Evaluating technology options to mitigate greenhouse gas emissions

Sustainability in Petrochemicals

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SUSTAINABILITY IN PETROCHEMICALS

Key Messages

- **Petrochemicals** are an important building block of a huge range of products that underpin modern daily life and economic activity.
- The potential to sustainably produce **methanol, olefins and ammonia/urea** has been investigated.
- As well as its use as a fuel, **methanol** may be used as a feedstock for a wide range of downstream products. It has a healthy and growing global market, particularly in China. Efficient, sustainable production of methanol could drive the decarbonisation of the petrochemicals industry.
- **Olefins** are crucial intermediates in the manufacture of a vast range of products. Ethylene and propylene are basic petrochemicals used primarily to manufacture plastics, while butadiene is used to create a variety of synthetic rubbers. Driven by population and fast economic growth, the manufacturing of such basic materials has moved from Europe and North America to East Asia, and so has the demand for olefins.
- Biomass and wind-sourced methane-to-olefin routes, while more costly, showed potential to decrease carbon emissions compared with the conventional naphtha-cracking route. Unabated coal-to-olefins exhibit a higher environmental impact, though the application of **carbon capture and storage** (CCS) would reduce these emissions markedly.
- A reduction in crude oil demand associated with transport fuels seems quite possible in the medium-term future, which would lower feedstock costs, improve their competitive advantage and, consequently, shift olefin production back towards heavier hydrocarbons.
- The use of **ammonia** to produce fertilisers is essentially driven by the demand for agricultural products. Combining hydrogen, derived from natural gas, with airborne nitrogen is the traditional process for ammonia production. Consequently, ammonia production and hence fertiliser production has traditionally been driven towards the cheapest source of natural gas. At the same time, food security issues incentivise local fertiliser production, leading to a tension between these two drivers, i.e. to produce fertilisers where natural gas is cheapest or where they are in greatest demand. Increasingly, the cost of the primary feedstock dominates, leading to production at otherwise stranded sources of natural gas or, in the case of China, where there is cheap coal.
- Of the alternative routes to ammonia production investigated, the biomass-based route was found to be the most environmentally attractive, followed by electrolysis based on wind power. However, given sustainability concerns, stakeholders, when consulted, felt uncomfortable proposing biomass as a resource to produce petrochemicals.
- While there are several promising options to **decarbonise** petrochemical production, there is no panacea. Each of the options are disadvantaged by barriers relating to cost, resource availability/depletion, water usage or, in the case of bio-based feedstocks, creating competition with other critical industries such as agro-industry and food security.
- A cost-effective process using **hydrogen** from a low-carbon source would offer an excellent opportunity to decarbonise petrochemical production.
- A unique challenge to the petrochemical industry is the need to **decarbonise heat**. While options exist to decarbonise electricity, heat is more difficult to decarbonise.
- The implementation of CCS has potential to lower carbon emissions in the production of petrochemicals and, clearly, CCS with thermal power plants would greatly assist in lowering the emissions associated with electricity generation.
- With **carbon capture and utilisation** (CCU), on the other hand, care must be taken to account for net emissions associated with the life cycle of any products. For example, one

route to methanol production is via hydrogenation of captured CO_2: even though the hydrogen may come from a low-carbon source, depending on the end product of the process, the CO_2 utilised is ultimately very likely to be released to the atmosphere. Similarly, urea may be produced from ammonia and captured CO_2, where again the CO_2 would also eventually be released.

- Given that the petrochemical industry will remain dependent on fossil fuels for some time, a strong **policy and regulatory framework** is required. Stakeholders consulted suggested carbon prices and emissions performance standards were the most popular policy options.
- The global nature of trade for petrochemicals necessitates a global approach to the application of policies or regulation. The need for a level playing field was considered essential.
- High levels of international trade create the potential for **'carbon leakage'**. The application of carbon pricing or emissions performance standards would need to be carefully managed.
- Given the 25 to 40-year economic lifetime of plants, technology lock-in can be a significant barrier to short and medium-term decarbonisation. A good example of this is the investment in coal-based petrochemical production in China. Even with a 2°C-consistent CO_2 price, the environmentally sustainable production of petrochemicals in China over the first half of this century appears challenging.

Background to the study

Since the Rio Earth Summit in 1992, economic development has increasingly proceeded hand-in-hand with sustainable development, i.e. balancing economic, environmental and societal responsibilities. The Paris Agreement adopted in December 2015 at the UNFCCC's Conference of the Parties (COP21) put forward a pathway to low-carbon development by giving signatory parties the opportunity to present their (intended) nationally-determined contributions without penalising their social and economic development.

Industry will reduce its carbon footprint by reducing its greenhouse gas (GHG) emissions and improving its energy efficiency goals. The global chemical industry currently contributes around 4.5% of total anthropogenic GHG emissions. Petrochemicals, a sub-sector of the global chemical industry, are an important building block of a large range of products that underpin modern daily life and economic activity. There is a drive to produce petrochemical products in a more sustainable manner and this study explores some of the possible options to achieve this outcome.

The study was undertaken at Imperial College London by a team from its Sustainable Gas Institute led by Dr. Adam Hawkes.

Scope of Work

The primary aim of this study is to establish a methodology to assess different aspects of the sustainability of petrochemical production. The report investigates a combination of industry drivers on the historic, current and future status of the petrochemical industry. Three categories of petrochemicals are analysed, namely methanol, olefins and ammonia/urea. For each, the following assessments were undertaken to gain insight into the sustainability prospects of the industry:

- **Market analysis.** An assessment of the historic and current status of market trade, including trends in end-uses, feedstocks, demand, production and international trade. Demand projections for each chemical are made based on collected data.
- **Process engineering characterisation** of the current and low carbon alternative routes and feedstocks to produce the key petrochemical productions.
- **Environmental life cycle assessment** of the various feedstocks and production methods for each petrochemical and a contribution analysis of the key environmental impacts.

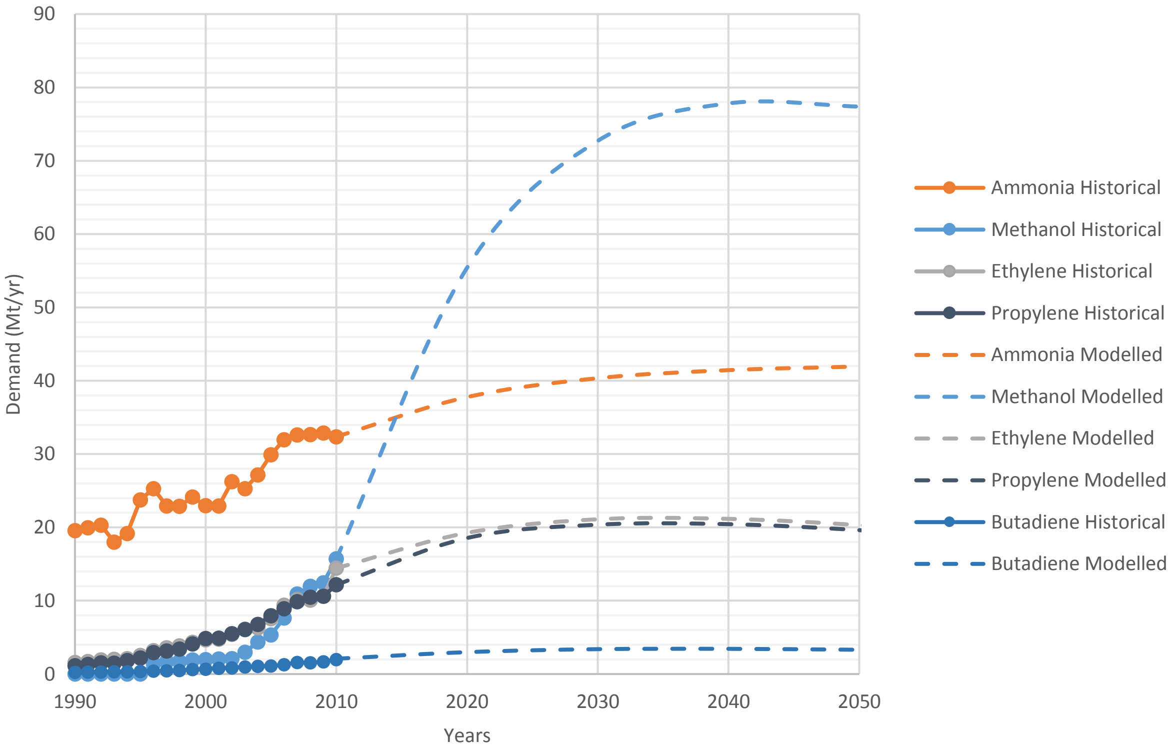
- **Market projection** of petrochemical production and technology mixes for a key region, China, for the time period 2010 – 2050.
- A series of **expert stakeholder interviews** on views of how the petrochemical industry may progress in terms of demand, costs, environmental impacts and policy drivers.

It is important to recognise that the study does not profess to cover all aspects of sustainability of petrochemicals, but rather a constrained range of environmental and socio-economic impacts.

Findings of the Study

A perspective is offered on the potential for the petrochemical industry to decarbonise and the mechanisms by which this may be enabled. Key findings relate to changing demands and costs, and decarbonisation options and mechanisms.

Changing demands and costs. Global demand for petrochemicals is likely to continue to grow, particularly for methanol, but also for ammonia and the olefins ethylene, propylene and butadiene. An example of projected demand growth is shown below for China, but regional variability is likely to be high. Whilst CO_2 emissions may be decoupled from economic growth and demand growth, for example via increased use of renewable energy to generate electricity, other environmental impacts such as water footprint may not. Consequently, with continued demand growth there will be continued environmental challenges.



Historical demand and projections of petrochemicals for China up to 2050.

Methanol may become an increasingly important petrochemical. It has a highly diverse range of end-uses, with a large proportion used currently as a component in transport fuel. In transport fuel, it may be added directly to gasoline or, when reacted with isobutylene, as methyl tertiary butyl ether (MTBE), a fuel additive. Given that the United States has eliminated MTBE's usage as a transport additive due to environmental concerns, it could well reduce elsewhere over time (e.g. in China). Even so, the potential of methanol as an intermediate chemical in a multitude of applications suggests that demand is still likely to increase in the future.

Methanol may be produced, for example, via the catalytic hydrogenation of CO_2, where the hydrogen comes from a low-carbon source. It can then be used as a feedstock for other bulk petrochemicals, in particular olefin production. Whilst, in general, methanol-to-olefin (MTO) processes are not economically feasible at present (except in China when produced from cheap coal), a change in feedstock price or regulation could provide the impetus for a rapid increase in demand.

Olefins are important intermediates in the production of a vast range of goods that underpin daily life and economic activity. Ethylene and propylene are used primarily to manufacture plastics, while butadiene is used to create a variety of rubbers.

Historically, the steam cracking of naphtha has been the starting point for olefin production, but with cheap natural gas liquids becoming increasingly available, naphtha is being replaced as a feedstock. There has been significant investment in olefin plant in the Middle East using natural gas liquids (NGLs) as a feedstock, freeing up the traditional feedstock of naphtha for gasoline manufacture. Additionally, a focus on self-sufficiency in both China and the United States has led to changing trade dynamics of olefins. China has rapidly expanded its coal-to-olefin capacity, and the United States has utilised NGLs associated with recent growth in shale gas production. This growth in China, the United States and the Middle East has the potential to create global excess capacity.

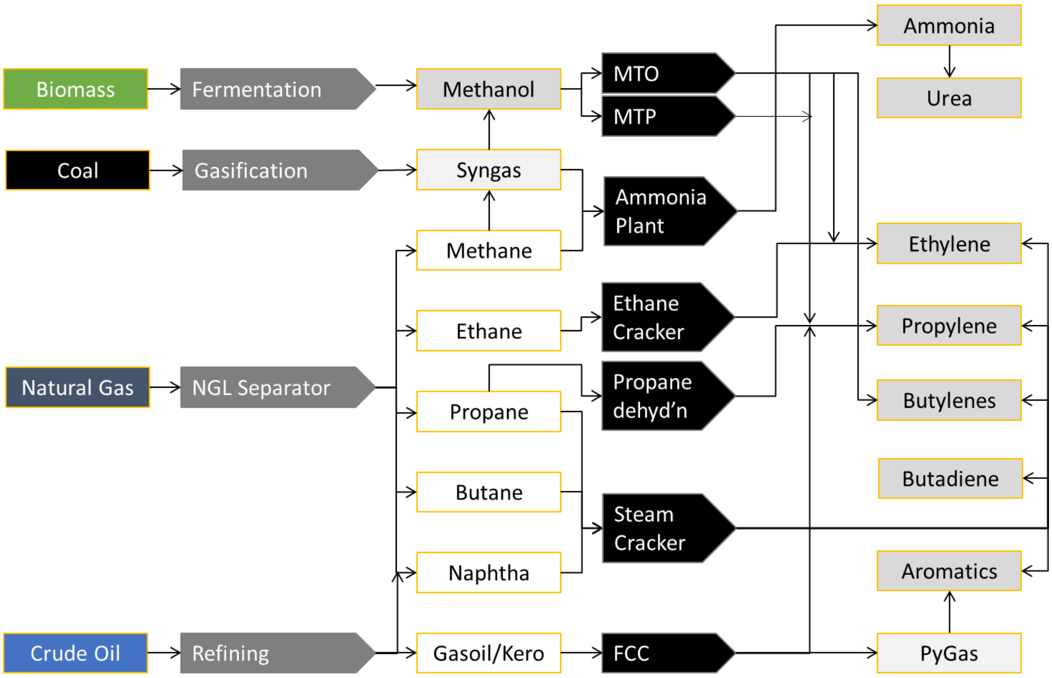
Ammonia demand is largely driven by fertiliser demand, which in turn is driven by demand for agricultural products. Natural gas is the key feedstock for ammonia production worldwide, driving production towards the cheapest source of that gas. At the same time, food security issues incentivise local fertiliser production, leading to a tension between these drivers. Increasingly, the cost of the primary feedstock is the key issue, leading to production at otherwise stranded sources of natural gas or, in the case of China, where there is cheap coal.

In the longer term, prices for each of the commodities considered are highly uncertain. Two opposing price drivers were frequently raised in the stakeholder interviews: the impact of reduced oil demand from transport and the impact of climate-related policy and regulation. The growth in renewable electricity generation and the potential growth in electric vehicle uptake may significantly reduce the future demand for oil. This could result in increased availability of oil to the petrochemical industry, thus reducing the price. Given that petrochemical products typically represent the minor share of products from a refinery, the majority being fuel products, this could spell a sea-change for refinery production business models. The impact is likely to be seen not only in terms of petrochemical prices, but also as a change to a heavier hydrocarbon feedstock, which will change processing needs.

A further note is that international drives towards recycling and re-use of products such as consumer plastics may reduce the demand for petrochemicals significantly and signify a future of high uncertainty and potential regional variability.

Decarbonisation options. First and foremost, unabated coal-based feedstocks typically have the highest environmental impact for all petrochemicals studied, in particular with respect to global warming potential: all other options for feedstocks and processes perform significantly better with the exception of unabated coal-based electrolysis routes.

As shown in the figure below, there are many promising options to decarbonise petrochemical production, including the use of bio-based or renewable feedstocks and the use of innovative catalytic processes. However, there is clearly no silver bullet and each option exhibits disadvantages or barriers relating to cost, resource availability or, in the case of bio-based feedstocks, creating competition with other critical industries such as agro-industry and food security.



Basic routes to petrochemical products. MTO: methanol-to-olefin, MTP: methanol-to-propylene, FCC: fluidised catalytic cracking.

Using hydrogen as a feedstock from a low-carbon source may represent a good opportunity for decarbonisation via gasification of low-carbon feedstocks or via low-carbon electrolysis. However, currently, these are not cost-effective and, while these technologies may help to meet climate change targets, they can lead to other environmental impacts, e.g. higher water usage, land-use change issues and metal resource depletions.

While bio-based feedstocks performed well in the environmental assessment of this study, feedback from the stakeholder interviews suggest their use is highly contentious. With the many competing applications/industries for bio-based feedstocks, it is debatable which is most appropriate/efficient for what is a limited resource. Many bio-based feedstocks are not molecularly similar to petrochemical products, resulting in a higher energy demand and, consequently, high cost/low efficiency.

A unique challenge to the petrochemical industry is the need to decarbonise heat. It is an energy intensive industry but, whilst there are many options for low-carbon electricity, low-carbon heat is difficult to access.

The implementation of **carbon capture and storage** (CCS) has some potential to lower carbon emissions in the production of petrochemicals and, clearly, CCS with thermal power plants would greatly assist in lowering the emissions associated with electricity generation.

With **carbon capture and utilisation** (CCU), on the other hand, great care must be taken to account for net emissions associated with the life cycle of any products. For example:

- CO_2 may be utilised as a feedstock for methanol production. However, there are many end-uses for methanol and the carbon that forms methanol is likely to be released eventually as CO_2 after end-use;
- CCS may also be used as part of the syngas production to make ammonia. However, most ammonia is used to produce urea, where the CO_2 is again eventually released, limiting potential for emission avoidance;

- The production of olefins may be a promising route for utilisation of CO_2, via methanol to olefins. However, the end-of-life of the plastic produced must be managed effectively to ensure emissions are minimised.

Technology and policy of decarbonisation. Given its dependence on fossil feedstocks and its need for high-grade heat, the petrochemical industry may take longer to decarbonise than the power sector. With increasing use of renewables, nuclear power and CCS, emissions from the power sector are being addressed. A decarbonised power sector would naturally help to decarbonise the petrochemical industry. Nonetheless, while there has been continual effort to reduce environmental impacts through improved efficiencies of petrochemical production, deep decarbonisation requires a strong policy and regulatory framework to be realised.

Petrochemical production based on low-carbon processes such as electrolysis faces significant economic barriers, which is why they do not appear in the projected sustainable petrochemical pathways for China. Modelling indicates that carbon pricing is likely to lead to increased gas use for petrochemicals production in China, for example for methanol and ammonia production. For ammonia production, biomass-based routes were also seen to be competitive in the longer term.

The most popular policy options according to the stakeholders interviewed were carbon prices and emissions performance standards. However, the global nature of trade for petrochemicals necessitates a global approach to the application of policies or regulation. High levels of international trade creates the potential for 'carbon leakage', where regionally differing carbon pricing may drive incentives to import rather than produce sustainable products locally. National emissions performance standards may also be effective, with stakeholders indicating that non-technology-specific regulations would have most appeal to industry. Here again, however, care must be taken to avoid the significant potential for carbon leakage, this time for example via border tariffs. The need for a level playing field was particularly highlighted by industrial stakeholders.

Technology lock-in from investments in unabated coal-based petrochemical production are a significant barrier to improving sustainability in China. In the short-to-medium term capacity investments in methanol and ammonia production in China are focused on coal as a feedstock. The resulting plant has a lifetime of 25-40 years, meaning that much of this capacity may still be operating in 2050. Therefore, even under the influence of a 2°C-consistent CO_2 price, the environmentally sustainable production of these petrochemicals over the first half of this century could be challenging.

In summary, there are substantial challenges to decarbonise petrochemicals given the high regional variability in costs, feedstocks and processes that contribute to a strong global trade. With ever-increasing demand, the implementation of an effective emissions policy is vital to meet climate targets. However, any emissions policy must be implemented with caution to avoid perverting the market and displacing one environmental impact (e.g. climate change) for another.

Expert Review Comments

A review was undertaken by a number of international experts. The draft report was generally well received, with reviewers remarking on its valuable contribution to an important topic that has been underexplored.

A large number of comments and suggestions were made by the reviewers, all of which were addressed by the authors, with corrections and additions to the text or a recognition that some recommendations for content lay outside the scope of the study.

Conclusions

- **Petrochemicals** are an important building block of a huge range of products that underpin modern daily life and economic activity;
- The potential to sustainably produce **methanol, olefins and ammonia/urea** has been investigated.
- As well as its use as a fuel, **methanol** maybe used a fuel or as a feedstock for a wide range of downstream products. It has a healthy and growing global market, particularly in China. Effective, sustainable production of methanol could drive the decarbonisation of the petrochemicals industry.
- **Methanol** has largely been produced from natural gas, though in China, where the rapid growth in production of methanol is expected to continue, coal-based processes dominate.
- Catalytic hydrogenation of CO_2 has been widely proposed as an alternative route to produce **methanol**, though its application depends very much on identifying an economic and environmentally-sustainable means of producing hydrogen. Hydrogen can be produced by a range of low-carbon methods, each with very different economic and environmental characteristics.
- The decarbonisation of grid **electricity** by using renewables or CCS, would enhance the reduction of carbon emissions from petrochemicals production.
- **Olefins** are crucial intermediates in the manufacture of a vast range of products. Ethylene and propylene are used primarily to manufacture plastics, while butadiene is used to create a variety of synthetic rubbers. As manufacturing of such goods has moved from Europe and North America to East Asia, so has the demand for olefins.
- While naphtha cracking has historically been the processes of choice for **olefin** production, both lighter NGLs and coal have recently gained market share.
- Biomass and wind-sourced **methane-to-olefin** routes, while more costly, showed greater potential to decrease carbon emissions compared with the conventional naphtha-cracking route. Unabated **coal-to-olefins** exhibit a relatively higher environmental impact, though the application of CCS would reduce these emissions markedly.
- In China, naphtha cracking complemented by **coal-to-olefins** are the incumbent technologies. Where a carbon price was imposed in the modelling exercise, there was a shift towards the cracking of lighter hydrocarbons rather than to the **methane-to-olefins** route based on the more environmentally-sustainable but higher cost and relative immature biomass or wind power options.
- It was generally felt that a reduction in crude oil demand associated with transport fuels was quite possible in the medium-term future, which would lower feedstock costs and shift **olefin** production back towards heavier hydrocarbons.
- The use of **ammonia** to produce fertilisers is essentially driven by the demand for cereal crops. With natural gas the traditional feedstock for ammonia, production is driven towards the cheapest source of that gas. At the same time, food security issues incentivise local fertiliser production, leading to a tension between these two drivers. Increasingly, the cost of the primary feedstock dominates, leading to production at otherwise stranded sources of natural gas or, in the case of China, where there is cheap coal.
- Of the alternative routes to **ammonia** production investigated, the biomass-based route was found to be the most environmentally attractive, followed by electrolysis based on wind power. However, given sustainability concerns, stakeholders, when consulted, felt uncomfortable proposing biomass as a resource to produce petrochemicals.
- When considering process options for China as energy prices evolve from 2010 to 2050, **petrochemical** production initially switches from coal to natural gas-based processes and

then to biomass-based processes. This trend appeared to be independent of CO_2 price. The high price of the relatively immature electrolysis-based routes negated their selection.

- While there are several promising options to **decarbonise** petrochemical production, there is no silver bullet. Each of the options have disadvantages, including barriers relating to cost, resource availability/depletion, water usage or, in the case of bio-based feedstocks, creating competition with other critical industries such as agro-industry and food security. The use of unabated coal-based feedstocks typically had the highest environmental impact, regardless of the petrochemical studied.
- Using **hydrogen** from a low-carbon source would offer an excellent opportunity to decarbonise petrochemical production. The gasification of low-carbon feedstocks and the electrolysis of water using low-carbon electricity are both possible low-carbon sources of hydrogen. Unfortunately, neither of these routes are currently attractive from a cost viewpoint.
- A unique challenge to the petrochemical industry is the need to **decarbonise heat**. While options exist to decarbonise electricity, low-carbon heat, high-grade is more difficult to achieve and, in fact, may simply add further environmental burden.
- The implementation of **carbon capture and storage** (CCS) has potential to lower carbon emissions in the production of petrochemicals and, clearly, CCS with thermal power plants would greatly assist in lowering the emissions associated with electricity generation.
- With **carbon capture and utilisation** (CCU), on the other hand, care must be taken to account for net emissions associated with the life cycle of any products. For example, one route to methanol production is via hydrogenation of captured CO_2: even though the hydrogen may come from a low-carbon source, depending on the end product of the process, the CO_2 utilised is ultimately very likely to be released to the atmosphere – even plastics degrade over time. Similarly, urea may be produced from ammonia and captured CO_2, where again the CO_2 would eventually be released.
- Given the likelihood that the petrochemical industry will remain dependent on fossil fuels for the medium-term future, a strong **policy and regulatory framework** is required if it is to decarbonise effectively. Low-carbon routes to the production of petrochemicals generally face significant economic barriers.
- Stakeholders consulted suggested carbon prices and emissions performance standards were the most popular policy options. However, the global nature of trade for petrochemicals necessitates a global approach to the application of policies or regulation. High levels of international trade create the potential for '**carbon leakage**', where regional carbon pricing may create incentives to import rather than produce sustainable products locally.
- Being non-technology-specific, **emissions performance standards** were likely to have most appeal to industry. Again, however, these could lead to carbon leakage, for example, via border tariffs. The need for a level playing field was considered essential.
- Modelling regarding China suggested that **carbon prices** would likely lead to increased gas use for methanol and ammonia production, while biomass-based routes were seen to be competitive routes to ammonia production in the longer term.
- Given the 25 to 40-year economic lifetime of plants, **technology lock-in** from investments in coal-based petrochemical production in China were potentially a significant barrier to improving sustainability. Even with a 2°C-consistent CO_2 price, the environmentally sustainable production of petrochemicals in China over the first half of this century appears challenging.
- There are substantial challenges to **decarbonise** petrochemicals, given the high regional variability in costs, feedstocks and processes that contribute to a strong global trade. Effective emissions policies were vital to meet climate targets, but need to be implemented with caution

to avoid perverting the market and substituting one environmental impact (e.g. climate change) with another.

Recommendations

To cost-effectively decarbonise the petrochemical industry, low-emissions routes must be pursued via a combination of effective policy implementation, improved processes and a closing of the gap in costs when compared with mature fossil fuel options.

From a technology perspective, lower carbon processes may be achieved by:

- Improved efficiency. Improving the efficiency of existing and novel processes makes more effective use of resources and reduces the environmental footprint per unit petrochemical produced;
- Process innovation. Innovation may be achieved, for example, by the development of better catalysts, with the potential to produce petrochemicals via a process that is cleaner, safer and more economic;
- Application of CCS. Where CCS may be applied in a process, it offers the potential to capture a high fraction of the CO_2 emitted, transporting it to a site where it may be safely and securely stored deep underground for millennia or longer;
- Bio-based feedstocks. While the identification of suitable bio-based feedstocks would reduce the energy intensity of conversion, it may introduce other challenges;
- Low-carbon hydrogen. Efforts could be made to develop a source of hydrogen with lower environmental and economic impact.

To assess potential decarbonisation targets, there is a need to identify the extent to which emissions may be minimised for each petrochemical. While this was out of scope for the current study, some insights were achieved via the focus on China. Where China uses unabated coal as its primary feedstock, its electricity generation is highly carbon intensive and, given much of China's infrastructure is relatively new, it will likely remain in service for decades. Conclusions would undoubtedly differ should the case study have focused, say, on a region with good availability of low-carbon electricity and/or high-grade heat. Identifying a 'best case scenario' with respect to emissions may help to set targets and drive research to improve the sustainability of the industry.

Suggestions for further work

It is clear there exists substantial challenges to decarbonise the petrochemical industry under changing but generally increasing demand, while meeting cost expectations. The current study examined three important petrochemicals and considered an extensive list of processes. Given the broad range of assessments included in this study, a deeper and more insightful analysis would be achieved if the focus was on a smaller set of products, e.g. olefins or methanol.

Exploring the full range of chemical processes options for methanol, for example, which may be used as a transport fuel, a fuel additive or as a source chemical for a whole range of other every-day products such as plastics, would still be a complex undertaking. A narrowing of scope, however, would enable more time to synthesise and compare results with other studies. The current study would serve as an excellent starting point to plan such an exercise. In relation to improvements of the methodology tested in this report, a number of recommendations are proposed.

A revised scope of assessments may include:

- Techno-economic, LCA and social impact characterisation of process options, feedstocks and decarbonisation methods.
- Comparative analysis between process routes across a chosen sub-set of the UN Sustainable Development Goals.

- A larger set of stakeholder interviews to strengthen and elicit the key challenges associated with the future petrochemical industry, with findings incorporated into the other sections of analysis.
- Identify key opportunities and barriers to petrochemical industrial development with respect to processes, feedstocks and policies.

Finally, this study has taken the view that social benefit can be maximised by minimising the cost of petrochemical production (after emissions costs are internalised), but future studies would benefit from a more nuanced and disaggregated view on social sustainability, including quantitative and qualitative measures of the social aspects of sustainability.

Sustainability in Petrochemicals

Impacts and perspectives from market, process, environmental and economic assessments

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Glossary

ABS:	Acrylonitirile-butadiene-styrene
ADP:	Abiotic resource depletion potential
AP:	Acidification
ASU:	Air separation units
BECCS:	Bioenergy with Carbon Capture and Storage
CAGR:	Compound annual growth rate
CAPEX:	Capital Expenditure
CCS:	Carbon capture and storage
CCU:	Carbon capture and utilisation
Conv:	Conventional
CTM:	Coal-to-methanol
DCB:	Dichlorobenzene
DME:	Dimethyl ether
EDC:	Ethylene dichloride
EOR:	Enhanced oil recovery
EP:	Eutrophication potential
ETS:	Emissions Trading Scheme
FAETP:	Freshwater aquatic ecotoxicity potential
FCC:	Fluidised catalytic cracker
GHG:	Greenhouse gases
GWP:	Global warming potential
HDPE:	High density polyethylene
HE:	Heat exchanger
HTP:	Human toxicity potential (HTP)
IIASA:	International Institute for Applied Systems Analysis
KPI:	Key performance indicator
LCA:	Life cycle assessment
LDPE:	Low density polyethylene
LI:	Log-inverse
LIT:	Log-inverse with time efficiency factor (LIT)
LL:	Log-log
LLDPE:	Linear low density polyethylene (LLDPE)
LLS:	Log-log-square
LN:	Linear
MAETP:	Marine aquatic ecotoxicity potential
MEG:	Monoethylene glycol
MTBE:	Methyl tertiary butyl ether
MTO:	Methanol-to-propylene
MTP:	Methanol-to-olefins
NCAR:	National Centre for Atmospheric Research
NGL:	Natural gas liquid
NLI:	Non-linear inverse
NLIT:	Non-linear inverse with time efficiency factor
NR:	Nitrile rubber
NVOC:	Non-volatile organic compounds

NVP:	Net Present Value
ODP:	Ozone depletion potential
P:	Power
PBR:	Polybutadiene rubber
PE:	Polymers polyethylene
PED:	Primary energy demand
PET:	Polyethylene terephthalate
PFD:	Process flow diagram
PO:	Propylene Oxide
POCP:	Photochemical ozone creation potential
PP:	Polypropylene
PS:	Polystyrene
PTA:	Purified terephthalic acid
PVC:	Polyvinyl chloride
ROI:	Return on investment
SBR:	Styrene butadiene rubber
SBR:	Styrene-butadiene rubber
SC:	System Costs
SGA:	Sales, General and Administrative
SL:	Semi-log
SMR:	Steam methane reforming
STPR:	Social Time Preference Rate
TAME:	Tertiary amyl methyl ether
TETP:	Terrestrial ecotoxicity potential
TRL:	Technology readiness level
VAM:	Vinyl acetate monomer
WACC:	Weighted average cost of capital

Executive summary

Petrochemicals are an important building block of a huge range of products that underpin daily life and economic activity. Production processes for these products have historically been closely associated with the oil and gas industry, but this pattern has been challenged in recent years. In particular, the global chemical industry contributes approximately 4.5% of total anthropogenic greenhouse gas (GHG) emissions, but to date there has been little progress on sector decarbonisation. Other drivers of change to the petrochemical industry include the regional variation in costs and availability of resources, and the drive for national self-sufficiency.

This report investigates a unique combination of these industry drivers on the historic, current and future status of the petrochemical industry to gain insight into the sustainability of petrochemicals. Three categories of petrochemicals are subject to analysis, namely methanol, olefins and ammonia/urea. For each of these petrochemicals, the following series of studies are formed and analysed in aggregate to gain insight in to the sustainability prospects of the industry:

- An assessment of the historic and current status of market trade, including trends in end-uses, feedstocks, demand, production and international trade. Demand projections for each chemical are made based on collected data.
- Process engineering characterisation of the current and low carbon alternative routes and feedstocks to produce the key petrochemical productions.
- Environmental life cycle assessment of the various feedstocks and production methods for each petrochemical and a contribution analysis of the key environmental impacts.
- Market projection of petrochemical production and technology mixes for a key region China, for the time period 2010 – 2050.
- A series of expert stakeholder interviews on views of how the petrochemical industry may progress in terms of demand, costs, environmental impacts and policy drivers.

