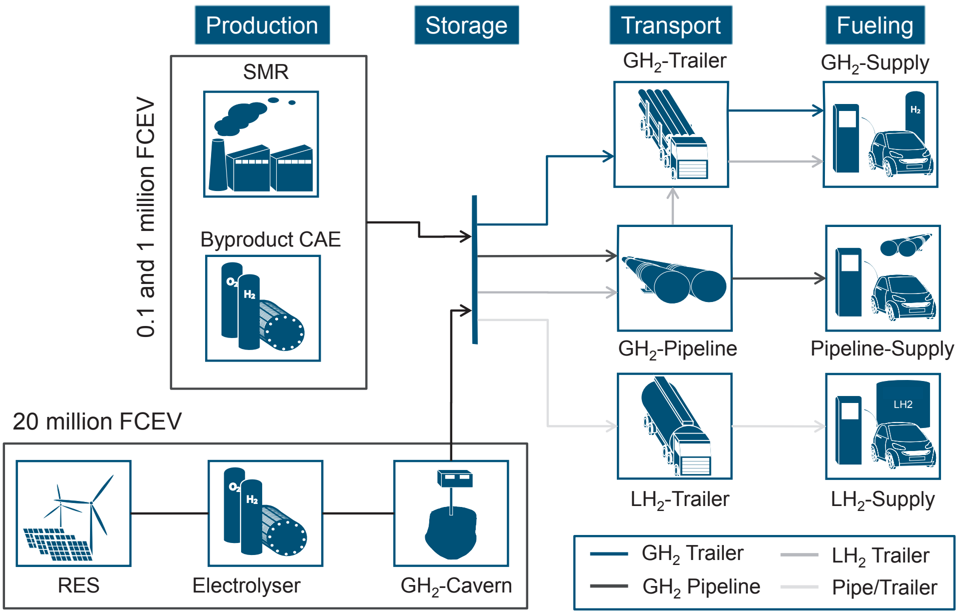
FCV Refueling Infrastructure

Geospatial Hydrogen Infrastructure Model



Electrochemical Process Engineering (IEK-3)

Hydrogen Supply Pathways



Electrochemical Process Engineering (IEK-3)

Final Geospatial Results: Scenario 20 million FCV

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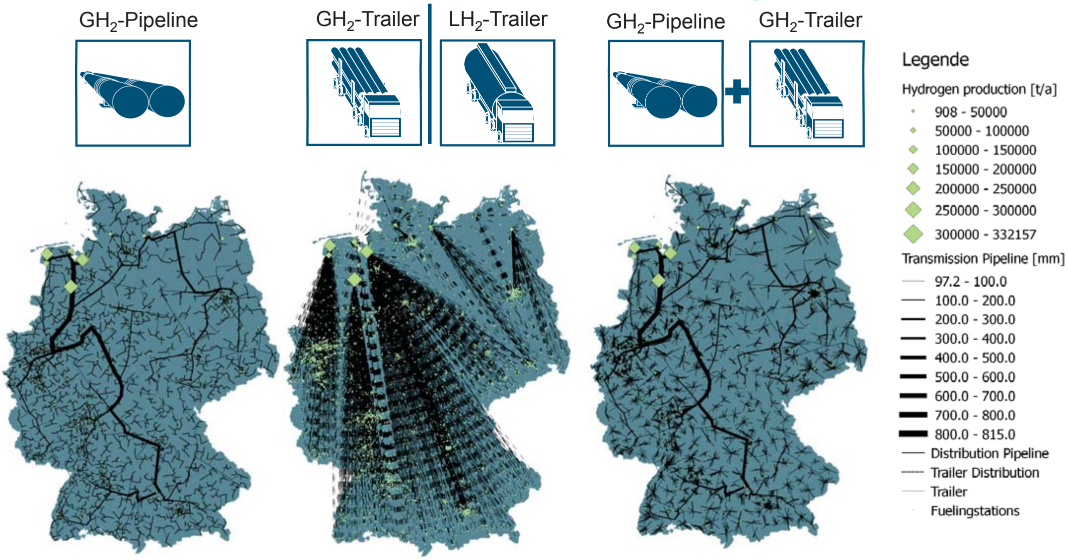
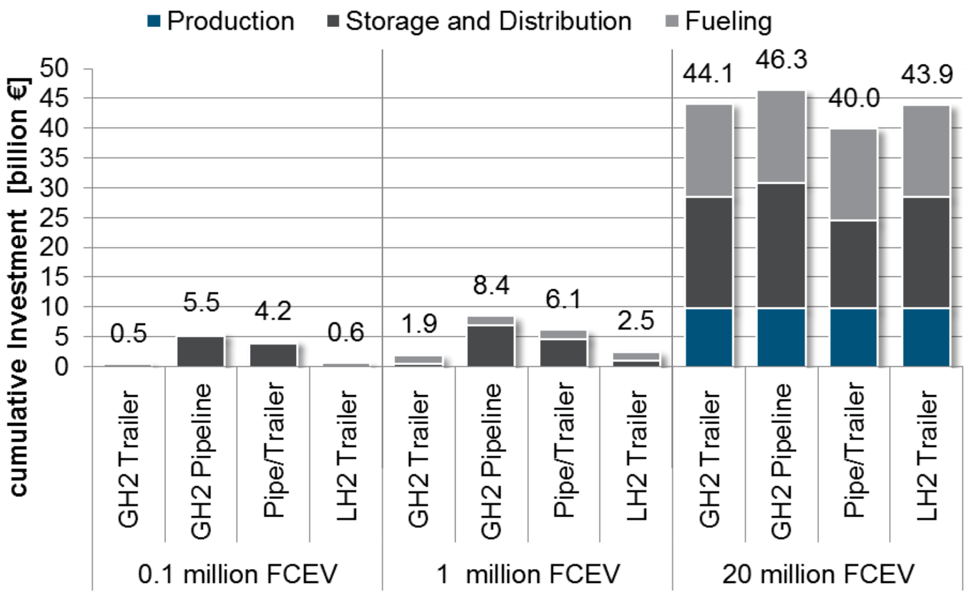
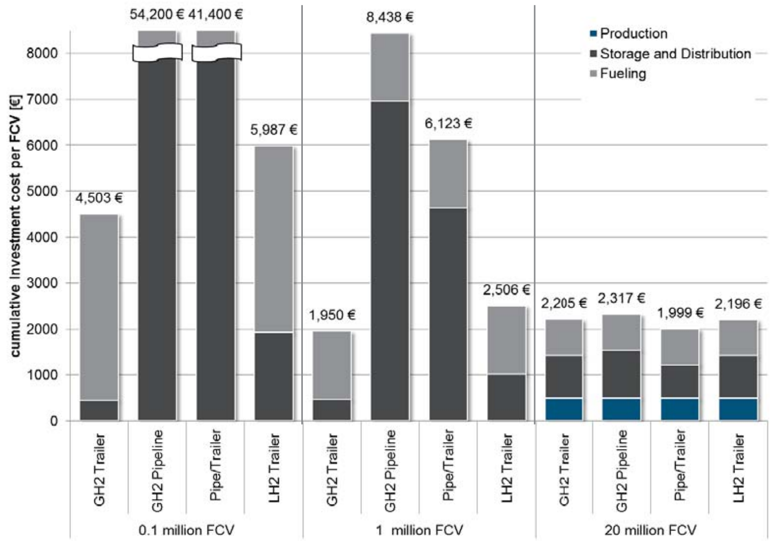


Total Investment

H₂ MOBILITY WASSERSTOFF TANKEN · JÜLICH FORSCHUNGSZENTRUM



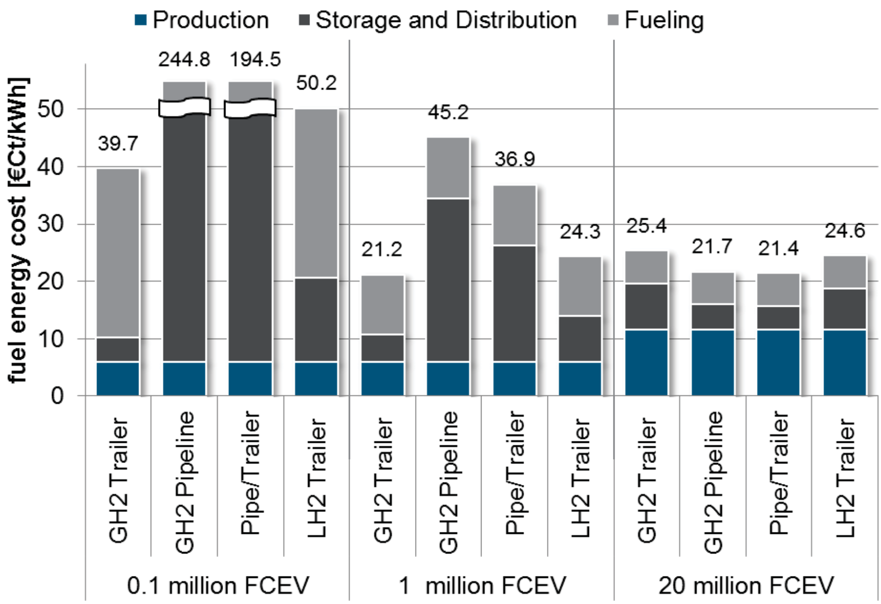
Cumulative Investment per Vehicle



- Pipeline → high costs for small vehicle penetrations
- Pipe/Trailer → lowest investment cost for 20 million FCV

