OME Worked Example for the TEA Guidelines for CO_2 Utilization

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GLOBAL CO_2 INITIATIVE
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eit Climate-KIC

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Foreword from CO_2 Sciences

Climate change is one of the largest challenges of our time. One of the major causes of anthropogenic climate change, carbon dioxide, also leads to ocean acidification. Left unaddressed, these two challenges will alter ecosystems and fundamentally change life, as we know it. Under the auspices of the UN Framework Convention on Climate Change and through the Paris Agreement, there is a commitment to keep global temperature increase to well below two degrees Celsius. This will require a variety of strategies including increased renewable power generation and broad scale electrification, increased energy efficiency, and carbon-negative technologies.

We believe that Life Cycle Assessment (LCA) is necessary to prove that a technology could contribute to the mitigation of environmental impacts and that Techno-Economic Assessment (TEA) will show how the technology could be competitively delivered in the market. Together they are a valuable toolkit for promoting carbon capture and utilization (CCU) technology development.

The work presented here was made possible through the vision of the Chairman of CO_2 Sciences Inc., Bernard David, and the expertise of the CEO of CO_2 Sciences Inc., Issam Dairanieh.

The Global CO_2 Initiative was launched during the 2016 meeting of the World Economic Forum with the goal of catalyzing innovative research in CO_2 utilization. Starting July of 2018, the Initiative will continue its work as *The Global CO_2 Initiative at the University of Michigan*.

Development of standardized CO_2 Life Cycle and Techno-economic Assessment Guidelines was commissioned by CO_2 Sciences, Inc., with the support of 3M, EIT Climate-KIC, CO_2 Value Europe, Emissions Reduction Alberta, Grantham Foundation for the Protection of the Environment, R. K. Mellon Foundation, Cynthia and George Mitchell Foundation, National Institute of Clean and Low Carbon Energy, Praxair, Inc., XPrize and generous individuals who are committed to action to address climate change.

Global CO2 Initiative@UM, August 2018

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List of abbreviations

APCr	Air Pollution Control Residue
BDF	Block flow diagram
C8S	Carbon8 Systems
CAPEX	Capital Cost
CAPM	Capital asset pricing model
CCS	Carbon capture and storage
CCU	Carbon capture and utilization
CEPCI	Chemical Engineering Plant Cost Index
CO_2	Carbon dioxide
COGM	Cost of goods manufactured
COGS	Cost of goods sold
EFW	Energy from Waste
ETS	Emission trading system
EU	European Union
FCI	Fixed capital investment
FOAK	First of a kind
GWP	Global warming potential
H_2	Hydrogen
IRR	Internal rate of return
ISBL	Inside battery limits
ISO	International standardization organization
LCA	Life cycle assessment
LCC	Life cycle costing
LCI	Life cycle inventory
LCOE	Levelized cost of electricity
LHV	Lower heating value
MADM	Multiple attribute decision making
MCDA	Multicriteria decision analysis
MODM	Multiple objective decision making
MSW	Municipal Solid Waste
NGO	Non-Governmental Organisation
NOAK	Nth of a kind
NOX	Nitrous Oxides
NPV	Net present value
OPEX	Operational Cost
OSBL	Outside/off-site battery limits
P&ID	Piping and instrumentation diagram
PEM	Proton exchange membrane
PFD	Process flow diagram
R&D	Research and Development
RDF	Refuse derived fuel
ROI	Return on investment
SA	Sensitivity analysis
SI-UNITS	International System of Units
TCI	Total capital investment
TEA	Techno-economic assessment
TRL	Technology readiness level
UA	Uncertainty analysis
USD	United States Dollars
WACC	Weighted average cost of capital

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1. Executive Summary

Reducing greenhouse gas emissions from heavy duty transportation remains challenging. OME_{3-5} is discussed as fuel technology for reducing the environmental footprint of heavy duty transportation, especially through reducing fuel carbon intensity as well as soot and NO_x emissions. OME_{3-5} can act as synergistic diesel blend and use existing infrastructure and engine technology.

Goal of this study was to identify economic opportunities and barriers for OME_{3-5}, derive R&D pathways and benchmark values. The analysed OME_{3-5} production process included seven system elements: membrane carbon capture, PEM water electrolysis as well as the synthesis of methanol, formaldehyde, trioxane, methylal (OME_1) and OME_{3-5}, combining and adjusting the findings of two prior studies from Michailos et al. (2018) and Schmitz et al. (2016).[1,2] Conventional diesel fuel and OME_{3-5} from conventional methanol are selected as benchmark products; lower heating value in GJ as functional unit.

The study concluded that the cost of goods manufactured (COGM) of OME_{3-5} produced from flue gas, water, electricity and steam via a seven step process on a 1 million tonne per year plant that resembles a small diesel refinery was 1.1 times higher than the 10-year average diesel price in Germany and 2,1 times higher than the 10-year average diesel price at the United States gulf coast. Further findings are that the energy of the output OME_{3-5} (based on lower heating value, LHV) equals 33% of the input energy (electricity and steam) and that the mass of the output OME_{3-5} equals 11% of the input mass of flue gas and water.

The results are judged to be uncertain relating to -30% to +50% due to the low technical maturity of membrane carbon capture and OME_{3-5} conversion. The results are found to be sensitive to location and time related factors (currency, CEPCI, location factor) as well as to the technical and economic specifications of the water electrolysis process, especially electricity consumptions, electricity price and electrolyser capex. Under the optimistic assumptions of free electricity and electrolyzer capex of 330 MW, the COGM of OME_{3-5} becomes competitive in Germany but not in the United States due to the higher diesel prices in Germany.

Overall OME_{3-5} fuel provides an intriguing emission and environmental impact reduction technology for heavy duty transportation; the early stage evaluation shows mixed results. Future success seems technically feasible, however it is dependent on extremely large amounts of very low cost low emission electricity, hydrogen or methanol. Core R&D priority remains the provision of these energy vectors, benchmark values are set by current diesel fuel. Main priorities for future research on techno-economics of OME_{3-5} are found to be detailed modelling of FA/TRI/OME_1/OME_{3-5}, more detailed electrolyzer capex models and choosing a specific location. Furthermore, additional methanol production pathways such as SMR-CCS should be analysed.

2. Technical Summary

GOAL	**CCU product**	OME$_{3-5}$ heavy duty transportation fuels	
	Intended application and reasons for study	The study serves as an example for the TEA practitioner that wishes to assess a novel CCU process concept at low technology maturity.	
	Brief description	The study analysis the economic opportunities and barriers for OME$_{3-5}$e-fuels via a seven step process starting from electricity and CO_2.	
	Intended audience	TEA practitioners in academia and industry	
	Commissioners and Assessors	Assessor: TU Berlin with support from MIT Energy Initiative Commissioner: EIT Climate-KIC, The Global CO_2 Initiative	
	Limitations of study	The study results in a comparison and trends, however no definite claims of superiority (comparative assertion) are derived, due to the early maturity and corresponding high uncertainty of results.	
SCOPE	**System boundary (i.e cradle to gate)**	Cradle to gate	
	Benchmark system	Diesel refinery	
	Plant size	Mass output: 1 000 000 t/a OME$_{3-5}$, corresponding energy output: 18.8 PJ/a OME$_{3-5}$	
	Functional Unit	Lower Heating Value (LHV) in Giga Joule (GJ)	
	System elements and technology maturity	**System elements**	**Technology maturity**
		Carbon capture via membrane	TRL 5
		PEM water electrolysis	TRL 9
		Methanol Synthesis	TRL 7
		Formaldehyde production	TRL 9
		Trioxane production	TRL 9
		OME$_1$ production	TRL 9
		OME$_{3-5}$ production	TRL 4
	Assessment indicators	Mass and carbon efficiency, energy efficiency, opex (direct/indirect), capex, cost of goods manufactured (COGM)	
INVENTORY	**Data Source**	☐Primary sources ☒Secondary sources ☒Stoichiometric data	☒Process modelling based data ☒Mixes sources ☐Other (please specify) …………………………………………
	Energy sources (select all that apply)	☒Grid mix ☐Power station with Carbon Capture ☐Wind ☐Solar	☐Nuclear ☐Hydro ☐Future (see timeframes) ☐Other (please specify) …………………………………………
	Base year	2016	
	Currency	US Dollar (USD)	
	Location	Germany, US (Gulf Coast)	
	Plant life time	Not applicable - DCFA not applied	
	CO_2 sources and price (if applicable)	CO_2 source: cement plant CO_2 price: capture cost Germany: 49 USD/t, US: 42 USD/t (only capture included in boundary)	
	H_2 sources and prices (if applicable)	H_2 source: PEM water electrolysis H_2 price Germany 4 415 USD/t, US 3 653 USD/t (included in boundary)	
CALCULATION OF INDICATORS	**Energy consumption** per functional unit	2.6 GJ electricity and 0.46 GJ steam per GJ$_{OME3-5}$	
	CAPEX per functional unit	Germany: 35 USD/ GJ$_{OME3-5}$, US: 29 USD/GJ$_{OME3-5}$ (base case)	
	OPEX per functional unit	Germany: 54 USD/ GJ$_{OME3-5}$, US: 47 USD/ GJ$_{OME3-5}$ (base case)	
	Price per functional unit	Germany: 89 USD/GJ$_{OME3-5}$, US: 76 USD/GJ$_{OME3-5}$ (base case)	
INTERPRETATION	**Sensitivity Analysis main factors**	Price of electricity, H_2 capex, location (DE/US), overall 8 scenarios	
	Uncertainty manipulated variables	Judgement by AACE class	
	Main Conclusions	OME$_{3-5}$ fuel provides an intriguing emission and environmental impact reduction technology for heavy duty transportation; the early stage evaluation shows mixed results. Future success seems technically feasible, however it is dependent on extremely large amounts of very low cost low emission electricity, hydrogen or methanol.	

3. Context of this study

Assessment studies of CO_2 capture and utilization (CCU) technologies (also see [3]) often rely on varying indicators and scopes, even for the same technology, making the comparison of environmental impact or economic potential difficult.[4,5] To avoid such apples and oranges comparison and to find a common assessment 'language', a Guideline for techno-economic assessment (TEA) and life-cycle assessment (LCA) was recently drafted in a multi-stakeholder process.[6] These TEA and LCA Guidelines for CCU build on existing standards and procedures such as the ILCD handbook,[7] ISO 14044[8] and Technology Readiness Levels,[9] providing more detailed guidance in the field of CCU. Furthermore, these Guidelines adapt the approach of TEA to LCA, enabling a more systematic integration of both assessment concepts. The common LCA sections of goal, scope, inventory and impact assessment (here called 'calculation of indicators') as well as the parallel interpretation are adopted and accompanied by a TEA report summarizing the results. This work represents one of three worked examples of these CCU Guidelines, focusing on early-stage TEA.

This study applies the Guidelines described in the accompanying report "Guideline for Techno-Economic Assessment of CO_2 Utilization", hereafter referred to as "the Guidelines". It is intended as supporting material to show how the TEA methodology can be specifically applied to tackle the issues surrounding CO_2 utilization processes. This study is a worked example with data collected from the literature. The aim of the study is not to prove whether the selected process is economically viable or to make process alterations to make it so, but to clearly demonstrate how the proposed Guidelines can be used to conduct a transparent TEA which can then be followed by others.