The primary themes from each section of analysis are brought out and discussed in aggregate to form a perspective on the potential for the petrochemical industry to decarbonise and the mechanisms by which this may be enabled. Key findings are summarised below, relating to changing demands and costs, decarbonisation options and mechanisms, as well as recommendations for further work.

Changing demands and costs

Global demand for petrochemicals is likely to continue to grow, in particular for methanol, but also ammonia and olefins ethylene, propylene and butadiene, as shown in Figure ES-1. An example of projected demand growth is given for a focus study region of China, but regional variability is likely to be high. Whilst CO_2 emissions may be decoupled from economic growth and demand growth, for example via increased renewable energy, other environmental impacts such as water footprint cannot and consequently there are likely to be other environmental barriers in the future with continued demand growth.

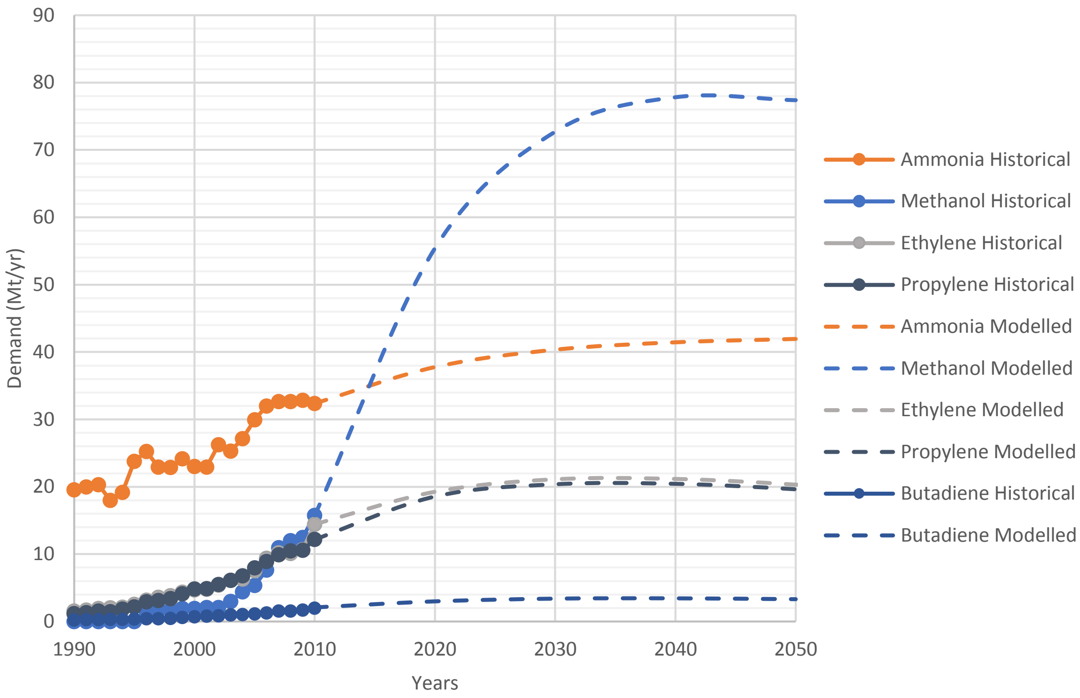

Figure ES-1. Historical demand and projections of petrochemicals for China up to 2050.

Methanol may become an increasingly important petrochemical. It has a highly diverse range of end-uses, a large proportion of which is currently as a component in transport fuel. Given that the US have eliminated this usage due to environmental concerns, it is anticipated it could also reduce elsewhere over time (e.g. China). However, the potential of methanol as an intermediate chemical in a multitude of applications suggests that there is likely to be increased and diverse demand in future. Methanol may be produced from low carbon feedstocks, for example via catalytic hydrogenation. It can then be used as a feedstock for other bulk petrochemicals, in particular olefin production as demonstrated in this study. Whilst methanol-to-olefin (MTO) processes are not generally economically feasible at present, a change in feedstock price or regulation could provide impetus for rapid demand increases.

Historically the steam cracking of naphtha has been starting point for olefin manufacture and has determined the pattern of trade. However, naphtha is being replaced as a feedstock with cheap natural gas liquids becoming increasingly available. This is particularly the case in North America with the advent of shale gas, as well as the Middle East where olefin production has ramped up significantly in recent years. As countries seek to become self-reliant they are also looking to coal and methanol as a petrochemical feedstock where costs are favourable.

There has been significant investment in olefin plant in the Middle East using natural gas liquids (NGLs) as a feedstock, freeing up the traditional feedstock of naphtha for gasoline manufacture. Additionally, a focus on self-sufficiency in both China and the US has led to changing trade dynamics of olefins. China has rapidly expanded its coal-to-olefin capacity, and the US has utilised NGLs associated with recent growth in shale gas production. This growth in China, the US and the Middle East has the potential to create an excess of global capacity.

Ammonia demand is largely driven by fertiliser demand, which in turn is driven by demand for cereal crops. Natural gas is the key feedstock for ammonia production worldwide, driving production towards the cheapest source of that gas. At the same time, food security issues incentivise local fertiliser production, leading to a tension between these drivers. Increasingly, the cost of the primary feedstock is the key issue, leading to production at otherwise stranded sources of natural gas, or where there is cheap coal in the case of China.

In the longer term, prices for all commodities considered are highly uncertain. Two opposing price drivers were discussed in the stakeholder interviews most frequently: the impact of reduced oil demand from transport and the impact of climate-related policy and regulation. The growth in renewable electricity generation and the potential growth in electric vehicle uptake may significantly reduce demand for oil. This could result in increased availability of oil to the petrochemical industry, thus reducing the price. Given that petrochemical products typically represent the minority of products from a refinery, the majority being fuel products, this could spell a sea-change for refinery production business models. The impact is likely to be seen in terms of petrochemical prices, but also as a change to a heavier hydrocarbon feedstock will change processing needs.

An important note is that the impact of international drives towards recycling and re-use of products such as consumer plastics may reduce demand for petrochemicals significantly and represents a high uncertainty and potential regional variability.

Decarbonisation options

There are various options for alternative process routes and feedstocks for the different petrochemical products, resulting in a range of expected environmental impacts. This study has focused on assessing conventional fossil-based routes and a selection of alternative processes and potentially low carbon feedstocks. There are many promising options for petrochemical production which may provide decarbonisation as shown in Figure ES-2. Conventional methanol production is based on synthetic gas, produced through coal gasification or steam methane reforming (SMR), whereas alternatives include catalytic hydrogenation of CO_2. The conventional process for olefin production is the thermal cracking of light hydrocarbons and naphtha, but methanol-to-olefins are increasing in prominence and may utilise low carbon feedstocks. For ammonia, natural gas and coal are typical feedstocks but these could be replaced by a low carbon hydrogen source.

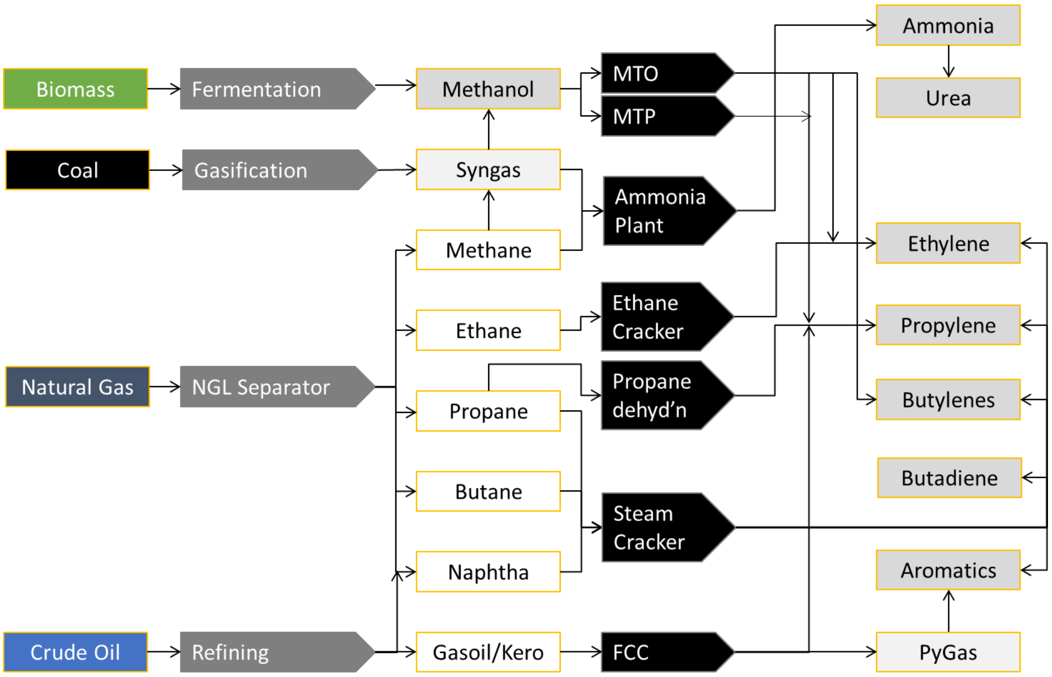

Figure ES-2. Basic routes to petrochemical products. MTO: methanol-to-olefin, MTP: methanol-to-propylene, FCC: fluidised catalytic cracking.

However, there is clearly no silver bullet environmentally benign option and each option exhibits multiple disadvantages or barriers, relating to cost, resource availability or in the case of bio-based feedstocks, creating competition with other critical industries such as food. Coal-based feedstocks typically have the highest environmental impacts, in particular global warming potential with the exception of coal-based electrolysis routes. All other options for feedstocks and processes perform significantly better.

Using hydrogen as a feedstock from a low carbon source may represent a good opportunity for the decarbonisation of methanol and ammonia production. Hydrogen may be derived via gasification of low carbon feedstocks or via electrolysis using low carbon electricity. However, currently these are neither cost-effective nor environmentally beneficial for many supply chains. Additionally, while these technologies may help to meet climate change targets, other environmental impacts are significantly higher given high energy intensities of the process, as well as water usage, land-use change and metal resource depletions.

Bio-based feedstocks perform very well in the environmental assessment of this study as shown in Figure ES-3 for methanol production routes in particular, but is a highly contested approach from the stakeholder elicitations. There are many competing applications/industries for bio-based feedstocks and it is debatable which is most appropriate/efficient for a limited resource. Many bio-feedstocks are not molecularly similar to petrochemical products, resulting in high energy intensity and consequently high cost/low efficiency. Competition with the energy sector for bio-feedstocks currently favours the energy sector, whilst competition for bio-feedstocks with food systems should be avoided to prevent adverse impacts in areas with high levels of poverty. With a projected increase in bio-based feedstocks for industry and energy (potentially in electricity, heat and transport provision), water impacts, land use changes and other environmental impacts may be significant and must be managed carefully in order to prevent shifting from one environmental impact to another.

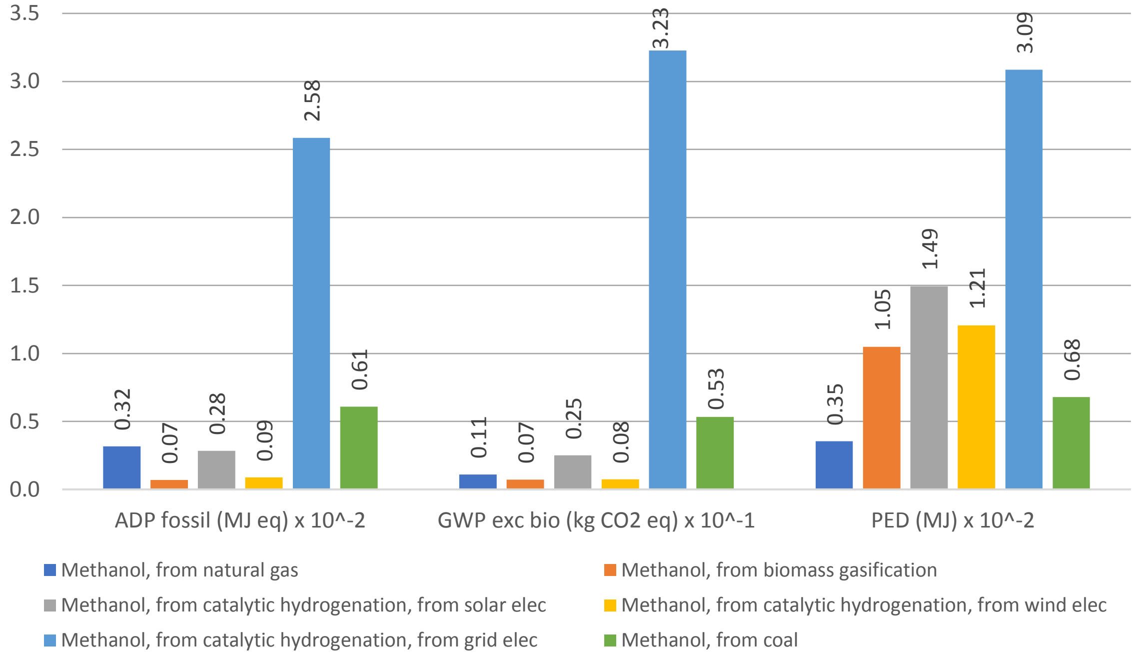

Figure ES-3 *Environmental impacts associated with methanol production routes, expressed per kg of methanol production. ADP: abiotic resource depletion potential, GWP: global warming potential, PED: total primary energy demand.*

A unique challenge to the petrochemical industry is the need to decarbonise heat. It is an energy intensive industry, but whilst there has been much progress in decarbonising electricity, there are several technical, infrastructural and economic barriers to decarbonising heat. For example, electrification of heat is relatively inefficient and also places additional strain on electricity grids. Additionally, the use of renewable energy sources will increase the demand on rare metals, which adds another environmental burden to the decarbonisation routes. The use of hydrogen as a heat source may have significant potential in the petrochemical industry given its generation within existing processes, but this will impact upon system efficiencies and cost.

The implementation of carbon capture and storage (CCS) or utilisation (CCU) has some potential for the petrochemical commodities, but great care must be taken to account for the life cycle of any products produced here.

- CCS may be used as part of the syngas production to make ammonia. Indeed, carbon dioxide separation is already part of the chain in various forms of syngas and hydrogen production. However, most ammonia is used to produce urea which uses carbon dioxide and is again released at end-use phase, limited potential for emission avoidance.
- Carbon dioxide may be utilised as a feedstock for methanol production. However the utilised carbon that forms methanol is likely to be released eventually as CO_2 after end-use and so any utilisation of CO2 in this way is

only temporary. Consequently, it is vital that this is accounted for and is not just assumed to be stored indefinitely.
- Depending on waste management option, the production of olefins may be a promising route for utilisation of CO_2, via methanol to olefins. However, the end-of-life of the plastic produced must be managed effectively to ensure emissions are minimised.

How to decarbonise: technology and policy

The petrochemical industry may remain more dependent on fossil fuels than the energy sectors (e.g. as fuel for electricity generation or transport), given the high efficiencies in using fossil feedstocks and requirement for high-grade heat. However, a decarbonised energy sector would naturally help to decarbonise the industry via utilisation of decarbonised electricity and heating infrastructure, for example.

Whilst there has been continual effort to lower environmental impacts through improved efficiencies of petrochemical production, deep decarbonisation requires strong policy and regulatory frameworks to be realised.

For example, petrochemical production based on low carbon routes such as electrolysis face very significant economic barriers. Thus they do not appear in the modelled sustainable petrochemical pathways for China produced herein. A CO_2 price does not promote electrolysis options even when they are supplied by renewable energy as they show marginal improvements in greenhouse gas performance on a life cycle basis. This outcome may change under alternative scenarios however: for example, a decarbonised electricity grid would result in better performance of all electrolysis options (including solar and wind electrolyser). Additionally, the outcome might be altered if better information were available on how the cost of electrolysers may change if the technology is scaled up.

Carbon pricing is likely to lead to increased gas use in petrochemicals in China. For the study on petrochemical pathways for China, a switch from coal to gas for methanol (shown in Figure ES-4) and ammonia production was observed. For ammonia production, biomass-based routes also were seen to be competitive in the longer term. However, as methanol is gaining importance as a petrochemical, there appears to be a substantial opportunity to increase gas use in its production. In China, where cheap coal is readily available, introduction of a carbon price (or equivalent measure) at a sufficient level would lead to increased gas use.

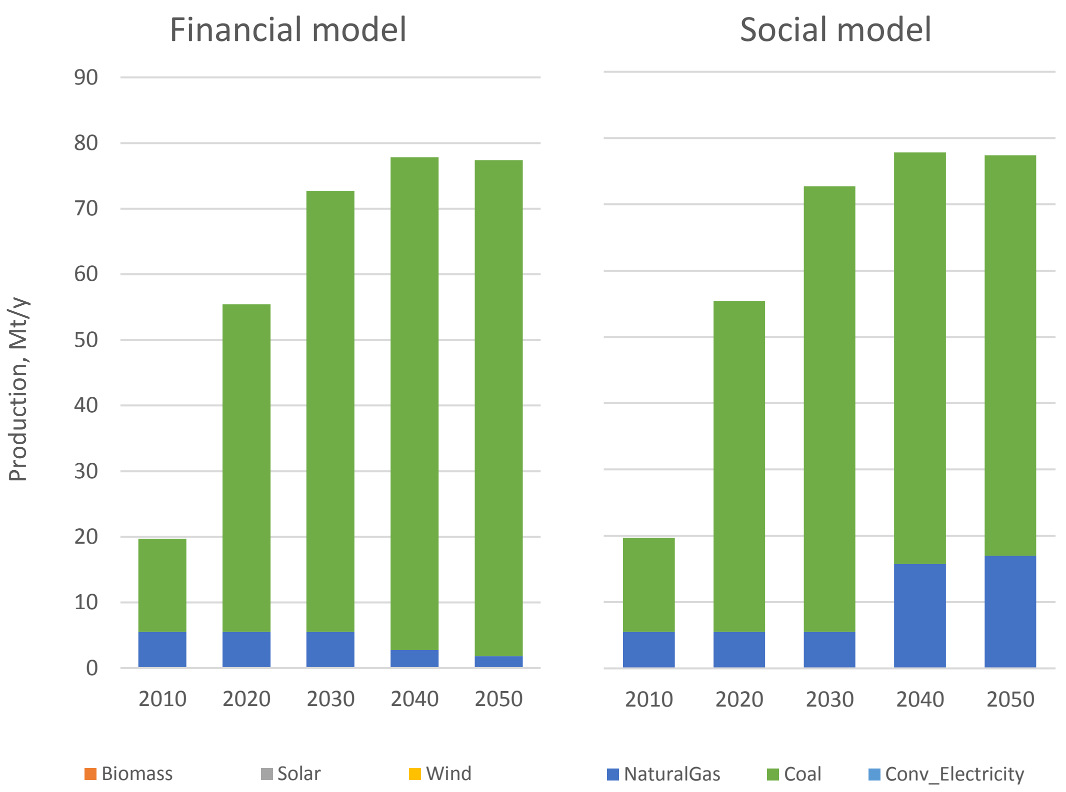

Figure ES-4 Projection of methanol production from the modelled technologies in China from the financial model without CO_2 price (left) and the economic model with CO_2 price (right)

The most popular policy options amongst the stakeholders interviewed were carbon prices and emissions performance standards. However, the global nature of trade for petrochemicals necessitates the application of global policies or regulation. High levels of international trade creates the potential for 'carbon leakage', where regional carbon pricing may create incentives to import rather than produce products sustainably. National emissions performance standards may also be effective and stakeholder views suggest that non-technology-specific regulations are most appealing to industry. However again much care must be taken to avoid the significant potential of carbon leakage, for example via border tariffs. Additionally, the need for a level playing field was highlighted particularly by industrial stakeholders.

Technology lock-in from investments in coal-based petrochemical production are a significant barrier to improving sustainability in China. In the short to medium-term capacity investments in methanol and ammonia petrochemical production in China are focused on coal as a feedstock (Figure ES-4). The resulting plant has a lifetime of at least 25 years and probably closer to 40 years, meaning that very significant amounts of this capacity will still be present in the Chinese petrochemical production matrix towards 2050. Therefore, even under the influence of a 2C-consistent CO_2 price, the environmental sustainability of these petrochemicals over the first half of this century looks challenging.

Recommendations for further work

It is clear that there exist great challenges to decarbonise the petrochemical industry under changing demand and meeting cost expectations. The enabling of low carbon routes must be realised by a combination of improved efficiencies and closing the gap in costs between these and the mature fossil fuel options. Improved efficiencies may be achieved by

- Process innovation, e.g. through catalysis
- Identification of suitable bio-based feedstocks which require lower energy intensity for conversion
- A low-environmental-and-economic impact source of hydrogen
- Decarbonising heat, for example using renewable feedstocks or with carbon capture

There is a need to identify how much emissions may be minimised for each petrochemical to assess potential decarbonisation targets. This study estimated environmental impacts based on a case study region of China, which has high carbon intensity of electricity, as well as other infrastructural resources. Consequently, the routes may exhibit significantly lower emissions if the case study region were different (i.e. where low carbon electricity and/or heat were available). An identification of a 'best case scenario' with respect to emissions may help to drive targets and further research to improve the sustainability of the industry.

In relation to improvements of the methodology tested in this report, a number of recommendations are made here. Given the broad range of assessments included in this study, a deeper and more insightful analysis would be achieved if the focus was on a smaller set of products, e.g. olefins or methanol. This would enable more time to synthesise and compare results with other studies. A revised scope of assessments may include:

- Techno-economic, LCA and social impact characterisation of process options, feedstocks and decarbonisation methods.
- Comparative analysis between process routes across a chosen sub-set of the UN Sustainable Development Goals.
- A larger set of stakeholder interviews to strengthen and elicit the key challenges associated with the future petrochemical industry. Allow time to iterate and incorporate the findings of the expert elicitations into the other sections of analysis
- Identify key opportunities and barriers to petrochemical industrial development with respect to processes, feedstocks and policies.

In summary, there exists a great challenge with respect to decarbonisation of petrochemicals with high regional variability in costs, feedstocks and processes, contributing to strong global trade. With ever-increasing demand, the implementation of emissions policy is vital to meet climate targets, but must be implemented with great care to avoid creating market perversions and replacing one environmental impact (e.g. climate change) with another.

1 Introduction

Petrochemicals are an important building block of a huge range of products that underpin modern daily life and economic activity. Production processes for these products have historically been closely associated with the oil and gas industry, but this pattern has been challenged in recent years due to a complex combination of macro- and micro-economic, technology, political and environmental factors. In particular, the global chemical industry contributes approximately 4.5% of total anthropogenic greenhouse gas (GHG) emissions, but to date there has been little progress on sector decarbonisation despite increasing global ambitions as evidenced by the Paris Agreement on climate change mitigation. Further important drivers of change to the petrochemical industry include the regional variation in costs and availability of resources, the drive for national self-sufficiency, and particularly important with respect to the topic of this report the imperative to produce these products in a more broadly sustainable manner.

Indeed sustainability has arguably become a mainstream consideration in the context of petrochemical developments. It is considered by companies when prioritising new investments, by shareholders considering investment portfolios, by governments sanctioning new developments, and by the broader community in the context of the social benefits and social acceptability of firms. However the methodology by which sustainability is assessed varies widely, with no generally accepted definition, and therefore methodology development and standardisation is needed. The UN Sustainable Development Goals represent the first step in this direction, with 17 different aspects and associated metrics defined, though the relative importance of the aspects covered remains a political decision.

The primary aim of this study is to establish a methodology to assess different aspects of the sustainability of petrochemical production. It is important to note that in this study we consider sustainability as the study of the impacts of products and processes over time on natural and societal resources, typically divided into the three 'pillars' of environment, economics and society. To this end, the report investigates a unique combination of the industry drivers on the historic, current and future status of the petrochemical industry to gain insight into the sustainability of petrochemicals. Three categories of petrochemicals are subject to analysis, namely methanol, olefins and ammonia/urea. For each of these petrochemicals, the following series of studies are formed and analysed in aggregate to gain insight in to the sustainability prospects of the industry:

- **Market analysis.** An assessment of the historic and current status of market trade, including trends in end-uses, feedstocks, demand, production and international trade. Demand projections for each chemical are made based on collected data.
- **Process engineering characterisation** of the current and low carbon alternative routes and feedstocks to produce the key petrochemical productions.

- **Environmental life cycle assessment** of the various feedstocks and production methods for each petrochemical and a contribution analysis of the key environmental impacts.
- **Market projection** of petrochemical production and technology mixes for a key region China, for the time period 2010 – 2050.
- A series of **expert stakeholder interviews** on views of how the petrochemical industry may progress in terms of demand, costs, environmental impacts and policy drivers.

It must be noted that this study does not profess to cover all the aspects of sustainability of petrochemicals, but rather a constrained range of environmental and socio-economic impacts. Sustainability, more broadly characterised, could be assessed across the vast range of metrics as presented with the seventeen UN Sustainable Development Goals. However, a restricted subset of sustainability aspects is included here to ensure tractability of the work, with recommendations made for targeted inclusion of further aspects in future studies. For readers interested in possible future methodologies covering a wider range of the facets of sustainability, a useful discussion of the relationship between the UN's Sustainable Development Goals (SDGs) and the energy system is presented in Nerini *et al* (2017)[1], which maps the SDGs onto energy system metrics. Such a mapping represents a possible starting point for an approach to assessing sustainability be more holistically. Another useful example of application of SDGs in an energy system transition study is the recent Sustainable Development Scenario released within the IEA World Energy Outlook 2017[2], where three of the seventeen areas of sustainability are considered to create an assessment of energy system transition that focuses on more than simply emissions reduction.

This report is organised following the methodology described above. Firstly, the market status and demand drivers for each of the bulk petrochemicals is presented, providing reasoning on the historical trends in production and consumption patterns. This is followed by the definition of petrochemical production process routes from both engineering and economic perspectives, based on flow sheets and published information regarding the processes. A detailed environmental lifecycle assessment of the routes is then presented, including consideration of a range of typical end-uses of the petrochemicals. The projection of production and technology mixes for the case study region of China is described, focusing on the contrast between a socially-optimal investment pathway, with a pathway that may materialise if driven only by the commercial attractiveness of the process options to firms. An assessment of six expert stakeholder interviews is presented, representing industry, academia and policy on perspectives of the future of the petrochemical industry. Finally, an overarching view of the characteristics of future petrochemical production pathways is described in the concluding section.

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[1] Nerini et al (2017) Mapping synergies and trade-offs between energy and the Sustainable Development Goals. Nature Energy 3 Pages 10–15.

[2] IEA (2017) World Energy Outlook. International Energy Agency, Paris, France.

2. The market status and demand drivers

This section outlines the key features of the petrochemical industry in relation to feedstocks, uses, demand and production over the last 2 decades. Projections of future petrochemical demand are then made based on this historical perspective, paying regard to both the quantitative relationships between demand and economic activity and, where relevant, the structural changes that are evident from recent history.

The commodities considered in this analysis are methanol, ethylene, propylene, butadiene and ammonia. Each can be produced via various different feedstocks and mechanisms, illustrated in Figure 1. The following sections examine the petrochemicals in turn, relating to their uses, feedstocks, demand, production and trade.

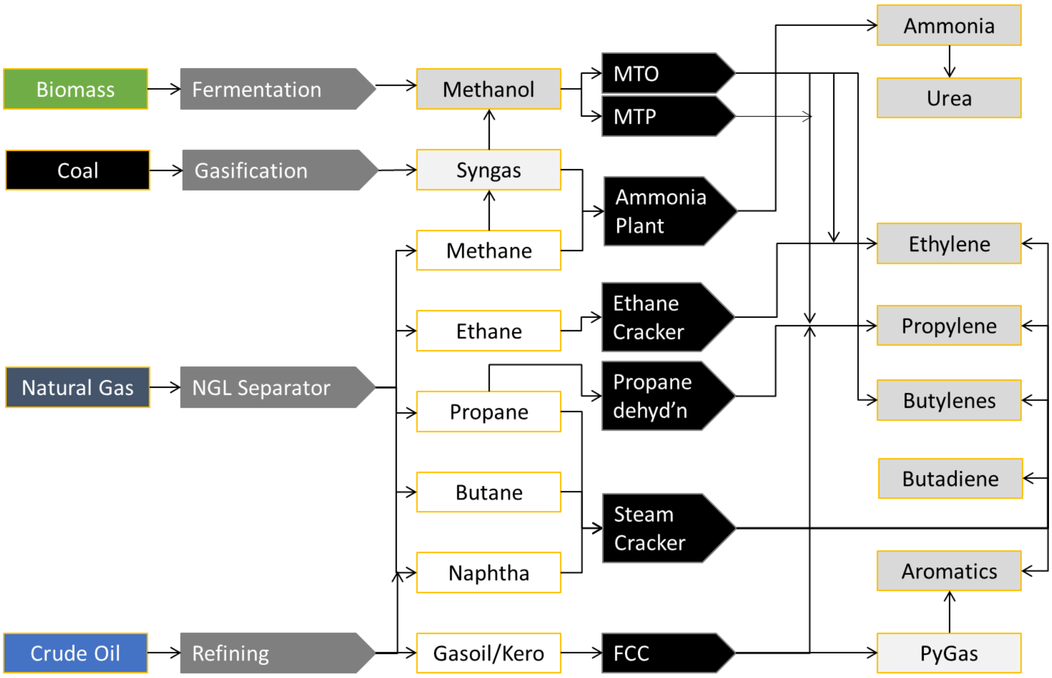

Figure 1 Basic routes to petrochemical products

2.1 Methanol

2.1.1 Uses

Methanol performs a range of different functions in the petrochemical and hydrocarbon supply chain, as shown in Figure 2. It is used as solvent and antifreeze directly in its own right, as a feedstock to products such as formaldehyde, as an intermediate in the production of olefins and as a transportation fuel, either directly as methanol or, more commonly, in a derivative.

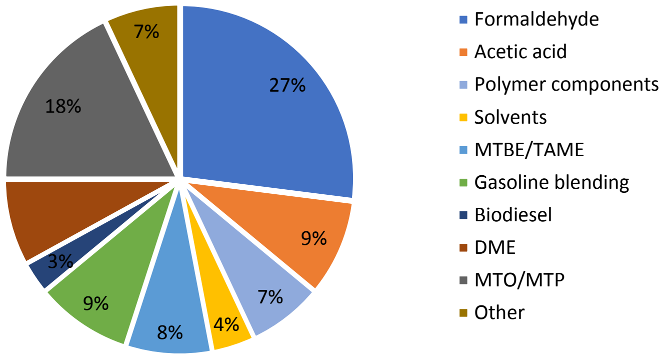

Figure 2 Methanol demand by end use in 2015[3]

Formaldehyde makes up over a quarter of the market for methanol as a feedstock for amino and phenolic resins for use as a preservative and resin binder in wood-based products. Acetic acid is one of the components of vinyl acetate monomer (VAM) and purified terephthalic acid (PTA), both of which have markets as polymers.

A growing segment of methanol use is as the feedstock for olefins synthesis in methanol to olefins (MTO) and methanol to propylene (MTP) plants. Chinese investment in MTO/MTP plants is a major source of Chinese methanol demand growth, the methanol being produced by coal-to-methanol plants which capitalises on the local availability of low cost coal.

However, the major single end market is as a transportation fuel accounting for over 28% of methanol demand. As methanol, or a MTBE/TAME, methanol is used an octane enhancer in gasoline; it is also blended directly or as DME in diesel. In China, the combination of low cost and a desire to increase fuel self-sufficiency, has seen its use as a transportation fuel increase significantly. In the US however, the use of methanol as MTBE in transportation fuel has been phased out due to concerns about its water solubility and potential to pollute the water table.

2.1.2 Feedstock

The feedstock for methanol production is synthesis gas (syngas) sourced from the steam reforming of natural gas or refinery products or coal (or biomass) gasification. Historically, natural gas has been the dominant feedstock and has made up to 85% of total methanol production capacity. However, the surge in demand for methanol in China has seen investment in coal to methanol (CTM) plants based on the low-cost coal reserves, and coal-based methanol capacity makes up as much as 35% of global capacity[4].