FCV: Fuel Cell Vehicle

Specific Fuel Costs



BEV Charging Infrastructure

Approach

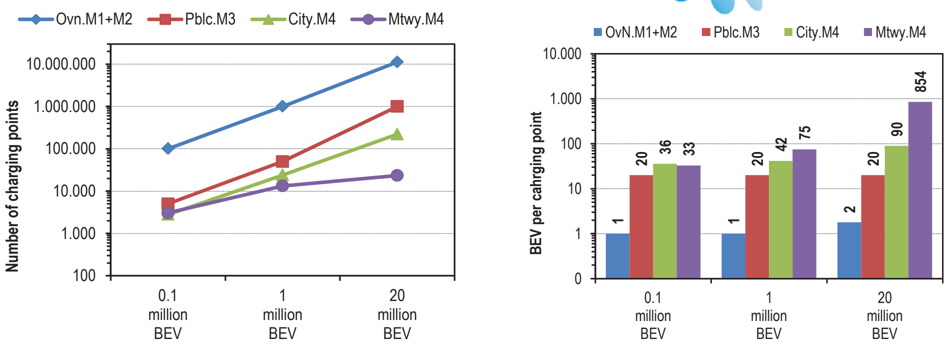
Analysis of charging in cities and on freeways, relevant parameters

- fleet size and distribution amongst settlement types
- share of overnight charging sites in garages or on-street and their actual utilization
- allocation of charged energy at overnight (Mode 1 & Mode 2), public (Mode 3) and commercial (Mode 4) charging points
- dimensioning of chargers according to charge time definitions
- net electricity cost
- annual mileage and BEV fuel economy

Parameter specifically for charging along freeways

- freeway lengths
- traffic volume classes

Number of Charging Points in Germany



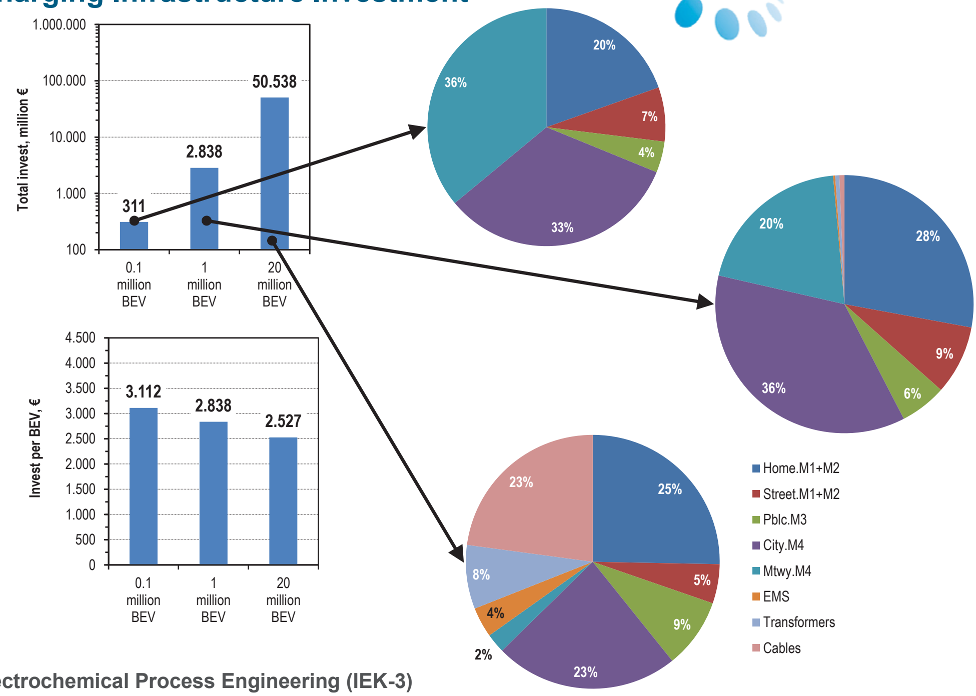
Number of overnight chargers (Mode 1 & 2) increases with BEV number but with decreasing ratio:

- 1 by 1 in the first two scenarios (all BEV have an overnight charging option)
- 1 by 2 in the last scenario (only 58 % of all BEV have an overnight charging option)

The ratio of BEV per Mode 4 charger increases due to decreasing charging frequency caused by higher driving range (battery capacity)

OvN.M1+M2: Home and on-street chargers (Mode 1 and 2); Publc.M3: Public convenience chargers (Mode 3); City.M4: quick chargers in cities (Mode 4); Mtwy.M4: Quick chargers along motorways (Mode 4)

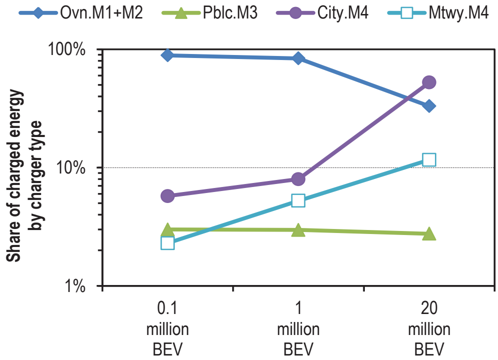
Total and Specific Charging Infrastructure Investment



Distribution of Charged Energy by Charger Type

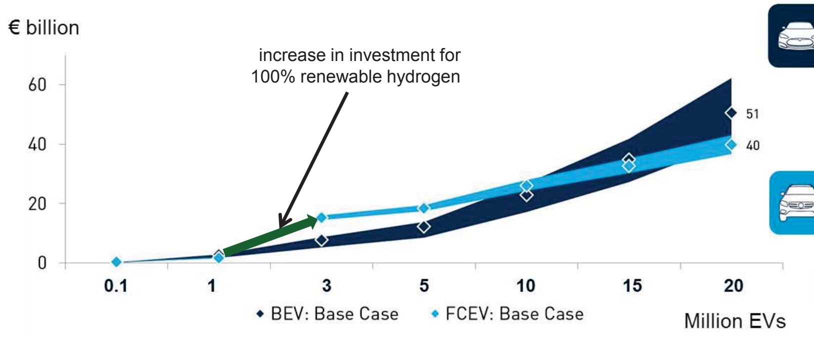
Assumptions for charging energy distribution by location:

- overnight charging decreases
- public Mode 3 charging is assumed low
- Mode 4 fast charging in cities and on motorways increases



Comparison of Results

Comparison of Cumulative Investment

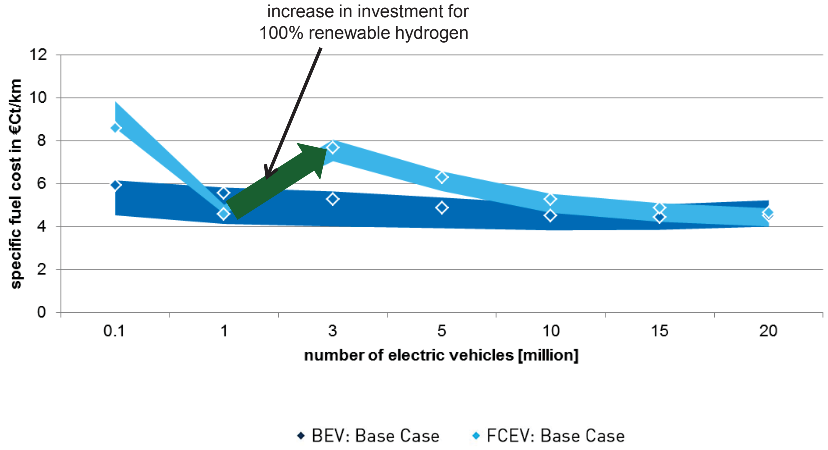


Sensitivity:

Top // larger batteries with 100 kWh dominate in the long run (base case +100 kWh)
Bottom // no fast charging at 350 kW in cities

Top // base case +20% investment in stations
Bottom // base case -20% investment in stations

Comparison of Specific Mobility Costs



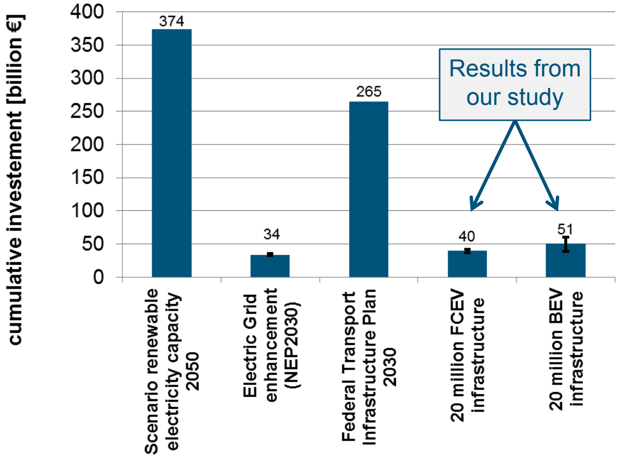
Sensitivity:

Top // larger batteries with 100 kWh dominate in the long run (base case +100 kWh)
Bottom // no fast charging at 350 kW in cities

Top // base case +20% investment in stations
Bottom // base case -20% investment in stations

vehicle purchase and operation costs excluded

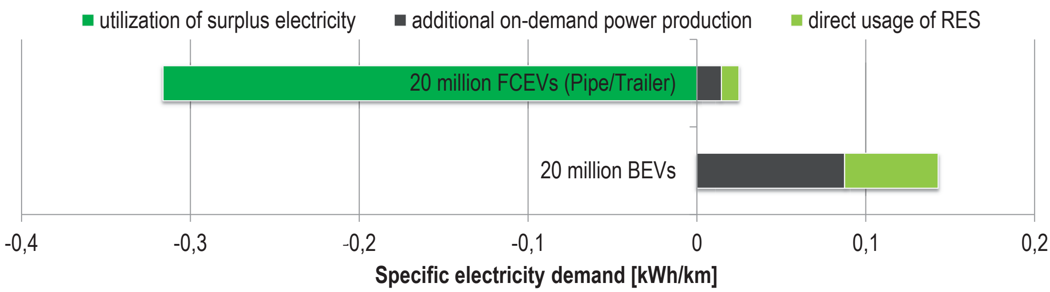
Comparison of Infrastructure Investment

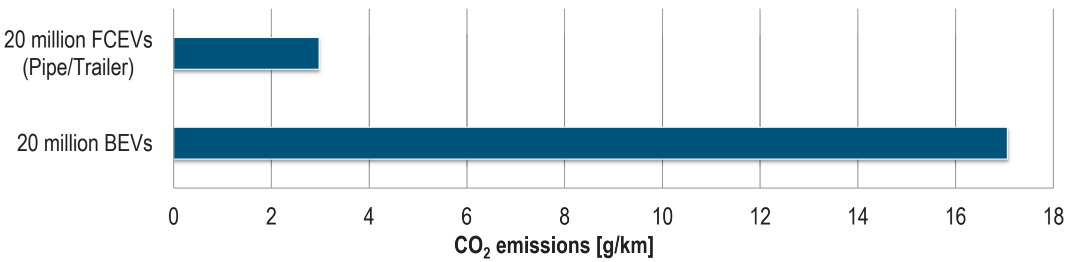


Renewable power capacities and specific invest:

- wind onshore 171 GW @ 1000 €/kW
- wind offshore 59 GW @ 2500 €/kW
- PV 55 GW @ 1000 €/kW

Comparison of Specific Electricity Demand and CO_2 Emissions





Conclusion

Conclusion

- With a major share of RE from wind and solar, even the **perfect grid doesn't help** avoid surplus. H_2 will be required to store energy to balance volatile electricity production and demand. At 80 % RE one third of the surplus electricity allows powering 50 % of the German fleet with H_2.
- The refueling infrastructure for FCVs is very (time) efficient. The more vehicles, the better the **economies of scale work in favor of the hydrogen infrastructure**.
- At 100.000 vehicles the cost for both infrastructures is about the same. At 1 million EVs the investment for hydrogen refueling stations is lower than that for the charging points.
- Investment in green H_2 production and storage drives the cost for the H_2 infrastructure temporarily above the investment for BEVs. For higher numbers of vehicles the increase of additional investments in infrastructure is steeper for BEVs than for FCEVs.
- The investment in an infrastructure for producing and storing 100% green H_2 to refuel 20 million FCEVs is around 11 billion € lower than the investment required for charging 20 million BEVs.

Thank you for your attention!

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Model-Based Product and Pathway Design for Tailor-Made Fuels from Biomass

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RWTH Aachen University, Aachen, Germany

The Cluster of Excellence “Tailor-Made Fuels from Biomass” (TMFB) at RWTH Aachen University aims at holistic co-optimization of biofuel production and combustion by considering the fuel’s molecular structure (or its composition in case of a mixture) as the single most important design degree of freedom. Conceptually, the challenge is to identify oxygenated fuel components, which enable high-efficiency and low-emission combustion, and their corresponding production pathways that facilitate efficient and sustainable conversion of lignocellulosic materials into liquid biofuel through selective catalytic refunctionalization of biomass monomers. In the present contribution, we give an overview on model-based strategies and tools for such integrated product and pathway design of both pure and multi-component fuels. More specifically, we cover the following aspects of our work:

i. computational fuel design, i.e., a variant of computer-aided molecular design (CAMD), and its relations with engine experimentation/optimization and (bio-)chemical pathway optimization (reaction engineering),
ii. key physico-chemical properties of oxygenated fuels and their role in maximizing engine efficiency and minimizing pollutant emissions,
iii. fast and reliable prediction of those properties (including the derived cetane number (DCN) as an important indicator for fuel auto-ignition quality) on the basis of the two-dimensional molecular structure by means of group contribution and quantitative structure-property relationship (QSPR) modeling,
iv. a generate-and-test CAMD framework for identification of pure compound fuel candidates with tailored properties that exploits the concept of targeted refunctionalization of bio-derived platform chemicals, and
v. a novel methodology for integrated product and pathway design of biofuel mixtures, where mathematical programming is employed to optimize a production process-related measure, i.e., the energy of fuel produced for a fixed amount of biomass, subject to a network of potential conversion pathways, predictive mixture property models, and a fuel specification chosen to unlock the potential of a highly-boosted direct-injection spark-ignition engine.

To illustrate the feasibility of the proposed methods and tools, we briefly review some selected important results obtained from case studies. Moreover, we refer to engine testing and optimization results that clearly demonstrate the potentials of the tailor-made fuels approach. Further results as well as details on the methodological approach can be found in the provided references.

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Model-Based Product and Pathway Design for Tailor-Made Fuels from Biomass

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TRENDS 2017 – Novotel Aachen – December 6th, 2017

The “Tailor-Made Fuels“-Approach at RWTH Aachen University

From Biomass to Biofuels

From Biofuels to Propulsion

Tailor-Made Fuels from Biomass

http://www.fuelcenter.rwth-aachen.de/

The “Tailor-Made Fuels“-Approach at RWTH Aachen University

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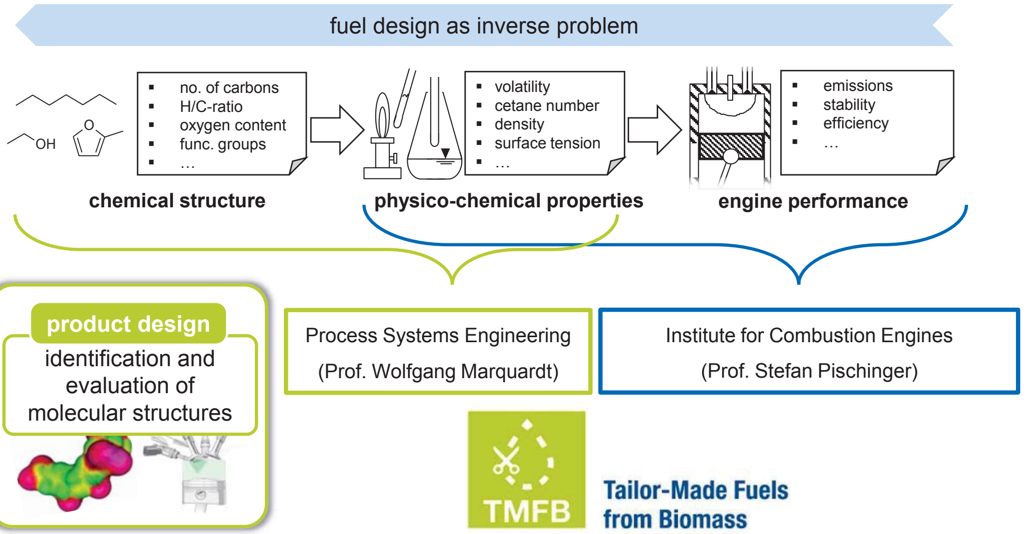
Manuel Dahmen and Wolfgang Marquardt
AVT – Process Systems Engineering, RWTH Aachen University

The “Tailor-Made Fuels“-Approach at RWTH Aachen University

Dahmen & Marquardt. *Energy & Fuels*, *30*(2), 1109-1134, **2016**.



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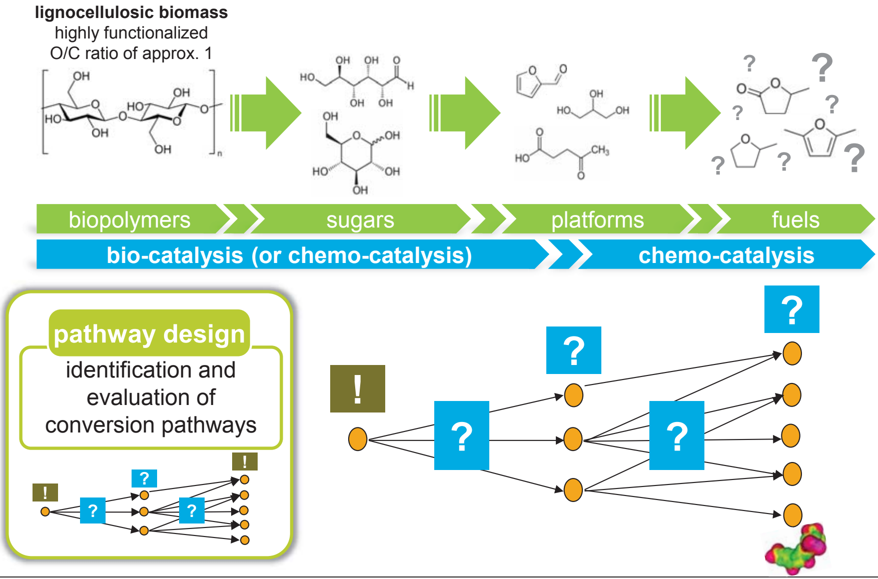
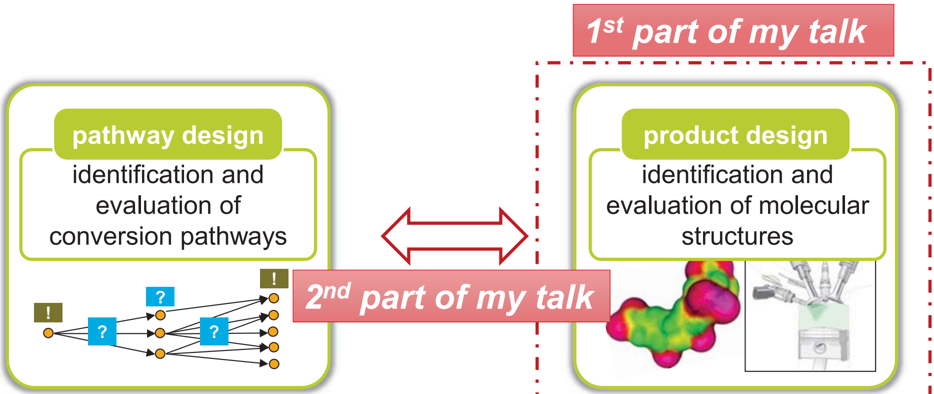
AVT – Process Systems Engineering, RWTH Aachen University

Processing Steps in the Synthesis of Oxygenated Biofuels



Product and Pathway Design of Tailor-Made Biofuels



Voll & Marquardt, *AIChE Journal*, 58(6),1788-1801, **2012**.