The study analyses an OME_{3-5} production concept based on CO_2 and electricity, including the process of CO_2 capture (membrane), water electrolysis (PEM) and the synthesis of methanol, formaldehyde, trioxane, methylal (OME_1) and OME_{3-5}. Recently OME_{3-5} has gained interest as a transport fuel, especially as option for heavy duty transportation. Electricity and CO_2 were included in the study to show how alternative energy and carbon resource could be used in transport fuels for heavy duty vehicles, potentially as an option to decrease the carbon intensity of freight. **This study uses a novel process concept at early technology maturity to outline the methodological challenges and approaches in early-stage assessment.** The intended application of this study is as a reference on how to apply the TEA Guidelines for CO_2 utilization to a comparative assessment between a CCU technology and a conventional technology. This report is for public use and targets the TEA practitioner who assesses a CCU process.

Blue-coloured text boxes are used to refer to the Guidelines as explanation of why certain decisions were taken or choices made and to refer to the reporting checklist that is found in the Guidelines. The Guidelines, together with this study was commissioned by The Global CO_2 Initiative/CO_2 Sciences and EIT Climate-KIC, a body of the European Union. In addition, this study was included in an earlier version in the proceedings of GHGT-14 conference.

4. Introduction

Decarbonization of some sectors, such as heavy duty road freight transportation, remain highly challenging. As road freight transportation is strongly linked to economic activity, demand and related greenhouse gas (GHG) emissions have seen a strong increase over the last decades, rising from 1.7 Gt/a in 2000 to 2.6 Gt/a in 2015 and are projected to increase to 4.3 Gt/a in 2030.[10,11] The majority of road freight transportation emissions are caused by heavy duty vehicles, which are more efficient for long distance transportation but have substantially higher per km emissions than light or medium duty vehicles. Besides avoiding journeys, model shift to lower-emission systems and lowering the energy intensity of transport, a fourth major strategy for emissions reduction is decreasing fuel carbon intensity. This means switching from diesel fuel to natural gas, biofuels, renewable electricity or hydrogen.[12] A recent whitepaper demonstrated hydrogen fuel cells to be the most promising technology for heavy duty freight with significant emissions reduction, however with very high initial cost.[11] E-fuels, building on existing infrastructure and making use of low-emission electricity, could combine both, low cost and emissions reduction and thereby provide an additional option for heavy duty freight. A recent review identified three promising e-fuel options, dimethyl ether, oxymethylene ether and Fischer-Tropsch n-alkanes, that have similar properties as conventional fossil diesel.[13]

Polyoxymethylene dimethyl ethers (PODME) or simply oxymethylene ethers (OME), are ethers with the structure $CH_3\text{-}O\text{-}(CH_2O)_n\text{-}CH_3$. Dimethyl ether (DME) can also be described as OME with n=0. OMEs show an excellent combustion behaviour and a drastic reduction in soot emissions due to a lack of C-C bonds.[13–16] Furthermore, a modification of the exhaust gas recycling in the engine also enables a significant reduction in NO_x emission. These emission reductions also occur in OME-diesel blends, where OME's emissions reduction effect is greater than its share in the fuel (synergistic blend).[17] The major disadvantage of OMEs is a lower energy density compared to diesel fuels (33% lower for DME and ~55% lower for $OME_{3\text{-}5}$ on a LHV mass basis).[13,14] For e-fuels, OMEs with three to five repeating units are preferred as these show similar behaviour and good miscibility with conventional diesel fuel. $OME_{<3}$ (including DME) have low boiling points and low flash points, requiring pressurized tanks and modifications at engines and infrastructures.[13] $OME_{>6}$ have high melting points, leading to potential clogging of the engine fuel systems.[13] Research and development on OME first started in the 1960ies with activities focusing on Polyoxymethylene (POM), the polymer of OME with 20 or less publications per year on average. Starting from the 2000s, research interest in Europe and also later in China increased focusing on OME_0 and OME_1 from oil and coal sources leading to rising numbers in publications and patents. Research on $OME_{3\text{-}5}$ started around 2006 with a constant annual increase leading to 12 publications in 2017 and various large scale research projects including the substance in their work today (see Figure 1, also see [18]).

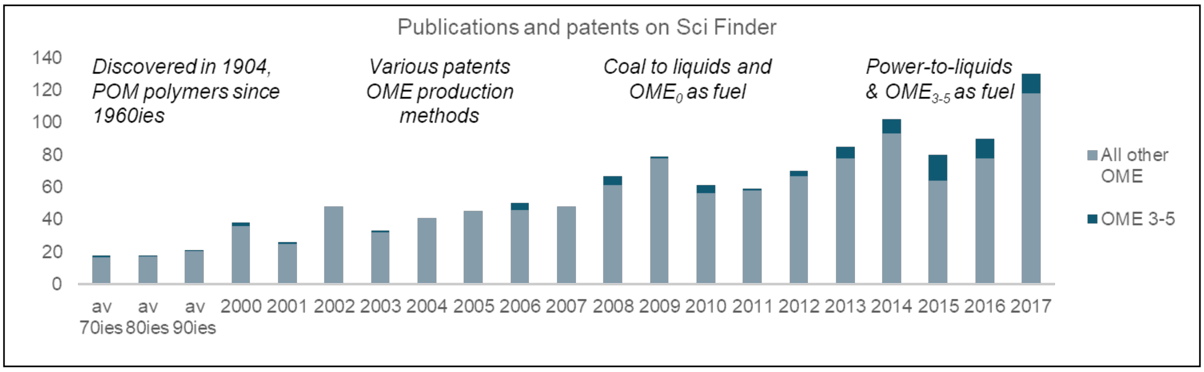

Figure 1. Publications and patents on Sci-Finder for $OME_{0\text{-}5}$ 1970-2017

$OME_{3\text{-}5}$ can be produced via two routes, the anhydrous and aqueous route, and requires two components: a formaldehyde monomer source, such as monomeric formaldehyde, para-formaldehyde or trioxane, and a capping methyl group, such as methanol, dimethylether (OME_0) or methylal (OME_1). The anhydrous route includes two intermediate production steps (production of trioxane and either OME_0 or OME_1). On each step water is separated from the product stream. The intermediate products are then reacted to oligomeric OME and other products, separated and fed back into the reactor. The aqueous route does not include intermediate steps and reacts methanol and formaldehyde or para-formaldehyde directly towards OME; water is separated after the synthesis. As both routes can be started from methanol, the formaldehyde can be produced in the process from methanol.[14,19] One recent publication mentions a 400 kt/a $OME_{3\text{-}5}$ production plant (OME_1 / para-formaldehyde route) in China operating since 2013,[18] which was not yet confirmed by another reference. Otherwise no larger scale production plants have been reported.

4.1 Technology maturity

The assessed system takes the anhydrous route and consists of seven elements (here called 'unit processes'): CO_2 capture, water electrolysis, methanol production, formaldehyde production, OME_1 production, trioxane production and $OME_{3\text{-}5}$ production. To derive the technology maturity, the technology readiness level scheme adapted for the chemical and process industries is used as presented in the TEA and LCA Guidelines.[6] The technology readiness level (TRL) was identified for each system element individually and the lowest TRL assigned to the overall system. CO_2 capture (membrane) was identified as TRL 5 as pilot-scale or commercial-scale plants are yet to come, but process design parameters can be derived from literature. CO_2/H_2 based methanol production was identified as TRL 7 based on the pilot-scale plant from Carbon Recycling International in Iceland and process designs available in the literature.[20] For the production of $OME_{3\text{-}5}$, the proof of concept has been accomplished and first process patents have been issued, however publicly available detailed property or process data was lacking,[2] which is why it was identified as TRL 4 and only a simplified process could be used for this assessment. The remaining unit processes were identified as TRL 9, as they are available at commercial scale and detailed process and property data was available in literature [21,22] (see Table 1). Overall this system can be assessed on TRL 4.

Table 1. Technology Readiness Level (TRL) of system elements

System element	TRL
CO_2 capture (membrane)	5
Water electrolysis	9
Methanol production (CO_2 / H_2 route)	7
Formaldehyde production	9
Trioxane production	9
OME_1 production	9
$OME_{3\text{-}5}$ production	4

5. Goal

Reference to Checklist (see Guideline Chapter 8)

A checklist of items to be included in each section of the report is included in **Chapter 8 Reporting** of the Guidelines, which for the goal is as follows:

Goal of the study

- ☐ State the intended application of the study
- ☐ State the reasons for carrying out the study
- ☐ State the intended target audience of the study
- ☐ State whether the results are to be used in comparative assertions disclosed to public
- ☐ State unambiguously the research question(s)

5.1 Goal perspective and principles

The study serves as an example for the TEA practitioner that wishes to assess a CCU process or product at low technology maturity. As the technology maturity of this process concept was identified as TRL 4, an R&D assessment perspective was taken, aiming to address academia and industrial stakeholders. The study results in a comparison and trends, however no definitive claims of superiority (comparative assertion) are derived, due to the early maturity and corresponding high uncertainty of results.

Goal of the study is to identify economic opportunities and barriers for OME$_{3-5}$ e-fuels as fuels for heavy duty vehicles and derive crucial R&D development pathways and benchmark values. As these opportunities might be varying by location, a hypothetical location in Germany, where OME$_{3-5}$ research is currently seeing very strong interest, is compared to a hypothetical location in the United States (gulf region) where cost for electricity is lower, resulting in a potentially lower OME$_{3-5}$ price. The analysed OME$_{3-5}$ is regarded as CCU fuel.

Reference to Guidelines B.1

Goal definition is described in Guideline B.1. The report serves to provide information and showcase good practices to a potential CCU practitioner, especially for academia and industrial stakeholders. Goal of the study is to identify economic opportunities and barriers for OME$_{3-5}$ e-fuels for heavy duty transportation.

5.2 Assessment scenarios

Given the limited data availability, a shortcut assessment was conducted with the limitation that this approach cannot provide precise results other than general tendencies. Germany (DE) and the United States (US) were chosen as locations and set the base year to 2016. Simple price scenarios were created representing a business as usual / base case and three optimistic cases, outlining the limits of future developments, resulting in 8 scenarios overall, see Table 2.

Table 2. Assessment scenarios

Scenarios	**High electricity price (current)**	**Low electricity price (zero)**
High electrolyzer capex (current)	DE base case	DE scenario A
	US base case	US scenario A
Low electrolyzer capex (future)	DE scenario B	DE scenario C
	US scenario B	US scenario C

The report is of public use and by accompanying the Guideline document. The process design and economic parameter value choices, underlying this analysis, are based on public domain literature, mainly on the Methanol worked example of the Guideline document. For these reasons, the results are not indicative of potential performance, but are meant to represent the most likely performance given the assumptions (time and location) and the current state of public knowledge.

Reference to Guidelines B.2

Assessment scenarios are described in Guideline B.2. The three scenarios are distinct as they differentiate in the key pricing parameters. The base case extends current trends, the alternative scenarios account for potential pricing changes. The scenarios are based on the finding of prior studies, including the findings of academic stakeholders.