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[3] M. Alvorado (2016). METHANOL, IHS. Accessed from: http://www.methanol.org/wp-content/uploads/2016/07/Marc-Alvarado-Global-Methanol-February-2016-IMPCA-for-upload-to-website.pdf

[4] Bloomberg L.P. (2017). Commodity production and demand regional data from Bloomberg Terminal, Accessed Dec 2017.

2.1.3 Demand, production and trade

Between 1996 and 2015, global methanol demand increased by a compound annual growth rate (CAGR) of 6.2%, significantly above the rate of GDP growth[4]. This is due to the growth of demand in China as shown in Figure 3, particularly as a feedstock for MTO/MTP and as a component in transportation fuels. Of the 55 mtpa growth in global demand, nearly 45 mtpa is from China.

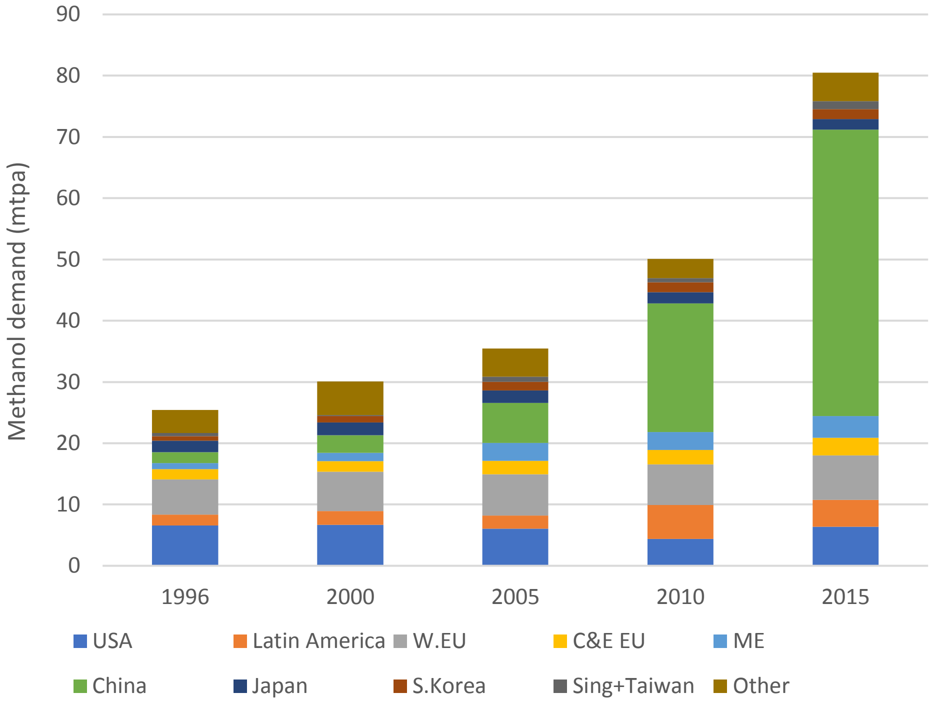

Figure 3 Methanol demand[4]. USA: United States of America, W.EU: West Europe, C&E EU: Central and Eastern Europe, ME: Middle East.

Three main regions with increased methanol production has been in China, the Middle East and North America as shown in Figure 4. Firstly, from representing only 7% of global production by volume in 2000, China now makes up nearly 55% of global production. Secondly, the production and export of methanol in the Middle East (Iran in particular) has been driven by a combination of use in the local transportation segment and the opportunity to monetise natural gas through methanol exports. Lastly, the abundance of shale gas in the US and Canada is now seeing investment in new methanol production and the de-mothballing of plants that had been rendered uneconomic by high relative gas prices in the decade first decade of the 21st century.

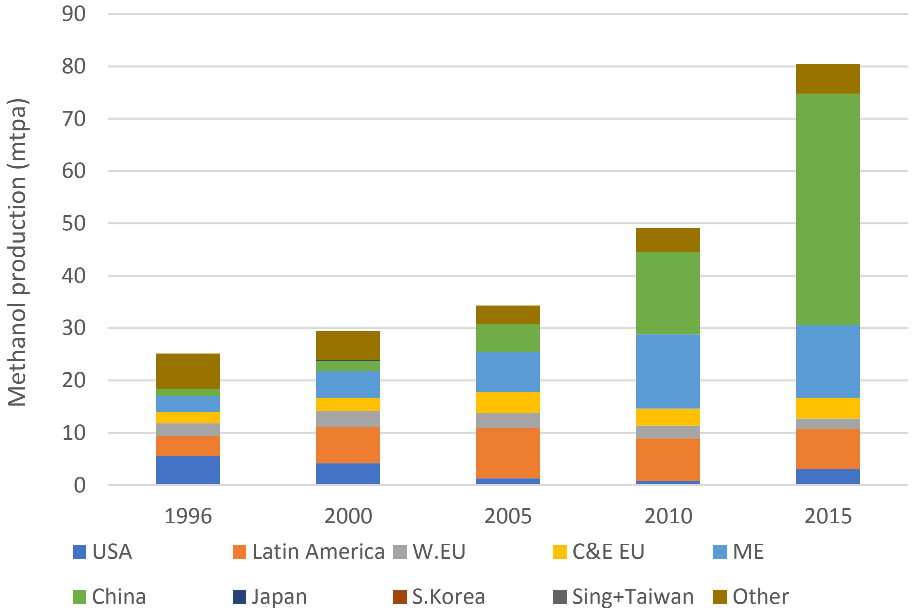

Figure 4 Methanol production[4]

While China continues to import methanol, investment in methanol production in China has limited import dependency over the last decade, unlike the trade pattern of olefins. As a result, the pattern of trade has remained consistently more diverse, with imports into most regions except Latin America, the Middle East and Central and Eastern Europe as shown in Figure 5.

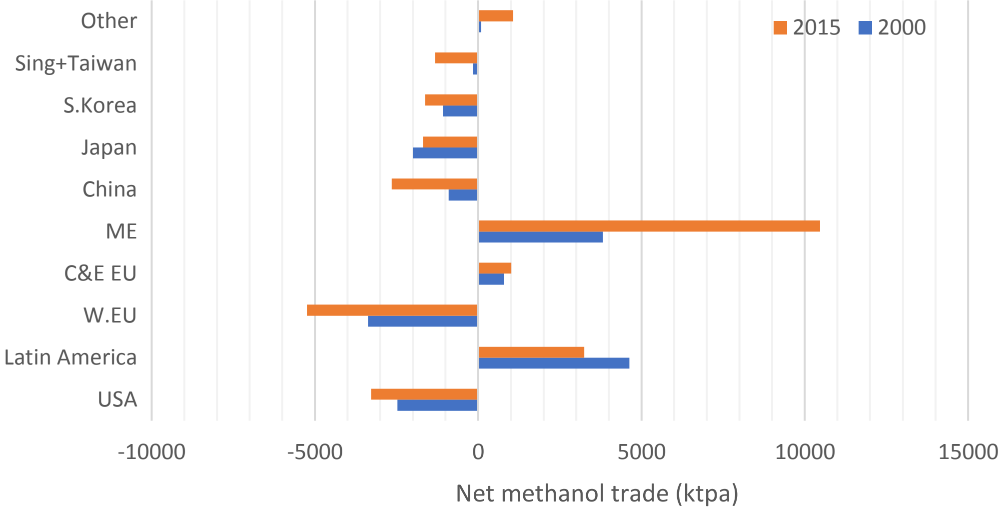

Figure 5 Net regional methanol trade in 2000 and 2015[4,5]

2.2 Ethylene

2.2.1 Uses

Ethylene is the largest volume olefin and its uses extend beyond polymers and resins to solvents, surfactants and alcohols. Ethylene is primarily used in the manufacture of the polymers polyethylene (PE), polyethylene terephthalate (PET), polyvinyl

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[5] United Nations. (2017). UN comtrade database. Accessed Dec 2017: https://comtrade.un.org/

chloride (PVC) and polystyrene (PS) (Figure 6). 60% of ethylene was used in the manufacture of various grades of polyethylene (polythene). Low density polyethylene (LDPE) and linear low density polyethylene (LLDPE) are used in film applications such as food and non-food packaging, shrink and stretch film, and non-packaging uses. High density polyethylene (HDPE) is used primarily in blow moulding and injection moulding applications such as containers, drums, household goods, caps and pallets. HDPE can also be extruded into pipes for water, gas and irrigation, and into film for refuse sacks, carrier bags and industrial and construction linings.

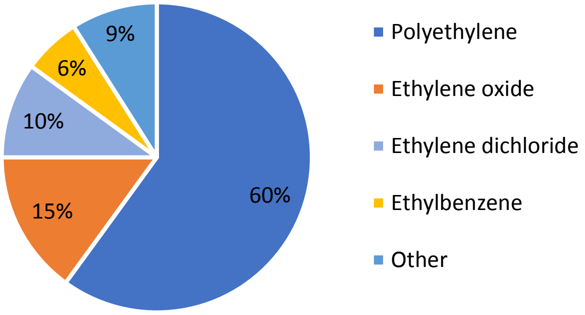

Figure 6 Ethylene demand by end use in 2015[6]

Ethylene oxide (EO) is primarily used to make ethylene glycol. Monoethylene glycol (MEG) is used to make polyester textiles and PET resins for bottles and polyester film. MEG is also used in antifreeze applications. Ethylene dichloride (EDC) is the intermediary for vinyl chloride monomer (VCM), nearly all of which used to make polyvinyl chloride (PVC), used mainly in the construction industry. Ethylbenzene is the intermediary for styrene, leading to polystyrene, and with butadiene to the synthetic rubbers: ABS (acrylonitirile-butadiene-styrene) and SBR (styrene butadiene rubber) – these are discussed in the section on butadiene[7]. Other ethylene derivatives include alpha olefins, detergent alcohols and plasticiser alcohols; vinyl acetate monomer (VAM); and industrial ethanol which is used as a solvent or in the manufacture of chemical intermediates such as ethyl acetate and ethyl acrylate.

2.2.2 Feedstock

Ethylene is produced from the steam cracking of hydrocarbon feedstocks. Historically the primary feedstock had been naphtha, placing petrochemical plants next to refineries. However, ethane has become the feedstock of choice for natural gas-rich regions such as the USA and the Middle East (Figure 7). Additionally, bioethanol is an important feedstock in Brazil.

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[6] J.S. Plotkin (2016). Beyond the Ethylene Steam Cracker, ACS Industrial Chemistry and Engineering. Accessed from: https://www.acs.org/content/acs/en/pressroom/cutting-edge-chemistry/beyond-the-ethylene-steam-cracker.html?_ga=2.116766915.455477633.1526565321-1451277039.1524741973

[7] Also, with cumene, drives benzene demand

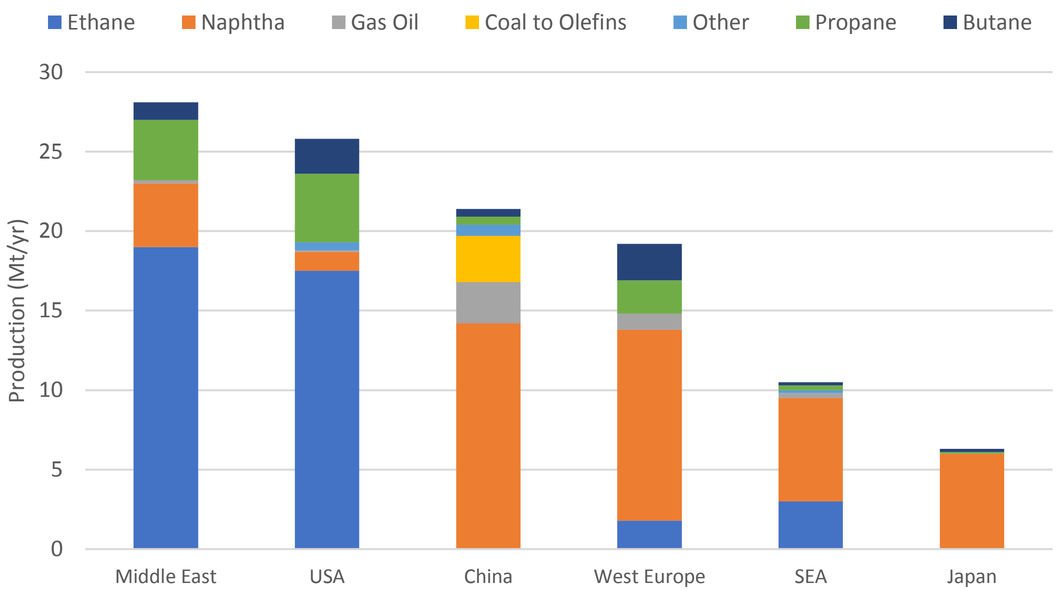

Figure 7 World ethylene production by feedstock[8]

China has invested in coal to olefins (CTO) plants that capitalise on low cost coal to reduce its dependence on imports of the monomer and polymers. On the basis of planned investment, by early in the next decade as much as 20% of ethylene produced in China could use coal as the primary feedstock. Small volumes (in a global context) are now also being produced from methanol (MTO).

2.2.3 Demand, production and trade

Between 1995 and 2015, global demand for ethylene doubled to over 140mtpa, with a CAGR of 3.6%. Growth is concentrated in the developing economies of Asia, where it is used for domestic consumption of plastics etc, and in the Middle East where it is primarily used to manufacture bulk plastics for export to Asia, consistent with a policy of seeking to maximise the hydrocarbon added value within the region (Figure 8).

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[8] Mitsubishi (2017). Global Supply and Demand of Petrochemical Products relied on LPG as Feedstock, Mitsubishi Chemical Techno-Research. Accessed from: http://www.lpgc.or.jp/corporate/information/program5_Japan2.pdf

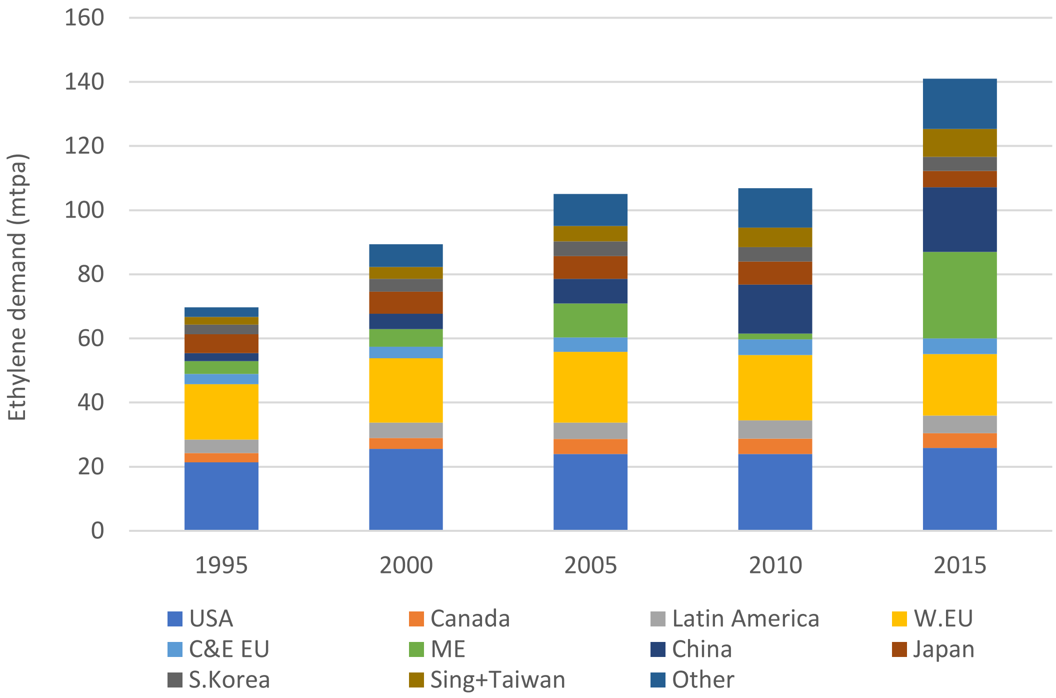

Figure 8 Growth in ethylene demand by region[4,5]

International trade in ethylene has been constrained by the high cost of liquefaction, shipping and handling. However, recently this changed as investment in refineries and petrochemical plants in the Middle East has sought to take advantage of the abundant reserves of low cost feedstocks, to become a key source of supply to China both in the form of ethylene and the finished bulk polymer.

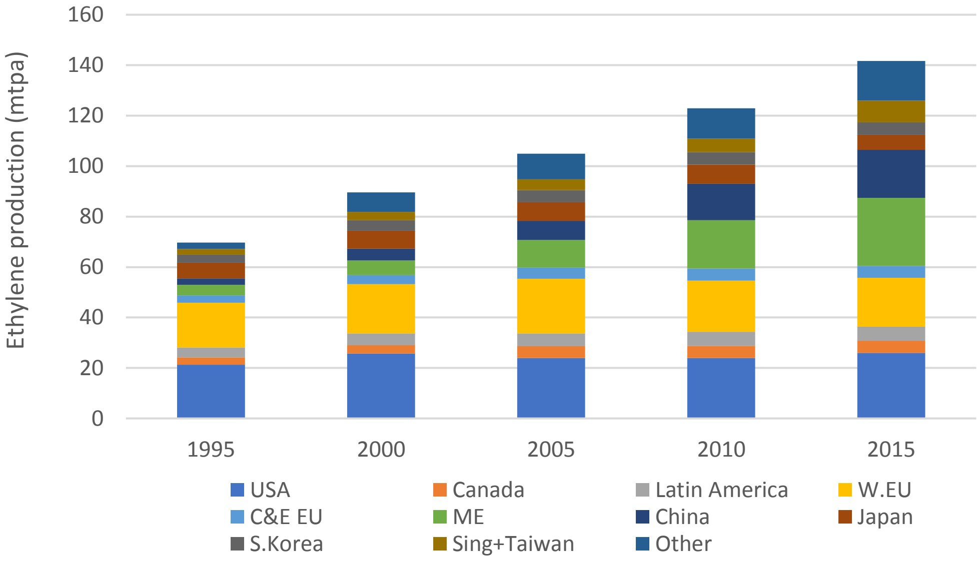

Figure 9 Ethylene production by region[4]

The supply position in North America is also undergoing change. The development of shale gas and shale oil has created new streams of NGLs and associated gas respectively and there is currently a substantial programme of investment in ethane pipelines and ethane crackers that will significantly increase the production of ethylene.

The development of the Chinese market is clearly reflected in the changing patterns of trade in ethylene between 1995 and 2015 as shown in Figure 10, with imports of 1.5mtpa in 2015. However, trade figures for the Middle East and China obscure the fact that most ethylene is traded in the form of the bulk polymer.

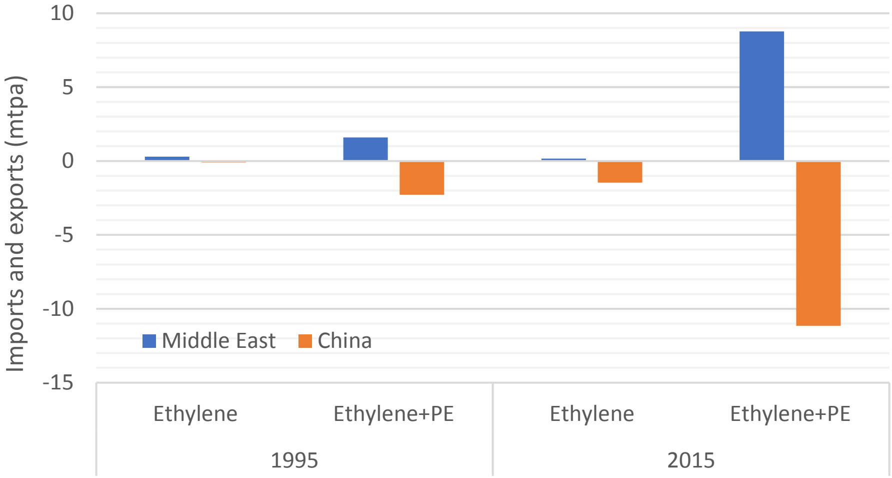

Figure 10 Ethylene and bulk polyethylene exports and imports[4,5]

Accounting for the trade in ethylene as a bulk polymer as well as the raw product underlines the importance of China as an importer for olefins in either form in the global traded market. The extent to which these imports may be replaced by domestic production as the investment programme in coal-to-olefins plants gather pace is therefore a critical issue in the medium term, and one that could be affected by the balance between Chinese policy on carbon emissions, other environmental issues and a desire to achieve self-sufficiency in petrochemicals.

2.3 Propylene

2.3.1 Uses

Propylene has a wide range of uses as shown in Figure 11, but primarily for manufacture of polypropylene (PP). Injection moulded PP is the basis of casings for domestic appliances, electronic items, luggage etc. Extruded PP is seen in piping, wiring and cabling. PP can also be used to form fibres for use in the textile industry, ropes and string. Propylene Oxide (PO), also derived from propylene, is the primary feedstock for polyurethanes, propylene glycol and for propylene glycol ethers which are found in paints, inks, resins etc.

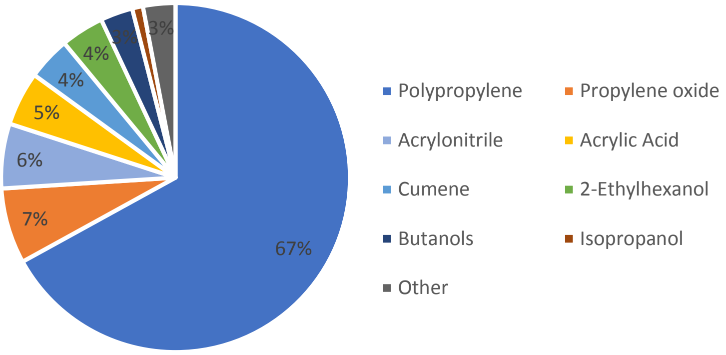

Figure 11 Propylene demand by end use 2015[9]

2.3.2 Feedstock

Propylene, unlike ethylene, has a range of sources as shown in Figure 12. Steam-cracking contributes over half of the production, typically associated with the production of ethylene through the cracking of naphtha and gasoil. However, propylene is also produced in significant quantities as a by-product of the production of high octane gasoline in fluidised catalytic cracker (FCC) refining units, well as from propane dehydrogenation (PDH).

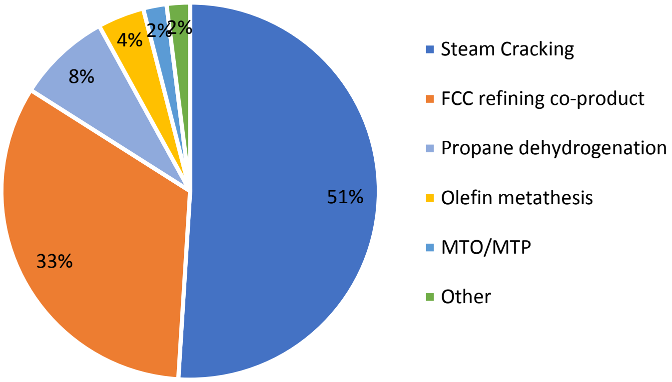

Figure 12 Propylene supply by process[9]

2.3.3 Demand, production and trade

Propylene attractiveness as a basis for a wide variety of products and historically relatively low-cost relative to other monomers has seen demand grow faster than ethylene, by 4.8% CAGR between 1995 and 2015[4], more than doubling to just under 94mpta.

The pattern of demand growth reflects that of ethylene, with near stagnant demand in North America and Europe and strong growth in the Far East based upon use in manufacturing as shown in Figure 13. Again - in the Middle East demand is driven by

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[9] J.S. Plotkin (2016). The Propylene Quandry. ACS Industrial Chemistry and Engineering. Accessed from: https://www.acs.org/content/acs/en/pressroom/cutting-edge-chemistry/the-propylene-quandary.html

use in petrochemical industry where most of the product is exported in the form of bulk polymers, primarily directed at Far Eastern markets.

Propylene and ethylene compete for polymer markets, and the relative price of the two products is an important determinant of the relative growth in demand. Historically, with naphtha a key feedstock, steam cracking output has been weighted towards the heavier product, propylene. However, the increasing use of NGLs as feedstock, in particular the ethane-rich NGLs of North American shales increasingly favours the production of ethylene, reducing the cost advantage of propylene.

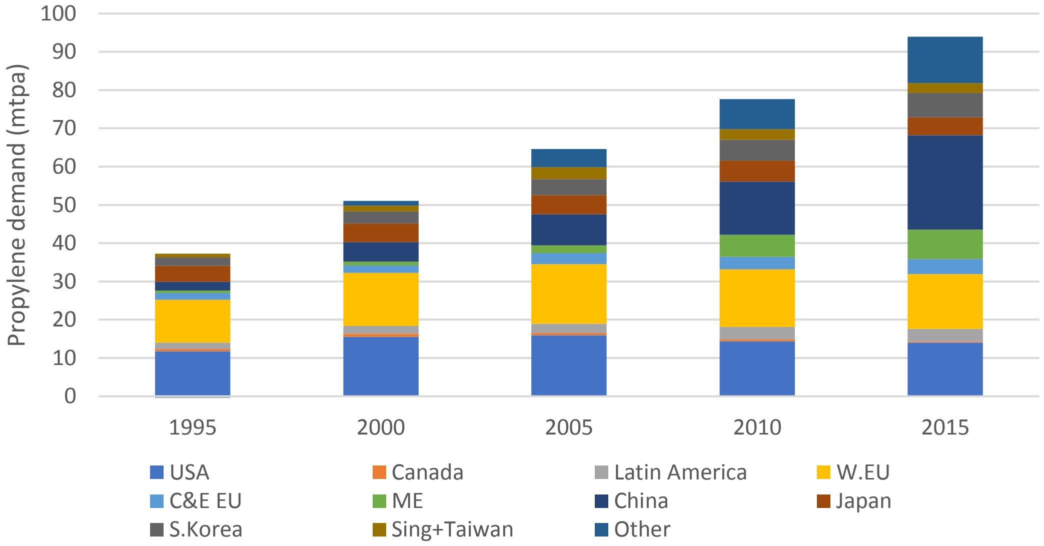

Figure 13 Growth in propylene demand by region[4,5].

The supply of propylene also closely mirrors that of ethylene, with increasing supply for export from the Middle East feeding demand in China in particular, albeit with China also increasing domestic production (Figure 14).

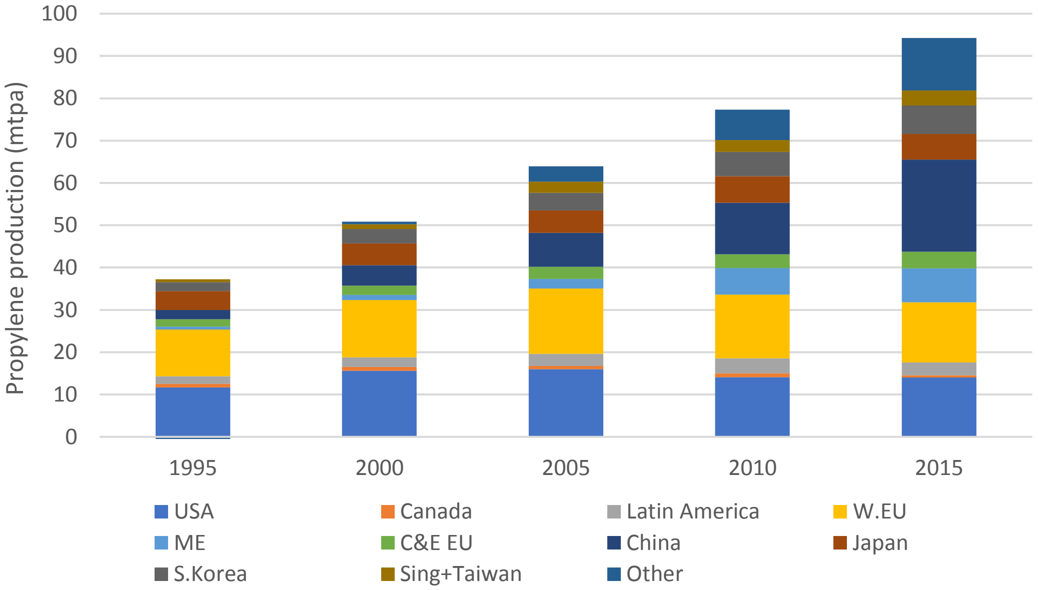

Figure 14 Propylene production by region[4]

The shift in trade of propylene reflects increasing demand into China, and the concurrent increased export capacity in neighbouring Japan and South Korea (Figure 15). The low export figures for the Middle East for the monomer hides the growing export volumes of polymers directed at Asia markets, China in particular.

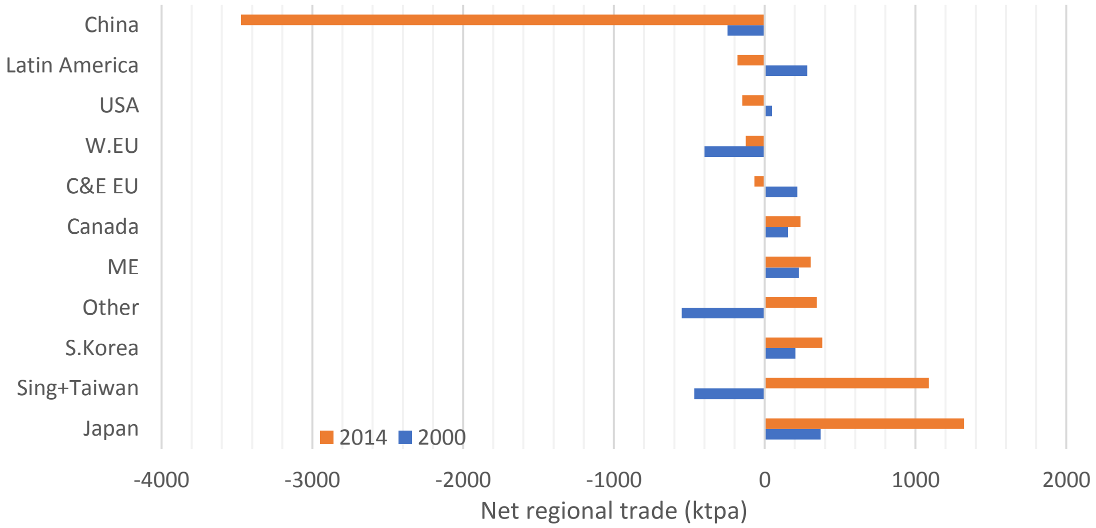

Figure 15 Net regional propylene trade[4,5]

2.4 Butadiene

Butadiene is predominantly used in the production of synthetic rubbers and latexes in competition with natural rubber. Demand has reflected car manufacture, and historically has been met from the stream cracking of naphtha. However, with lighter NGL's now increasingly used for olefins, this has seen a tightening of the availability of butadiene. The investment in MTO and CTO plants in China has to some extent compensated for this trend.

2.4.1 Uses

The main use of butadiene is in the manufacture of synthetic rubbers. Styrene-butadiene rubber (SBR) and polybutadiene rubber (PBR) is used to make synthetic tyres and rubberised plastic materials. Polychloroprene (Neoprene) is used in fabrics, whilst nitrile rubber (NR) is used in hoses, gaskets and gloves.

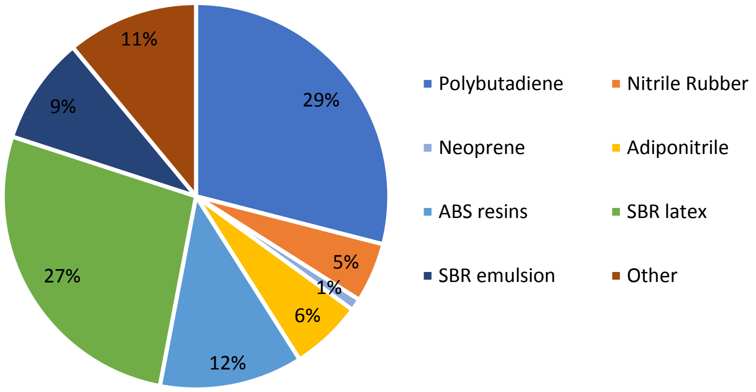

Figure 16 Butadiene demand by end use in 2015[10]

2.4.2 Feedstock

Almost all of the global supply of butadiene is extracted from the mixed C4 stream from steam cracking[10]. The balance comes from the recent investment in MTO and CTO projects in China.