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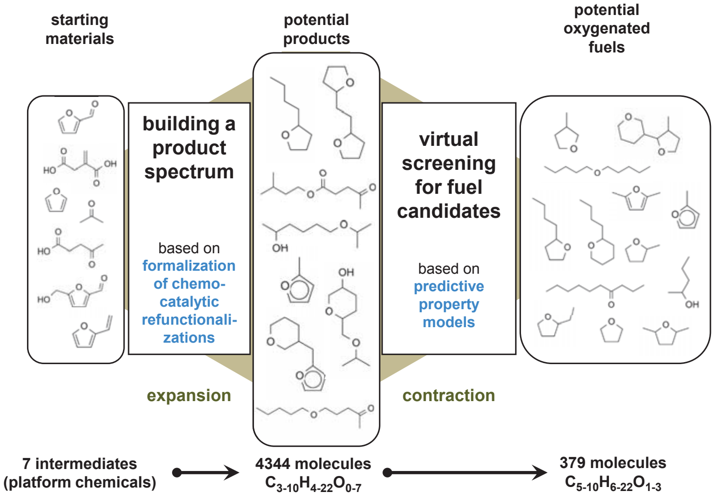
Hechinger, Voll & Marquardt. *Computers & Chemical Engineering*, 34(12), 1909-1918, **2010**.
Dahmen & Marquardt. *Energy & Fuels*, *31*(4), 4096-4121, **2017**.

Model-Based Fuel Design (The TMFB Approach)



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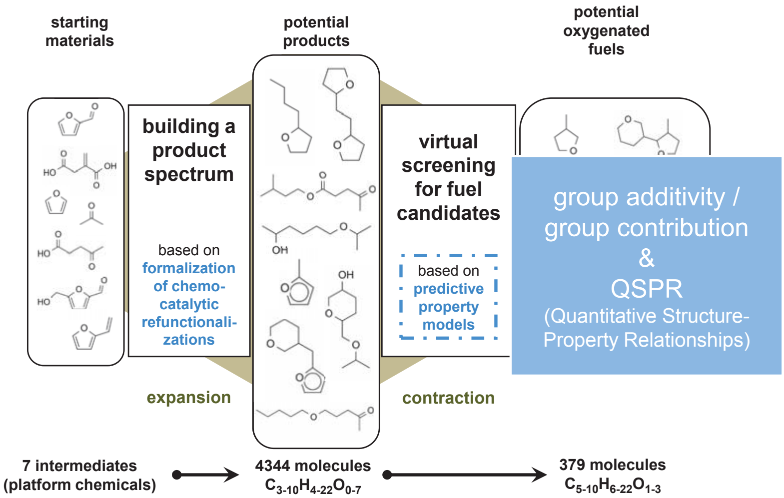
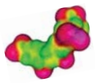
Model-Based Fuel Design (The TMFB Approach)



Dahmen & Marquardt. *Energy & Fuels*, *30*(2), 1109-1134, **2016**.

Fuel Property Modeling

Quantitative Structure-Property Relationship (QSPR)



ab-initio calculation
(topological, connectivity, eigenvalue indices, fingerprints etc.)

property y = *function*(**molecular descriptors** d_i)

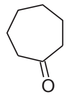
$$y = \alpha_1 d_1 + \alpha_2 d_2 + \alpha_3 d_3 + m$$

Multivariate Data Analysis

Principal Component Analysis (PCA)
Partial Least Squares (PLS)

Artifical Neural Networks
Support Vector Regression

Structural Group Contribution Method (GCM)



6x $-CH_2-$
1x $>=O$

property y = *function*(**group occurrences** n_i)

$$y = n_{CH2} g_{CH2} + n_{>=O} g_{>=O} + m$$

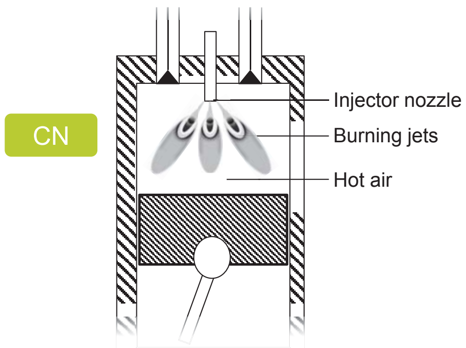
Model Structure &
Group Decomposition Scheme &
Parameter Uncertainty

Systematic model reduction
Model discrimination (Akaike's Information)

Model Validation
Y-Randomization, Cross-Validation, External Validation

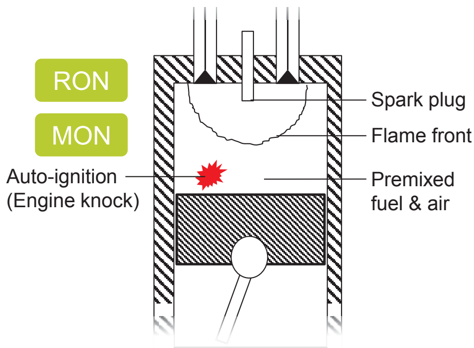
The Need for a Predictive Auto-Ignition Model

Compression Ignition (CI) Engine („Diesel"-Engine)



Fuel must auto-ignite briefly after its injection

Spark-Ignition (SI) Engine („Otto"-Engine)

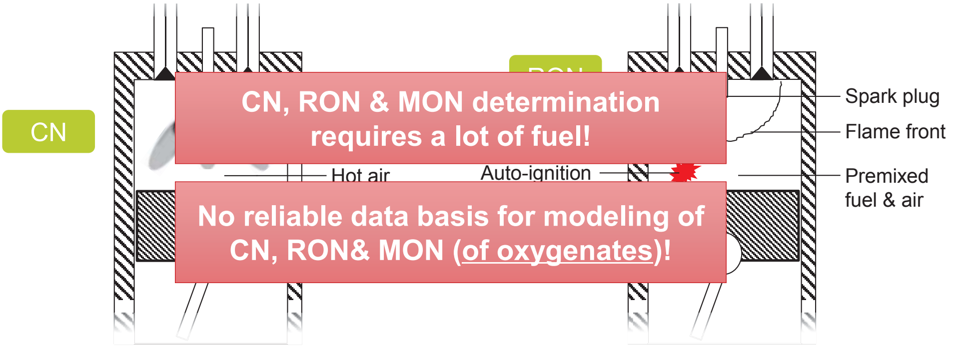


Fuel must withstand auto-ignition.

The Need for a Predictive Auto-Ignition Model

Compression Ignition (CI) Engine
(„Diesel“-Engine)

Spark-Ignition (SI) Engine
(„Otto“-Engine)



Fuel must auto-ignite briefly after its injection

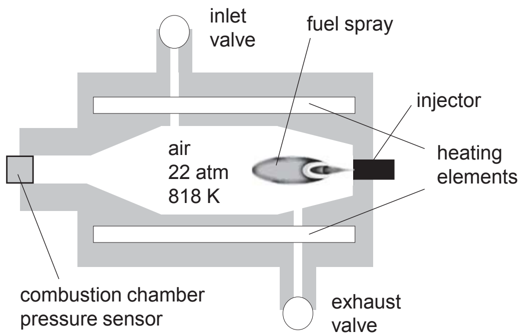
Fuel must withstand auto-ignition.

Rapid Auto-Ignition Screening

Ignition Quality Tester
(constant volume combustion chamber)

high CN & high RON fuels under same conditions

<200 ml fuel
32 repetitions
<20 mins



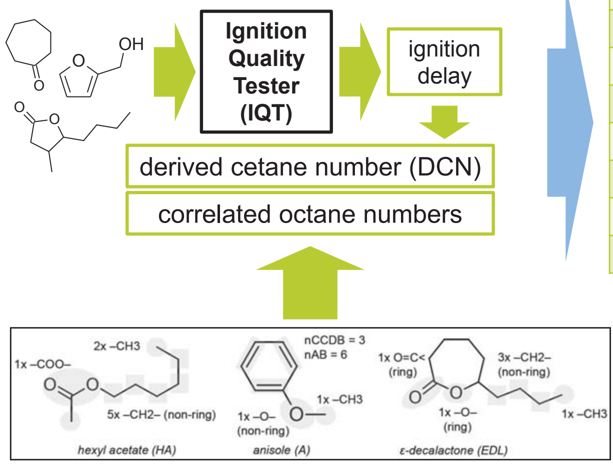
correlated octane number

ignition delay

derived cetane number (DCN)

ASTM D6890 “Standard Test Method for Determination of Ignition Delay and Derived Cetane Number (DCN) of Diesel Fuel Oils by Combustion in a Constant Volume Chamber”

Group Contribution Modeling of the IQT Auto-Ignition Delay

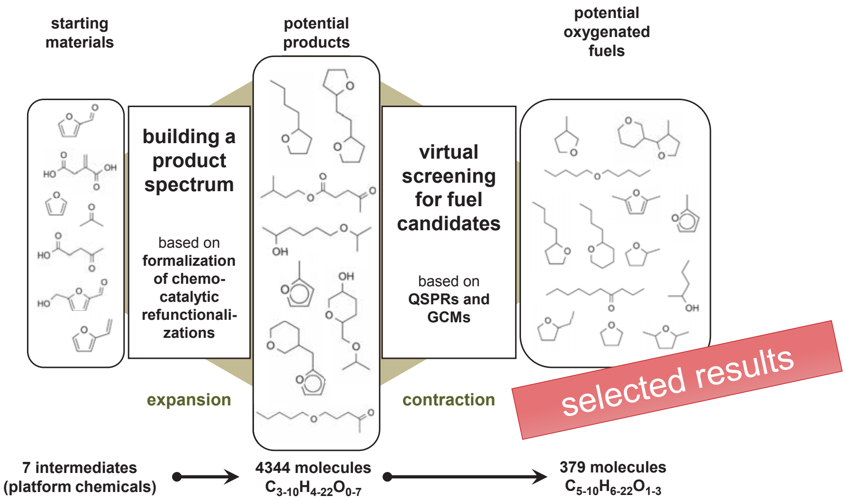


alkanes	ethers
iso-alkanes	furans
cyclo-alkanes	tetrahydrofurans
olefins	pyranes
aromatics	esters
alcohols	lactones
ketones	acetals
esters	polyfunctionals

Group Contribution Model for the IQT Ignition Delay

Dahmen and Marquardt, *Energy & Fuels* 29(9), 5781-5801, **2015**.