6. Scope

Reference to Checklist (see Guideline Chapter 8)

Scope of the study

- ☐ State functional unit clearly and unambiguously according to Guideline and report changes due to solving of multi-functionality
- ☐ State system boundaries according to Guideline
- ☐ State relevant issues with data quality and assumptions
- ☐ State technology readiness level (TRL) of processes and sub-processes
- ☐ Report production or storage capacity
- ☐ Report geographical scope
- ☐ State software system (and version) and data library (and version) used
- ☐ State type of review and provide additional information about reviewers

6.1 Product system and functional unit

The produced OME_{3-5} is assumed to be used as fuel in the market segment for heavy duty transportation fuels, following the study goal. Energy was selected as basis for comparison and GJ (Lower Heating Value, LHV) as functional unit, as the key utility of fuels is energy content.

Reference to Guidelines B.3

The definition of product systems and functional units is described in **Guideline B.3**. As the structure and characteristics of $OME_{3\text{-}5}$ are different to its benchmark diesel, the functional unit is derived from the product performance – its energy content in lower heating value. While fuel can have a range of different applications such as power generation, heating and transport, this study focusses on transportation, specifically on heavy duty transportation and in the segment of low-carbon intensity fuel options. A description of a customer group is left out as this study takes a R&D perspective.

6.2 System elements and boundaries

The scope of this study includes all operations from flue gas to $OME_{3\text{-}5}$ output, representing a hypothetical e-fuel production company. In the scope seven system elements were included (see Figure 2) and by accounting for the input economic impacts this represents a cradle to gate boundary. Only the anhydrous route was included in this study, as the aqueous route was lacking detailed techno-economic data at the time of assessment. To make the study comparable, the assumed anhydrous route taken from an existing study, the $OME_{3\text{-}5}$ conversion element (striped) is relying on estimated thermodynamic data. This study adopted an output of the product system of 1 Mt/a $OME_{3\text{-}5}$ of Schmitz et al. (2016)[2] and a gate-to-gate assessment approach.

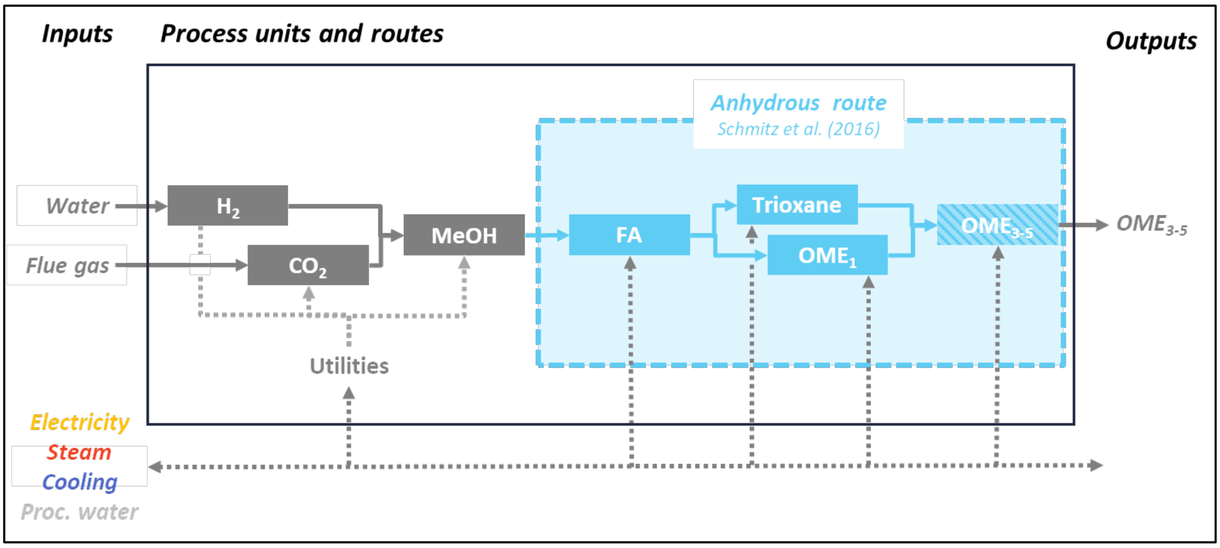

Figure 2. Product system for $OM_{E3\text{-}5}$ assessment

Multifunctionality was not regarded as an issue here, as the product systems major valuable output is $OME_{3\text{-}5}$, the other outputs of water, oxygen, cleaned flue gas, purge gas and CO_2 were regarded as waste streams and released into the environment.

Reference to Guidelines B.4

System elements and boundaries are addressed in Guideline B.4. The product system is represented in a graphical scheme (see Figure 2). Specifications for input flows are shown together with the results (see Figure 4). As the technology includes several steps, some at an early maturity, the system elements were defined to each represent one process unit. The system boundaries are derived from a hypothetical e-fuel production company located at an industrial park with available flue gas, water, electricity, heating and cooling infrastructure. It was assumed that the company's value proposition is the production of OME$_{3-5}$ from flue gas and electricity. Upstream process such as flue gas emitting production processes and downstream processes such as combustion were excluded as they would not be core of the hypothetical company's business.

6.3 Benchmark systems

As nearly all energy for heavy duty transport is supplied by diesel, it was selected as benchmark product and a conventional refinery as benchmark system. As benchmark value, gas station prices were selected providing a simple comparison for the consumer. These rather low quality data seemed sufficient for this analysis following the iterative approach and more detailed data would have not changed the outcome. These gas station prices would represent a tax-free introduction of e-fuels, however OME$_{3-5}$ production cost would have to reach values significantly lower than that. In addition, the benchmark of OME$_{3-5}$ produced from methanol is used as benchmark as reported in the study of Schmitz et al. (2016).[2]

Reference to Guidelines B.5

Benchmarks are discussed in Guideline B.5. Diesel is currently the most common product in the application and was therefore selected as benchmark. Customer needs were addressed indirectly: while a range of options for e-fuels exist, some were ruled out as transition fuels in recent literature, mainly due to more complicated handling and higher cost of change (see introduction).

6.4 Assessment indicators

To provide a general overview of the technical and economic performance, mass and carbon efficiency, energy efficiency (in the form of work), opex (direct and indirect) and capex as well as the resulting cost of goods manufactured (COGM) were used as assessment indicators.

Reference to Guidelines B.6

Assessment indicators and methods are found in Guideline B.6. The indicators were selected to address the goal (identify economic opportunities and barriers and derive development pathways and benchmark values) and can be used also in early maturity stages (taking into account high indicator uncertainty). The selected indicators are commonly used in academia and industry and reflect both - economic and technical fields.

6.5 Plausibility checks

In addition, two plausibility checks (“sanity checks”) were performed for sizing the OME_{3-5} plant with regards to energy output and CO_2 supply. Assuming the substitution of diesel through OME_{3-5}, the energy output of a conventional refinery was selected as relevant benchmark. Assuming the OME_{3-5} mix as in Burger et al. (2013),[23] the OME_{3-5} plant with an output flow of 1 Mt/a OME_{3-5} would provide an energy output of 18.8 PJ/a, which roughly equals the size of the 10th percentile of refineries in the United States and which seems like a small but reasonable capacity (see Figure 3, left).[24] Regarding CO_2 supply, the plant would require 1.2 Mt/a pure CO_2, of which 419 sources exist with an overall potential of 1.2 Gt/a CO_2. However, excluding all fossil fuel power plants, which might be shut down to reduce GHG emissions, only 26 emission sources would be left with an overall potential of 58 Mt/a. Regarding the CO_2 supply, the proposed plant seems still valid, but on the upper end of the potential (see Figure 3, right).

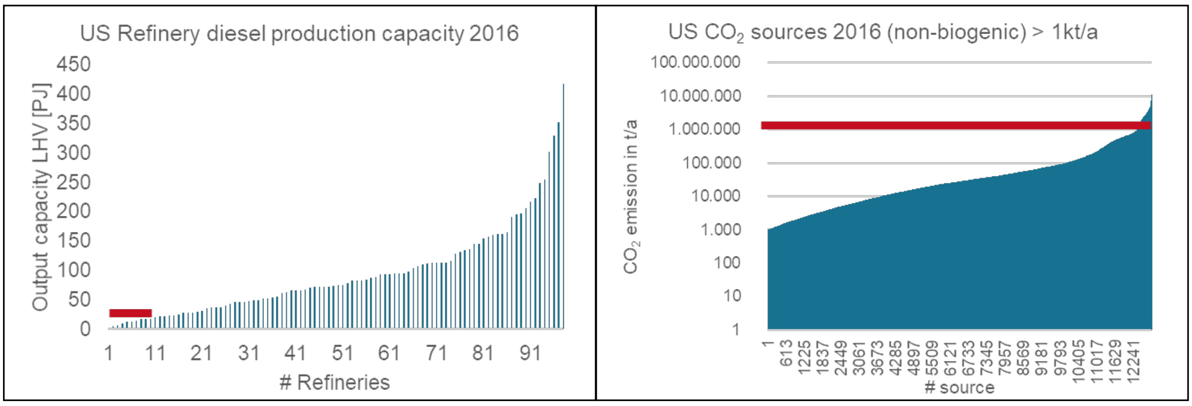

Figure 3. Output energy capacity (left) and CO2 demand (right) of the product system compared to conventional and supply systems

Reference to Guidelines

Plausibility checks are recommended to conduct for defining goal and scope of a study (see in the Guideline Chapter B.3.2, p. 30)

7. Inventory

This study extends the existing worked example of methanol and builds on the simulations and inventory presented there. Focus in this description are the additional processing steps of OME conversion.

Reference to Checklist (see Guideline Chapter *8)*

Inventory of the study

- ☐ State types and sources of the data including the quality
- ☐ State the technical data in SI units and in a technical parameter list
- ☐ State economic data in an economic parameter list
- ☐ State all economic decisions and assumption made

7.1 Types of data and interim quality control

Generic data reflecting a typical scenario from secondary sources (process simulations, data from peer-reviewed publications, industry reports as well as public and proprietary databases) were used to create the inventory; for the system elements capture, electrolysis and methanol conversion detailed technical data were obtained from process simulations from the methanol worked example. For OME production, detailed technical data could not be obtained at the time of assessment, which is why less detailed, generic data from a secondary source were used. As a result, only aggregated data for steam, cooling water, process water and waste water were included and reporting by system element was not possible. While an inventory for the anhydrous OME route could be created, the efforts for the aqueous OME route were not successful as available publications did not include sufficient data at the time of assessment.

As OME conversion has become an increasingly popular field of research it can be expected that more detailed technical data will be available in the near future. While the quality of data for OME production was rather low, it was judged to be sufficient as OME production was not found to be a major contributor to sensitivity. It is important to keep in mind that this study can only derive tendencies, but not precise figures. However, deriving economic opportunities and barriers, as it is the goal of this study, seems reasonable from this inventory given the low technology maturity.

Reference to Guidelines B.8

Multiple iterations for data quality were carried out, however more detailed data could not be not obtained due to the rather early technology stage. The low level of detail for OME conversion is however judged sufficient for the assessment goal as the overall results are not very sensitive to changes from these inputs. However, further detailed analysis is not meaningful with this inventory, see Guideline B.8.