2.4.3 Demand, production and trade

Butadiene rubbers compete directly with natural rubber, and demand on a year by year basis varies to compensate for variations in the natural rubber production due to weather – rainfall and floods in particular.

The location of demand for butadiene is largely determined by tyre production. The rapid growth in vehicle manufacture in China has increased butadiene demand by 2.3 mtpa between 1995 and 2015, equivalent to over half the global increase in demand (Figure 17). There has been a reduction in demand from the US concurrent with reduced US vehicle manufacturing and a shortage of feedstock.

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[10] J.S. Plotkin (2016). The Continuing Quest for Butadiene, ACS Industrial Chemistry and Engineering. Accessed from: https://www.acs.org/content/acs/en/pressroom/cutting-edge-chemistry/the-continuing-quest-for-butadiene.html

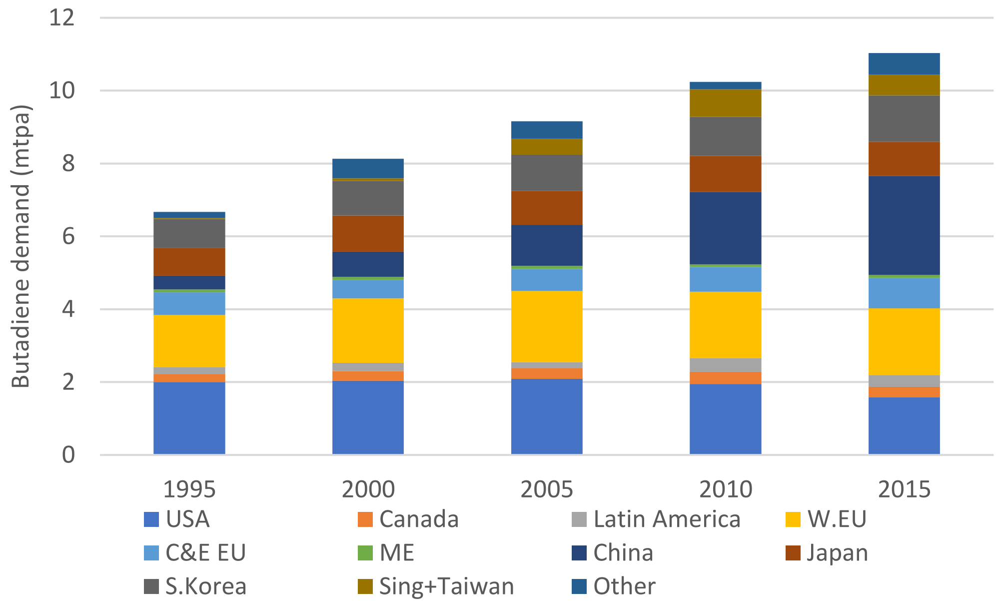

Figure 17 Growth in demand for butadiene by region[4,5].

With increasing use of lighter NGLs as feedstock for steam cracking in the Middle East and North America, the availability of butadiene has become constrained. This has reinforced the drive towards CTO and MTO in China which, combined with oxidative dehydrogenation of butenes, has limited China's reliance on imports.

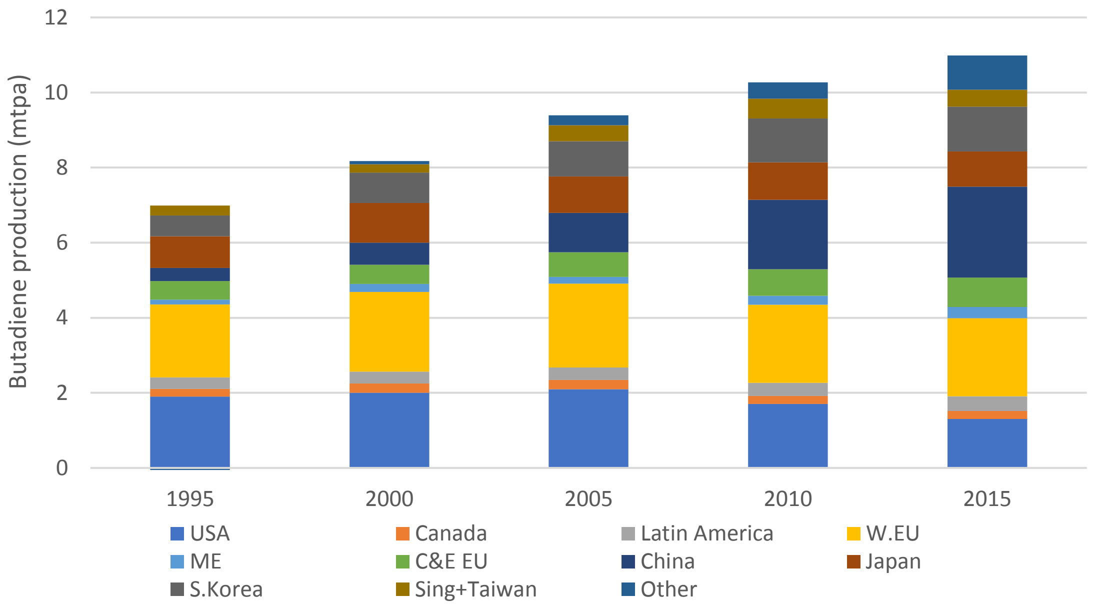

Figure 18 Butiadiene production by region[4]

The changes in feedstock are reflected in the shift in the pattern of trade shown in Figure 19. The US has become a net importer and exports from Western Europe have declined. The balance has been made up by increasing exports from the Middle East.

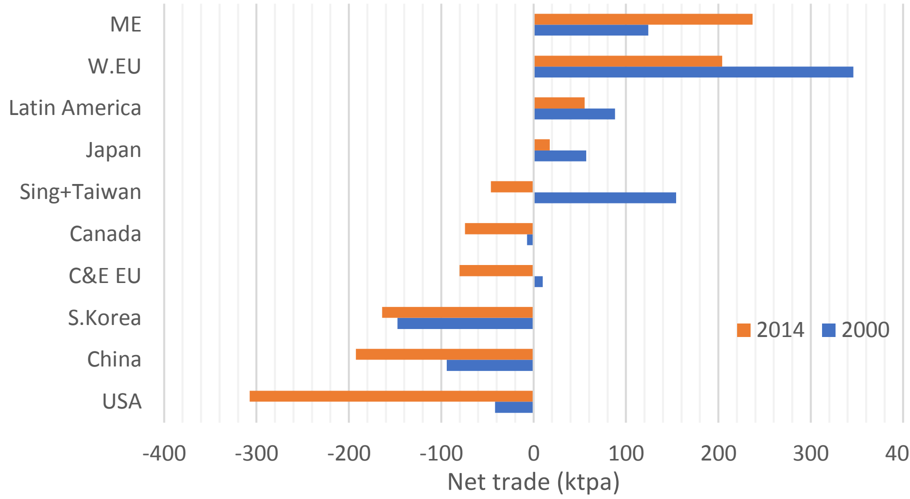

Figure 19 Net regional butadiene trade[4,5]

2.5 Nitrogen Fertilisers

2.5.1 Uses

Ammonia is the feedstock to all nitrogen fertilisers. Only 10% of the application of ammonia is direct, with most converted into ammonia derivatives. More than half of the global consumption of fertiliser is in the form of urea, just under half in the form of various ammonium salts, with the balance in the form of compounds with phosphates and potassium, or the direct application of ammonia (Figure 20). Note that all quantities are measured in terms of tonnes nitrogen as the various formulations contain different percentages of nitrogen, and require different feedstock quantities and the conversion ratio is not one-for-one.

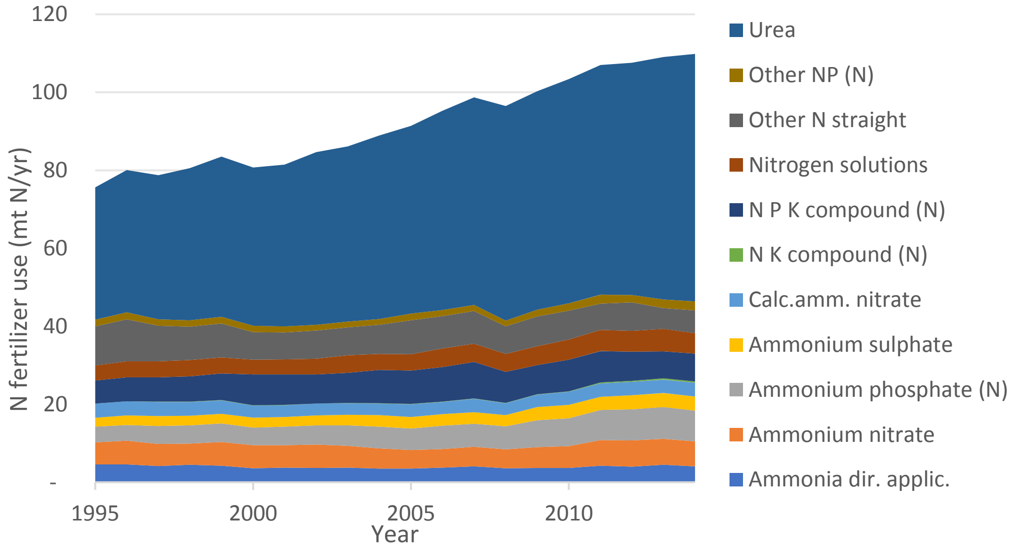

Figure 20 Fertiliser use[11,12]

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[11] Food and Agriculture Organization of the United Nations (2014). FAOSTAT. Fertilizers (Dataset). Accessed 17 May 2018: http://data.fao.org/ref/d1a87a6c-37a8-43be-bfdc-c5cb398a1956.html?version=1.0

[12] International Fertilizer Association (2017). IFADATA IFA Statistics (Dataset). Accessed from: https://www.fertilizer.org/En/Statistics/Statistics.aspx?WebsiteKey=411e9724-4bda-422f-abfc-

Of the circa 180 mtpa[12]of ammonia production in 2014, some 20% is used in industrial applications split evenly between use as a feedstock for explosives, use in the textile industry and other chemical and feedstock uses.

2.5.2 Feedstock

The feedstock for ammonia production is predominantly natural gas as shown in Figure 21. However, where coal is low cost and/or there is no access to natural gas, coal is used as a feedstock through coal gasification, e.g. in China.

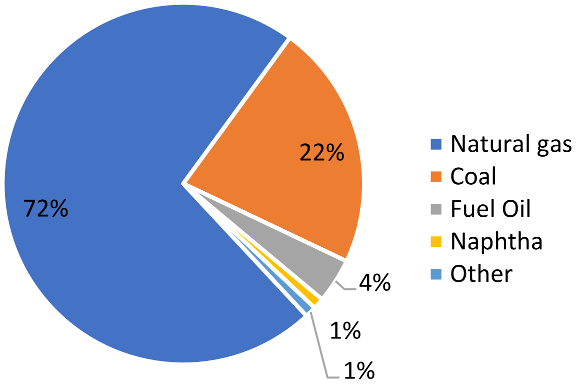

Figure 21 Feedstock for ammonia in 2015[11]

2.5.3 Demand, production and trade

China and India together make up 45% of the global use of nitrogen, and their growth in use between 1995 and 2014 has been close to the global average of a CAGR of 2.0%. The fastest growing areas for fertiliser use are C&E Europe, predominantly Russia, Latin America and Africa, as these regions seek to bring more land under cultivation and increase the yields from existing stock.

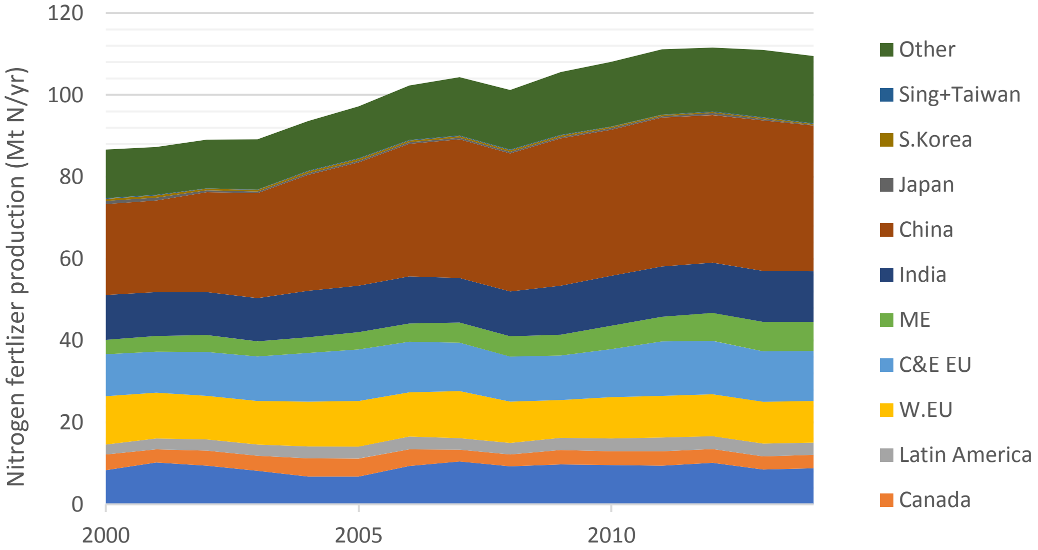

Figure 22 Fertiliser demand by region[11,12]

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Increasing crop production requires a higher intensity of production in the absence of underutilised arable land, hence growth in fertiliser demand. As the intensity of crop yield per hectare increases, so does fertiliser use per hectare. Figure 23 also suggests diminishing returns from incremental application at a national level. In Asia, the area for cultivation has remained broadly constant, but the intensity of use has increased threefold since 1960. By contrast in Africa the area under cereal cultivation has more than doubled, but with only a 30% increase in yield per hectare.

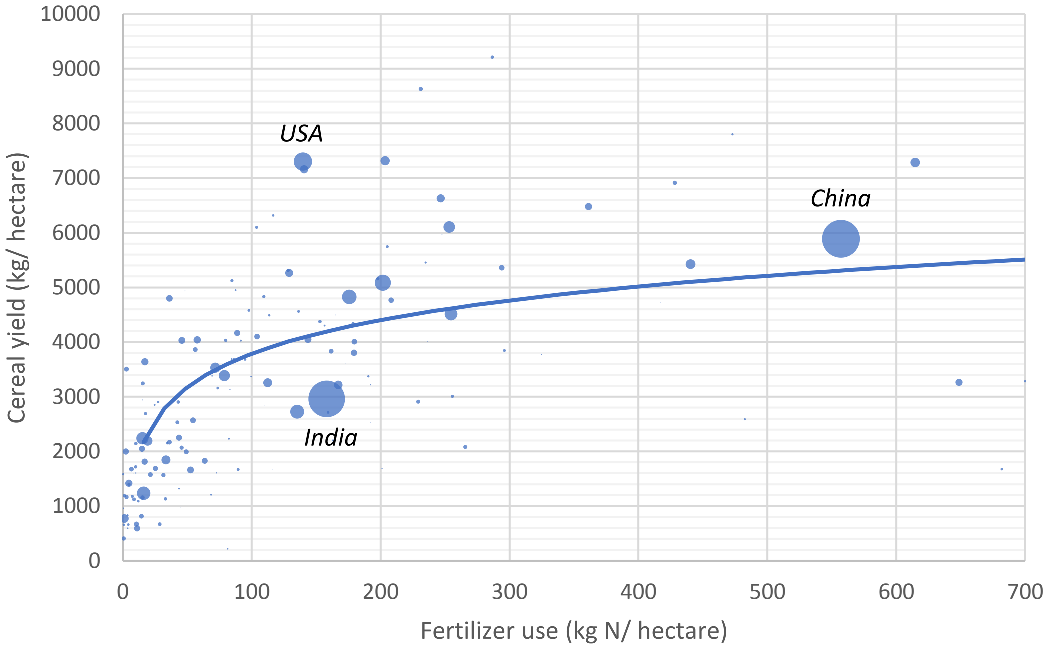

Figure 23 The dependency of crop yield on fertiliser intensity[11]. Bubble size reflects national population and the solid line is a logarithmic regression trendline.

Regional supply closely follows demand, though the availability of low cost feedstock in the Middle East, Russia and Trinidad has encouraged the export of ammonia and fertiliser plants. Cross border trade in nitrogen fertilisers has been increasing: international trade in 2000 was 17% of total consumption, and by 2014 had grown to 24%. On the demand side, the increase in imports has been driven by the strong growth in fertiliser use in countries such as Brazil, Mexico and India, and through the period 2000-2010 by the USA, due to the high relative cost of natural gas in the USA over that period.

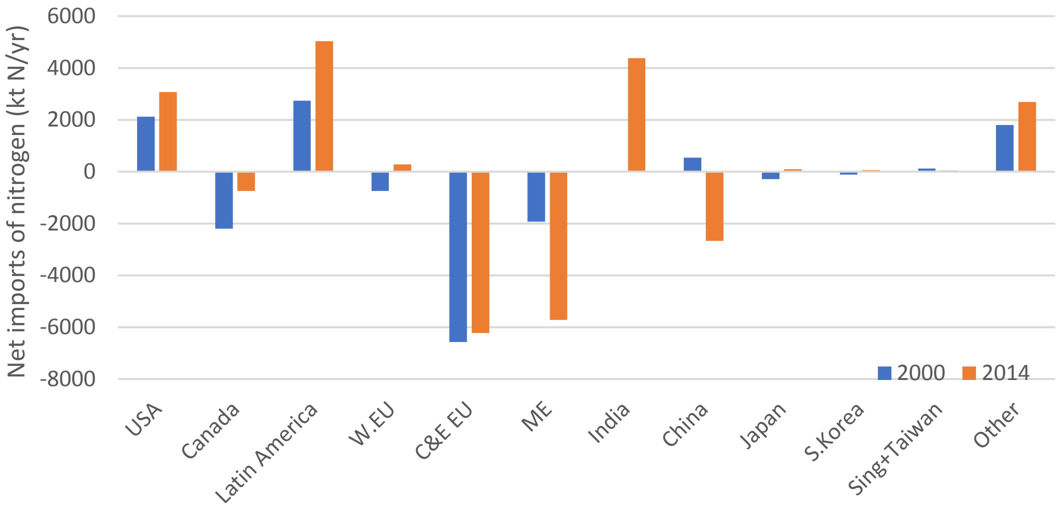

Figure 24 Net imports of nitrogen[11,12]

This import demand has been met by the traditional exporter, Russia, and now the Middle East and China. Looking forward, countries such as the USA, Brazil, Tanzania and Mozambique are looking to build fertiliser plants to meet local demand as new low cost natural gas supplies come on stream over the next decade. These plants will likely compensate for the reduction in natural gas feedstock availability as fields in countries such as Trinidad mature.

2.6 Demand projection

In this section, demand projections are made for each of the above petrochemicals based on the relationship between historical demand and the structural drivers of this demand. The data collected on demand, production and trade of each petrochemical as described above has been used as input for the demand projections. Petrochemicals considered in the study are methanol, ethylene, propylene, butadiene and ammonia. Regional regressions are made for different regions in the following categories: Canada, China, India, Japan, Latin America, Middle East, Russia, South East Asia, South Korea, USA, West and North Europe, all the remaining regions i.e. others and world. The data collected was for a timeframe of 1995 – 2015 and was included for regression, against the macroeconomic variables of population and GDP.

Core drivers are those developed within the latest Shared Socioeconomic Pathways of development (that project GDP, population and urbanisation for each country in the world on a common basis). The Shared Socio-Economic Pathways (SSPs) provide projections of socio-economic macro drivers (such as population, GDP and urbanisation) developed by the International Institute for Applied Systems Analysis (IIASA) and the National Centre for Atmospheric Research (NCAR)[13]. There are five sets of SSPs, each one representing a different narrative in terms of global development. Low, medium and high challenges to mitigation and adaptation are represented respectively by SSP1, SSP2 and SSP3, while SSP4 portrays low challenges

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[13] IIASA (2016). SSP Database (Shared Socioeconomic Pathways) - Version 1.1, [Online]. Available: https://tntcat.iiasa.ac.at/SspDb/dsd?Action=htmlpage&page=about [Accessed 29/ 11/ 2017]

to mitigation and high challenges to adaptation and SSP5 the opposite trend i.e. high challenges to mitigation and low challenges to adaptation[14]. SSP2, which has been used for these projections, is defined as a 'middle of the road' pathway, consistent "with typical patterns of historical experience observed over the past century"[15].

The following linear and non-linear regression functions were tested to correlate petrochemical demand with population and GDP[16]:

- Linear (LN): $demand\ pc = a\ \times GDP\ pc + b$
- Log-log (LL): $\ln(demand\ pc) = a + b \times ln(GDP\ pc)$
- Semi-log (SL): $demand\ pc = a + b \times \ln(GDP\ pc)$
- Log-inverse (LI): $\ln(demand\ pc) = a - b/(GDP\ pc)$
- Log-log-square(LLS): $\ln(demand\ pc) = a + b \times ln(GDP\ pc) - c \times \ln(GDP\ pc)^2$
- Power (P): $demand\ pc = a\ \times\ GDP\ pc^b + c$
- Non-linear inverse (NLI): $demand\ pc = a\ \times\ e^{b/GDP\ pc}$
- Non-linear inverse with time efficiency factor (NLIT): $demand\ pc = a\ \times e^{b/GDP\ pc}\ \times (1-m)^{T-2010}$
- Log-inverse with time efficiency factor (LIT): $\ln(demand\ pc) = a + b/GDp\ pc + \ln(T - 1969)$.

The parameters *a*, *b* and *c* are constants to be estimated during the regression, while *m* is the time efficiency factor.

Each regression function was assessed and an optimisation software (MathWorks Curve Fitting Toolbox™ [17]) was employed to perform the regression and estimate the R-squared value for each trend. The mathematical representations were selected using an optimisation approach based on the minimisation of the squared error sum. As such, the obtained projections should be interpreted as the best fit of the average trend in the demand during the analysed period. Although extemporaneous discontinuities might not be captured, such as those observed in the ethylene and propylene demand in China approaching 2015, the approach interprets well the average historical demand behaviour. In doing so, it can give a plausible trend that

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[14] K. Riahi, D. P. van Vuuren, E. Kriegler, J. Edmonds, B. C. O'Neill, S. Fujimori, N. Bauer, K. Calvin, R. Dellink, O. Fricko, W. Lutz, A. Popp, J. C. Cuaresma, S. Kc, M. Leimbach, L. Jiang, T. Kram, S. Rao, J. Emmerling, K. Ebi, T. Hasegawa, P. Havlik, F. Humpenöder, L. A. Da Silva, S. Smith, E. Stehfest, V. Bosetti, J. Eom, D. Gernaat, T. Masui, J. Rogelj, J. Strefler, L. Drouet, V. Krey, G. Luderer, M. Harmsen, K. Takahashi, L. Baumstark, J. C. Doelman, M. Kainuma, Z. Klimont, G. Marangoni, H. Lotze-Campen, M. Obersteiner, A. Tabeau & M. Tavoni (2017). The Shared Socioeconomic Pathways and their energy, land use, and greenhouse gas emissions implications: An overview. Global Environmental Change, 42, 153-168.

[15] B. C. O'Neill, E. Kriegler, K. L. Ebi, E. Kemp-Benedict, K. Riahi, D. S. Rothman, B. J. van Ruijven, D. P. van Vuuren, J. Birkmann, K. Kok, M. Levy & W. Solecki (2017). The roads ahead: Narratives for shared socioeconomic pathways describing world futures in the 21st century. Global Environmental Change, 42, 169-180.

[16] B. J. van Ruijven, D. P. van Vuuren, W. Boskaljon, M. L. Neelis, D. Saygin & M. K. Patel (2016). Long-term model-based projections of energy use and CO2 emissions from the global steel and cement industries. Resources, Conservation and Recycling, 112, 15-36.

[17] MathWorks, Inc (2018). Curve fitting toolbox: for use with MATLAB®: user's guide. Version 1. Natick, MA : MathWorks, 2001 [Online]. Available: https://uk.mathworks.com/help/curvefit/product-description.html [Accessed 29/ 05/ 2018]

the demand could follow as a result of the population and welfare evolution in the country.

Four functions were chosen across the commodities and regions: LN, SL, NLI and P functions. Linear functions fit particularly well with historical trends related to expanding markets or developing regions, whereas semi-log functions broadly fit well with developed regions as shown in Table 1. This assumption has been adopted for projections up to 2050, but should be revised for studies beyond the year 2050. The selection of the regression functions are summarised in the following table, by commodity and by region.

Table 1 Selection of demand regression functions by study regions and petrochemical commodities

Study region	**Butadiene**	**Ethylene**	**Methanol**	**Propylene**	**Ammonia**
Canada	SL	SL	LN	SL	P
China	SL	LN	NLI	NLI	P
Japan	SL	SL	SL	SL	P
Latin America	SL	SL	SL	SL	P
Middle East	SL	NLI	SL	SL	P
Others	SL	SL	SL	SL	P
India	-	-	-	-	P
Russia	SL	LN	SL	LN	P
SE Asia	SL	SL	LN	SL	P
South Korea	SL	NLI	SL	SL	P
USA	SL	SL	SL	SL	P
W and N Europe	SL	SL	LN	SL	P
World	SL	SL	SL	SL	P

The following figures are the results of the case study region of China, as well as for the USA, the Middle East, and North and west Europe. The fitted regression curves for China are shown in the Appendix, whilst the historical demand and projections up to 2050 are shown in **Error! Reference source not found.**, Figure 26, Figure 27 and Figure 28

The demand of all the reported commodities show a strong correlation with the regional GDP and also highlights the pronounced growth that China has undertaken in the past 25 years. The general demand growth presented in this study, which is broadly in agreement with the expert elicitations presented in section 6, evolve differently depending on the region. In particular, growing economies, such as China, would show a rapid expansion followed by a stabilisation trend towards 2050. On the contrary, established markets such as Europe and US exhibit low growth rates and generally an early saturation.

Among the exceptions to the general growing trend in the petrochemical demand, it is worth mentioning the case of methanol in the US as well as ammonia in China. The methanol demand in the USA, linked to the trend shown in the historical data, shows a connection with the decisions of the country to eliminate its use as a fuel due to environmental concerns. For ammonia demand in China, the projected decrease is due to population reduction towards 2050, due to the strong links with the fertiliser industry and food demand.

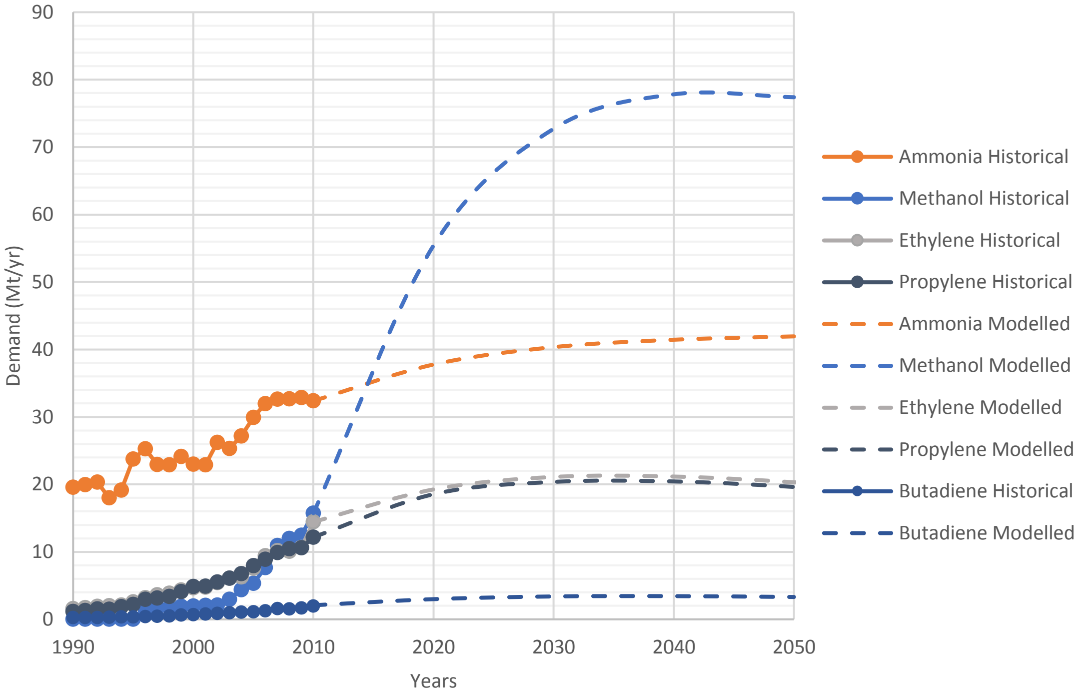

Figure 25. Historical demand and projections of petrochemicals for China up to 2050.

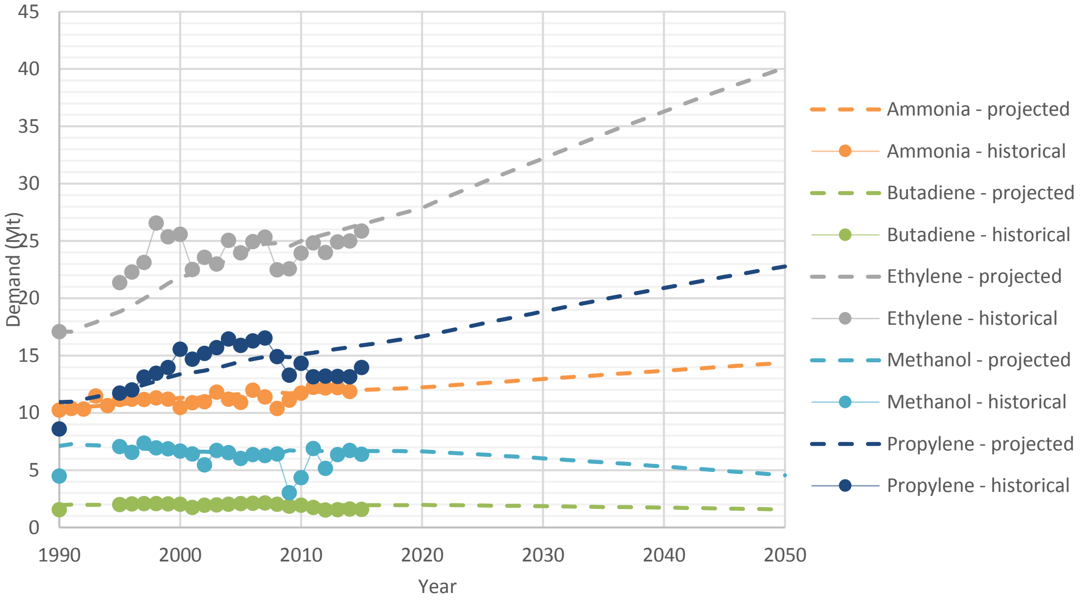

Figure 26. Historical demand and projections of petrochemicals for USA up to 2050

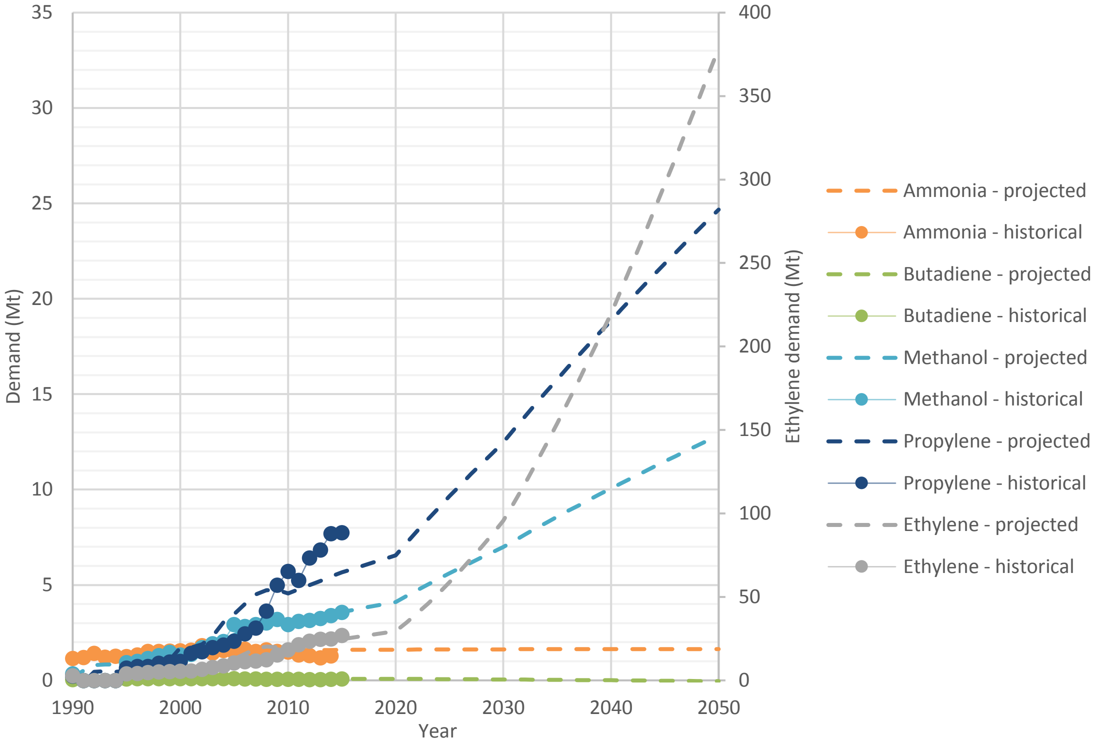

Figure 27. Historical demand and projections of petrochemicals for the Middle East up to 2050. Note that the trend for ethylene demand is shown on the secondary axis given the large projected increase.