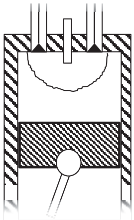
Model-Based Fuel Design (The TMFB Approach)



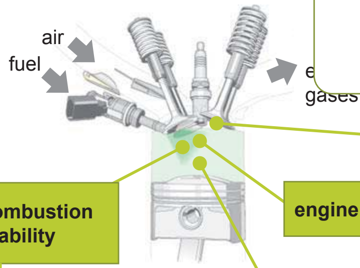
Dahmen & Marquardt. *Energy & Fuels*, *30*(2), 1109-1134, **2016**.

Results from Fuel Design
Tailored Fuels for the Spark-Ignition (SI) Engine

Spark-Ignition (SI) Engine
(„Otto“-Engine)



Dahmen & Marquardt. *Energy & Fuels 30*(2), 1109-1134, **2016**.



chemical kinetics
oxygen content (**local C/O-ratio**)
mixture homogeneity
volatility,
enthalpy of vaporization,
surface tension,
viscosity

soot emissions

combustion stability

engine efficiency

Group contribution model for DCN

cold-start operability

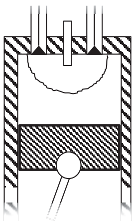
mixture homogeneity
volatility,
enthalpy of vaporization,
surface tension,
viscosity

well impingement & misfiring
volatility (vapor pressure)
enthalpy of vaporization

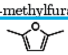
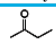
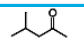
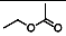
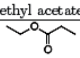
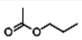
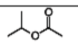
knock-resistance
ignition delay
charge cooling
enthalpy of vaporization

Results from Fuel Design
Tailored Fuels for the Spark-Ignition (SI) Engine

Spark-Ignition (SI) Engine
(„Otto“-Engine)



Dahmen & Marquardt. *Energy & Fuels 30*(2), 1109-1134, **2016**.

	compound	boiling point [°C]	DCN	lower heating value [MJ/kg]	enthalpy of vaporization [kJ/kg(air)]	density [kg/m³]	intermediates
furans	 2-methylfuran						furfural
furans	 2,5-dimethylfuran	112.9	9.8	32.1			
ketones	 2-butanone						2,3-butanediol
ketones	 methyl isobutyl ketone	114.7	19.0	34.8	32.0	808	lactic acid, 1,3-propanediol
esters	 ethyl acetate	104.6	13.7	23.2	47.5	920	ethanol, acetic acid
esters	 ethyl propanoate	113.0	17.4	26.1	42.2	902	ethanol, lactic acid
esters	 propyl acetate	107.2	17.4	25.8	41.6	886	acetic acid, 1,3-propanediol, lactic acid
esters	 propanyl acetate	111.8	10.3	26.0	38.7	811	acetic acid, lactic acid

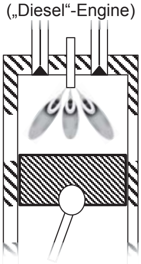
2-methylfuran (RON 102) vs. RON95
- **strong decrease in soot emissions**
- **efficiency +18%** at full load

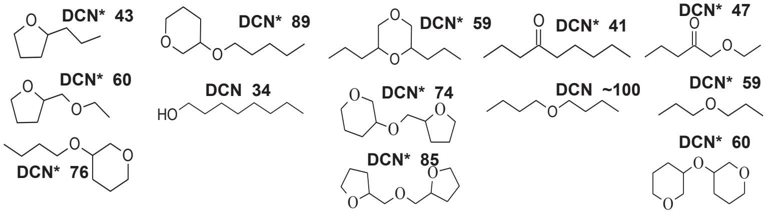
Hoppe et al., *International Journal of Engine Research* 17 (1), 16-27, **2016**.

2-butanone (RON 117) vs. RON95
- **strong decrease in soot emissions**
- **efficiency >+18%** at full load

Results from Fuel Design
Tailored Fuels for the Compression-Ignition (CI) Engine

Compression Ignition (CI) Engine
(„Diesel"-Engine)





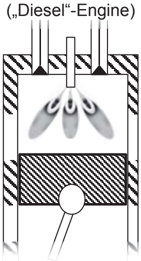
*** prediction** Dahmen & Marquardt, *Energy & Fuels* 29(9), 5781-5801, **2015**.

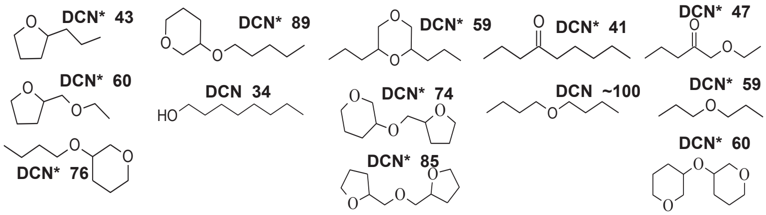
Acyclic & cyclic ethers and large ketones
are most promising candidates for CI ("Diesel") engines.

Dahmen & Marquardt. *Energy & Fuels*, *30*(2), 1109-1134, **2016**.

Results from Fuel Design
Tailored Fuels for the Compression-Ignition (CI) Engine

Compression Ignition (CI) Engine
(„Diesel"-Engine)



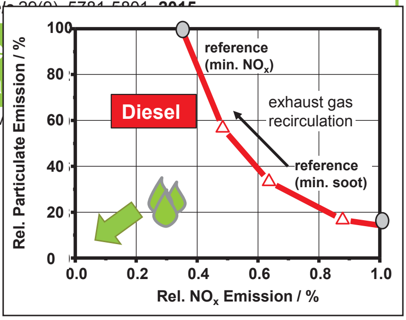


*** prediction** Dahmen & Marquardt, *Energy & Fuel*...

Acyclic & cyclic ethe...
are most promising candida...

Dahmen & M...

Dramatically lower soot emissions – even at EURO 6 engine-out NOx emissions!



Hoppe et al. *International Journal of Engine Research* 17 (1), 16-27, **2016**.
Heuser et al. *SAE Technical Paper* 2013-01-1253, **2014**.

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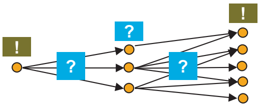
Product and Pathway Design of Tailor-Made Biofuels

1st part of my talk

pathway design

identification and evaluation of conversion pathways

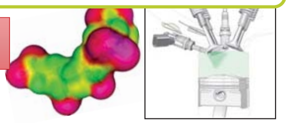


Voll & Marquardt, *AIChE Journal*, 58(6),1788-1801, **2012**.

2nd part of my talk

product design

identification and evaluation of molecular structures



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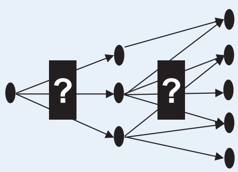
Hechinger, Voll & Marquardt. *Computers & Chemical Engineering*, 34(12), 1909-1918, **2010**.
Dahmen & Marquardt. *Energy & Fuels*, *31*(4), 4096-4121, **2017**.

Integrated Product and Pathway Design

Biomass

CO_2 H_2

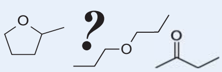
network of possible conversion pathways:



target values for physico-chemical properties:

- cetane number
- octane number
- volatility
- heating value
- density
- viscosity
- surface tension
- …

biofuel mixture with tailored properties



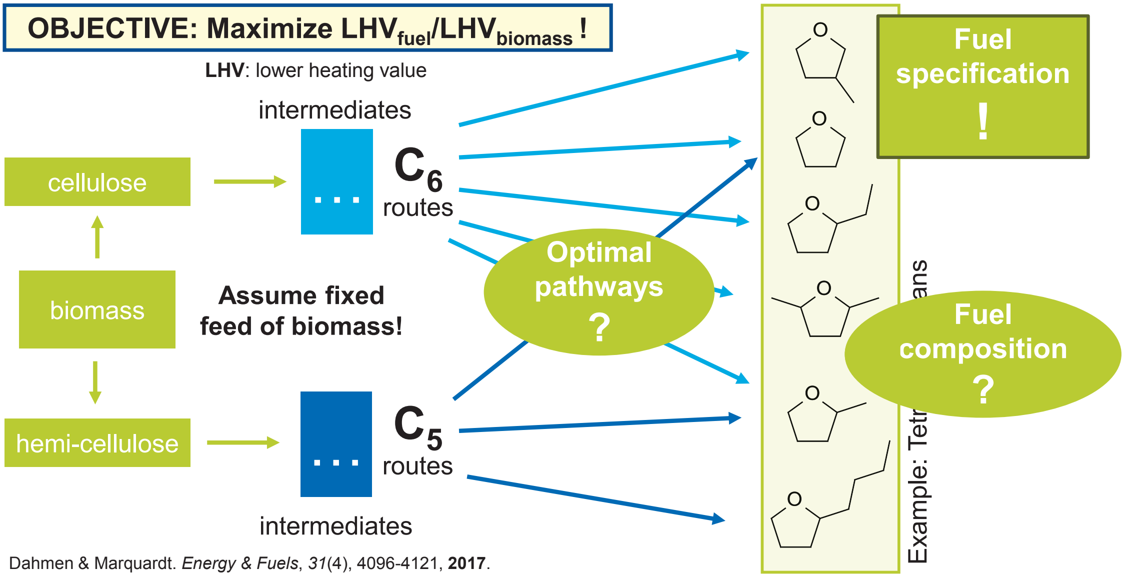
Design fuel and its optimal production pathways at the same time!