7.2 Technical inventory

For the steps of CO_2 capture, hydrogen and methanol production, data and assumptions were adopted the methanol worked example, in particular from Aspen Plus models, see Michailos et al. (2018).[1] For the steps of formaldehyde production and OME production, data and assumptions were adopted from Schmitz et al. (2016) and Burger et al. (2013).[2,23]. Both models report aggregated values but are based on detailed process models. The energy content of the resulting OME_{3-5} mixture was assumed to reach 19,05 GJ_{LHV}/t as in the priory mentioned literature references. The product system still holds potential for optimization such as the recycling of carbon dioxide from FA production to CO_2 capture, heat integration or improved separation and recycling of water. All data was documented per functional unit: GJ of OME_{3-5} output (see Figure 4).

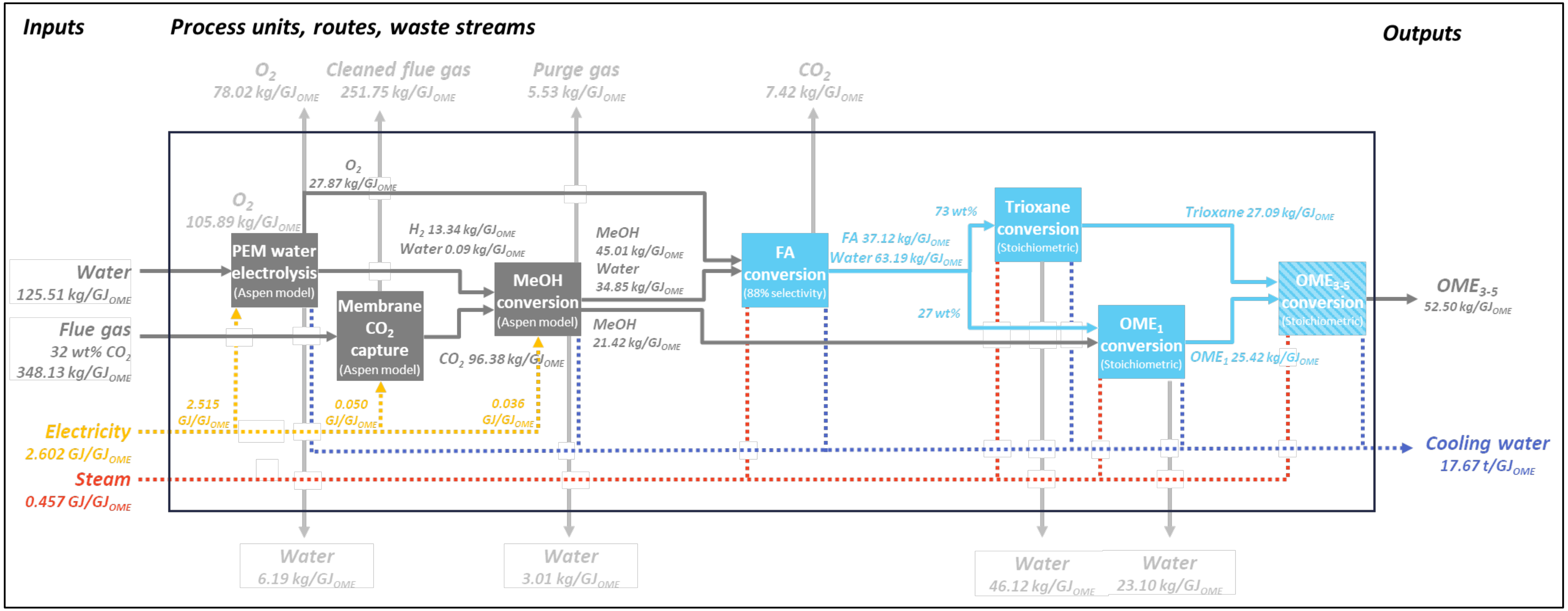

Figure 4. Product system for OME_{3-5} production from flue gas, water and energy

7.3 Economic inventory

7.3.1 General assumptions

The economic data was documented in US Dollar (USD), for the year 2016 and for the regions US gulf coast and Germany; currency, temporal and location adjustments were conducted. Process and location relevant production cost of CO_2 and hydrogen were considered as CO_2 capture (membrane) and compression as well as water electrolysis (PEM) and H_2 compression were included in the assessment scope. Opex and capex calculation approaches follow Buchner et al. (2018).[25]

The price of diesel fuel for Germany is the average price for consumers reported by MWV, the German Oil Economy Association.[26] The price of diesel fuel for the US is the US-average retail price for ultra-low sulphur diesel reported by the US EIA.[27] The $OME_{3\text{-}5}$ prices from market methanol were taken from the study of Schmitz et al. (2016) with an adjusted methanol price reported by ICIS. As 2016 marks a year of exceptionally low diesel and methanol prices, a 10 year average prices were taken for both regions.

Table 3. Benchmark values

	adjusted value		original value		comment	Reference
Diesel						
Diesel DE 10y-a	39.81	USD/GJ	1.2746	EUR/l		[26]
Diesel US 10y-a	24.42	USD/GJ	3.2761	USD/gal	source key: EMD_EPD2DXL0_PTE_NUS_DPG	[27]
$OME_{3\text{-}5}$ MeOH						
$OME_{3\text{-}5}$ MeOH DE 10y-a	40.31	USD/GJ	407.09	USD/t	Methanol, FOB Rotterdam contract price	[2,28]
$OME_{3\text{-}5}$ MeOH US 10y-a	41.89	USD/GJ	429.51	USD/t	Methanol, FOB USG contract price	[2,28]

7.3.2 Direct OPEX

The calculation of direct operational expenditure (OPEX - direct), was based on unit operations and simple thermodynamic calculations (mass and energy consumption and their respective unit prices) as recommended for TRL 4. Input flue gas was assumed to be free of charge, prices for deionised water, steam and cooling water were taken from Baerns et al. (2013).[29] Catalyst replacement costs were included at a replacement rate of 6.8 $g/GJ_{OME3\text{-}5}$ as in the methanol worked example. Electricity prices for very large industrial consumers were used in Germany 47.36 USD/MWh, in the US 38.65 USD/MWh; for a more detail discussion see chapter 7.4. See Table 4 for an overview of direct opex values.

Table 4. Opex assumptions

Direct OPEX			Reference
Flue gas	0.00	USD/t	
Deionised water	2.77	USD/t	[29]
Cooling water	0.07	USD/t	[29]
Process water	0.05	USD/t	[29]
Waste water treatment	0.44	USD/t	[30]
Steam	22.14	USD/t	[29]
Catalyst for methanol conversion	105 377	USD/t	[31]
Electricity - DE	47.36	USD/MWh	[32]
Electricity - US	38.65	USD/MWh	[33]

7.3.3 Indirect OPEX

Indirect operational expenditure is derived from factors of major direct OPEX and CAPEX units as recommended for TRL 4. The calculation of labour cost is discussed in more detail below. Maintenance cost are assumed to be 3% of $ISBL_{capex}$, tax and insurance 1.5% of $ISBL_{capex}$, interest is assumed as 6% of working capital (WC_{capex}) (see Table 5), replacement is only assumed for the elements CO_2 capture and water electrolysis as in the methanol worked example. Ideally, positions can be based on detailed data for each system element, which is the case for CO_2 capture, water electrolysis, methanol conversion and utilities. However, for FA to OME_{3-5}, the only available data is for n^{th} of a kind total cost of capital (NOAK-TCI) and only for a black box consisting of the four system elements FA, TRI, OME_1 and OME_{3-5} conversion. This is why for this black box "forced detail" (see Guideline B.6.3.2) is applied, deriving WC_{capex} and $ISBL_{capex}$ from TCI assuming the same distribution.

Table 5. Indirect Opex positions

Indirect opex		Reference
Maintenance	3% * $ISBL_{capex}$	[34,35]
Tax & insurance	1.5% * FCI_{capex}	[34,35]
Interest	6% * WC_{capex}	[34,35]
Labour cost	see below	

For labour cost, the estimates of the reference studies were adjusted. While the methanol worked example uses a functional unit counting method from Turton et al. (2012), Schmitz et al. (2016) uses a shortcut approach based on number of plants from Towler, Sinnot (2009).[34,36] Following the functional unit based approach as in the methanol worked example, the labour cost is estimated based on each step, specifically reaction, separation, heating, cooling, pumping and throttling. The number of steps for CO_2 capture, water electrolysis, methanol synthesis and corresponding utilities was taken from models used in the methanol worked example.[1] The number of steps for FA and Trioxane were taken from Franz et al. (2016), for OME_1 from Drunsel (2012) and for OME_{3-5} from Burger et al. (2013).[21,23,37].

The number of regular staff $N_{reg.staff}$ is estimated using the number of functional units with solid handling $N_{fu.sol}$, the number of functional units with non-solid handling $N_{fu.nso}$ and the number of shifts N_{shifts}.

$$. = (6.29 + 31.7 \quad . \quad + 0.23 \quad . \quad)^{0.5} * \quad t\ h$$

The overall cost of labour π_{labour} is derived from the number of regular staff . and wages $\pi_{wage.reg}$ for both locations (DE and US), resulting in the cost of staff $\pi_{staff.reg}$ as well as additional cost of supervision $\pi_{staff.sup}$ (assumed to be 25% of $\pi_{staff.reg}$), direct overhead (50% of $\pi_{staff.reg}$ and $\pi_{staff.sup}$) and general overhead (65% of $\pi_{staff.reg}$, $\pi_{staff.sup}$ and direct overhead). The factors for supervision, direct and general overhead can be summed up to a single factor of 2.0938.

$$\pi_{labour} = \pi_{staff.reg} + \pi_{staff.sup} + \pi_{direct\ OH} + \pi_{general\ OH}$$

$$\pi_{labour} = 2.0938 * N_{staff.reg} * \pi_{wage.reg}$$

As wage for regular staff at a chemical plant the average wage for the pharmaceutical and chemical industry of 56 173 EUR was assumed for Germany, which equals wage group EG10 in the collective labour agreement valid until late 2017;[38,39] A wage of 63 825 USD reflecting the average wage for chemical plant operators was assumed for the United States.[40] Overall assuming a wage of 60 000 USD/a as recommended in Sinnot, Towler (2009) seems to be a useful starting point.

7.3.4 CAPEX

Regarding CAPEX, the total invested capital (TIC) approach was selected according to Buchner et al. (2018) [25] with slight modifications and nth of a kind plant adaption from Michailos et al. (2018).[1] Regarding CO_2 capture, water electrolysis, methanol synthesis and utilities of the prior, a component factored approach was selected to estimate the equipment cost: starting from a published equipment cost of a process unit at a specific capacity, the cost was scaled with an exponential factor applicable to the technology to derive the equipment cost at the relevant scale following Michailos et al. (2018). From purchased equipment cost, all further cost positions until total invested capital TIC were estimated via factors (see Table 6). In addition, decreasing TIC from learning was included (nth of a kind plant TIC_{NOAK}), by applying learning curves reasonable to the system element following Michailos et al. (2018).