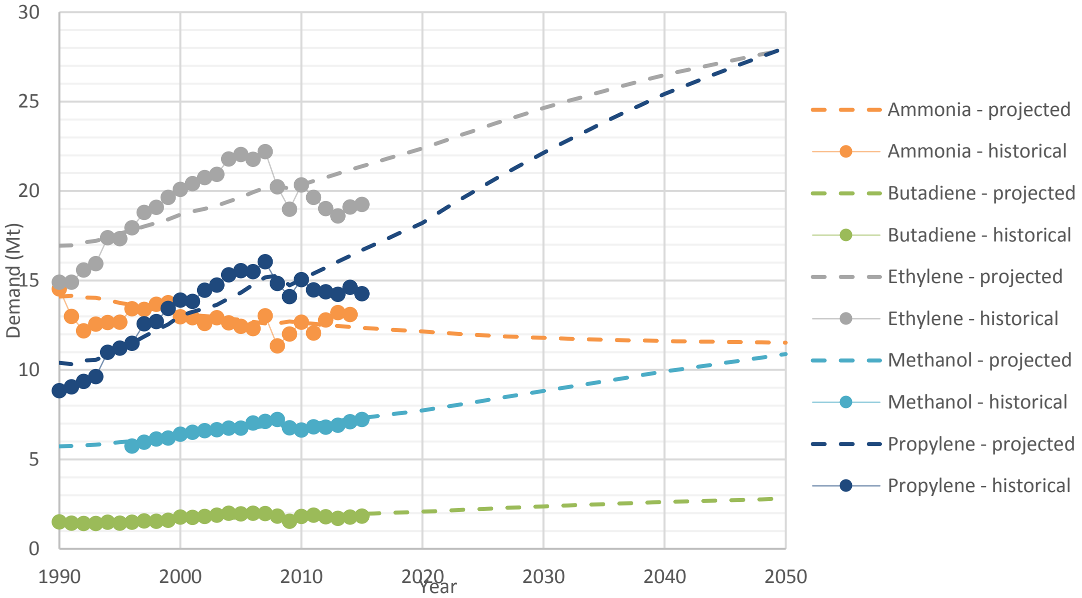

Figure 28. Historical demand and projections of petrochemicals for West and North-East Europe up to 2050.

2.7 Summary

This section has described historical trends and current status of petrochemical commodities relating to feedstocks, uses, demand and production across different regions of the world. Projections of demand for each commodity are to increase significantly for the case study region, albeit by different rates across products. A number of key narratives arise from this chapter, which are summarised below.

With the cost of methanol feedstock being the majority of the cost of manufacture of methanol, the location of methanol production follows the lowest cost feed. This primarily gives preference to low cost natural gas, whereas coal dominates in China. Methanol has a highly diverse range of end-uses, but a large proportion is as a component in transport fuel. Given that the US has eliminated this due to environmental concerns, this may also reduce elsewhere over time. However, the potential of methanol as an intermediate chemical in a multitude of applications suggests that the potential for increased and diverse demand globally is high.

The global focus of ethylene manufacturing has moved from European and North American economies to those of East Asia, and so has demand for ethylene and its derivatives. Historically the steam cracking of naphtha has been starting point for olefin manufacture and has determined the pattern of trade. However, naphtha is being replaced as a feedstock as cheap natural gas liquids become increasingly available. As countries seek to become self-reliant they are also looking to coal and methanol as a petrochemical feedstock.

There has been significant investment in olefin plant in the Middle East, which is increasingly focussing on NGLs as a feedstock. This may lead to freeing up the traditional feedstock of naphtha for gasoline manufacture. Additionally, a focus on self-sufficiency in both China and the US has led to changing trade dynamics of olefins. China has rapidly expanded its coal-to-olefin capacity, and the US has utilised NGLs associated with recent growth in shale gas production. This growth in China, the US and the Middle East has the potential to create an excess of global capacity. Petrochemicals increasingly compete at a global level, resulting in drives toward lower cost feedstock, increased plant efficiency and integration.

Demand for ammonia is primarily driven by extent and intensity of cereal farming. As yields per hectare increase to meet the increasing demand for grain, fertiliser use increases as a compound of crop tonnage and tonnage per hectare. Historically fertiliser production has been close to the point of use, driven by a combination of economic and policy considerations. However, as the cost of the principal feedstock natural gas has fallen, global trade in nitrogen products has risen significantly.

3. Process engineering characterisation

This section defines the process engineering features and core techno-economic characteristics of a set of production routes for each category of petrochemicals. For each product, the conventional process route is set out, alongside alternative routes with potentially improved greenhouse gas (GHG) and sustainability credentials.

An engineering assessment of the potential avenues for inclusion of renewable energy and the use of CO_2 derived from carbon capture in each process is also undertaken. Note that the study did not include an assessment of CCS in conjunction with conventional methods, but more information can be found in a dedicated 2017 IEAGHG report in relation to methanol and ammonia[18]. The following section is divided into 3 sub-sections: methanol production, olefin production and ammonia/urea production. Note that for olefin production, this section and the proceeding analyses consider only ethylene and propylene.

3.1 Methanol

For each methanol production route a brief overview of the plant, process flow diagram (PFD), mass balance, energy balance and key performance indicator is outlined.

3.1.1 Conventional methanol synthesis

Conventional methanol production is based on synthetic gas, produced through coal gasification or steam methane reforming (SMR). In order to increase the productivity and decrease environmental impact, the produced carbon dioxide is separated and mixed with synthetic gas. The process flow diagram (PFD), with recycled carbon dioxide, is illustrated in the following figure, not including the production of syngas.

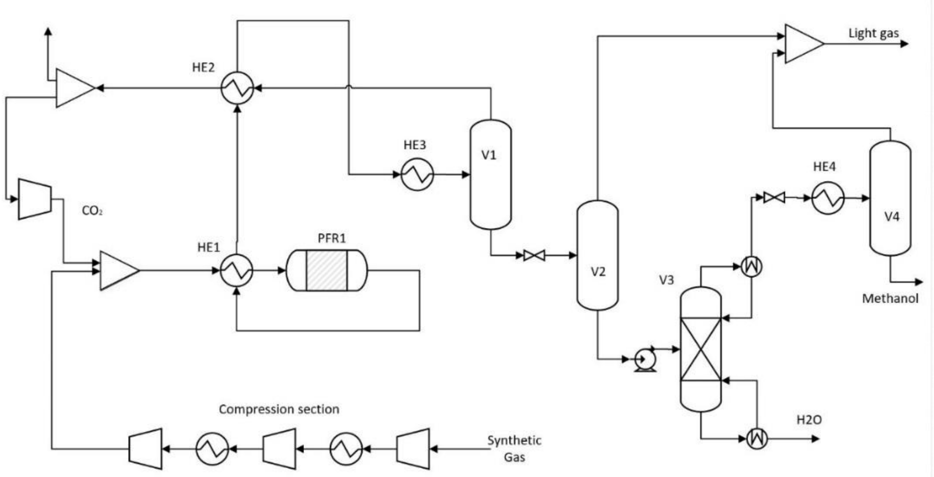

Figure 29 Process Flow Diagram of syngas to methanol[19]

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[18] IEAGHG (2017). Techno-Economic Evaluation of Hyco Plant Integrated to Ammonia/Urea or Methanol Production with CCS. February 2017. Available from: http://ieaghg.org/exco_docs/2017-03.pdf

[19] C. F. R. Machado, , J.L. de Medeiros & O. F. Q. Araújo (2014). et al.A comparative analysis of methanol production routes: synthesis gas versus CO2 hydrogenation. Proceedings of the 2014 International Conference on Industrial Engineering and Operations Management Bali, Indonesia.

The syngas feed stream is heated to 200-300°C and compressed to 50-100 bar. The carbon dioxide recycle is mixed and fed to the cooled fixed bed plug flow reactor (PFR1). A series of reactions occur here to produce methanol from carbon monoxide, carbon dioxide and hydrogen[20]:

$$CO + 2H_2 \Leftrightarrow CH_3OH$$
$$CO_2 + H_2 \Leftrightarrow CO + H_2O$$
$$CO_2 + 3H_2 \Leftrightarrow CH_3OH + H_2O$$

Heat exchangers HE1 and HE2 perform energy integration, with cooling temperature set to maximise recovery of methanol in the flash separation unit V1 and low pressure V2. The gas phase stream leaving the flash separation unit (V1) is recycled and mixed with syngas, in case of carbon dioxide utilisation. The liquid phase, rich in methanol, is flashed at low pressure (V2) and then fed to a distillation column (V3). The bottom stream is mainly water, and distillate is cooled (HE4) and decompressed to 1 bar. The product stream is then flashed to ensure high purity. The top stream of V2 and V4 are mainly light gas, which are mixed and disposed.[19] Key metrics associated with conventional methanol synthesis are described further in the Appendix.

3.1.2 Methanol from catalytic hydrogenation

The catalytic hydrogenation of CO_2 has a technology readiness level (TRL) of 5-6: it has been demonstrated at pilot scale, although one study cites two companies with commercialised technologies[21]. The process reacts carbon dioxide collected from flue gas (through CCS technology) with hydrogen, which may come from a low carbon source. The process flow diagram (PFD) is illustrated in the following figure, not including the production of hydrogen.

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[20] *G.H. Graaf, J.G.M Winkelman (2016). Chemical Equilibria in Methanol Synthesis Including the Water–Gas Shift Reaction: A Critical Reassessment*. Industrial & Engineering Chemistry Research ***2016*** 55 *(20), 5854-5864 DOI: 10.1021/acs.iecr.6b00815*

[21] CO2 Sciences and The Global CO2 Initiative (2016), Global Roadmap for Implementing CO2 Utilization. The Innovation for Cool Earth Forum (ICEF). Accessed from: https://assets.ctfassets.net/xg0gv1arhdr3/27vQZEvrxaQiQEAsGyoSQu/44ee0b72ceb9231ec53ed180cb759614/CO2U_ICEF_Roadmap_FINAL_2016_12_07.pdf

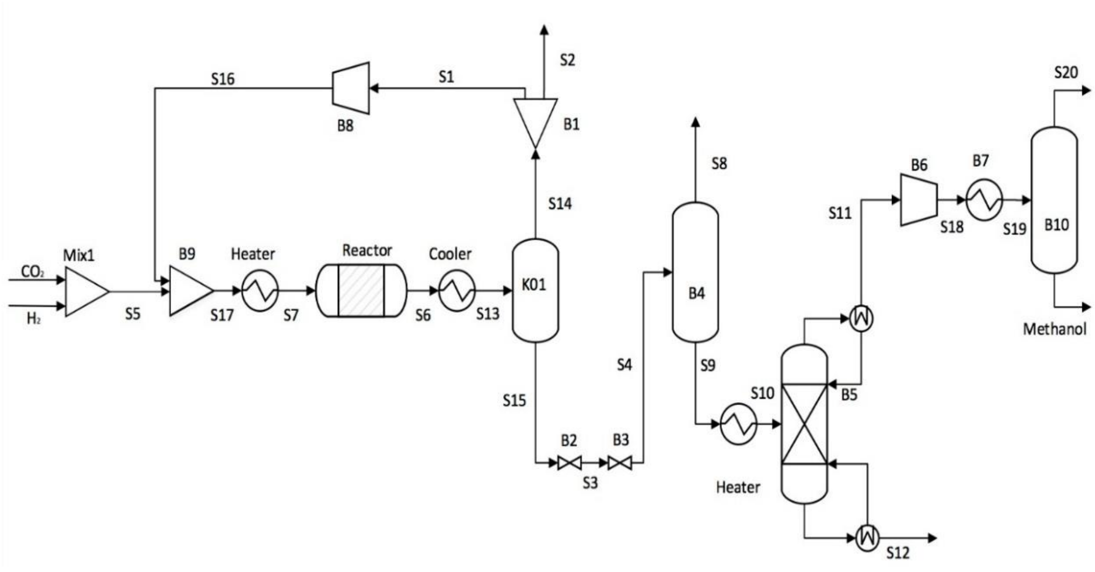

Figure 30 PFD of CO_2 to methanol[19]

Reagents, CO_2 and H_2, are fed at 60 bar, and mixed with the recycle stream. The stream is heated to 210^{o}C and injected to the fixed bed adiabatic reactor. The reaction pathway depends on the catalyst and operating conditions but an indicative mass and energy balance associated with Figure 30 is detailed in the appendix. The outlet stream is separated through a flash separator (K01); the vapour fraction is recycled. The pressure in the liquid fraction is reduced by 10 bar (B2) then 1.2 bar (B3). Vapour fraction is removed through another flash separator (B4). The resulting liquid fraction is heated to 80^{o}C (Heater) and subsequently fed to a distillation column (B5), with operating at 70-100^{o}C and 1 bar. The top stream, rich in methanol, is compressed to 1.2 bar (B6) and cooled to 40^{o}C (B7). The vapour fraction is removed through a flash separator (B10) and the product is collected in the liquid form. A mass and energy balance of this system as well as key process metrics is available in the Appendix.

3.2 Olefins

3.2.1 Ethane and propane cracking

As shown in Figure 9, the main feedstocks for ethylene and propylene production are ethane, propane and naphtha. The conventional process is thermal cracking in the presence of steam, which inhibits coking and improves ethylene/propylene selectivity. The growth in shale gas production has led to a similar growth in investment in new ethane cracking technology. Typical technology locations include US Gulf Coast, the Middle East, China and Southeast Asia and the North Rhine Region of Europe. A diagram of the cracking process is shown in the figure below.

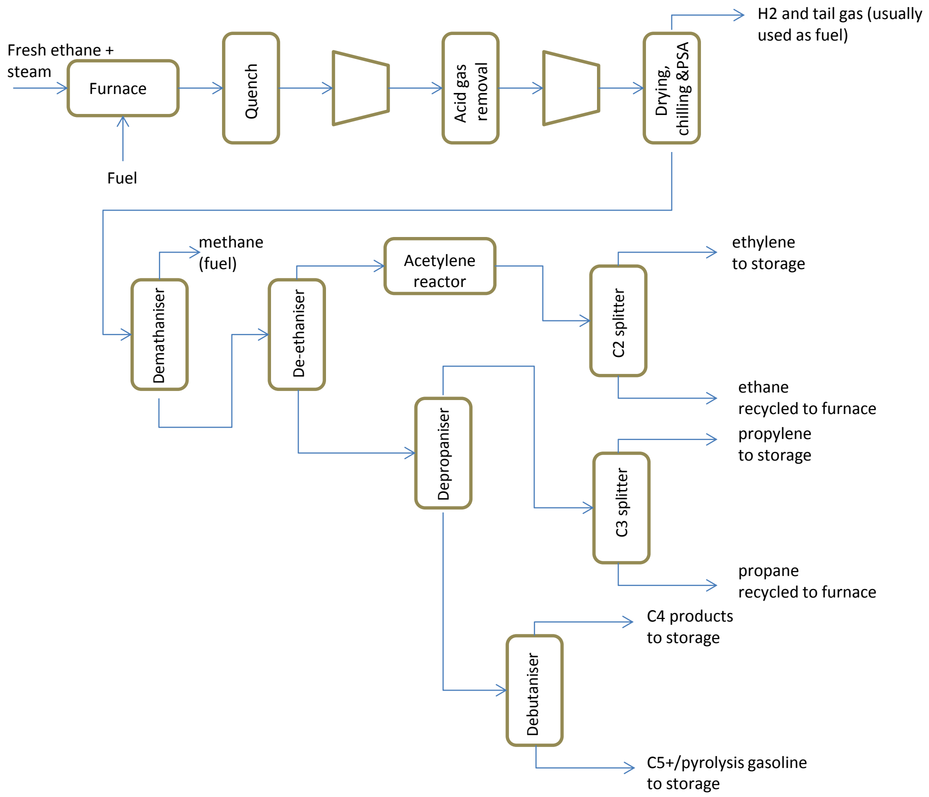

Figure 31 Flowsheet for conventional olefins process

The core unit operation is the steam cracking (furnace) reactor, which is then followed by gas clean up, compression and separation, with recycles of unreacted hydrocarbons and re-use of some fuel gas in the process. The reactor inlet temperature and the outlet temperature typically vary from 850K to 950K and from 1050K to 1200K respectively. The dilution ratio between the steam and the hydrocarbon feedstock typically varies between 0.3 and 0.9 kg-steam per kg-hydrocarbons. This part of the process is known as the “hot side”. After the cracking reaction, water is directly added to quench the cracker effluent. Besides ethylene and other hydrocarbon products, undesired acid gas can also be found in the reactor effluent due to impurities in the raw material. It should be removed from the process stream to enhance final product purity as well as to prevent corrosion of downstream equipment.

The cleaned and compressed process stream then passes through a sequence of drying and cooling steps. The distillation system contains several columns to recover individual products and reactants to recycle. The number of columns depends on the product specifications. Due to the presence of very light components (e.g. hydrogen and methane), the distillation columns operate at relatively low temperatures and are described as the cold side of the process. The basic distillation trains in the typical ethylene process consist of five columns, the demethaniser, deethaniser, the C2 splitter, depropaniser and a C3 splitter. If the C4 product is desirable, a debutaniser column can be placed after the depropaniser for the separation of the C4 and the pyrolysis gasoline.

3.2.2 Methanol-to-Olefin Process

The prevalent alternative to conventional cracking is the methanol-to-olefin processes. The flowsheet for this process is illustrated below, derived from Jasper and El-Halwagi (2015)[22].

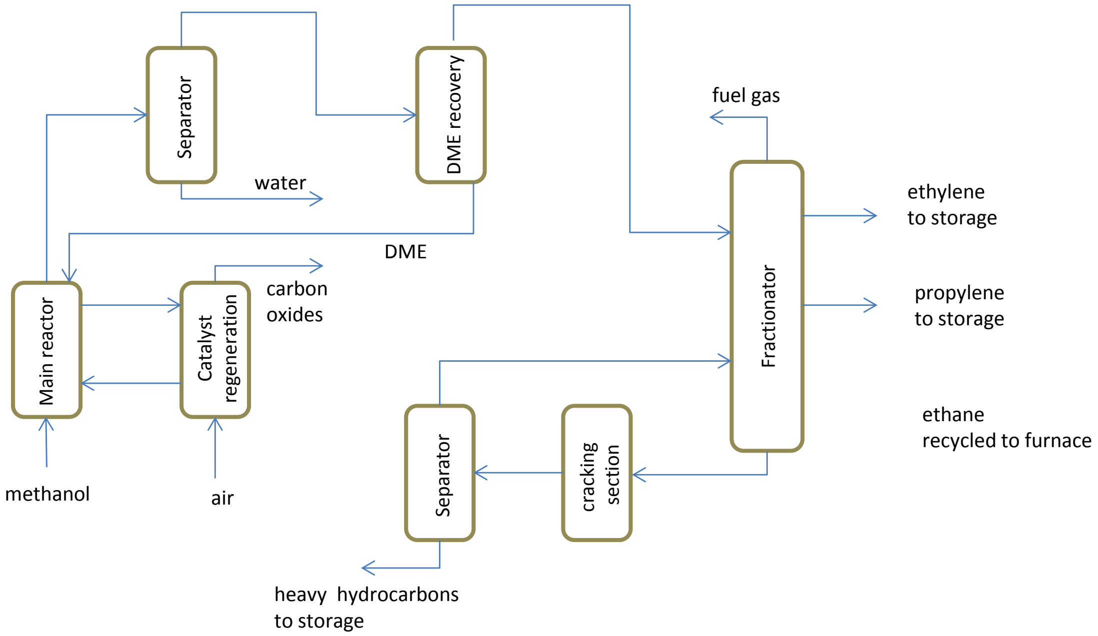

Figure 32 Flowsheet for methanol-to-olefins process

In general, the process has 3 sections (1) methanol production; (2) methanol to olefin reaction; and (3) product purification and separation. Methanol is discussed in the previous section, so here we assume methanol is a primary feedstock.

The key MTO reactions take place in two steps:

1) Dehydration of methanol to dimethyl ether (DME) and water:

$$2CH_3OH \rightarrow CH_3OCH_3 + H_2O \qquad (1)$$

2) Cracking of DME to ethylene and propylene:

$$CH_3OCH_3 \rightarrow C_2H_4 + H_2O \qquad (2)$$

$$3CH_3OCH_3 \rightarrow 2C_3H_6 + 3H_2O \qquad (3)$$

The proportions of olefins produced depend on process conditions and the catalysts used. Production depends on the catalyst, reaction parameters and the technology. Typical overall conversions of the methanol are up to 100% with high selectivity to olefins.

Regarding the process details, the core reactor is a fluidised bed catalytic reactor using a zeolite catalyst. The latter experiences coke build-up and needs to be regenerated. The reactor product is distilled to remove water and then to recover

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[22] S. Jasper & M.M. El-Halwagi (2015). A Techno-Economic Comparison between Two Methanol-to-Propylene Processes.", Processes, 3(3), 684-698.

unreacted DME which is recycled. The remaining stream is rich in olefins and proceeds to a separation and upgrading section, where the desired olefins are removed and heavier hydrocarbons are cracked into the lighter desired ones. Some by-product heavier hydrocarbons are removed as by-products. Further process and economic characteristics of MTO processes are detailed in the Appendix.

3.3 Ammonia and Urea

3.3.1 Conventional ammonia production

Conventional ammonia production is based on two main steps, hydrogen and nitrogen production, and the Haber-Bosch step to ammonia. Typically, hydrogen is produced via natural gas reforming, which produces the carbon monoxide/dioxide stream for the following urea process. The process flow diagram (PFD) for ammonia production is illustrated in the following figure.

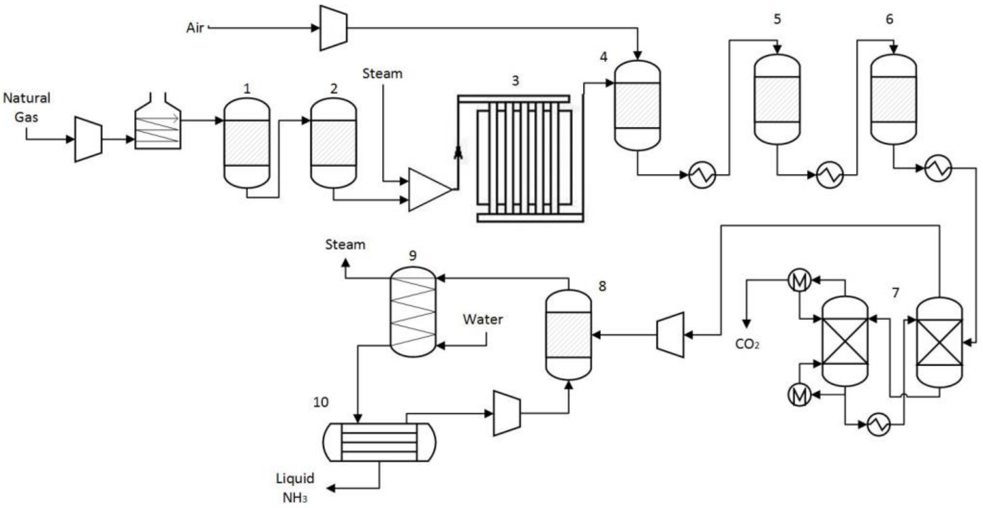

Figure 33 PFD of ammonia production

Natural gas feed is completely desulphurised to prevent deactivation of the catalyst. Sulphur removal is performed on a mixed oxide of cobalt and molybdenum on an inert alumina supported catalyst, this step converts sulphur compounds in the feedstocks to gaseous hydrogen sulphide (1), which are then adsorbed and removed by passing it through beds of zinc oxide where it is converted to solid zinc sulphide (2). The desulphurised natural gas is reformed, on a nickel catalyst, with steam into raw synthetic gas (primary steam reforming, 3); main components are hydrogen, carbon dioxide, carbon monoxide and nitrogen. Secondary steam reforming reacts oxygen, from air, with hydrogen and the resulting mixture is passed over a nickel catalyst (4). The steam and the heat produced from the reaction reform most of the residual methane.

In the gas purification section, the CO and CO_2 are converted into H_2 with steam (shift reaction). The reaction is done in two stages. First (5), the high temperature shift reaction, the gas is mixed with steam and passed over an iron chromium(III) oxide catalyst in order to decrease CO concentration. Then (6), the low temperature shift reaction, the gas mixture is passed over a copper zinc catalyst, where CO concentration is further reduced. Carbon dioxide is removed through a scrubber (7).

The ammonia is synthesised through the Haber-Bosch process, in which H_2 and N_2 (from air) are converted into ammonia by passing them through an iron oxide catalyst (8) (core of Fe_3O_4, surrounded by FeO and an outer shell of iron metal). The conversion per pass is less than 20%, thus the unconverted part is recycled to the reactor after separation of the liquid product. The outlet stream is stepwise cooled (9) to condense (10) ammonia and recycle the unreacted gas.

3.3.2 Alternative ammonia production

Currently the most economically favourable option to decarbonise the production of ammonia is to use lower carbon feedstocks with the conventional Haber-Bosch process. Hydrogen can be produced through alkaline water electrolysis and nitrogen via air separation units (ASU). Both units are considerably more expensive, in terms of investment and operating cost, than the conventional process.

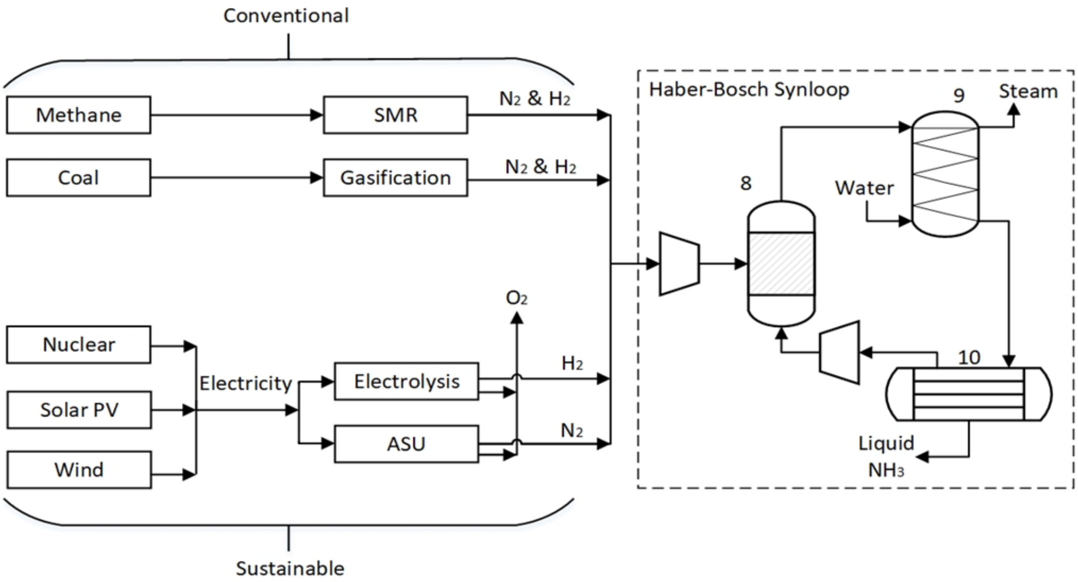

Figure 34 PFD of conventional and alternative ammonia production

The Haber-Bosh synloop to produce ammonia, costs roughly a third of the CAPEX in a conventional plant[23,24]. The ASU unit, which produces pure N_2, costs one-fourth of the capital required for an entire conventional ammonia plant. Alkaline water electrolysis is considered a mature technology, but, nonetheless its electricity consumption is very substantial, resulting in a hydrogen production cost considerably higher relative to fossil fuel derived H_2. There are multiple sources of electricity, to power the electrolyser, to choose from, which also results in different product costs. The cheapest alternative may be to use off-peak electricity from

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[23] J.R. Bartels (2008). A feasibility study of implementing an Ammonia Economy. Graduate ThesisTheses and Dissertations. Paper 11132.

[24] M. Appl (1999). Ammonia principles and industrial practice. Weinheim,Wiley-VCH. ISBN 3-527-29593-3

power plants; as published by Ryazantsev et al.[25] and Petri et al.[26] However, the synloop requires continuous operation, thus an intermittent supply of off-peak feed would significantly reduce the efficiency of operation. The utilisation of an intermittent feed would necessitate either a local buffer storage or an innovation in ammonia production plant design. Additionally, the cost of off-peak electricity is highly variable across regions and its suitability as cheap energy source depends on energy pricing regulation.

3.3.3 Urea production

Urea has been produced from carbon dioxide on an industrial scale for nearly a century and present the largest markets for CO_2 outside enhanced oil recovery (EOR)[27]. It is produced via a two-step process that involves the exothermic reaction of liquid ammonia, derived from natural gas, and CO_2 to form ammonium carbamate, followed by the endothermic decomposition and dehydration of ammonium carbamate to yield urea, *via* the Bosch-Meiser process[28].

The process flow diagram (PFD) is illustrated in the following figure:

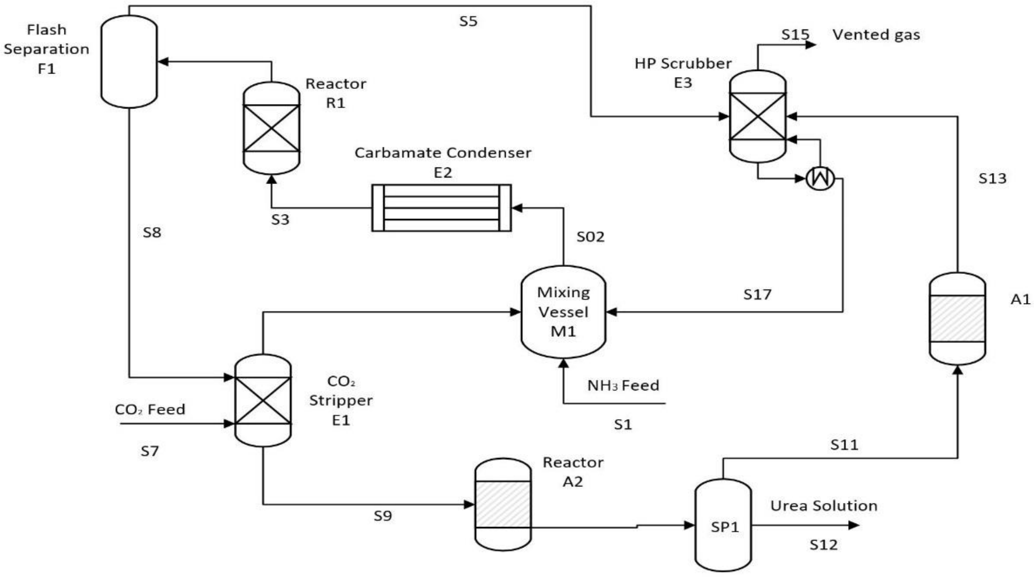

Figure 35 PFD of CO_2 to urea

The carbon dioxide stream (S7) is fed to the stripper (E1), to separate the urea solution coming from the reactor. Within the stripper, ammonium carbonates decompose, liberating more ammonia and carbon dioxide. Heat is supplied to the urea solution passing through the tubes counter-currently down past the rising CO_2-stripping gas. The stream leaving the stripper is rich in urea and is sent to the urea

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[25] E. Ryazantsev & A. Chabak (2006). Hydrogen production, storage, and use at nuclear power plants. Atomic Energy,101:876-881.