Dahmen & Marquardt. *Energy & Fuels*, *31*(4), 4096-4121, **2017**.

Integrated Design of Multicomponent Fuels

OBJECTIVE: Maximize $LHV_{fuel}/LHV_{biomass}$!

LHV: lower heating value



Dahmen & Marquardt. *Energy & Fuels*, *31*(4), 4096-4121, **2017**.

Integrated Design of Multicomponent Fuels

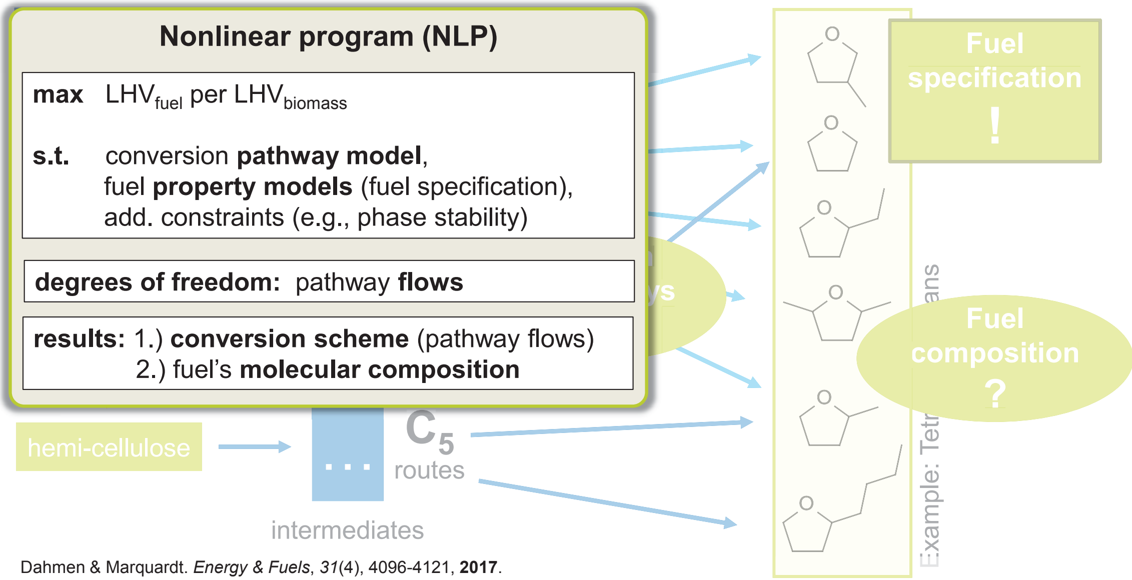
Nonlinear program (NLP)

max LHV_{fuel} per $LHV_{biomass}$

s.t. conversion **pathway model**,
fuel **property models** (fuel specification),
add. constraints (e.g., phase stability)

degrees of freedom: pathway **flows**

results: 1.) **conversion scheme** (pathway flows)
2.) fuel's **molecular composition**



Dahmen & Marquardt. *Energy & Fuels*, *31*(4), 4096-4121, **2017**.

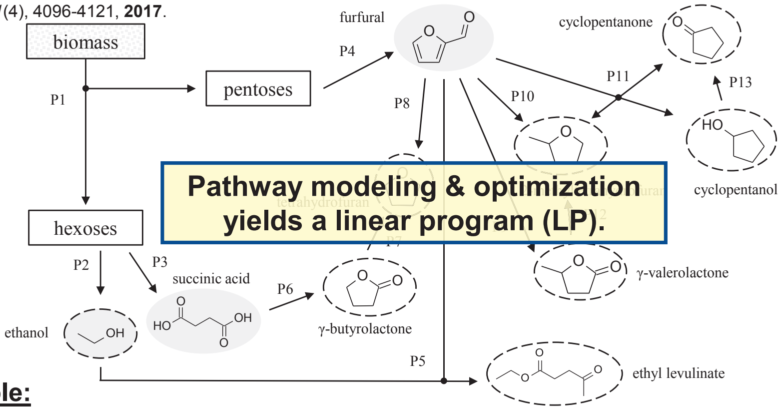
Pathway Modeling & Optimization

Dahmen & Marquardt. *Energy & Fuels*, *31*(4), 4096-4121, **2017**.

Reaction **N**etwork **F**lux **A**nalysis (RNFA)
Voll & Marquardt, *AIChE Journal*, 58(6),1788-1801, **2012**.

Consider **selectivity** and **conversion** of all pathways!

Balance $\mathbf{H_2}$ and $\mathbf{CO_2}$!



Basic optimization example:

$$\max_{\mathbf{f},\mathbf{b}} \sum_{i \in PC} b_i$$
$$\text{s.t.} \quad \mathbf{A} \cdot \mathbf{f} = \mathbf{b},$$
$$\mathbf{f} \geq 0, \mathbf{b} \geq 0$$

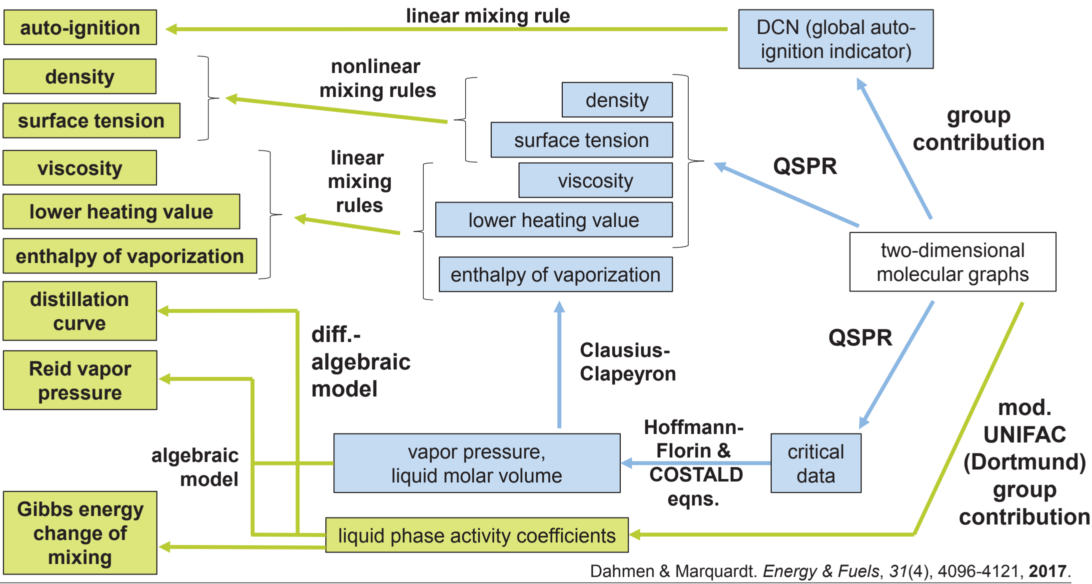
Maximize **sum of product flows** (palette compounds (PC) only)

$\mathbf{b}$: product flows [kmol/h]
$\mathbf{f}$: flows over pathways [kmol/h]
$\mathbf{A}$: stoichiometric matrix

Palette compound:
Compound that **can** be part of a rationally formulated blend.

Fuel Property Modeling – Mixture Properties

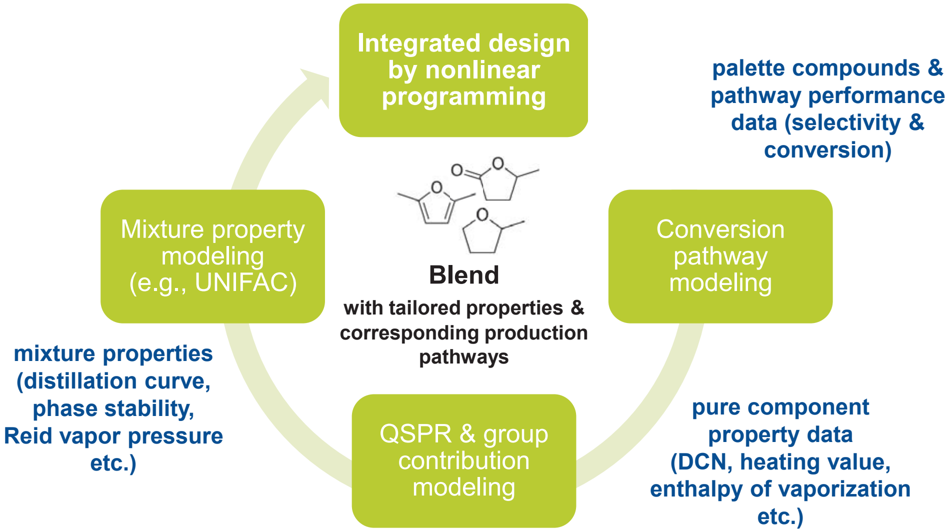
green: depends on mixture composition
blue: depends on a pure compound



Dahmen & Marquardt. *Energy & Fuels*, *31*(4), 4096-4121, **2017**.

Putting it all together

Dahmen & Marquardt. *Energy & Fuels*, *31*(4), 4096-4121, **2017**.