Regarding formaldehyde, trioxane, OME_1 and OME_{3-5} conversion, a simpler TIC_{NOAK} estimation is adopted from Schmitz et al. (2016). TCI_{NOAK} were derived from by a short method from a refinery with a capacity of 5 Mt/a that costs 780 million USD and scaled down to 1 Mt/a with an exponent of 0.65. A short method approach was judged reasonable given the low technology maturity. For formaldehyde conversion, 17.00 USD/t_{FA} was adopted from Schmitz et al. (2016), largely corresponding to capex.[2]

Table 6. CAPEX assumptions

Units	Prices	Units	Prices
Inside battery limits (ISBL)		**Total invested capital (TIC)**	
Purchased Equipment Cost (PEC)	1	OSBL - Outside battery limits	0.12*ISBL
Purchased Equipment Installation	0.39	IC - Indirect cost	1.07*(ISBL+OSBL)
Instrumentation and controls	0.26	TDIC - Total direct and indirect cost	ISB+OSBL+IC
Piping	0.31	CPC - Process contingency	0.05*TDIC
Electrical Systems	0.1	CPJ - Project contingency	0.15*TDIC
Buildings (including services)	0.29	FCI - fixed capital investment	TDIC + CPC + CPJ
Yard Improvements	0.12	WC - Working capital	0.15*FCI
ISBL	2.47 * PEC	Location factor DE/US	1.1
		TIC_{FOAK}	FCI + WC

Reference to Guidelines B.9

We collected technical and economic data for each system element and each input and output. All technical data was related to functional units, while this was not possible for some of the economic data as they were in some cases only available in aggregated form (for multiple system elements). We collected the economic data either as country-average or global average which is in line with the goal to derive a rather global than local set of opportunities and barriers, see Guideline B.9.

7.4 CO_2 cost and credits, hydrogen and electricity

To make TEAs for CCU technologies more comparable, further information are provided to increase transparency for deriving a CO_2 price. As this study is an extension of the methanol worked example, the same scope, data and assumptions regarding CO_2 were used, which can be found there. As in the methanol study it was assumed to use flue gas from a hypothetical cement plant, capture CO_2 through a membrane-based process including a follow-up compression. Transport was not necessary to include as it was assumed that the capture occurs at the same hypothetical site. Overall the product system was assumed to capture 1 840 000 t_{CO2}/a. As the study differentiates between two locations and an overall 8 scenarios, different cost of CO_2 capture were obtained. The cost of CO_2 capture (COGM) result in 48.75 USD/t_{CO2} for the DE base case and 41.07 USD/t_{CO2} for the US base case, and drop in the scenarios B, C, D due to the lower assumed cost of electricity (see Table 7). These cost are country-specific but not location-specific. Furthermore, these costs represent the cost of capture only and not the cost of CO_2 avoided. The latter includes further effects such as further processing steps or substitution of inputs or outputs.

Reference to Guidelines B.10

In this study CO_2 capture and compression were included in the scope, deriving cost that are related to the full process and to the country and resulting in 35 to 49 USD/t_{CO2} depending on the scenario, see Guideline B.10.

Regarding hydrogen production, this study follows the methanol worked example that assumes a PEM water electrolysis process using currently available technology (for technical assumptions please refer to methanol worked example). It was challenging to derive valid capital cost for PEM water electrolysis, as the required system performance is about three orders of magnitude larger than current systems, leading to a large uncertainty. Overall equipment cost of 1 121 USD/kW were assumed, based on a reported stack price of 1.660 USD/kW and an assumed scaling factor of 0.95, reflecting the very limited economies of scale for PEM systems. For the low electrolyzer price scenario, a stack price of 330 USD/kW was assumed.[41] The cost of hydrogen (COGM) resulted in 4 445 USD/t in the DE base case and in 3 687 USD/t in the US base case, and dropped in the scenarios B, C, D due to the lower assumed cost of electricity as well as due the lower assumed capex (see Table 7). Analysing additional hydrogen production processes remains subject to future research.

Table 7. Cost of CO_2 and H_2

Scenario	COGM CO_2 captured USD/t	COGM H_2 USD/t
DE base case	48.95	4 445
DE scenario A	48.95	2 963
DE scenario B	42.10	1 965
DE scenario C	42.10	483
US base case	41.48	3 687
US scenario A	41.48	2 440
US scenario B	35.90	1 663
US scenario C	35.90	417

The study's results are particularly sensitive to the electricity price and a range of price assumptions are possible from the levelised cost of electricity (LCOE) for certain electricity generation technologies to grid prices for extra-large consumers. As LCOE price do not factor in intermittency of renewable energies and would require additional battery storage or intermittent hydrogen production, we excluded them for this analysis. Instead we chose cost of electricity for extra-large consumers, for Germany 47.36 USD/MWh based for extra-large industrial consumers excluding deductible taxes on data from IEA reported by UK BEIS [32] and for the US 38.65 USD/MWh based on US EIA data for companies with a consumption larger than 100 000 MWh reported in US EIA electricity report T8 (see Table 4).[33]

Reference to Guidelines B.11

The cost of hydrogen used in this study represents a cost of a full and process, including compression, but excluding transport and storage as in the methanol worked example. Process assumptions are country specific and focus on currently available technology in the base case and cost predictions for other scenarios. The assumed process is three orders of magnitude larger than today's versions, which creates substantial uncertainty. The chosen PEM technology is however the most mature renewable hydrogen technology available and this uncertainty cannot be circumvented. A future hydrogen scenario is included through low capex PEM based from forecasted data.

The electricity demand is calculated specific to the process and by system element for CO_2 capture, hydrogen generation and methanol synthesis. Electricity demand of downstream processes is excluded as data was not available, however it can be neglected as it only plays a minor role and the vast majority of energy demand is represented by steam and cooling. The electricity price is collected as grid mix, market-average and specific to consumption pattern from reported country-specific market data. See Guideline B.11.

Reference to Guidelines B.12

Only OME related assumptions are reported as the rest is already covered in the methanol worked example. Key technical and economic parameters necessary for calculation are reported in TEA flow diagram (figure 4) and assumptions regarding OPEX (table 1), capex (table 2) and cost of CO_2 (table 3). The calculation model can be requested by the interested readership for further information. See Guideline B.12.

8. Calculation and results

Reference to Checklist (see Guideline Chapter *8)*

Calculation of indicators

- ☐ State calculation procedures including any assumptions and estimates
- ☐ Explain methodology of financial analysis
- ☐ Include results of technical assessment
- ☐ Include results of economic assessment

Reference to Guidelines B.13

For calculation a single excel file was used, comprising of the sheets changelog, assumptions, benchmark values, TEA of system elements and results / sensitivity. The calculations were linked between the sheets and data gaps marked with comments. Result graphs were produced in Powerpoint with the Addon ThinkCell and based from a separate result excel file that allowed easy updating. See Guideline B.13.

8.1 Technical indicators

Overall mass efficiency for $OME_{3\text{-}5}$, $\dot{\eta}_{mass,OME,overall}$, expresses how much input mass ends is converted to the desired product. The indicator is calculated as the ratio of $OME_{3\text{-}5}$ output mass flow and all input mass flows.

$$\eta_{mass,OME,overall} = \frac{\dot{m}_{OME3-5}}{\sum_{inputs}\dot{m}_{input}} = \frac{\dot{m}_{OME3-5}}{\dot{m}_{flue\ gas} + \dot{m}_{H2O}}$$

Carbon efficiency for $OME_{3\text{-}5}$, $\dot{\eta}_{mass,OME,C}$, expresses how much carbon input is converted to the desired product. The indicator is calculated as the ratio of carbon in $OME_{3\text{-}5}$ output mass flow and carbon atom input mass flow.

$$\eta_{mass,OME,C} = \frac{\dot{m}_{OME3-5,C}}{\sum_{inputs}\dot{m}_{C}}$$

The energy efficiency $\dot{\eta}_{energy,OME}$ is calculated as the ratio of work from $OME_{3\text{-}5}$ fuel available for combustion on a lower heating (LHV) value basis and energy flow inputs, in this case work from electricity and work from heat energy of steam adjusted by carnot efficiency of 44% (optimistically assuming 50 bar saturated steam at 527 K and ambient temperature of 293 K). Work from potential and kinematic energy is judged to be of minor influence for the product system in focus and neglected in this calculation.

$$\eta_{energy,OME} = \frac{\dot{w}_{OME3-5}}{\sum_i \dot{w}_i} = \frac{\dot{w}_{OME3-5}}{\dot{w}_{electricity} + \dot{w}_{steam}} = \frac{\dot{w}_{OME3-5}}{\dot{w}_{electricity} + \eta_{carnot} * \dot{q}_{steam}}$$

All indicators are calculated for the product system corresponding to TRL 4 (preliminary process development).[5,6]

Table 8. Results of technical indicators

	TRL 4
$\eta_{\text{mass,OME,overall}}$	0.11
$\eta_{\text{mass,OME,C}}$	0.87
$\eta_{\text{energy,OME}}$	0.36

The here discussed product system reaches a mass efficiency of 11%, meaning that one tenth of all input mass is converted to the desired $OME_{3\text{-}5}$; other large outputs streams are flue gas stream (53% of input mass) and water (17% of input mass). The carbon efficiency reaches 87%, meaning that seven out of eight carbon atoms in the flue gas are converted to the desired $OME_{3\text{-}5}$. The energy efficiency reaches 36%, meaning that one third of all electricity and steam energy input is stored chemically in the desired $OME_{3\text{-}5}$ fuel; the major share of energy input is required in water electrolysis.

8.2 Economic indicators

8.2.1 Direct OPEX

Direct operational expenditure is calculated following the technical inventory and the reported prices for each input. The results for the base case DE and base case US are reported in Table 8.

Table 9. Direct OPEX results

	CO_2 capture	H_2O elect.	MeOH	Utilities	FA, TRI, OME_1, $OME_{3\text{-}5}$	total	
Base case DE							
Raw materials	0.00	0.35	0.72	0.00	0.00	1.06	$\text{USD/GJ}_{\text{OME3-5}}$
Energy and utilities	0.66	33.09	0.48	0.10	6.76	41.08	$\text{USD/GJ}_{\text{OME3-5}}$
Base case US							
Raw materials	0.00	0.35	0.72	0.00	0.00	1.69	$\text{USD/GJ}_{\text{OME3-5}}$
Energy and utilities	0.54	27.00	0.39	0.09	6.76	34.78	$\text{USD/GJ}_{\text{OME3-5}}$

8.2.2 Indirect OPEX

Following the assumptions and procedures presented in 7.3, an overall staff of 122 employees is estimated, resulting in labour cost of 1.23 $\text{USD/GJ}_{\text{OME3-5}}$ for Germany and 1.26 $\text{USD/GJ}_{\text{OME3-5}}$ for the United States (see Table 9). In comparison, the shortcut approach used in Schmitz et al. finds labour cost of 0.79 $\text{USD/GJ}_{\text{OME3-}}$

$_5$ (assuming eight plants, five shifts, four workers per shift, one technician and one manager per plant), excluding direct and general overheads. Including overheads increases the labour cost to 1.96 USD/GJ$_{OME3-5}$. Overall, both methods result in cost ~ 1-2 USD/GJ$_{OME3-5}$ and the final results are not sensitive to changes in the choice of method for labour cost estimation.