[26] M. Petri, Y. Bilge & A. Klickman (2006).. US work on technical and economic aspects of electrolytic, thermochemical, and hybrid processes for hydrogen production at temperatures below 550C. Int J of Nuclear Hydrogen Production and Application, 1:79-91.

[27] N. MacDowell, N. Florin, A. Buchard, J. Hallett, A. Galindo, G. Jackson, C. S. Adjiman, C. K. Williams, N. Shah & P. Fennell (2010).. "An overview of CO2 capture technologies." Energy & Environmental Science 3.11 (2010): 1645-1669.

[28] M. Fréjacques (1948).., Theoretical Basis of the Industrial Synthesis of Urea, Chem. Ind., 60, 22-35.

purification section. In the adiabatic urea reactor (R1), an aqueous solution of NH_3 and CO_2 and vapours flow upward through the reactor. Remaining gases condense and the carbamate decomposes in the reactor to provide heat for the slightly endothermic reaction of carbamate to urea. The urea solution goes through a flash separation unit (F1) to separate out the unreacted gas, then is fed back to the stripper E1.

The unreacted gases leave the flash separation unit (F1) from the top and are fed to the scrubber (E3) where recycled carbamate solution, from the evaporation/ recirculation section (S13), are passed over the top of a packed bed and fills the tube side section of vertical tubes. The gases rise up through the tubes and pass up through the packed section before leaving the top of the vessel. The contact with the carbamate solution absorbs the unreacted NH_3 and CO_2, while the inert gases of O_2, N_2, and others (S15) vent out from the top. At the bottom, recirculated cooling water flowing inside tubes removes the heat of absorption from the carbamate solution. Carbamate solution (S17) flows out of the vessel.

Solution (S17) and the top vapour stream from the stripper (S8) are fed to the carbamate condenser (E2), where the ammonia feed (S1) is used as pumping fluid. In the condenser, ammonium carbamate is formed. The vapour-liquid mixture (S03) falls through tubes and the heat of reaction is removed by generation of 3.5 bar steam on the shell side. The mixture goes to the bottom of the reactor for urea production. Finally, the bottom stream (S09) from the stripper (E01) is sent to the recover urea section. The recycled stream after recovering the urea (S13) is passed back to the high-pressure scrubber to complete the loop.

3.4 Summary

This section has presented the techno-economic characteristics of the range of conventional and alternative petrochemical production processes. Process flow diagrams have been presented showing the key components of each of methanol, olefin and ammonia/urea production, and a complete set of fully-referenced further technical and economic data for each of the processes can be found in Appendix A2.

It is from observation of this data alone, that substantial differences are likely to exist in terms of the sustainability of each. In terms of energy use and emissions, many use renewable forms of energy, have different greenhouse gas emissions profiles, and some consume CO_2. In terms of economic profile there are also very substantial differences, from capital cost to operational cost balance (which influences key investment metrics such as net present value), through to consumption of different fuels such as coal, gas and biomass.

The following section presents the full life cycle environmental characterisation of these processes. This is combined with the data from this section to form a complete technology characterisation, which then feeds through into the financial and economic assessment presented in Section 5.

4. Environmental assessment of process and feedstock options

This section examines the environmental impacts the different process options under a life cycle perspective as well as the main contributors to environmental burdens associated with each petrochemical. The petrochemicals considered are ethylene, propylene, methanol and ammonia. For these petrochemicals, an environmental assessment is conducted from cradle-to-gate, which includes the extraction and production of raw materials, transport and production of the petrochemical until factory gate. Furthermore, a series of case studies considering end-user products are examined to determine the environmental impacts of these options. Such products are: polypropylene, high density polyethylene (HDPE), dimethyl ether (DME), urea N fertiliser and urea-formaldehyde resin.

The LCA study follows the ISO 14040/14044 methodology[29,30], which describes the four-step method to undertake an environmental life cycle assessment. Namely, these are: goal and scope; inventory analysis; impact assessment; and results interpretation. The following sections describe first the goal and scope, then the inventory and the impact assessment before the analysis of the results.

4.1 Goal and scope

The goal of the study is to determine the environmental impacts of the typical routes to petrochemical production and to compare these results to alternative lower carbon routes. The case study region in which production is assumed to occur is China, congruent with the rest of this report. The study is conducted from cradle-to-gate, which includes the extraction and production of raw materials and utilities, the transport of raw materials to manufacturing installations and the production of the petrochemicals until factory gate or end users, depending of the product. Figure 36 summarises the life cycle stages considered in this study.

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[29] ISO (2006a).. ISO 14040-environmental management - life cycle assessment - principles and framework. Geneva.

[30] ISO (2006b).. ISO 14044-environmental management - life cycle assessment - requirements and guidelines. Geneva.

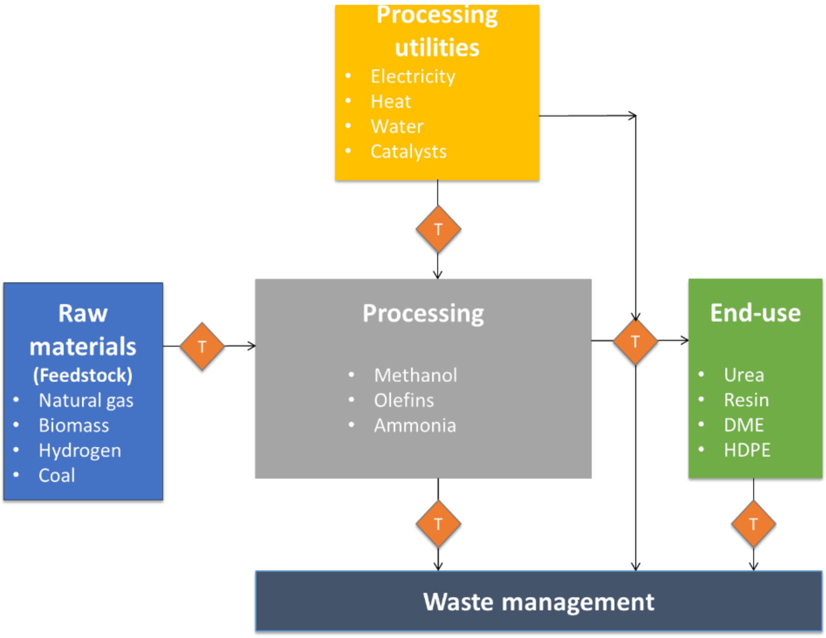

Figure 36 life cycle stages

The functional unit is defined as '1 kg of product at factory gate or user stage', which is the same for each product and each case study respectively.

There are several combinations of conventional and alternative feedstocks and processes as described in the previous section. The feedstocks considered are: natural gas, naphtha, coal, biomass and hydrogen from electrolysis, by solar, wind and central grid. A full list of the combinations of processes and feedstocks are given in the Appendix and are outlined at the start of each section below. For olefin production, sometimes both ethylene and propylene are co-produced in the same process. Where this occurs, the total emissions are allocated to each product by the mass of each product: the total emissions were divided proportionally by the mass of co-products and assigned to each co-product.

4.2 Inventory assessment

For each system, the life cycle of the total process was considered and data collected for each stage where possible. Overall, direct emissions associated with material handling and processing are considered, as well as indirect emissions associated with infrastructural equipment manufacture. Where possible, data is aligned with the process information given in the previous section. The most reliable data sources are used to determine the additional indirect emissions, including from Ecoinvent[31], NREL[32] and Plastics Europe[33]. Tables of inventories for each set of production

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[31] G. Wernet, C. Bauer, B. Steubing, J. Reinhard, E. Moreno-Ruiz & B. Weidema (2016). The ecoinvent database version 3 (part I): overview and methodology. The International Journal of Life Cycle Assessment, 21, 1218-1230.

[32] NREL (2012). US Life Cycle Inventory Database. In: National Renewable Energy Laboratory (ed.) [Online]. Available: www.lcacommons.gov/nrel/search. [Accessed 29/ 04/ 2018]

[33] Plastic Europe (2017). Eco-Profile Program. Available: www.plasticseurope.org/plastics-sustainability-14017/eco-profiles.aspx. [Accessed 29/ 04/ 2018]

processes are given in the Appendix for further information. The environmental impacts are assessed for the case study region China, thus feedstocks and emissions are assumed to be derived from domestic production. In particular, an important characteristic is the Chinese electricity grid. An average Chinese grid mix was considered, which is assumed to be approximately 75% coal sourced[34].

4.3 Impact characterisation

The life cycle models were created, estimating emissions masses, and then characterisation of emissions was implemented with the well-known impact assessment methodology, CML2001[35]. This method enables the conversion of specific chemical emissions into impacts of different environmental indicators. Additionally, an estimate of total primary energy demand (PED) was included. A total of 12 indicators are included for analysis, as described below.

- *Abiotic resource depletion potential (ADP) elements:* the level of depletion of non-fossil fuel materials such as rare earth metals, measured in mass of antimony equivalents. Characterisation factors are based on current levels of depletion and availability.
- *Abiotic resource depletion potential (ADP) fossil:* the level of depletion of the fossil fuel resources oil, gas and coal, expressed as MJ embodied energy equivalent.
- *Acidification potential (AP):* The level of acidification caused by emissions of acids or acidifying compounds to air, water and soil, expressed as a mass of sulphur dioxide equivalent.
- *Eutrophication potential (EP):* the level of eutrophication, or over nitrification, or water sources (both fresh water and sea water) by nutrients such as phosphates and nitrates, expressed in mass of phosphate equivalent.
- *Freshwater aquatic ecotoxicity potential (FAETP):* the damage to fresh water organisms due to emission of toxic substances, expressed in mass of dichlorobenzene equivalent.
- *Global warming potential (GWP):* the average radiative forcing associated with emissions of greenhouse gases, expressed in mass of carbon dioxide equivalent.
- *Human toxicity potential (HTP):* the impact to human health due to emission of toxic substances to air, water and soil, expressed in mass of dichlorobenzene equivalent.
- *Marine aquatic ecotoxicity potential (MAETP):* the damage to marine organisms due to emission of toxic substances, expressed in mass of dichlorobenzene equivalent.

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[34] K. Treyer & C. Bauer (2016). Life cycle inventories of electricity generation and power supply in version 3 of the ecoinvent database—part II: electricity markets. The International Journal of Life Cycle Assessment, 21, 1255-1268.

[35] Universitat Leiden (2016). CLM-IA Characterisation Factors. In: CML – Department of Industrial Ecology. (ed.) Available: www.universiteitleiden.nl/en/research/research-output/science/cml-ia-characterisation-factors. [Accessed 29/ 04/ 2018]

- *Ozone depletion potential (ODP):* the damage to the stratospheric ozone layer due to emissions to air, expressed in mass of refrigerant R11 equivalent.
- *Photochemical ozone creation potential (POCP):* the impact on the creation of tropospheric ozone (summer smog) which harms ecosystems and human health, expressed in mass of ethylene equivalent.
- *Terrestrial ecotoxicity potential (TETP):* the impact of emissions of toxic substances such as metals to soil, expressed in mass of dichlorobenzene equivalent.
- *Primary energy demand (PED)*: the total energy input to the product, expressed in MJ.

Out of these 12 environmental indicators, three were selected as the primary focus of this study: GWP, ADP fossil and PED. All other indicators are assessed and important conclusions are included in the main body of this report, but an assessment of each indicator is included in the Appendix.

In the following section, results of the environmental assessment are described for each category of petrochemical products.

4.4 Methanol

As summarised in Figure 37, six routes of methanol production via different feedstocks were considered. Results for each indicator vary significantly across the options, often spanning orders of magnitude. No single option represents the lowest impact for every route, thus there is no clear “best” option from an environmental perspective. In terms of GWP, the route deriving methanol from biomass gasification and catalytic hydrogenation from wind electrolysis are the lowest as shown in Figure *38*. The latter option also performs best for 3 other categories: acidification potential, human toxicity potential and terrestrial ecotoxicity potential. However, the conventional route of methanol from natural gas has the lowest impact over 6 other categories: ADP elements, eutrophication, FAETP, MAETP, ODP and PED (see detail in Appendix).

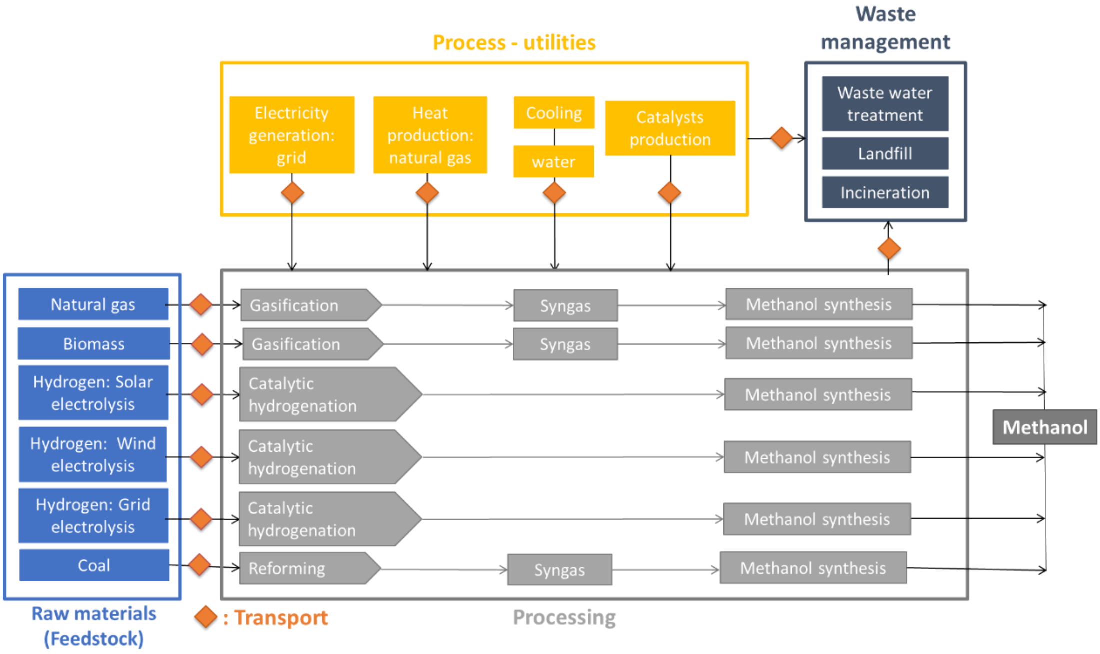

Figure 37 Methanol routes and its correspondent life cycle stages

Global warming potential (GWP)

As seen in Figure *38*, GWP values range from 0.7 to 32 kg CO_2 eq./kg. Catalytic hydrogenation using wind electrolysis and from biomass results in very low emissions, due to the relatively low carbon intensity of power generation as well as the use of a waste CO_2 stream that would otherwise be emitted. In comparison, conventional methanol from natural gas is 1.1 kg CO_2 eq./kg, whereas the route using solar PV increases to 2.5 kg CO_2 eq./kg. Notably, methanol from catalytic hydrogenation from grid electrolysis is the highest emissions at 32 kg CO_2 eq./kg, with methanol from coal at 5.3 kg CO_2 eq./kg.

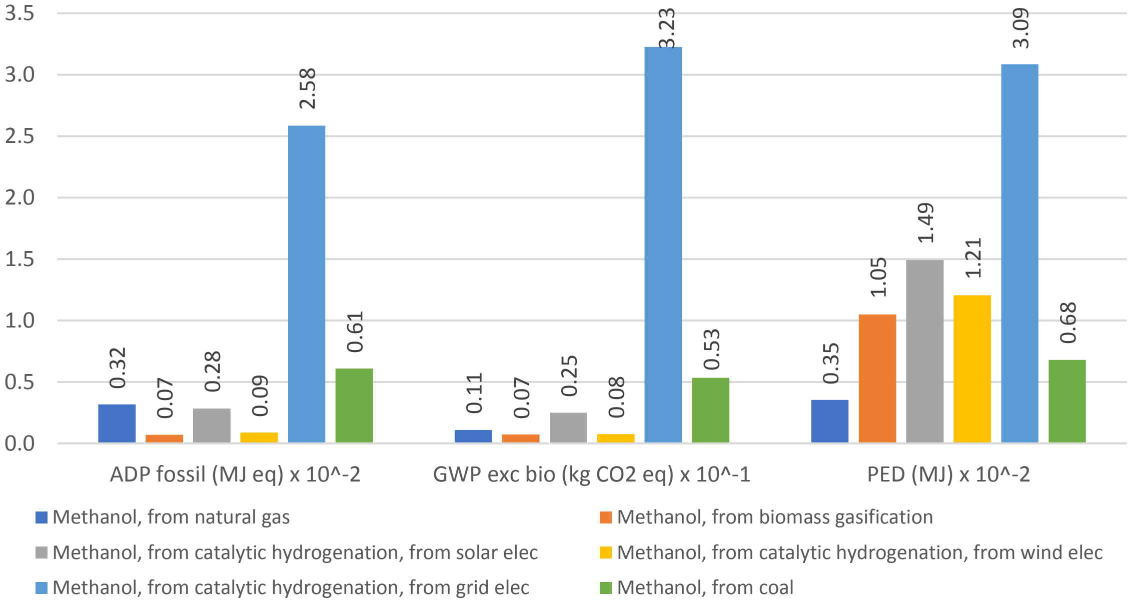

Figure 38 *Environmental impacts associated with methanol production routes, expressed per kg of methanol production*

Abiotic resource depletion potential (ADP) fossil

The largest impact on fossil fuel depletion comes from catalytic hydrogenation via grid electrolysis, at 258 MJ/kg (see Figure *38*). This is due to the grid mix being coal-dominated and the relative inefficiency of the catalytic hydrogenation route. Methanol from biomass gasification gives the lowest ADP fossil score due to its limited reliance on natural gas for heating or electricity. However surprisingly, whilst the wind fuelled electrolysis route gives a low ADP fossil impact, the solar electrolysis route is similar to methanol from natural gas, due to the grid electricity used to construct the solar panels and ancillary equipment.

Primary energy demand (PED)

The fossil fuel-derived methods of methanol production result in the lowest total primary energy demand, given the embodied energy within these resources and the comparative lower efficiency of the alternative systems (details in Figure *38*). Methanol from natural gas results in the lowest PED at 35.3 MJ/kg, with methanol from coal the second lowest, but almost double at 68 MJ/kg. This is due to the increased energy intensity and lower efficiency associated with coal conversion. The highest impact is from the catalytic hydrogenation using grid electricity at 308 MJ/kg, due to the intensity of the Chinese fuel mix, as well as the efficiency loss associated with the catalytic hydrogenation.

4.4.1 *Key contributors*

Generally, the lowest impacts are associated with methanol production by catalytic hydrogenation from wind electrolysis, as well as from biomass gasification. All process routes have different emissions profiles and contributions from different stages in their supply chain.

For methanol production from natural gas, the majority of emissions are associated with the extraction and conditioning of raw materials, namely of natural gas, as shown in Figure 39. The depletion of fossil fuel, the energy intensity of the conversion to methanol and the process emissions are the main contributors to GWP.

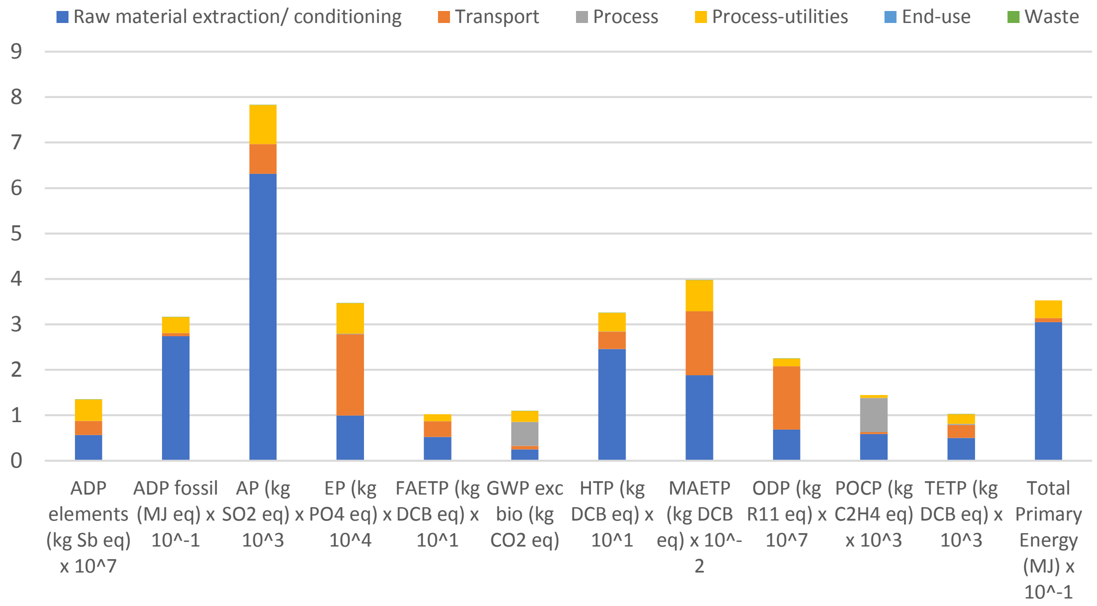

Figure 39 Environmental impacts associated with 1 kg methanol production from natural gas.

Methanol production from biomass offers an improvement in environmental impacts across 5 categories: GWP, ADP fossil, as well as acidification, ozone depletion and photochemical ozone creation potentials. Whilst there is much less reliance on fossil fuels, the process is more energy intensive, as shown by the increased PED. As seen in Figure 40, the main contributor to the environmental impacts of this route is the utilities used during the gasification and methanol production steps: 60% of which comes from electricity requirement during syngas production. Given the high carbon-intensity of the Chinese grid (due to the proportion of electricity generated by coal), there is significant potential for these impacts to be significantly reduced, via reduced reliance on electricity or via decarbonisation of electricity.

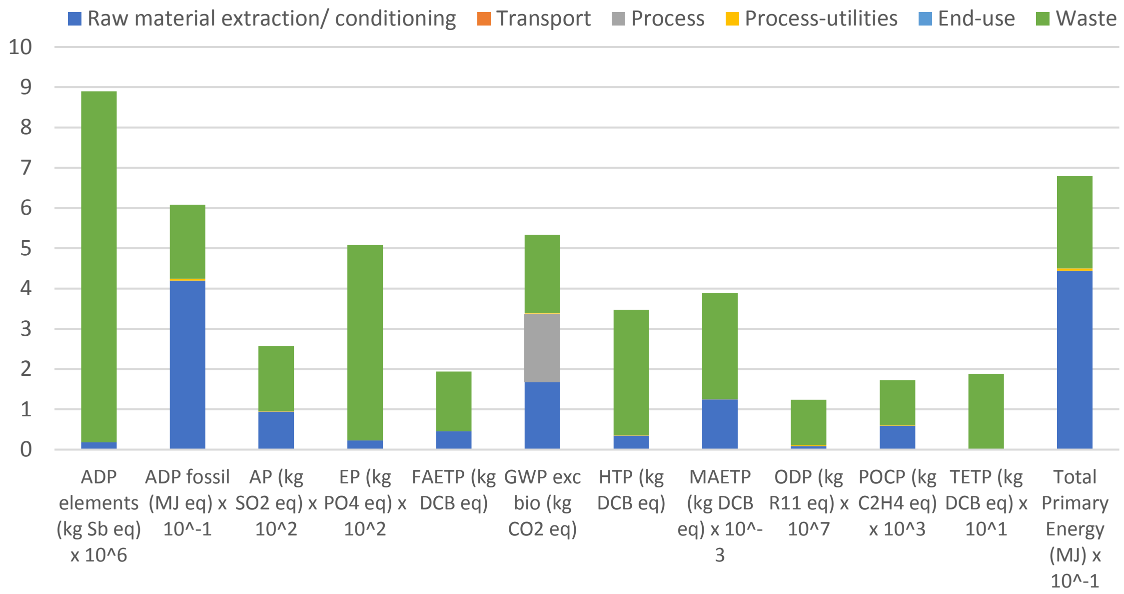

Figure 40 Environmental emissions associated with 1 kg methanol production from biomass gasification

Environmental emissions are highest from catalytic hydrogenation using grid electricity and methanol production from coal gasification. Given the high carbon intensity of the Chinese electricity mix, the production of hydrogen using grid electricity for electrolysis is high carbon as well as high in other environmental impacts due to the coal content. Additionally, this process route is relatively energy intensive, meaning that the high carbon intensity is magnified. Furthermore, the methanol production route from coal performs poorly, with the exception of PED. The majority of emissions across all categories are caused by emissions produced during coal extraction, the potential emissions associated with liquid effluent and the high carbon intensity of the grid, as shown in Figure 41.

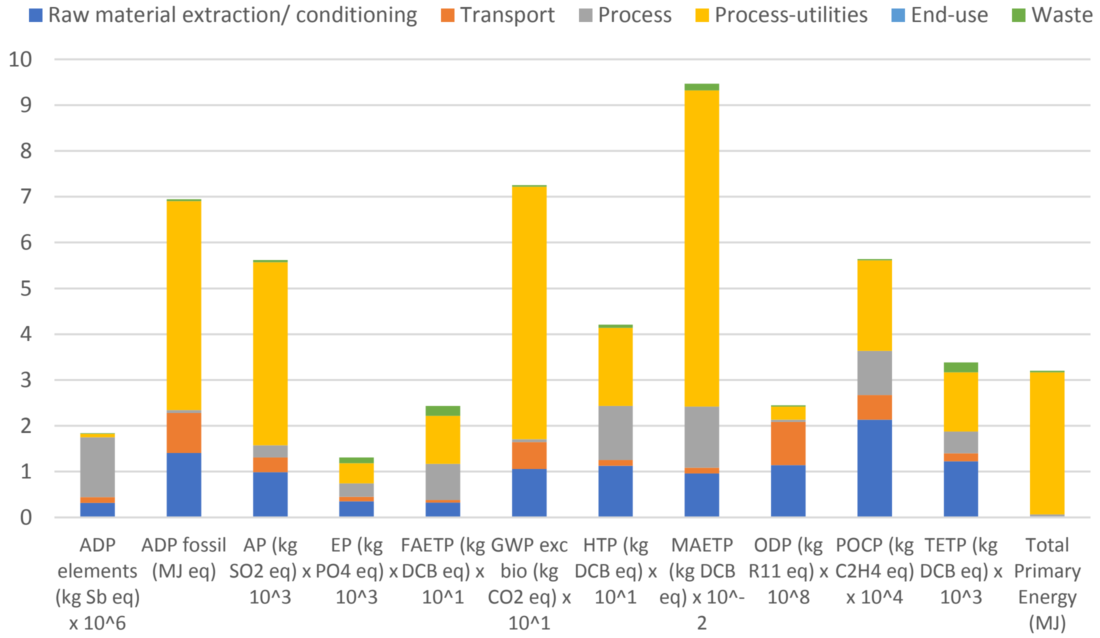

Figure 41 Environmental emissions associated with 1 kg methanol production from coal

4.5 Olefins

Figure 43 exhibits the results for the different routes to ethylene while Figure 44 shows those for propylene production. It should be noted that the majority of the process options for ethylene and propylene are the same, since most of the processes produce both products (see Figure 42). Given that the emissions are allocated by mass, for the MTO routes the propylene emissions are 26% greater than the ethylene but the relative change in impact between each option remains the same.

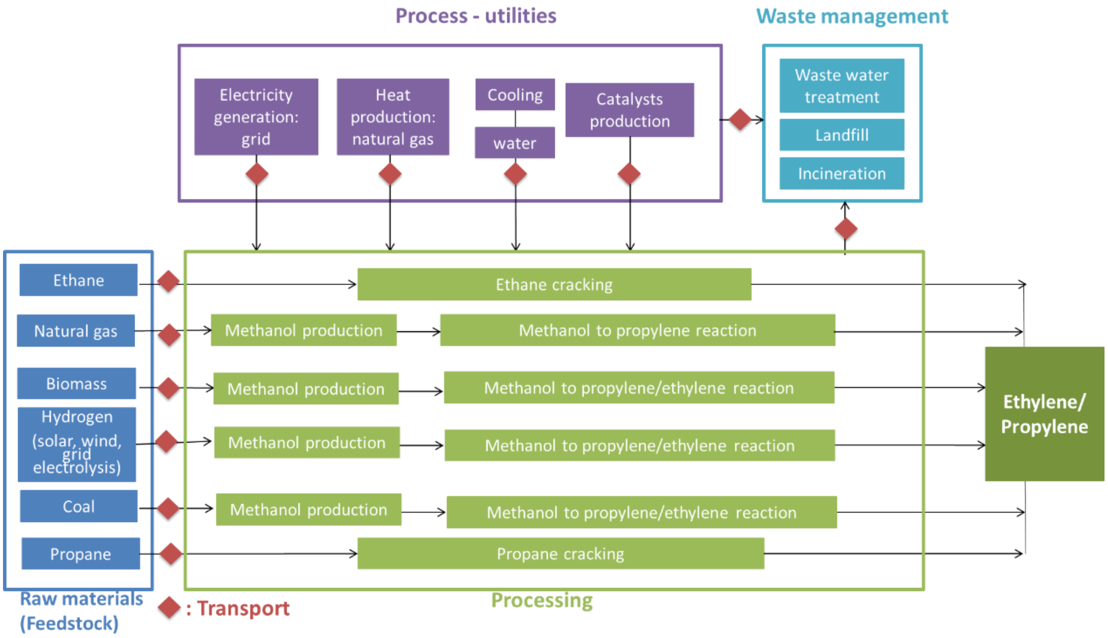

Figure 42 Ethylene and propylene routes and their correspondent life cycle stages

For ethylene and propylene, the production via naphtha cracking yielded the lowest environmental impacts for 9 out of 12 impacts (for full details on all environmental indicators see Appendix). However, it is the authors' opinion that the underlying dataset is of limited quality and transparency and therefore should not be considered to be the most environmentally benign option. Given the energy intensity and reliance on crude oil, it is most likely that naphtha cracking yields similar environmental impacts to those from natural gas. Further work is required to determine the impacts associated with naphtha cracking; the results are presented but should be considered with caution. However, cracking of ethane also performs well for many of the environmental impacts.

Considering the aforementioned issues, for GWP, the MTO options utilising hydrogen from wind electrolysis and biomass gasification have the lowest impacts. For propylene production, similar trends are shown given the similarity in processes.