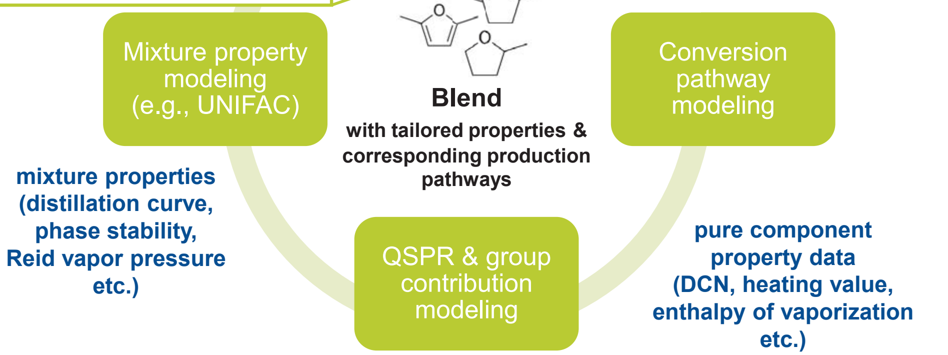


Putting it all together

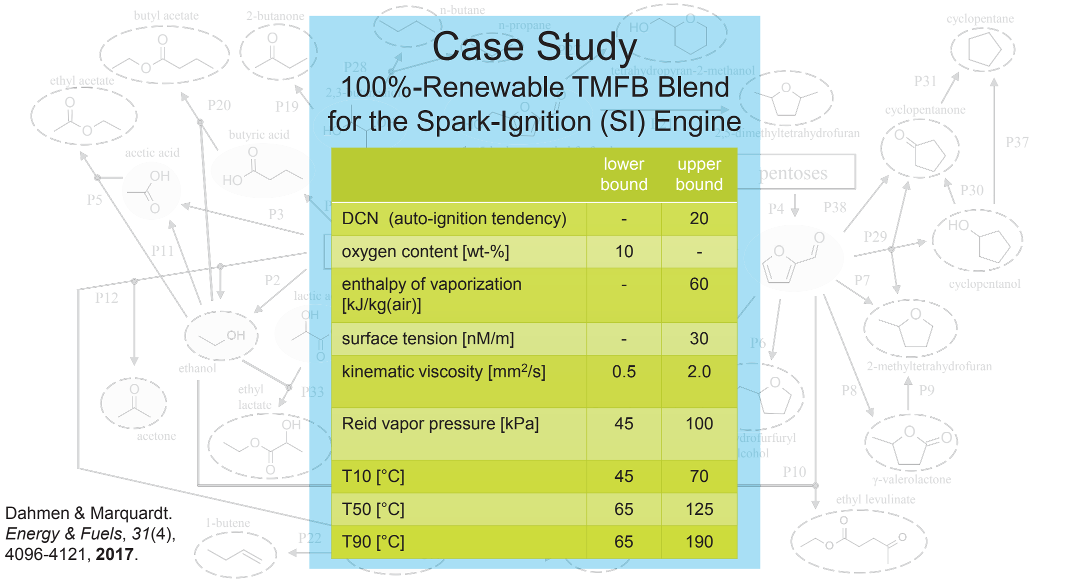
Dahmen & Marquardt. *Energy & Fuels*, *31*(4), 4096-4121, **2017**.

Nonlinear program (NLP)

- Nonlinearity due to fuel property models
- Matlab implementation
  (incl. QSPR & GC models, UNIFAC model)
- Solution strategy based on Matlab's *fmincon* SQP solver



Conversion Pathway Map (CPM) of the Case Study



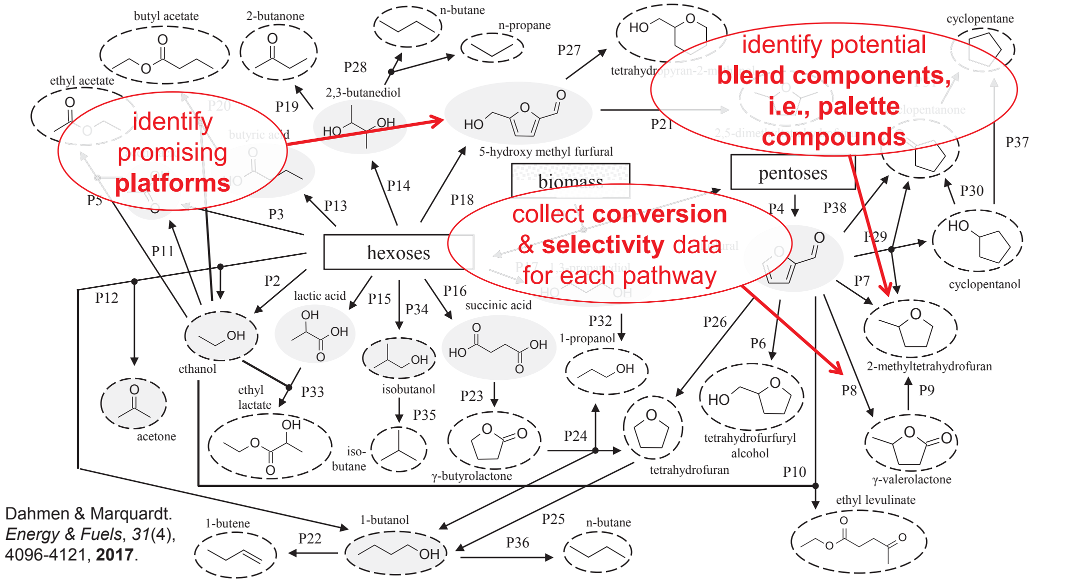
Case Study

100%-Renewable TMFB Blend for the Spark-Ignition (SI) Engine

	lower bound	upper bound
DCN (auto-ignition tendency)	-	20
oxygen content [wt-%]	10	-
enthalpy of vaporization [kJ/kg(air)]	-	60
surface tension [nM/m]	-	30
kinematic viscosity [mm²/s]	0.5	2.0
Reid vapor pressure [kPa]	45	100
T10 [°C]	45	70
T50 [°C]	65	125
T90 [°C]	65	190

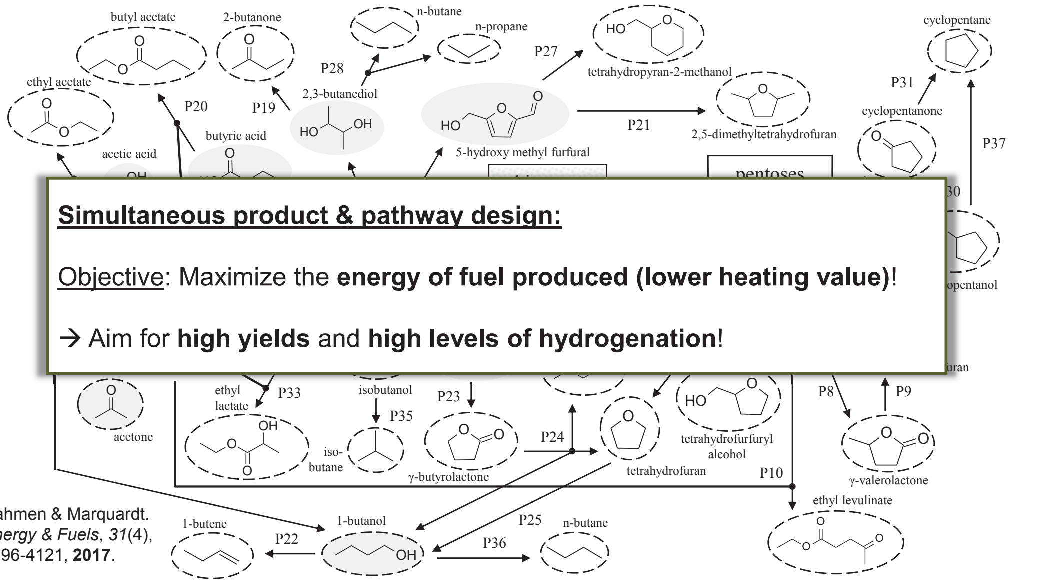
Dahmen & Marquardt. *Energy & Fuels*, *31*(4), 4096-4121, **2017**.

Conversion Pathway Map (CPM) of the Case Study



Dahmen & Marquardt. *Energy & Fuels*, *31*(4), 4096-4121, **2017**.

Conversion Pathway Map (CPM) of the Case Study



Simultaneous product & pathway design:

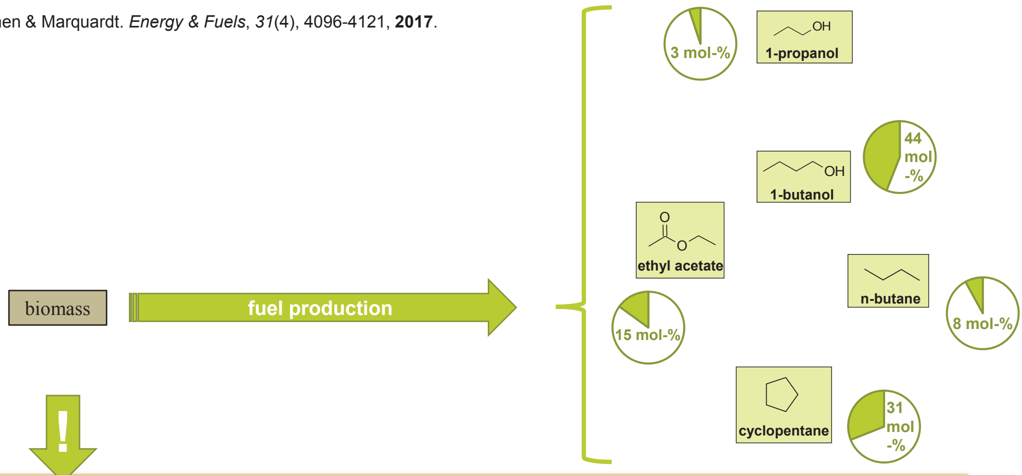
Objective: Maximize the **energy of fuel produced (lower heating value)**!

→ Aim for **high yields** and **high levels of hydrogenation**!

Dahmen & Marquardt. *Energy & Fuels*, *31*(4), 4096-4121, **2017**.