Table 10. Labour cost, number of regular staff

	CO_2 capture	H_2O elect.	MeOH	Utilities	FA	TRI	OME_1	OME_{3-5}	total	
$N_{fu.sol}$	0	0	0	0	0	0	0	0		
$N_{fu.nso}$	31	5	20	19	11	12	4	4		
N_{shifts}	5	5	5	5	5	5	5	5		
$N_{staff.reg}$	18	14	17	16	15	15	13	13	122	
$\pi_{labour.DE}$	0.18	0.14	0.17	0.16	0.15	0.15	0.14	0.14	1.23	USD/GJ$_{OME3-5}$
$\pi_{labour.US}$	0.19	0.14	0.17	0.17	0.15	0.16	0.14	0.14	1.26	USD/GJ$_{OME3-5}$

Following 7.3, indirect OPEX are calculated. Labour cost are calculated for each system element. All other positions are calculated for CO_2 capture, water electrolysis, methanol synthesis and utilities and one FA/TRI/OME_1/OME_{3-5} black box, as the capex estimate only exists for the combination of these processes. For the purpose of brevity only the total values for base case DE and base case US are presented in Table 10.

Table 11: Indirect OPEX results

	Base case DE	Base case US	
Maintenance	4.16	3.78	USD/GJ$_{OME3-5}$
Replacement	1.16	1.05	USD/GJ$_{OME3-5}$
Labour	1.23	1.26	USD/GJ$_{OME3-5}$
Tax & insurance	3.75	3.40	USD/GJ$_{OME3-5}$
Interest	2.25	2.04	USD/GJ$_{OME3-5}$
Total	12.54	11.54	USD/GJ$_{OME3-5}$

Reference to Guidelines B.15

Opex were calculated distinct for direct and indirect opex. Direct opex was related to material, energy and utility consumption, building on the level of detail provided by the technical inventory. Most indirect opex positions were calculated as factors. Calculating fixed opex position in more detail, as presented for personnel cost where a unit counting approach was used, did not add significant detail in this case. Market-average price data (10-year average) was used as recommended for research and development. See Guideline B.15.

8.2.3 CAPEX

The calculation of CAPEX for the system elements CO_2 capture, water electrolysis, methanol conversion and utilities follow the methanol worked example. First, core components of each system element were identified. Second cost and capacity data were collected for each component. Third for each component the cost was adjusted to the required capacity through the scaling exponent method, resulting in the total purchased equipment cost (TPEC). Fourth the total capital investment (TCI) was calculated through the factorial method, including inside battery limits (ISBL), outside battery limits (OSBL) that includes the balance of the plant (BOP) cost, indirect cost (IC) and working capital (WC). Calculation is discussed there in more detail in the methanol worked example,[1] results can be found in Table 12.

Capex for FA, TRI, OME_1 and $OME_{3\text{-}5}$ conversion were estimated as black box following a short method as described in Schmitz et al. (2016).[2] For deriving consistent intermediate results for example on ISBL, a "forced detail" approach is applied. Starting from the TCI_{NOAK} presented in Schmitz et al. (2016) of 274 million USD for an US location, an ISBL of 156 million USD can be derived, reversing the assumptions. Overall capex of 45.03 $USD/t_{OME3\text{-}5}$ (case DE) and 42.03 $USD/t_{OME3\text{-}5}$ (case DE) are calculated, see Table 11.

Table 12. CAPEX for FA, TRI, OME1, OME$_{3\text{-}5}$ conversion, forced detail

	Base case US	**Base case DE**	
ISBL Total purchased equipment cost (TPEC)	156.339.153		USD
OSBL	18.760.698		USD
Indirect cost (IC)	23.450.873		USD
Total direct and indirect cost (TDIC)	198.550.725		USD
Process contingency	9.927.536		USD
Project contingency	29.782.609		USD
Fixed Capital Investment (FCI)	238.260.870		USD
Working Capital (WC)	35.739.130		USD
NOAK TCI	274.000.000		USD
Location factor	1.0	1.1	
NOAK LF TCI	274.000.000	301.400.000	USD
CAPEX TRI, OME1, OME3-5 conversion	0.63	0.63	USD/GJ$_{OME3\text{-}5}$
CAPEX FA conversion	1.58	1.73	USD/GJ$_{OME3\text{-}5}$
Total CAPEX	2.21	2.36	USD/GJ$_{OME3\text{-}5}$

Reference to Guidelines B.14

In accordance to the assessment goal of identifying opportunities and barriers, AACE estimate class 4 and 5 methods were used and assumptions were presented in the inventory chapter. The early maturity of the OME production elements required the calculations only to stay at a lower level of accuracy (short method), while the methods for the Methanol elements reached a higher level of detail (scaling exponent and factored method). Methods from other studies and from major TEA textbooks were used, adjustments were discussed were taken. OSBL were calculated dependent on ISBL and both stated. Forced detail was used for reasons of comparison, but used with caution and caused no impact on indicator calculation. Learning curves were considered for NOAK TCI. Contingency of 15% on total direct and indirect cost was added. See Guideline B.14.

8.2.4 Cost of goods manufactured (COGM)

The cost of goods manufactured are calculated from the sum of direct OPEX, indirect OPEX and CAPEX of each individual system element. Results are shown in *Table 12*.

$$\pi_{COGM,OME3-5} = \sum_{system\ elements} \pi_{opex,direct} + \pi_{opex,indirect} + \pi_{capex}$$

Table 13. COGM results

	CO_2 capture	H_2O elect.	MeOH	Utilities	FA/TRI/ OME_1/ OME_{3-5}	total	
Base case DE							
OPEX direct	0.66	33.44	1.19	0.10	6.76	42.15	USD/GJ_{OME3-5}
OPEX indirect	1.27	7.06	1.89	1.21	1.12	12.54	USD/GJ_{OME3-5}
CAPEX	2.79	18.81	6.68	4.04	2.36	34.69	USD/GJ_{OME3-5}
COGM	4.72	59.31	9.77	5.35	10.24	89.38	USD/GJ_{OME3-5}
Base case US							
OPEX direct	0.54	27.35	1.11	0.09	6.76	35.84	USD/GJ_{OME3-5}
OPEX indirect	1.17	6.39	1.73	1.11	1.13	11.54	USD/GJ_{OME3-5}
CAPEX	2.29	15.45	5.49	3.32	2.21	28.75	USD/GJ_{OME3-5}
COGM	4.00	49.19	8.32	4.52	10.10	76.14	USD/GJ_{OME3-5}

The overall COGM sum up to 89 USD/GJ $_{OME3-5}$ (base case DE) and 76 USD/GJ $_{OME3-5}$ (base case US); the largest two contributing factors for both locations are water electrolysis direct opex (33 / 27 USD/GJ_{OME3-5}) and water electrolysis capex (19 / 15 USD/GJ_{OME3-5}). The contribution of OPEX (direct, indirect) and capex of OME_{3-5} production for the DE and US base case are shown in Figure 2 and Figure 3.

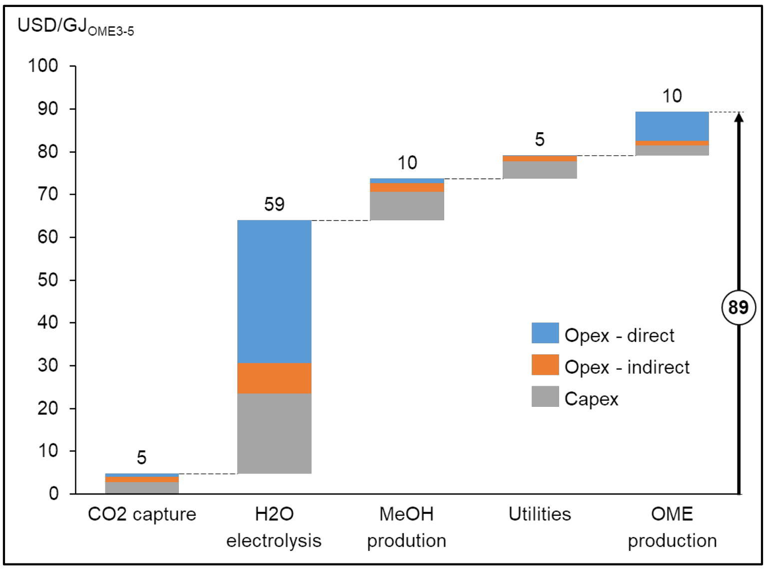

Figure 2. COGM for DE base case

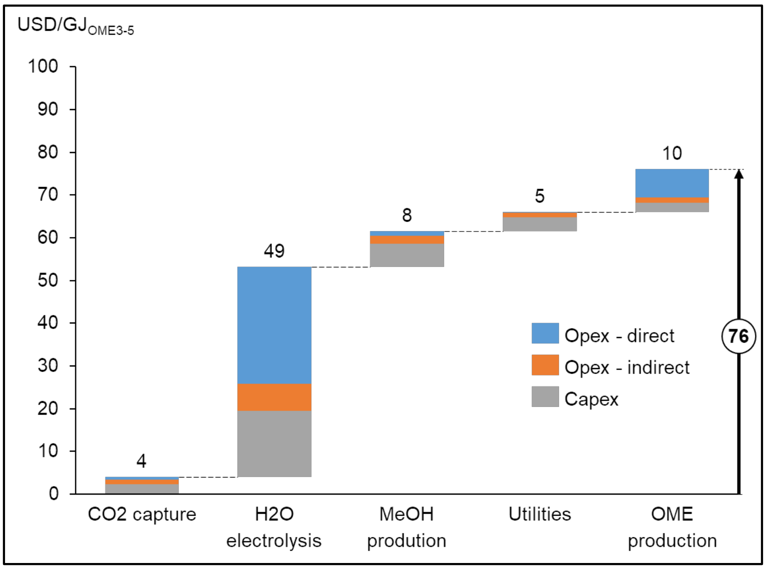

Figure 3. COGM for US base case

This analysis finds that the price of CO_2 and electricity based OME_{3-5} is ~110 % higher than diesel at a German gas station and ~210 % higher than diesel at a US gas station. While Schmitz et al. (2016) find that OME_{3-5} based on market purchased methanol could reach a price only 18% higher than diesel; this study finds that the price for OME_{3-5} based on market methanol could actually be even cheaper in the case of Germany, but not for the US.[2] A comparison with the selected benchmarks is shown in *Figure 4*.