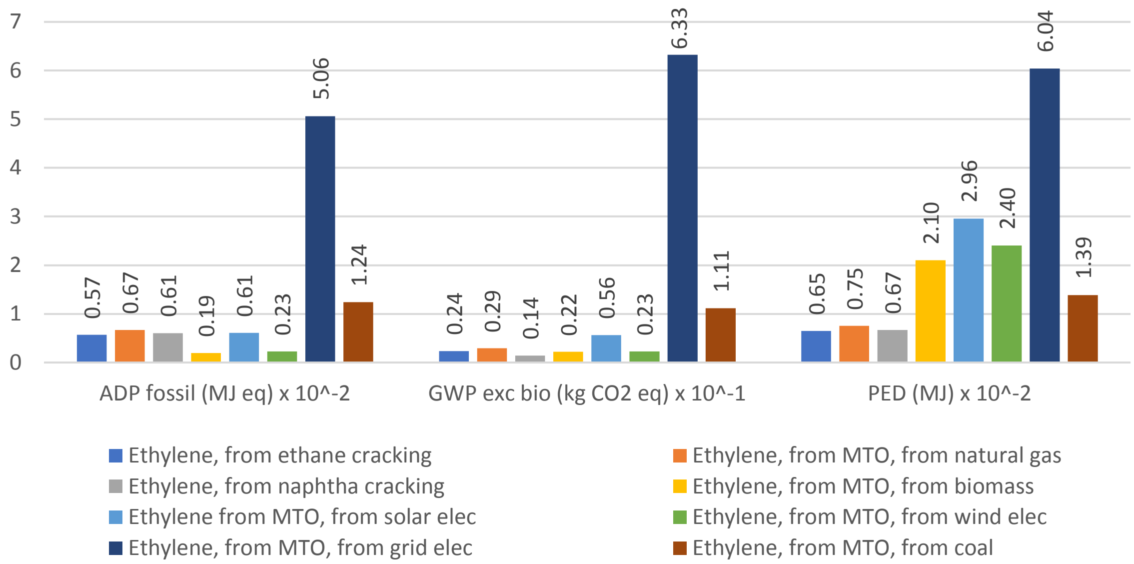

Figure 43 Environmental impacts of different routes to ethylene production. Based on 1 kg ethylene production and mass allocation where applicable

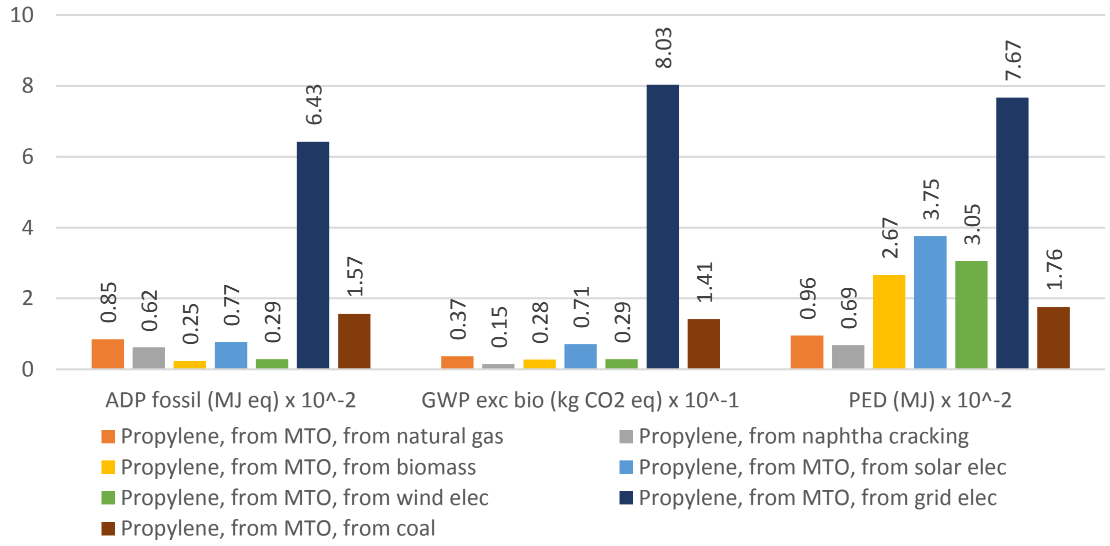

Figure 44 Environmental impacts of different routes to propylene production. Based on 1 kg propylene production and mass allocation where applicable

Global warming potential (GWP)

As seen in Figure 43 and Figure 44, the lowest GWP is exhibited by the wind electrolysis and biomass gasification routes, at 2.25 and 2.2 kg CO_2 eq./kg respectively for ethylene and 2.9 and 2.8 for propylene. Note that this analysis excludes the naphtha cracking option as the lowest due to the concerns about data quality previously mentioned. However, in the case of ethylene from ethane cracking, GWP is nearly 10% higher at 2.35 kg CO_2 eq./kg, whereas propane cracking exhibits emissions of 2.8 kg CO_2 eq./kg. Consequently, there is little GWP benefit associated with the lower carbon feed sources. The GWP of ethylene and propylene from solar electrolysis is a factor of 2.5 higher for both ethylene and propylene options.

The reason for the lack of carbon benefit is that there is no allowance for the utilised waste CO_2 used during catalytic hydrogenation, given that it is likely to be emitted eventually once the petrochemical product has been further used. When this 'negative emission' is accounted for, both wind and solar electrolysis routes become net negative emitters.

Abiotic resource depletion potential (ADP) fossil

In terms of ethylene production, results of ADP fossil range from 19 to 506 MJ/kg. The lowest comes from the alternative option using hydrogen from biomass gasification (see Figure 43). Conventional routes from natural gas and naphtha are similar at approximately 57-67 MJ/kg, whereas the coal and grid electrolysis options again represent the highest figures at 120 and 506 MJ/kg respectively.

Total primary energy (PED)

Olefin production from naphtha and natural gas exhibit the lowest total primary energy demand, given their embodied calorific value and high thermal efficiencies. The alternative routes, which include MTO are 2-7 times more energy intensive. The highest PED comes from the use of grid electricity to produce methanol via catalytic hydrogenation, followed by coal to methanol processes. Figure 43 and Figure 44 summarise the environmental impacts.

4.5.1 Key contributors

As described, the lowest environmental impacts are from ethane/propane cracking, from biomass and via wind electrolysis. The impacts associated with conventional production are dominated by the raw material extraction and the energy intensity of the conversion processes of propylene from propane, as shown in Figure 45.**Error! Reference source not found.** On average across the impacts, extraction and conditioning accounts for 66% of total impacts, the remainder largely from processing. Key areas of emissions reduction potential are from the processing, which occur due to the use of natural gas and electricity. Substitution via low carbon alternatives has potential where a local source is available. Note that the direct process emissions for this conventional route were not publicly available and so this is likely to be a slight underestimate of total emissions.

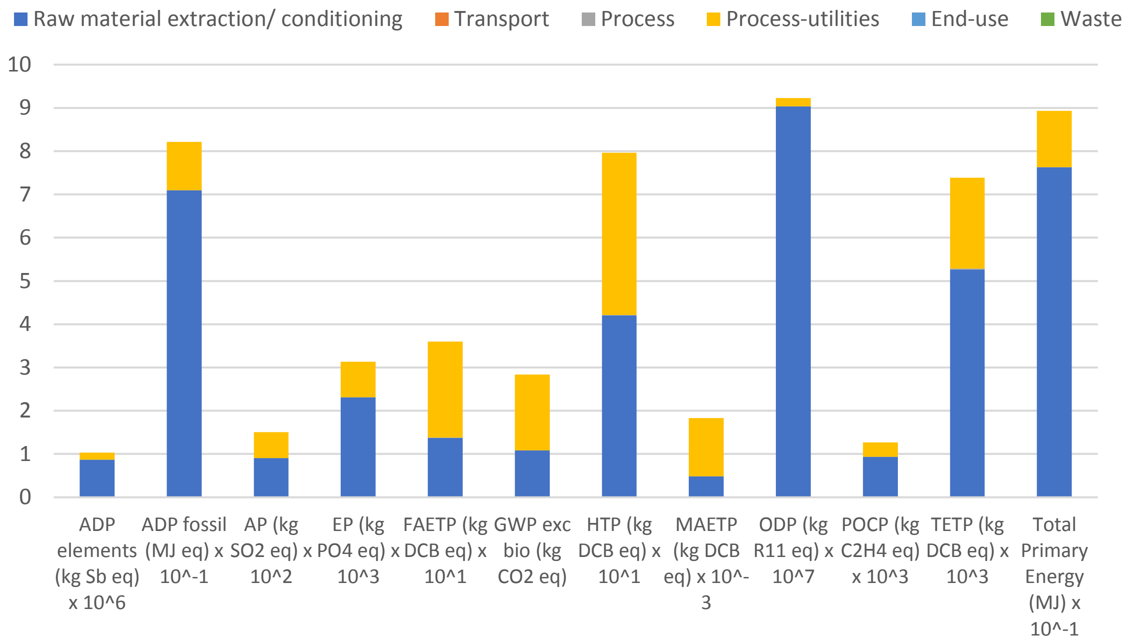

Figure 45 Environmental impacts associated with propylene production from propane cracking.

The route considering coal to methanol to olefins generally represents a higher impact option for all categories besides the primary energy demand, given the embodied energy within the fossil fuel. Metal and particulate emissions associated with extraction and processing of coal and the wastewater treatment are the key impacts to toxicities, acidification and eutrophication, as shown in Figure 46. The high GWP and ADP fossil derives from the extraction of a carbon intensive feedstock. Given the connection of the emissions with the feedstock management and the maturity of these process steps, there is relatively limited potential to reduce emissions further from this option.

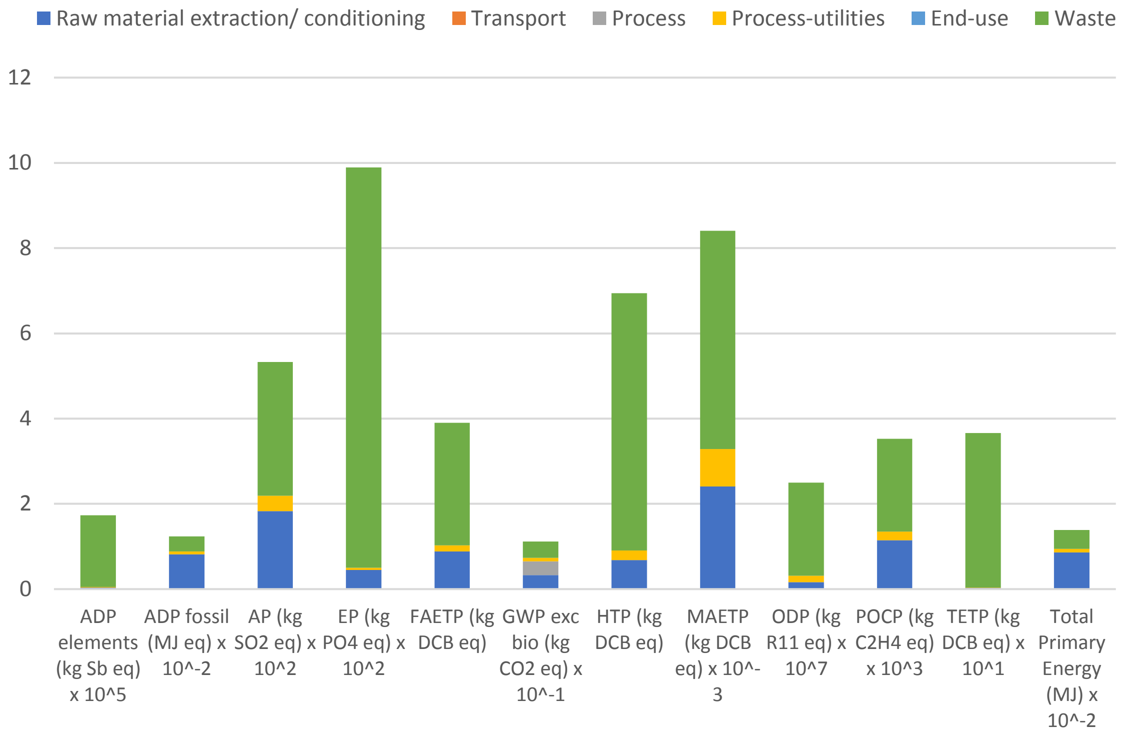

Figure 46 Environmental impacts associated with Propylene production from MTO, from coal gasification, categorised by different life cycle stages. Emissions have been allocated by co-product mass across different olefin products

4.6 Ammonia

As shown in Figure 47, the environmental assessment of ammonia production includes five routes, namely the conventional route using natural gas, three electrolytic routes powered by solar, wind and grid electricity, and biomass gasification.

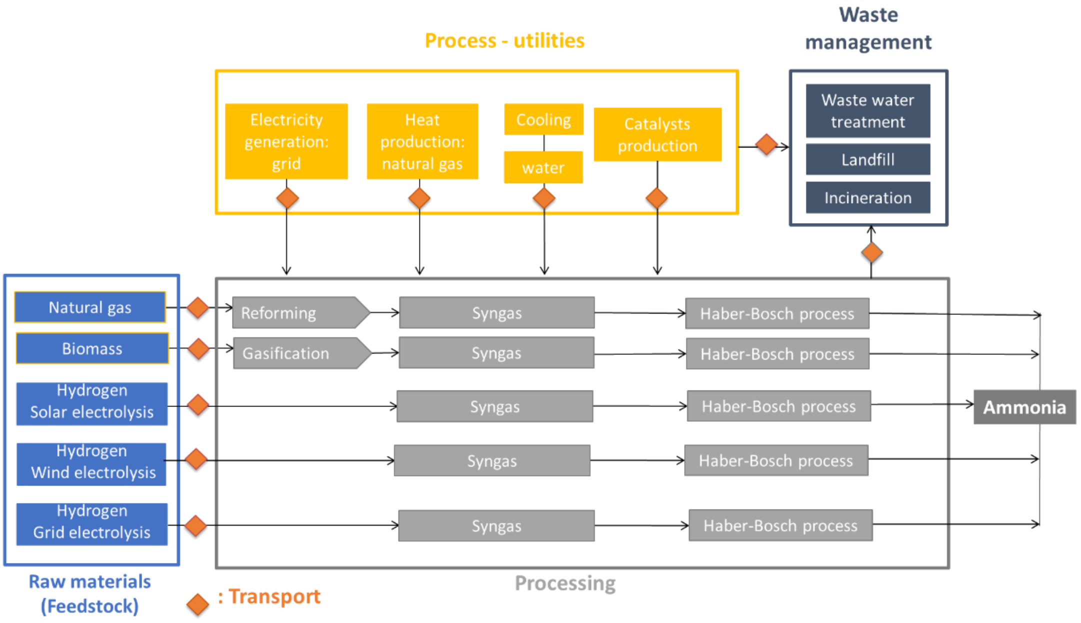

Figure 47 Ammonia routes and their correspondent life cycle stages

Figure 48 shows the environmental impacts of the five ammonia production routes. Overall, the grid powered electrolytic route exhibits the highest impact in 10 out of 12 categories. The main reason is the large amount of emissions such as carbon dioxide and sulphur dioxide from the life cycle of the electricity generation, which in this case is mainly coal based.

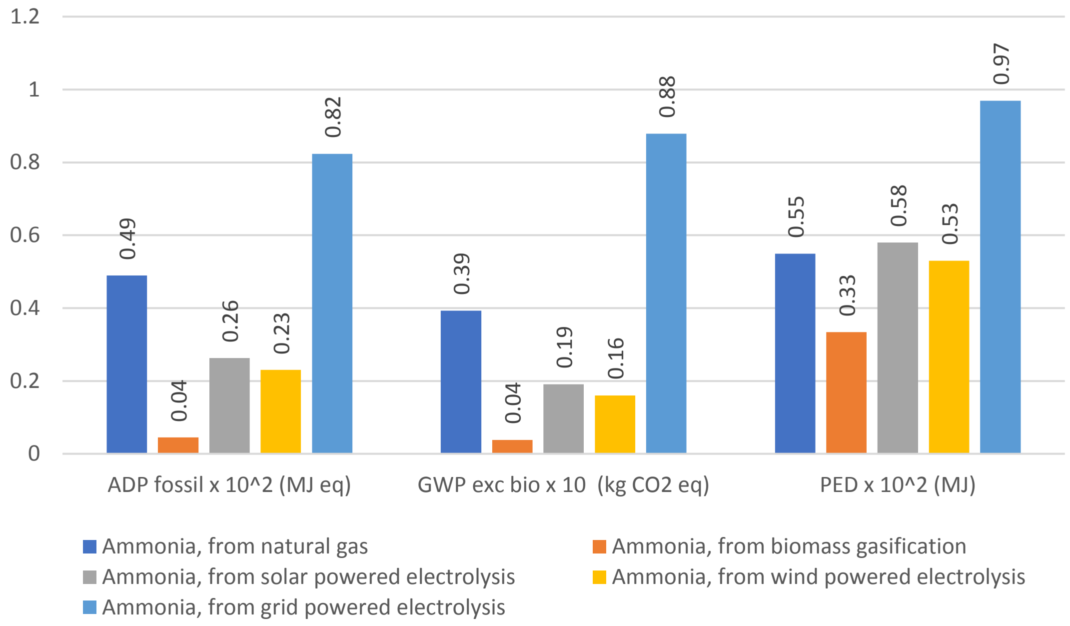

Figure 48 Comparison of the environmental impacts of ammonia production routes. Impacts are expressed per functional corresponding to 1 kg of ammonia

The best option is found in the biomass route production, with the lowest impacts across all the categories due to relatively low energy requirements and use of biogenic carbon. The second lowest impact option is the electrolytic route powered by wind. In this case, the low impact renewable energy system helps to reduce the burden of the before-mentioned issue of the electrolytic route – high electricity demand. This has been remarked in previous studies related to hydrogen generation, where in the case of electrolytic routes, the power source is the key to manage the environmental impacts[36].

Interestingly, the conventional route from natural gas exhibits a significantly better performance than from solar electrolysis in 7 out of 12 impacts: ADP elements, HTP, EP, FAETP, MAETP, ODP and PED. However, the solar powered electrolytic route displays improved performance in key metrics of GWP and ADP fossil, as well as AP, POCP and TETP (see detail in Appendix).

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[36] R. Bhandari, C. A. Trudewind & P. Zapp (2014). Life cycle assessment of hydrogen production via electrolysis – a review. Journal of Cleaner Production, 85, 151-163.

Global Warming Potential

The GWP impacts range from 0.4 kg CO_2 eq./kg NH_3 in the case of biomass gasification route to 8.9 kg CO_2 eq./kg NH_3 for grid powered electrolytic route. The solar and wind powered electrolytic routes are the second and third best options, with 1.6 and 1.9 kg CO_2 eq./ kg NH_3, respectively. GWP of the conventional route from natural gas is 3.9 kg CO_2 eq. This impact is mainly led by carbon dioxide emitted across all the life cycle stages of the routes, in particular from the coal based electric grid.

Abiotic depletion potential (ADP) fossil

ADP fossil follows the same trend as GWP; the best option is biomass gasification route and the worst is the grid powered electrolytic route. Wind and solar powered electrolytic routes are the second and third best options, followed by the conventional route.

Primary energy demand (PED)

PED shows similar trends again, with the biomass gasification route as the best alternative not only in terms of low score but also due to a higher share of renewable sources (87.5%). The wind and solar powered electrolytic routes are the second and third best options, with almost equal share between renewable and non-renewable sources. The worst option is the grid powered electrolytic route, followed by the conventional route, with over 95% of non-renewable sources.

4.6.1 Key contributors

Three key routes that perform well across the range of impacts are discussed here: ammonia from natural gas, biomass gasification and solar powered electrolysis. Figure 49 exhibits the environmental impacts and life cycle stage contribution of the conventional route of ammonia production. Three life cycle stages are mainly responsible for all impacts. The raw materials stage, which mainly refers to the extraction and production of natural gas, is the major contributor of 5 out of 12 impacts (ADP fossil, AP, ODP, POCP and PED). This is for two reasons; first, the nature of the fossil fuel-based feedstock leading to high ADP fossil and PED. Second, methane, carbon dioxide and sulphur dioxide associated with the natural gas supply chain affect impacts such as GWP, AP and POCP.

The process – utilities stage contributes to almost all the impacts, but it mainly drives ADP elements, due to the resources extracted and indirectly to the energy required to produce the chemical and catalyst. Finally, the process stage also leads GWP and TETP, mainly due to the emission arising from the coal-based electricity production.

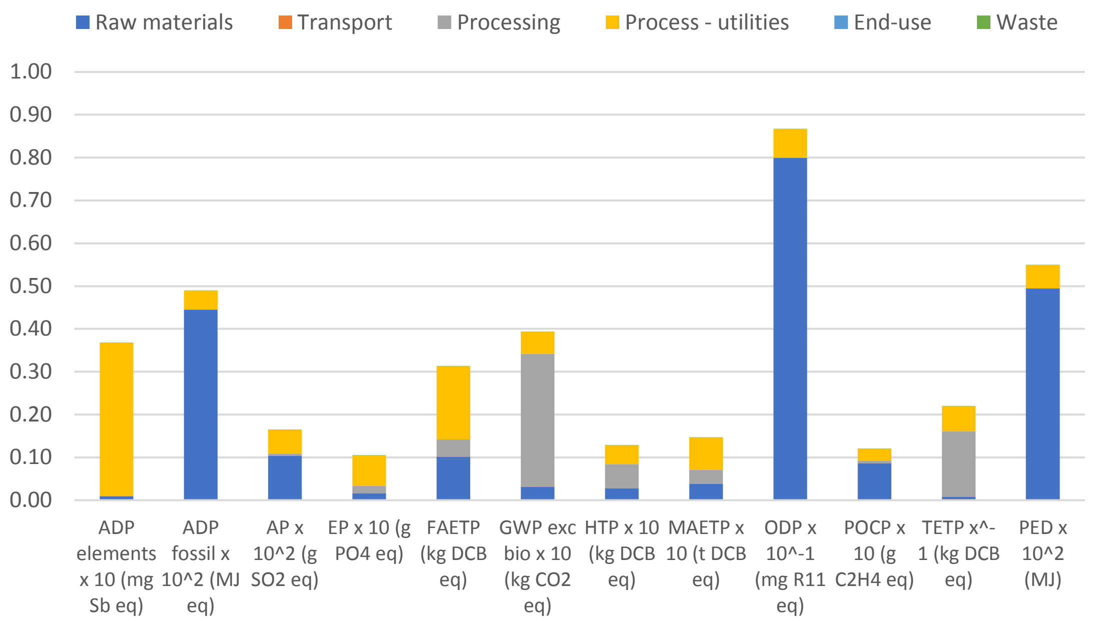

Figure 49 Environmental impacts and life cycle stage contribution of the ammonia production from natural gas (conventional route)

The solar powered electrolytic route is dominated by the raw material stage (see Figure 50). The electrolysis requires significant quantities of electricity, produced from the solar panel and ancillary equipment. The efficiency of electrolysis, material resource requirements and energy intensity of the equipment manufactured cause the large contribution from this stage. It is important to note that all the electrolytic routes have a high uncertainty level due to the lack of full inventories specifying the emissions generated in the life cycle of the electrolyser. Therefore, this process only accounts for the energy and utility requirements, while other routes have more robust inventories.

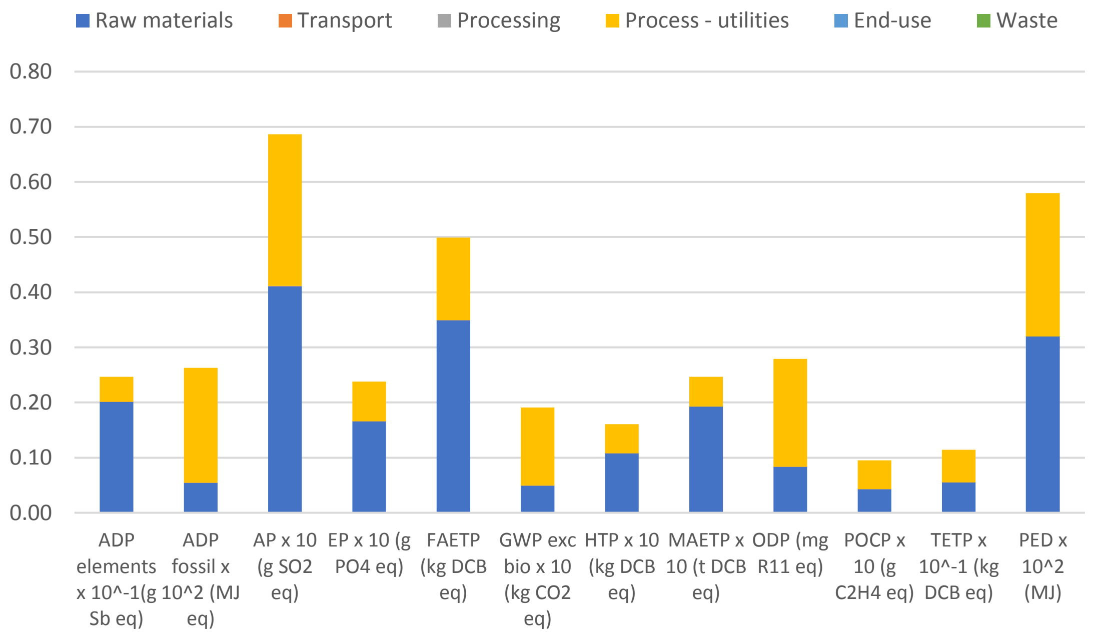

Figure 50 environmental impacts and life cycle stage contribution of the ammonia production from solar powered electrolysis

4.7 Urea

Figure 51 exhibits the environmental impacts of the urea production routes, which are the same five discussed in the previous section. Similar to ammonia, the biomass gasification route is the least impactful across all the processing routes in 11 out of 12 categories (see Appendix). The grid powered electrolytic route is the highest emitter in nine out of 12 categories, including GWP. The wind powered electrolytic route is the second-best option, with some of the best performances in impacts such as GWP, eutrophication potential and photochemical ozone creation. Interestingly, the conventional and the solar powered electrolytic routes are similarly impactful.

Global warming potential (GWP)

The order of impact magnitude across the options is the same as for ammonia production, as the additional impacts associated with urea production and use are the same for all routes. Consequently, urea produced from ammonia from biomass gasification performs the best 4.3 gCO2eq./kg, closely followed by the wind and solar electrolysis routes at 5 and 5.1 gCO2eq./kg. Conventional production via natural gas exhibits emissions 20% higher than the lowest routes, but 30% lower emissions than the coal and grid electrolysis routes.

Abiotic depletion potential (ADP) fossil

Wind and solar powered electrolytic routes exhibit impacts 1.8 and 1.5 times higher than the biomass gasification route. The use of electricity in the life cycle of the solar and wind power systems drives the contribution to this impact, due to a grid highly dependent on coal. This is also the reason of the poor performance of the grid electrolytic route, with the highest impact (52 MJ/kg urea).

Primary energy demand (PED)

The low efficiency in the electricity use makes the grid powered electrolytic route the worst option when PED is assessed. As explained at ADP fossil, the high-energy demand based on non-renewable sources (coal) make this route the worst. The most interesting outcome is the relatively similar scores across the conventional route and the solar and wind powered electrolytic routes, with a variation of around 8% between them. However, the type of energy source varies as the conventional route has a higher share of non-renewable sources.

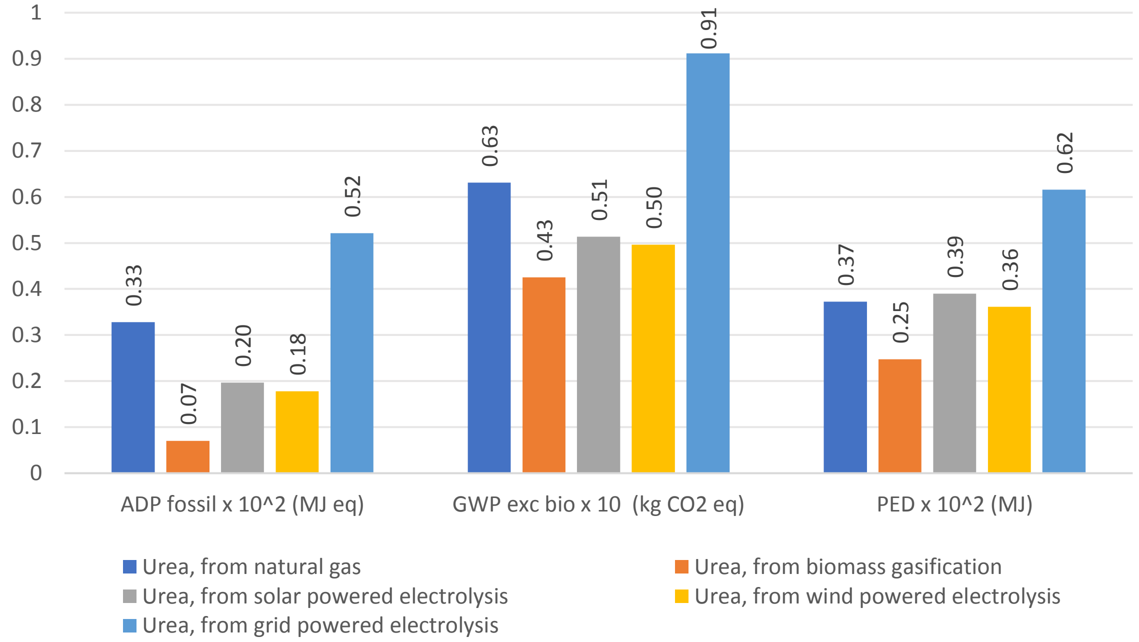

Figure 51 Comparison of the environmental impacts of urea production routes. Impacts are expressed per functional corresponding to 1 kg of urea

4.7.1 Key contributors

Figure 51 shows the environmental impacts of the conventional natural gas route for urea production; there is broad mix of contributions across the life cycle stages. For instance, the raw materials and processing stages are each the main contributor of four out of 12 impacts. In the case of the raw materials, this is mainly due to the life cycle of the natural gas production, which was explained in the previous section, while in the case of the processing stage, the extension of the processing line, which here accounts for the emissions coming from ammonia and urea processing, is the main responsible. Interestingly, the second largest contributor is the use stage, which plays a key role in impacts such as AP, EP and GWP. This is mainly due to the emission from the use of urea as nitrogen base fertiliser, especially nitrous oxide, which has a GWP of 298 gCO_2 equivalent. Additionally, significant nitrites emissions add to acidification and eutrophication impacts.

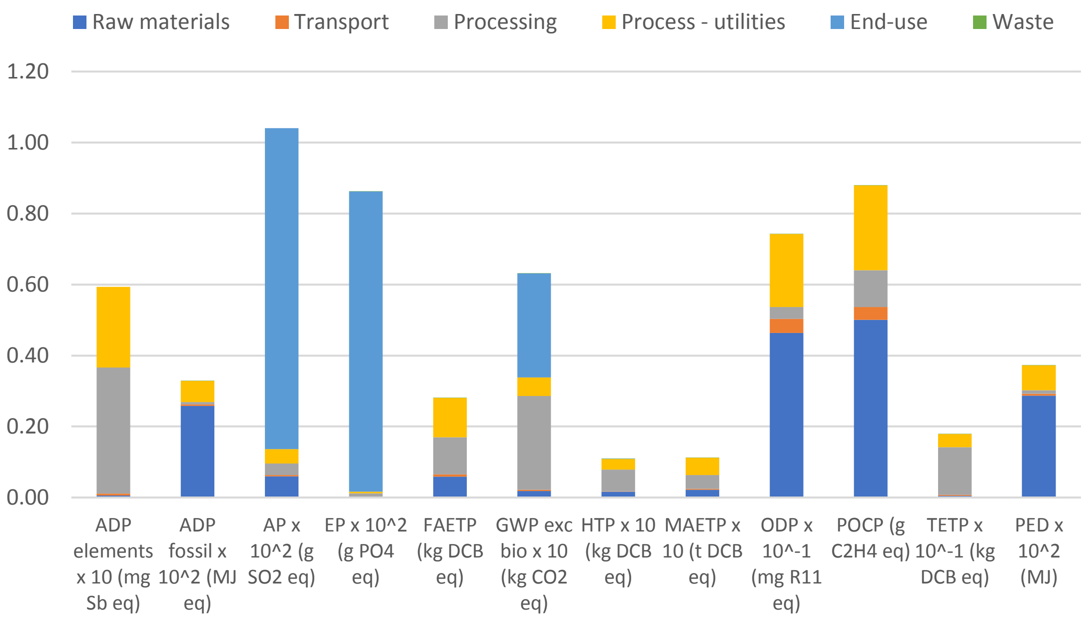

Figure 52 Environmental impacts and life cycle stage contribution of the urea production from natural gas (conventional route)

The production of urea using wind-powered electrolyser is equally driven by the raw material, processing, process-utility and use stages (see Figure 53). It is particularly interesting to see how the high demand of materials in the life cycle of the wind power added to the high demand of electricity, greatly affect ADP element. As discussed, it is also remarkable how the avoidance of fossil fuel-based feedstock greatly reduces the contribution of the raw materials stage and the absolute value of impacts such as ODP, POCP and ADP fossil. As result, this has shifted the contribution of the stages, explaining a greater contribution of the process-utility stage across all the impacts.