Solution – Maximization of the Energy of Fuel Produced

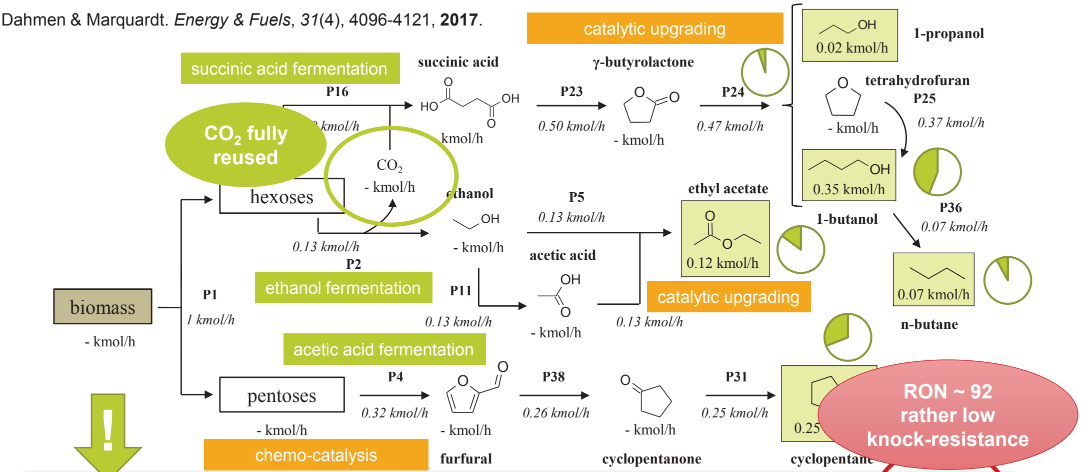
Dahmen & Marquardt. *Energy & Fuels*, *31*(4), 4096-4121, **2017**.



energy of fuel produced MJ_{fuel} / $MJ_{biomass}$	mass of fuel produced kg_{fuel} / $kg_{biomass}$	hydrogen demand mol_{H2} / mol_{fuel}	LHV energy efficiency MJ_{fuel} / ($MJ_{biomass}$+MJ_{H2})	CO_2 from biomass g / MJ_{fuel}	derived cetane number (DCN)
0.75	0.39	4.6	0.57	0.0	18.8

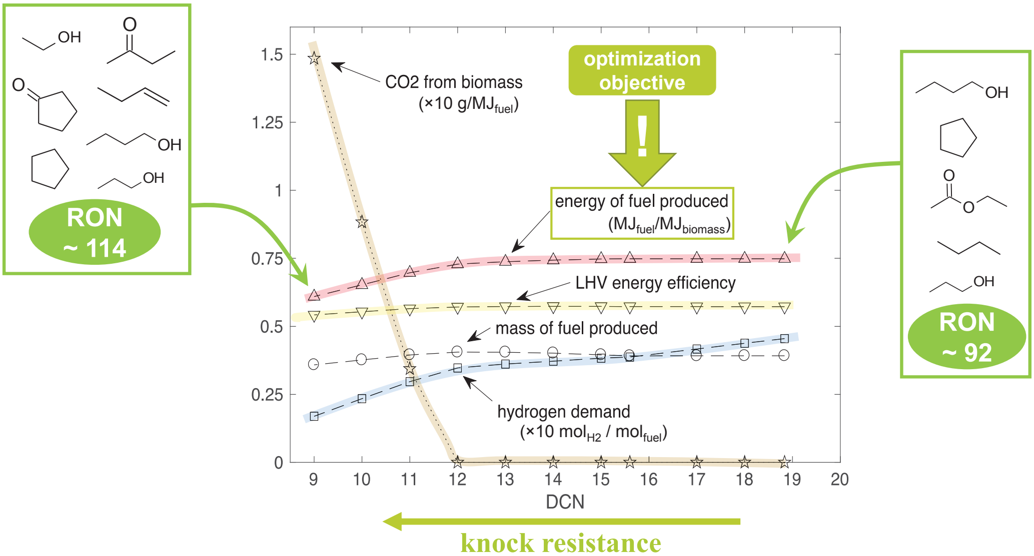
Solution – Maximization of the Energy of Fuel Produced

Dahmen & Marquardt. *Energy & Fuels*, *31*(4), 4096-4121, **2017**.



energy of fuel produced MJ_{fuel} / $MJ_{biomass}$	mass of fuel produced kg_{fuel} / $kg_{biomass}$	hydrogen demand mol_{H2} / mol_{fuel}	LHV energy efficiency MJ_{fuel} / ($MJ_{biomass}$+MJ_{H2})	CO_2 from biomass g / MJ_{fuel}	derived cetane number (DCN)
0.75	0.39	4.6	0.57	0.0	18.8

Trade-off Analysis: DCN vs. Energy of Fuel Produced



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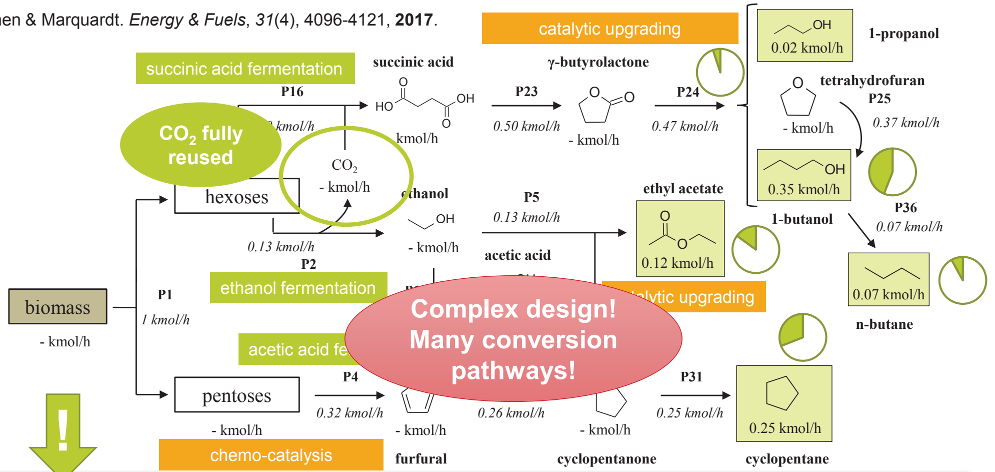

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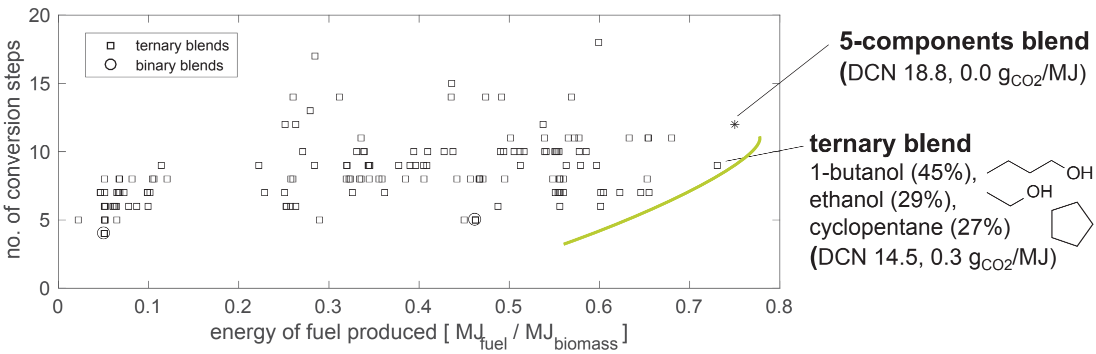
More Choices & Less Complex Designs

All optimal binary & ternary designs!

maximize: energy of fuel produced $\mathbf{MJ_{fuel}}$ **/** $\mathbf{MJ_{biomass}}$
s.t.: pathway & property models (**DCN≤15**),
number of palette compounds = 2 or 3

Few blends exhibit both desired **physicochemical** properties and attractive **process-related** properties!



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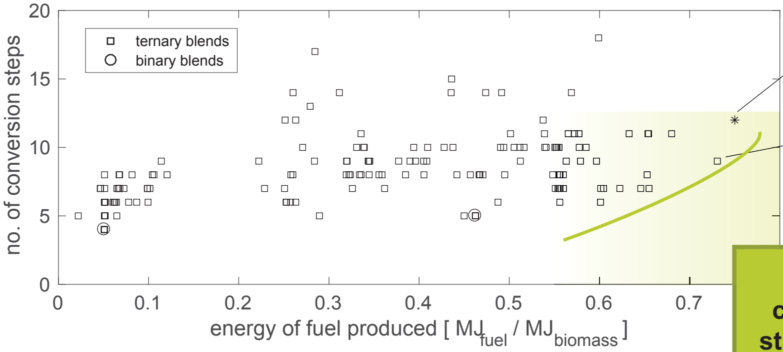
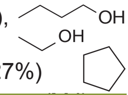


5-components blend
(DCN 18.8, 0.0 g_{CO_2}/MJ)

ternary blend
1-butanol (45%),
ethanol (29%),
cyclopentane (27%)



Product/pathway combinations for early-stage process screening!

Dahmen & Marquardt. *Energy & Fuels*, *31*(4), 4096-4121, **2017**.

Summary & Perspective

- **Tailor-made oxygenated fuels** can significantly **improve spark-ignition engine efficiency** and can greatly **simplify exhaust gas aftertreatment.**

- **Model-based design methodology for the identification of tailored biofuel (blends)**
  - **Targeted generation of candidate structures**
  - **Development of property models, e.g. DCN (ignition delay)**
  - **Pathway model based on selectivity & conversion data**
  - **Simultaneous product & pathway design**

  → **Product/pathway combinations** for further investigation by means of **early-stage process screening** and/or **conceptual process design**

- **Perspective**: From the **molecular level** to the **process level (Prof. Alexander Mitsos)**
  Early-stage process screening: Process Network Flux Analysis (PNFA)
  Effort for separation of intermediates, byproducts and solvents (short-cut models)

  → **First economic assessment**

  Ulonska, Skiborowski, Mitsos & Viell. *AIChE Journal*, *62*(9), 3096-3108, **2016**.

Thank you for your attention!

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Cluster of Excellence
Tailor-Made Fuels from Biomass
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