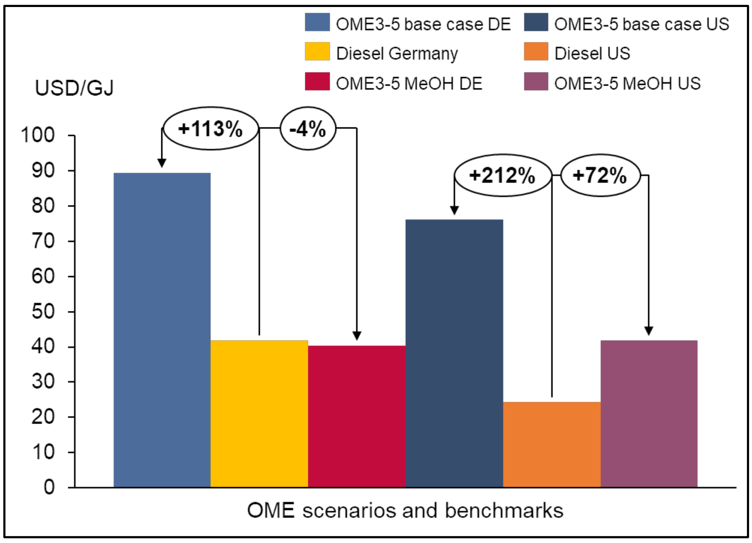

Figure 4. OME scenarios and benchmarks

Reference to Guidelines B.16

No profitability indicator is calculated due to the early maturity of the technologies and the goal of the study. A comparison of COGM with benchmark sales prices was used to analyse whether or not a profit can be expected. As both base cases show significantly larger values, profitability calculation was omitted. Normalisation of values, while generally being useful was not applied in this case due to the multiple cases and benchmarks that were compared. See Guideline B.16.

9. Interpretation

Reference to Checklist (see Guideline Chapter *8)*

Interpretation

- ☐ Include and describe the results
- ☐ Include and describe uncertainty and sensitivity analysis
- ☐ State assumptions and limitation associated with the assumptions, methods and interpretation of results
- ☐ Include conclusions
- ☐ Include recommendations, if any

9.1 Uncertainty analysis

Reliable quantitative data for uncertainty analysis was not available due to the low technology maturity of the OME conversion process. Uncertainty in this analysis depends on each system element and its maturity. CO_2 capture and FA/TRI/OME_1/ OME_{3-5} conversion are judged AACE class 5, translating into an accuracy of -30% to +50%. Hydrogen, methanol and utilities are judged AACE class 4 with an accuracy level of -20% to +30%.[42] The major source of uncertainty is the black box model of FA/TRI/OME_1/OME_{3-5} conversion in the assessment model. Modelling these four conversions on the same level of detail as the other system elements would result uncertainty, but requires a large amount of additional technical input data that was not available at the time of assessment. Modelling on the same level of detail would result in a more detailed electricity and steam requirements, allowing heat integration and potentially also a reduction of opex; more detailed modelling would also increase the granularity of equipment allowing for a better estimate of capex and potentially capex optimization based on operating conditions.

9.2 Sensitivity analysis

9.2.1 Local sensitivity analysis

The sensitivity of the results is analysed discussed for three indicators: mass efficiency, energy efficiency and COGM. The analysis of COGM scenarios can also be regarded as sensitivity analysis, but is discussed in the scenario chapter. Local sensitivity method is applied due to the nature of the goal, the early technology maturity of the system elements and the low number of available data points.

The overall mass efficiency is 11% - a rather low value. This is not be necessarily bad, as the occurring waste products are water, oxygen and flue gas – all have limited environmental impacts (but a thorough analysis is required to make a final statement). Potentially the output of waste streams can be reduced by recycling processed flue gas or output water. For local sensitivity the two factors consumption of water and flue gas were varied, see Figure 5. Overall a decrease of flue gas or water consumption increases mass efficiency. The effect is rather small, as much stronger increases in mass efficiency are required to significantly change the indicator.

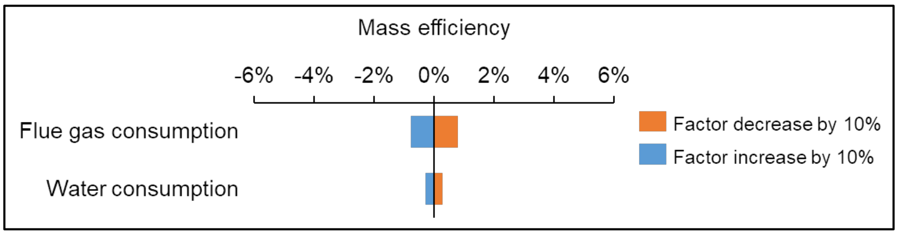

Figure 5. Mass efficiency change varying factors by +/- 10%

The product system in focus uses carbon quite efficiently – the obtained carbon efficiency of 87% is not far from the ideal value of 100% and only a minor waste stream of CO_2 occur in the formaldehyde production. A further improvement or carbon efficiency is possible, especially through reusing also the occurring CO_2 emissions, raising carbon efficiency to 94%. For local sensitivity analysis the two CO_2 content in the flue gas and the capture rate were varied. A decrease of CO_2 content in the flue gas leads to an increase in carbon efficiency; a decrease of the capture rate however leads to a decrease of carbon efficiency. Carbon efficiency is relatively sensitive to both factors.

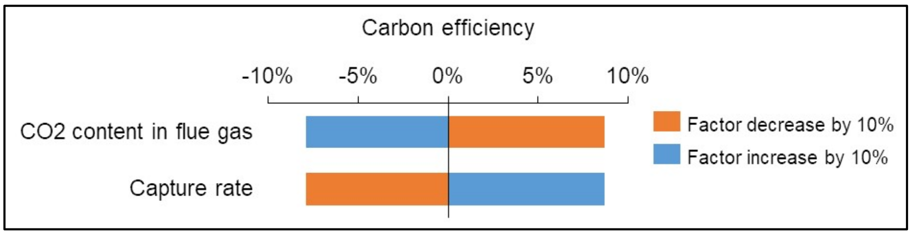

Figure 6. Carbon efficiency change varying factors by +/- 10%

For local sensitivity analysis, the energy consumptions of system elements were varied. Only two factors contribute to a significant change of energy efficiency (change larger than 1%), electricity consumption of electrolysis and steam consumption of OME conversion, see Figure 6. Energy efficiency could be further increased by integrating heat flows, for example at the moment low pressure steam generation in the formaldehyde process is not taken into account.

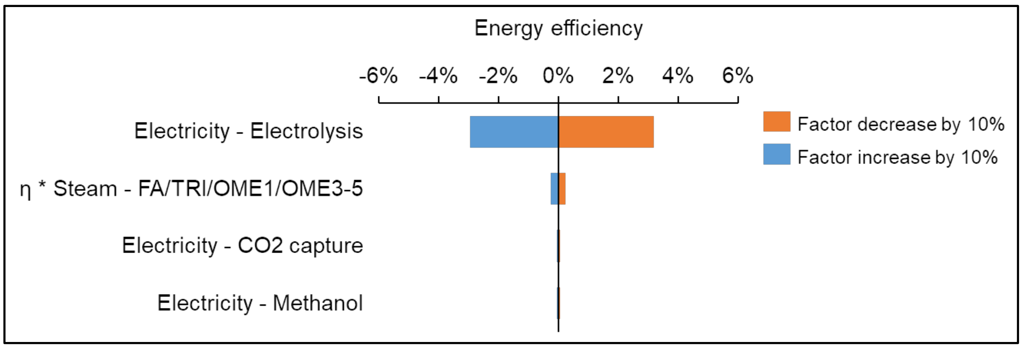

Figure 7. Energy efficiency change varying factors by +/- 10%

All major economic assumptions were varied by (increase and decrease by 10%) and the effect on COGM analysed. Overall five factors contributed to a significant change of COGM (more than 1%), see the 'tornado diagram' Figure 7. COGM is the most sensitive to changes in currency, chemical engineering plant cost index (CEPCI), electricity consumption, location factor and electrolyzer capex. Currency, CEPCI and location are all related to either time of analysis or location of the site, highlighting the importance of regional and time series influences in assessments.

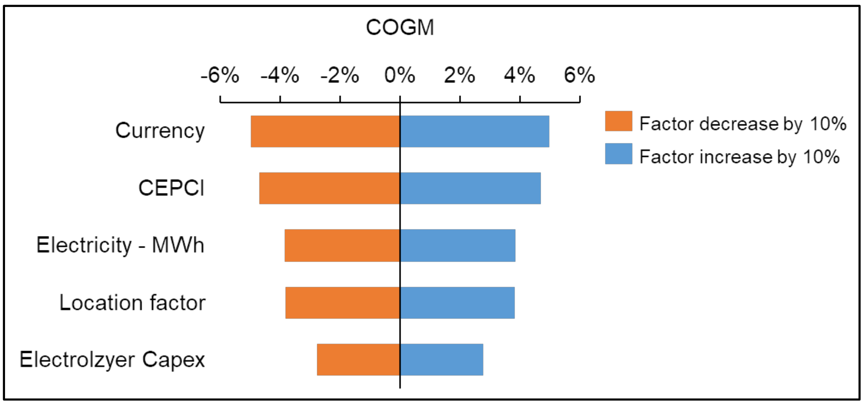

Figure 8. COGM change varying factors by decrease or increase of 10%

9.2.2 Scenario analysis

In the following four scenarios (base case and 3 price scenarios A, B, C) are analysed for two locations (Germany and US gulf coast). In the following scenarios four out of five significant impact factors for COGM are varied (currency, electricity price, location factor, electrolyser capex).

The four scenarios are presented in Figure 8 and Figure 9. The analysis shows for both locations that electrolysis is the major technical and economic barrier for implementing the assumed product system (see base case). The optimistic electrolyser capex assumption to 330 USD/MW reduces its share largely (see scenario A), however current cost of grid electricity would still result in too high COGM. Assuming free electricity reduces the COGM even stronger (see scenario B), but remaining high electrolyzer capex would lead to too high COGM. In the case of a drastic reduction of both, electricity cost and electrolyzer capex, competitive COGM can be achieved in Germany (13% lower than diesel prices), however not in the US (23% higher than diesel prices).

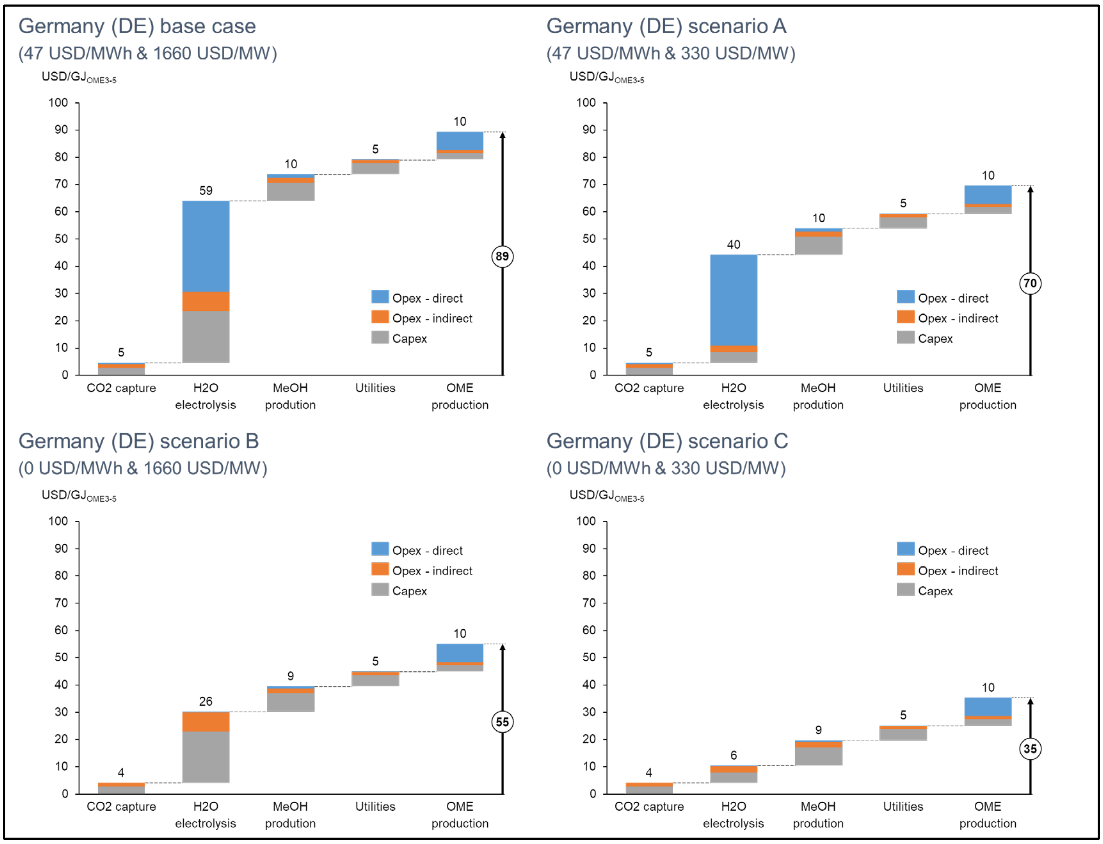

Figure 9. Germany (DE) scenarios detailed view

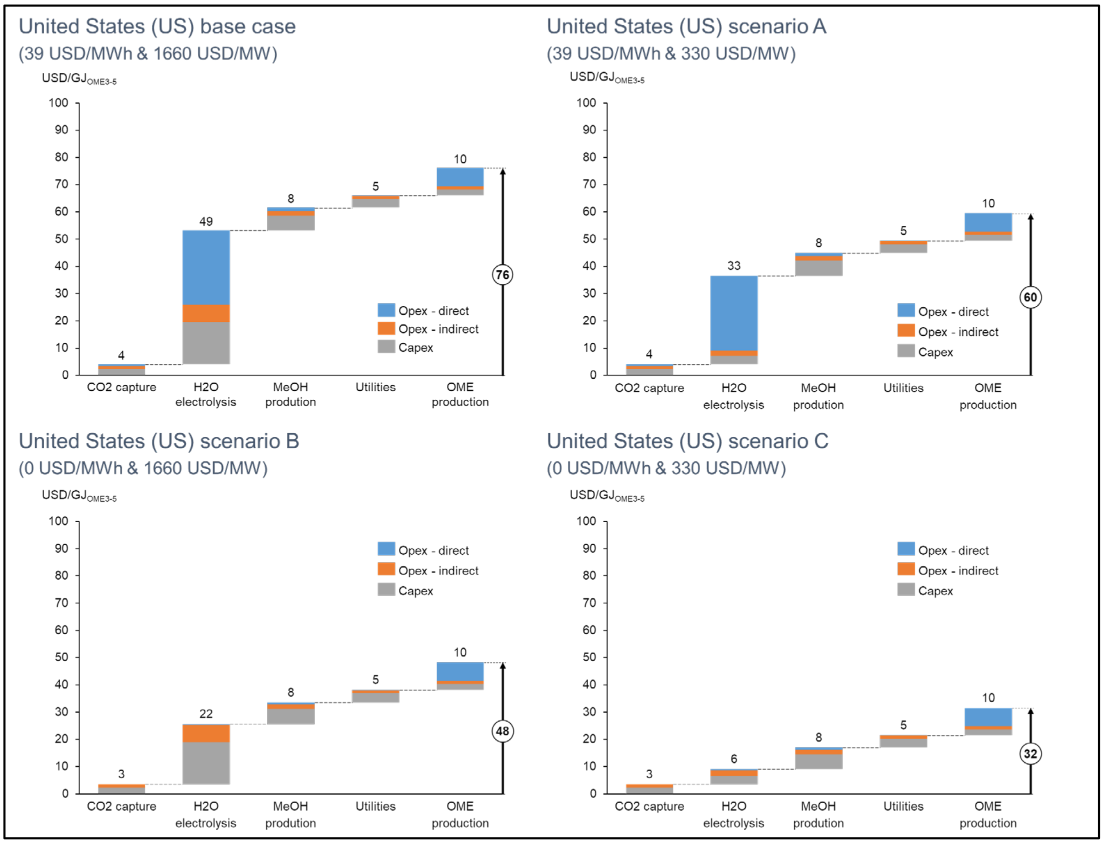

Figure 10. United States (US) base case and scenarios A, B, C

When comparing the total values of all four scenarios with the benchmark values (see Figure 10 and Figure 11), the analysis shows even the optimistic cases do not result in competitive COGM for the United States. In contrast, in Germany the highly optimistic scenario D is competitive to the 10-year average diesel price, as the German price for diesel is higher. The main reasons for higher diesel prices in Germany is suspected to be higher fuel taxes. A comparison of tax-free COGM and taxed diesel prices remains valid from the authors perspective as it is yet unclear if and how OME fuels would be taxed as they provide additional environmental services such as the reduction of soot and NO_x and the reduction of carbon intensity of heavy duty transportation. It should however be noted that even the highly optimistic scenario D is not competitive to the 2016 diesel prices in Germany, as this year fell into a low price period. Another interesting result is the lower price of Methanol-based OME_{3-5} compared to diesel prices in Germany. Upgrading conventionally produced methanol could provide a economically feasible first step for OME_{3-5} production for Germany. Future studies might also want to include additional methanol synthesis pathways such as steam methane reforming with carbon capture and storage (SMR-CCS).

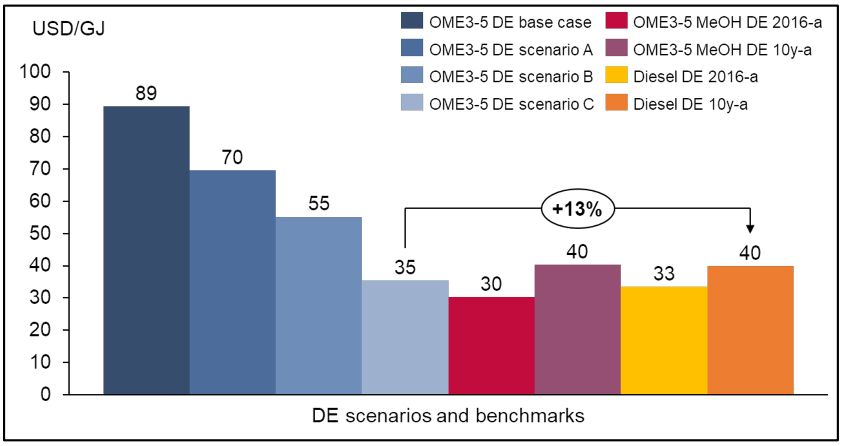

Figure 11. Germany (DE) scenario and benchmark values overview

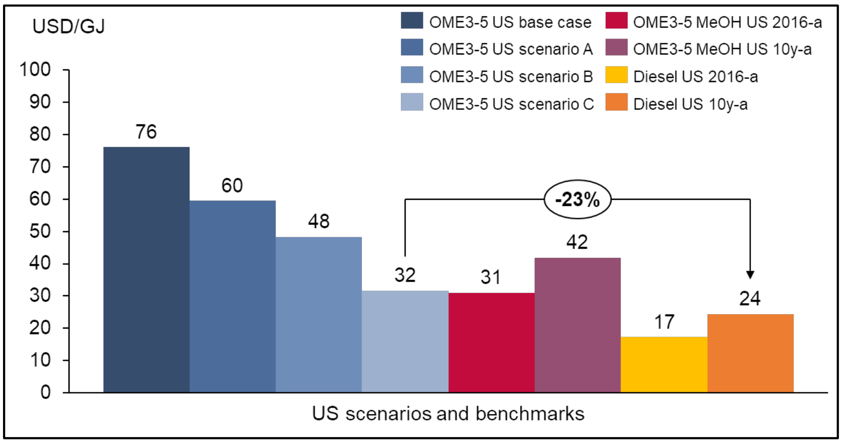

Figure 12. United States (US) scenario and benchmark values overview

9.2.3 Priorities for future research

Following the uncertainty and sensitivity analysis, priorities for improving future assessment results are derived and clustered by lack of quality and significance as recommended in the Guidelines (see Figure 12). The OME conversion model, the electrolyser capex model and location data are judged to be lacking quality and while being significant for the model results – improving them should be a high priority in future research. The technical electrolyzer model and using company specific electricity prices are also judged to be significant for model results, however the current available quality seems sufficient for the goal of the study (mid priority for future research). Process optimisation, applying strategies for heat integration and waste reduction, as well as a time series comparison with benchmark values would also help to improve results, however changes in these fields are not expected to be highly significant for the assessment results.

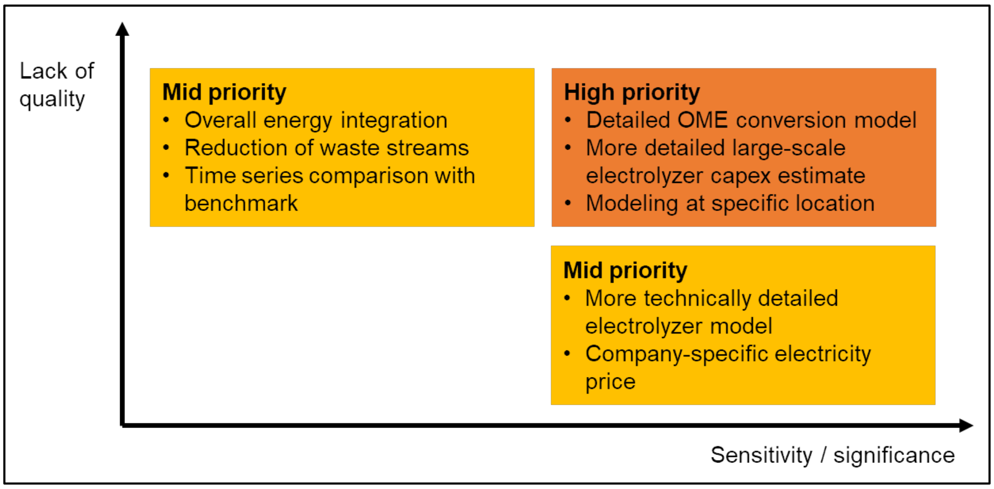

Figure 13. Priorities for future research

Reference to Guidelines B.18

Output uncertainty was identified by system element by AACE class judgement. Local sensitivity analysis was conducted on three output indicators. Major identified factors are factors based on the site location (currency, CEPCI, location factor), electricity consumption and electrolyzer capex. Conclusions for sensitivity and future research priorities are presented. See Guideline B.18.

10. Concluding remarks

Overall $OME_{3\text{-}5}$ fuel provides an intriguing emission and environmental impact reduction technology for heavy duty transportation. The early stage evaluation shows mixed results of COGM that are not competitive but within reach if deployment of renewable electricity continues at its strong momentum, if low-emission hydrogen or methanol can be produced at very low cost in large scales and if political and industrial action continue to push for emissions reduction in transportation. Core R&D priority remains the provision of these energy vectors, benchmark values today are set by diesel fuel in the future probably by hydrogen fuel cell trucks.

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