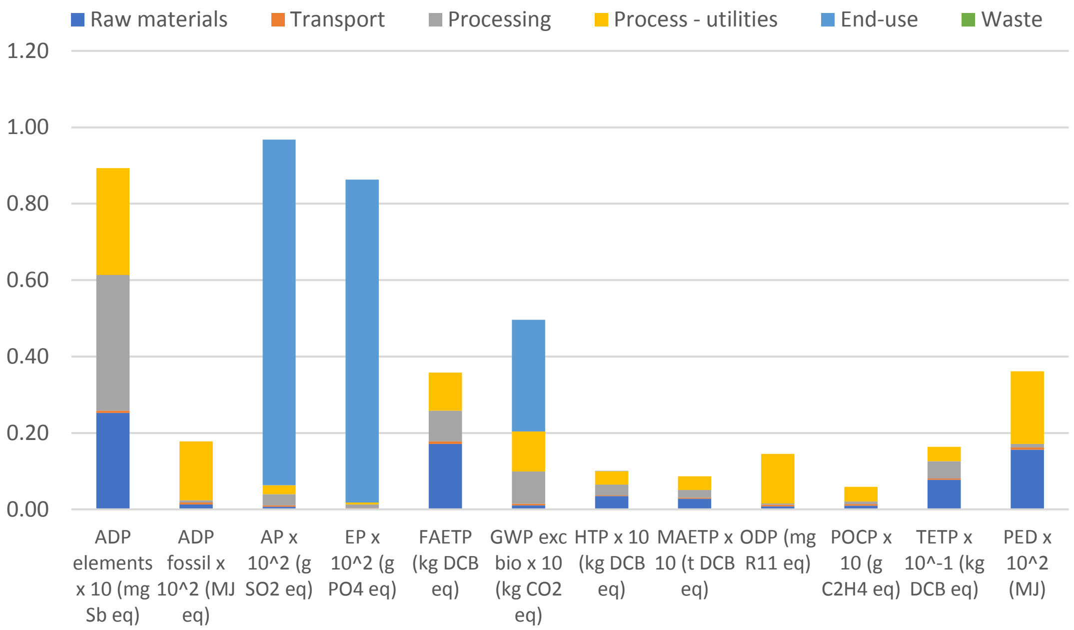

Figure 53 Environmental impacts and life cycle stage contribution of the urea production from wind-powered electrolytic

4.8 End-use and the impact of waste management

Whilst the focus on the study has been on cradle-to-gate impacts, end-use and the impact of different waste management options may have a significant effect on total life cycle emissions, in particular with respect to recycling. To test for this, different waste management options associated with end-of life of HDPE pipe were investigated. The following additional stages in the life cycle were taken in addition to the ethylene life cycle process:

- Production of polyethylene from ethylene
- Extrusion of HDPE pipe from HDPE pellets
- Transport to waste facility
- Waste management
  - Incineration
  - Landfill
  - Recycle

For incineration and landfill of HDPE, the Ecoinvent[31] database was used to for the emissions inventory. For incineration and landfill, it is important to note that no allowance was made for energy recovery other than to fuel its own process. This may result in an overestimate of emissions, but this is a typical assumption and overall the exported heat/electricity from incineration plants is relatively small compared to the process energy.

In terms of the recycling process, the emissions associated with waste collection and transport, handling and separations, and production of recycled pellets were modelled. The data source was based on the NREL life cycle inventory database[37], but converted to reflect Chinese fuel mixes and feedstock conditions. The following waste management options were given as four separate scenarios: Incineration (100%); Landfill (100%); Recycle (50%) and landfill (50%); Recycle (100%).

The life cycle environmental impacts associated with 1 kg HDPE pipe are estimated and shown in the Appendix. Incineration and landfill routes exhibit similar impacts for 9 out of 12 indicators, but incineration results in far higher GWP results, by approximately 70%, due to the combustion of embodied hydrocarbons in the plastic. Incineration also produces far higher terrestrial ecotoxicity.

The impact of recycling is to eliminate some/most of the virgin material extraction and processing duty. Thus, those indicators with large contributions from these stages are significantly reduced, most notably GWP, abiotic resource depletion (ADP) fossil and primary energy demand (PED). However, the recycling phase includes significant impacts in itself, primarily due to high electricity demand, as well as some

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[37] NREL (2012).. US Life Cycle Inventory Database. In: National Renewable Energy Laboratory (ed.) [Online]. Available: www.lcacommons.gov/nrel/search [Accessed 29/ 05/ 2018].). www.lcacommons.gov/nrel/search

transport and waste emissions. This prevents the GWP being increased by more than 50%.

Figure 54 shows the contribution of different life cycle categories to the four waste management scenarios described above. As can be seen, the contribution to the large increase for the incineration scenario is from the carbon dioxide emissions associated with the plastic combustion. For the landfill scenario, emissions are chiefly from the fuel usage (process utilities) as well as the raw material extraction and processing. When 50% of the material is recycled, this results in almost 50% reduction in raw material extraction emissions and a slight reduction in fuel usage. Given that the recycling stage has high fuel usage, total fuel usage is not significantly lowered. Therefore for the 100% recycle option; the vast majority of emissions arise from the fuel duty associated with the recycling and extrusion processes. It should be noted that, if energy recovery from incineration were carried out with high efficiency and resulted in the avoided burden of additional fossil-fuel generated energy services, the GWP of incineration would improve significantly. Eriksson and Finnveden[38] suggest that this could result in a similar or better GWP profile than for landfill.

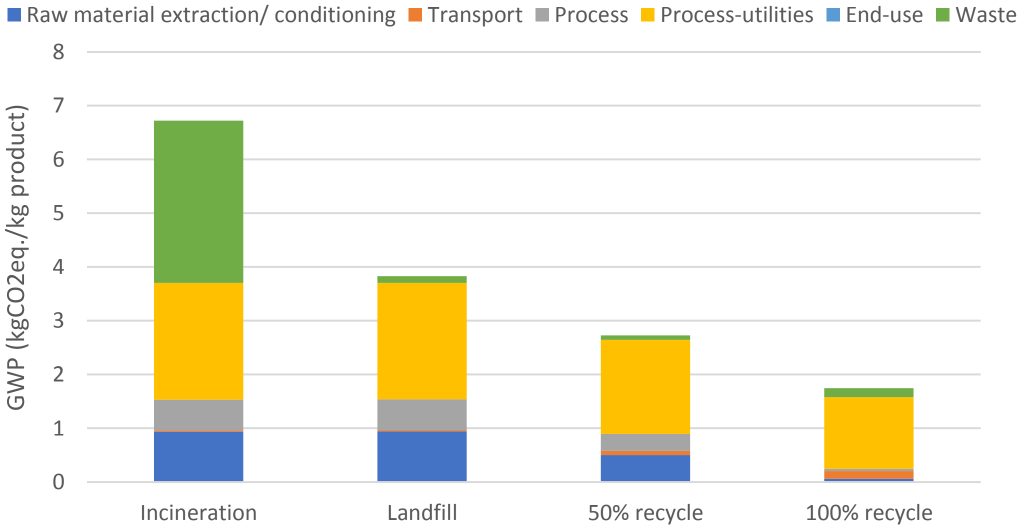

Figure 54 Life cycle global warming potential for 1 kg HDPE pipe, for different waste management options, split by life cycle stage.

In summary, the waste management options associated petrochemical products may have a large impact on total environmental impacts and must be considered carefully. Incineration exhibits significantly higher impacts in some of the categories. This may be reduced slightly by offsetting via waste heat recovery, but this is expected to be minimal. There is a clear positive impact across all impacts associated with recycling and the use of recycled material over virgin material. As a method for decarbonisation, reuse and reprocessing of waste plastic products may provide large benefits. In order to decarbonise further, the supply of low carbon heat and electricity is required.

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[38] O. Eriksson and G. Finnveden (2009). Plastic waste as a fuel - CO2-neutral or not? Energy & Environmental Science; 2: 907-914.

4.9 Summary

Overall, the range of production routes across the petrochemicals exhibit large differences in environmental impacts. However, very few routes exhibit the lowest impacts across the board of indicators. Ammonia production from biomass, as well as methanol from biomass, produces the most promising reductions, in particular with respect to GWP and ADP fossil. Additionally, the low carbon nature of electrolysis from wind results in low GWP impacts for all related routes. The routes from biomass and wind electrolysis, offer reductions in GWP but are typically more energy intensive processes in general, hence their higher PED values. This has an impact on total system efficiency and cost, due to the greater resource usage.

For the routes where large GWP reductions are achieved, there appears to be a trade-off between GWP and other environmental impacts. The alternative routes (e.g. catalytic hydrogenation) are more energy intensive. This is not a problem in terms of GWP because the energy conversion routes may be sufficiently low carbon. However, this may be a problem for other environmental impacts which are exacerbated by the increased energy intensity. For example, the toxicities due to the release of heavy metals from solar panel production: as these routes require more energy input from the solar panels, higher toxicity emissions ensue.

For these alternative routes to be beneficial in terms of GWP, it is vital that any electricity used comes from a sufficiently low carbon source. For example, whilst wind electrolysis performs well and offers significant GWP reductions, solar electrolysis routes offer limit reduction. In the case of using a grid-mix electrolysis, the emissions are by far the highest: therefore great care must be given to the feedstock sources. In the case of a high coal-electricity mix such as China, the energy-intensive alternative routes are often an order of magnitude greater in impacts than the conventional methods.

Additionally, there is potential to reduce emissions much further for the low carbon routes, via the decarbonisation of electricity and, perhaps more importantly, heat. The greater energy intensity of routes such as electrolysis to catalytic hydrogenation require higher heat and electricity loads. Consequently, increases in process efficiency will have a large positive impact on emissions. Additionally, in this study the large heating requirements are still provided by natural gas rather than a lower carbon source. Where low carbon heating sources are available, this would decrease emissions still further. Whilst decarbonisation of electricity has progressed in recent years, decarbonisation of heat is a key industrial challenge that would assist other industrial activities to decarbonise as well. There are a number of low carbon heat options but these currently represent high-cost options, for example via decarbonised electrification or the utilisation of low carbon hydrogen for heat. Further work to identify and incorporate the lowest-cost/environmental heat source would add value to this study.

The options that use coal as a feedstock or use the coal-heavy electricity grid perform poorly due to: toxic emissions during extraction and processing, NO_x and

SO_x emissions, and CO_2 emissions from combustion. Consistently, the coal feedstock options are the highest emitters, besides the use of grid electricity for the energy intensive alternative routes.

Notably for olefin production, the supposedly low carbon routes do not offer significant advantages in terms of GHG reductions. This is partly due to the fact that the embodied fossil carbon remains within this intermediate product and has not yet been emitted to atmosphere, negating the typical benefits seen between fossil and renewable options.

These results show the importance of using broader set of impacts and not only global warming potential, to first avoid shifting impacts from one category to another one, and then to broaden the scope of the decision-making process.

5. Petrochemical technology pathways for China

This section discusses potential petrochemical pathways in terms of technology uptake in the case study region of China between 2010 and 2050 for the production of methanol, ethylene, propylene and ammonia.

The methodology is first described, with respect to the projection of production and the financial and the economic modelling to project the technology mix. Finally, the output of the model is described in terms of technology mix obtained in a socio-economically optimal pathway, CO_2 prices required to achieve this pathway, and cumulative environmental impacts. It is important to note that this study has taken a simplified approach with respect to the social sustainability indicator. Whilst there are many vital social indicators in determining the most sustainable solutions, this short project determines the 'socially optimum' pathway based on where petrochemicals are produced at least cost after greenhouse gas emissions externality is internalised.

5.1 Methodology

5.1.1 Projection of production

As described in Section 2.6, projections of the macro drivers of demand are a central tool in projecting future demand for and production of petrochemicals. The profiles for China of population and GDP according to SSP2 are reported in Figure 57.

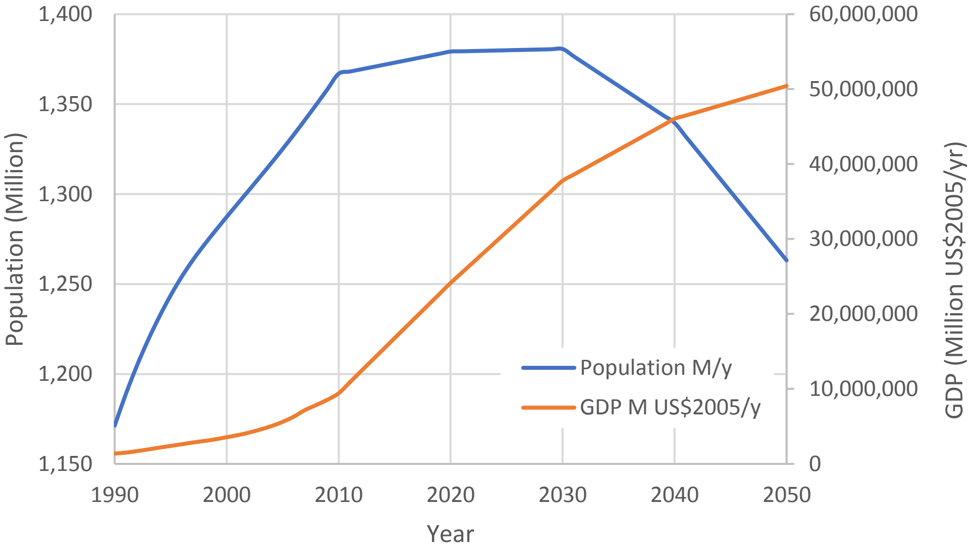

Figure 55 Historic and projected population (million total inhabitants) and GDP of China (million US$ 2005)

The same methodology as described in Section 2.6 for demand projection has been adopted here for projecting production. Historical production is based on the data collected and described in Section 2, and Table 2 summarises the best-fit regression functions used for the production projection.

Table 2 Selection of production regression functions by commodity. See Section 2.6 for details, noting that the regressions presented here are for production, not for demand (and one would not expect the production and demand regressions to be necessarily identical for a single region)

Study region	Methanol	Ethylene	Propylene	Ammonia
China	NLI	NLI	NLI	P

Figure 56 shows historical production and projections of the modelled commodities in China up to 2050.

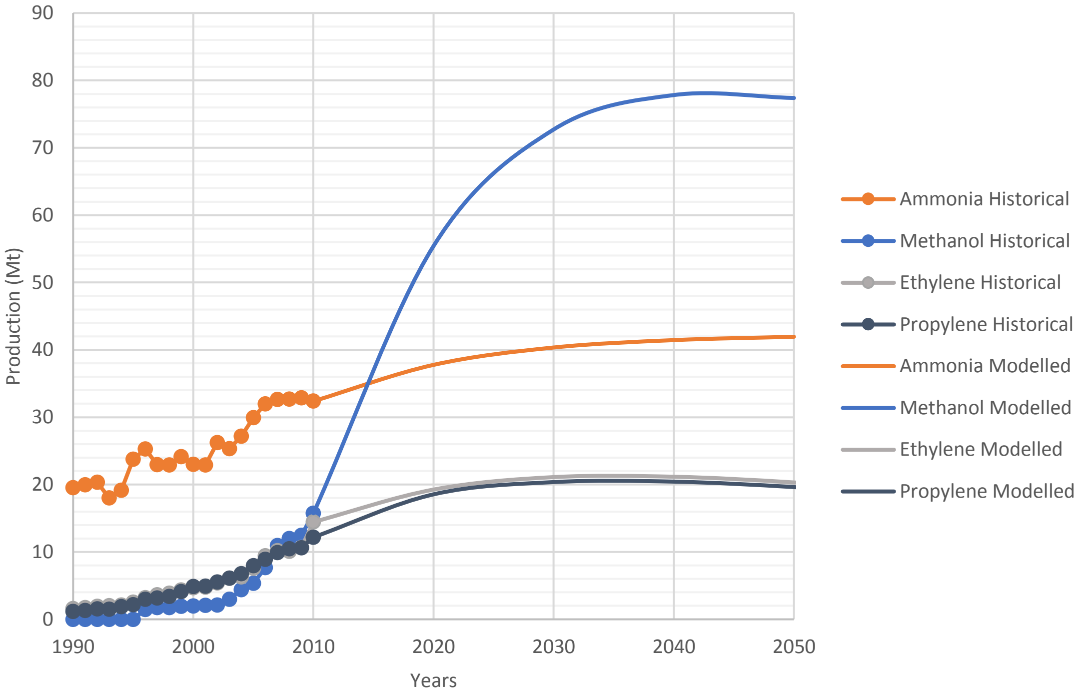

Figure 56 Historical production and projections (Mt) for each commodity up to 2050 for China.

5.1.2 Financial and economic models

The methodology used to produce pathways of petrochemical production process adoption, is based on a linear programming approach solved with the Excel Simplex Solver. The modelling framework calculates a KPI (Net Present Value, System Costs) for all the available technologies. For each commodity the analysis includes traditional technologies, alternative processes and feedstocks defined in the previous process and environmental characterisation sections. The KPI estimation relies on the techno-economic and environmental analysis discussed previously.

The models simulate the uptake of new technologies from 2010 to 2050. In every period, it applies the following steps:

1. Estimate the production gap, which is the difference between the projected domestic production and the installed capacity of all the technologies. Note that in the baseline year, the installed capacity is assumed to meet current production and any increase must be met by additional capacity.

2 It ranks the technologies according to a descending order with a selected KPI
3 Starting from the top ranked technology, the model adds up capacity of the same technology until a maximum technology uptake is met. When the model hits the maximum capacity limit, it moves to the second technology in the ranking and, in a similar way, it adds up capacities until the maximum uptake of the same technology is met. The procedure is repeated for every technology according to the ranking sequence until the production gap is fulfilled.
4 Move to the next period and repeats steps 1, 2, 3

The LP modelling framework was developed for 2 separate objective functions: named the financial model and the social model. In the financial model, the prioritisation of investments in new technologies depends on their relative profitability. The social economic model was developed to represent the view of a social decision-maker driven by cost reduction when investing in new technologies. Both are described below. It should be noted that both the economic and financial models assume the same production profile. This approach neglects the effects of mitigation policies on the commodity production, as they are generally interlinked with a complex pattern of factors and might eventually affect the global market equilibrium in unpredictable ways.

The financial model. The financial model aims to imitate the industrial perspective, therefore, it uses the NPV (Net Present Value) to compare the relative profitability if an investment among the technologies available. The NPV is calculated as the cumulative sum of the discounted cash flows of a project over its lifetime. Cash flows are the net between revenues and costs, reduced by the taxation, which was assumed 36% of the income.

Costs belong to four categories:

1. Fixed operating and maintenance costs are due to the general maintenance of an industry and generally correspond to periods of plant closures; they are assumed equal to 10% of the plant capital expenditure.
2. Sales, General and Administrative costs (SGA) are related to the expenses incurred during the distribution of the products and are assumed equal to a fixed proportion of the variable costs
3. Feedstock costs are associated to the feedstocks used in the process
4. Variable operating costs include the costs due to fuels and internalisation of environmental externalities in the form of CO_2 costs. CO_2 costs are based on the outputs from the environmental life cycle assessments, see Section 4 for further details.

In the first year of the investment, the net cash flow is the net between the fixed-capital investment and loan. The fixed-capital cost represents the plant capital expenditure (or the plant CAPEX), building and infrastructure costs, offices and administration, contingencies, and development and pre-operational activities.

The financing scheme was assumed to carry on for 7 years, using a basis for the debt of 60% of the company equity and being subjected to a 9% financing cost.
The discount factor was set to 10%, being the highest weighted average cost of capital (WACC) of the best performing petrochemical companies operating in 2016[39].

The economic model. The economic model reflects the social decision-maker perspective, as such it uses the System Costs (SC) to compare the relative merit of the technologies (rather than NPV in the financial model). SC is a discounted sum of fixed operating and maintenance costs (1), SGA (2), feedstock costs (3), variable operating costs (4) and the fixed-capital costs. The economic model uses a discount rate equal to an intergenerational equity-adjusted social discount rate of 3%. This is the Social Time Preference Rate (STPR) recommended for investments covering time periods greater than 30 years [40].

Both the financial and economic models include a series of constraints to represent the technical feasibility of the technologies considered for the production of petrochemicals. The decision variables, i.e. the newly installed capacities per technology, are modelled as linear variables to keep the model computationally tractable in Excel.
The model constraints are classified as follows:

- logic constraints which imply the non-negativity of the decision variables, such as the newly installed capacity of each technology
- maximum capacity addition constraints, which imply an upper bound to the newly installed capacities per year and per technology
- technical constraints which link the production of petrochemicals to the installed capacity in a year through technoeconomic parameters such yields and maximum number of operating hours in a year.

5.1.3 Model input

The inputs to the model with respect to energy consumption and efficiencies were taken from the process engineering characterisation of the options, as outlined in Section 3 (much of the data from this section is in the Appendix).

The projected costs for feedstocks, fuel and CO_2 prices for China are reported for 10 year periods between 2010 and 2050 in Table 34 alongside base year references. Fossil fuel price trend follows the IEA 450 ppm projections. The projection profile for all the petrochemical feedstocks follow the same trend as for oil, whilst the solid and gaseous energy vectors follow the profile of coal and natural gas. The CO_2 price follows the MARKER scenario obtained from MESSAGE-GLOBIOM - SSP2-2.6[41], model. This model run used the SSP2 socio-economic driver projections for demand (i.e. consistent with this study). It also used the representative concentration

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[39] R. Berger (2017). The Chemicals Industry 2016 - Lofty expectations… but will it deliver? Focus. Available at: https://www.rolandberger.com/en/Publications/pub_the_chemicals_industry_2016.html?country=null
[40] HM Treasure (2013). The Green Book, Appraisal and Evaluation in Central Government, London, UK.
[41] Science for Global Insight (2016). SSP Database (Shared Socioeconomic Pathways) - Version 1.1. [Online]. Available: https://tntcat.iiasa.ac.at/SspDb/dsd?Action=htmlpage&page=scatter

pathway corresponding to a radiative forcing of 2.6 W/m^2 (RCP2.6), consistent with mitigation limiting the increase of global mean temperature to 2°C[42,43].

Table 3 Cost of consumables, CO_2 and fuels as assumed in the study, based on 2010 USD.

Product							
Cost	Reference	Unit (2010 USD)	2010	2020	2030	2040	2050
Ethylene	IHS[44]	USD / t	1203	1195	1504	1473	1473
Propylene	IHS	USD / t	1391	1381	1739	1703	1703
Methanol	WP2.1	USD / t	532	528	665	651	651
Ammonia	WP2.1	USD / t	597	593	746	731	731
Feedstock							
Biomass	Liu et al.[45]	USD / MJ	0.0052	0.0053	0.0056	0.0057	0.0057
Coal	Liu et al.	USD / MJ	0.001	0.0012	0.0012	0.0012	0.0012
Electricity_grid	WEO 2014[46]	USD / MJ	0.0148	0.0195	0.0265	0.0239	0.0239
Natural gas	Liu et al.	USD / MJ	0.0044	0.0047	0.0060	0.0062	0.0062
Naphtha	https://www.opisnet.com	USD / t	392	389	490	479	479
Ethane	T. Ren Energy (33) 817 - 833[47]	USD / t	200	200	250	245	245
Propane	UN ComTrade[48]	USD / t	367	365	459	450	450
Water	WP2.1	USD / t	5.32	5.32	5.32	5.32	5.32
Electricity_solar	IRENA, 2015[49]	USD/MJ	0.0361	0.0232	0.0167	0.0167	0.0167
Electricity_onshore_wind	IRENA, 2015	USD/MJ	0.0194	0.0157	0.0139	0.0139	0.0139
Mitigation scenario							
CO_2	MESSAGE-GLOBIOM RCP2.6	USD / t	0	31.681	41.84	52.004	84.710

The 2010 base year stock of installed technologies in China was characterised for each commodity based on the market analysis detailed in Section 2. A decommissioning profile of the 2010 stock was also assumed: half of the 2010 stock

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[42] D. P. van Vuuren, J. Edmonds, M. Kainuma, K. Riah, A. Thomson, K. Hibbard, G. C. Hurtt, T. Kram, V. KreyJean-Francois Lamarque, T. Masui, M. Meinshausen, N. Nakicenovic, S. J. Smith & S. K. Rose ().The representative concentration pathways: an overview. Climatic Change (2011) 109: 5.https://doi.org/10.1007/s10584-011-0148-z

[43] D. P. van Vuuren, E. Stehfest, M. G. J. den Elzen, T. Kram, J. van Vliet, S. Deetman, M. Isaac, K. Klein, G. A.H of, A. Mendoza Beltran, R Oostenrijk & B. van Ruijven (2011). RCP2.6: exploring the possibility to keep global mean temperature increase below 2°C. Climatic Change, 109: 95. https://doi.org/10.1007/s10584-011-0152-3

[44] IHS Chemical, World Petrochemical Conference

[45] P. Liu, D. I. Gerogiorgis & E. N. Pistikopoulos (2007). Modeling and optimization of polygeneration energy systems. Catalysis Today, Volume 127, Issues 1–4, Pages 347-359. https://doi.org/10.1016/j.cattod.2007.05.024. P.

[46] OECD/IEA (2014). World Energy Outlook (2014). https://www.iea.org/publications/freepublications/publication/WEO2014.pdf)

[47] T. Ren, M. K. Patel & K. Blok (2008). Steam cracking and methane to olefins: Energy use, CO2 emissions and production costs. Energy, 33 (5), 817-833. https://doi.org/10.1016/j.energy.2008.01.002. T.

[48] UN ComTrade (2018). UN Comtrade Database [Online]. Available: http://www.un.org/en/databases/index.html [Accessed 29/ 05/ 2018] UN ComTrade, http://www.un.org/en/databases/index.html

[49] IRENA (2016).The Power to Change: Solar and Wind Cost Reduction Potential to 2025. www.irena.org/publications/2016/Jun/The-Power-to-Change-Solar-and-Wind-Cost-Reduction-Potential-to-2025

would be decommissioned in 2040 and only a third of the initial stock would remain in 2050. This decommissioning profile reflects the long lifetime expected of the plants in the petrochemical industry and reflects the considerations of the experts interviewed in Section 6.

5.1.4 Model output

The financial and economic models are applied to generate potential pathways of petrochemical process route choices for methanol, ammonia and olefins for China. The outputs are as three cases as follows:

- First, a **baseline** case is produced from the financial model, without a CO_2 price imposed. This represents the choices made by economically-rational decision makers under business as usual assumptions.
- Then, a **socio-economically optimal** case is simulated; this case uses the economic model, including the influence of the CO_2 price trajectory from the MARKER scenario described above. It is assumed that this pathway represents the preferred outcome from the point of view of a socially-motivated decision maker.
- Finally, a **mitigation** case is simulated, using the financial model, were a local CO_2 price is applied in a way to obtain the same decarbonisation pathway as in the socio-economically optimum.

As explained in Section 5.1.2, each case assumes the same production profile, thus assumes that mitigation policies do not impact production. The models calculate a set of technical variables (final energy consumption), environmental variables (ADP elements, ADP fossil, AP, EP, FAETP, GWP, HTP, MAETP, ODP, POCP, TETP, Primary Energy Demand) and economic variables (costs and revenues of each single technology, NPV, SC, levelised cost, return on investment (ROI)).

5.2 Methanol pathways

There are 6 technologies selected for methanol production, as summarised in Table 4. In 2010, the production of methanol relies for 35% on natural gas; the remaining uses coal[50] feedstock.

Table 4 Technologies modelled

Feedstock	Route
Natural gas	Methanol synthesis (Liu et al., 2007)
Biomass	Methanol synthesis (Liu et al., 2007)
Water (solar – electrolysis)	Methanol synthesis [51]
Water (wind – electrolysis)	Methanol synthesis
Water (wind – electrolysis)	Methanol synthesis

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[50] S.Su, Li-Wang, L. & Li, Xiang-Rong & S.Sun, Zuo-Yu. (2013). Flow chart of methanol in China. Renewable and Sustainable Energy Reviews, Elsevier, vol.. 28(C), pages. 541-550.

[51] D. Mignard, M. Sahibzada, J.M. Duthie & H.W. Whittington. (2003). Methanol synthesis from flue-gas CO2 and renewable electricity: a feasibility study. International Journal of Hydrogen Energy, 28, pp 455-464.

Coal	Methanol synthesis (Liu et al., 2007)

The results of the baseline financial model without CO_2 price and the social model with CO_2 price are shown in Figure 57. It must be noted that these results are illustrative and not conclusive, given the simplicity of the projections and technology models, as well as the uncertainty in medium-term pathway projections. For the financial model without CO_2 price, the trend of the new investments in the methanol production in China shows a preference towards the most profitable technologies, which are based on the use of coal. The implementation of the CO_2 price (consistent with a 2C target and SSP2) modifies the trends for the future installations, shifting the portfolio of feedstocks from coal to natural gas in order to offset both the decommissioned capacity as well as the need to meet the projected increasing production profile. However, this shift is very slow, with substantial coal-based capacity commissioned in the short term, resulting in a largely coal-based production stock remaining in 2050. The result here is largely driven by technology lock-in, where coal-based processes are commissioned early on to meet rapidly increasing Chinese production requirements, leaving little room for alternative technologies to enter the market.

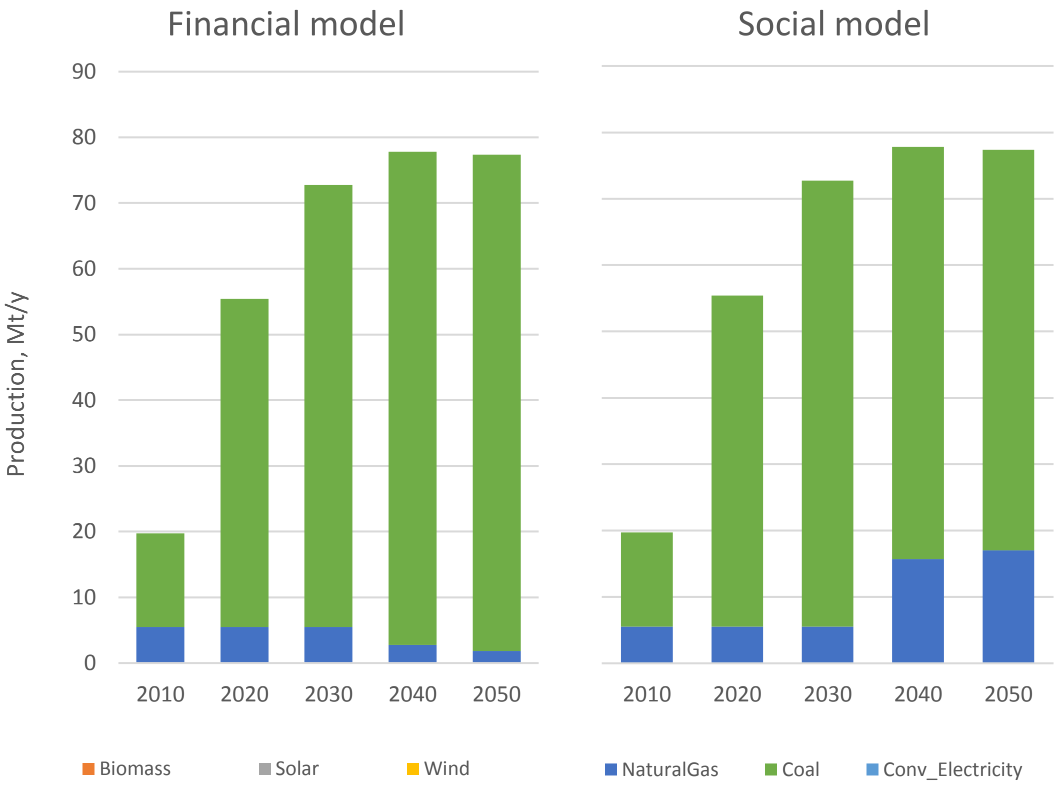

Figure 57 Projection of the production from the modelled technologies in China from the financial model without CO_2 price (left) and the economic model with CO_2 price (right)

As described above, the mitigation case is produced by running the financial model to determine the CO_2 price trajectory required to result in the same outcome as the socio-economically optimal sensitivity. This CO_2 price is shown in Table 5.

Table 5 CO_2 price for mitigation policy

	2010	2020	2030	2040	2050
CO_2 price, USD / t	0	41	52	126	225

These prices are higher than the MARKER scenario price in the period 2040-2050, indicating that a global cap-and-trade CO_2 price alone would not be sufficient for methanol production in China to achieve a socio-economically optimal 2C consistent pathway. Indeed, the significant presence of coal in the system even at 2050 is almost certainly not consistent with a 2C pathway. This again highlights the importance of technology lock-in in the long-term sustainability of a rapidly expanding petrochemicals market.

5.2.1 Environmental Impacts

Total annual CO_2 emissions associated with methanol production in China are shown in Figure 58 for the baseline and mitigation case between 2010 and 2050. The large rise in emissions is driven by the substantial production rate increase whilst levelised emissions (emissions per unit of production) remain relatively constant, except for a small decrease between 2030 and 2050 for the mitigation case. Additionally, cumulative total environmental impacts for this time period alongside the proportional variation between cases is shown in Table 6. The shift from coal-based to gas-based processes results in an improved outcome across all environmental indicators. However, these improvements are generally limited to less than 10%, as they are constrained by coal-based technology lock-in occurring in the near-term, as well as the lack of penetration of more environmentally benign options. In particular the anticipated total reduction in GHG emissions expressed as global warming potential (GWP) is 8%.

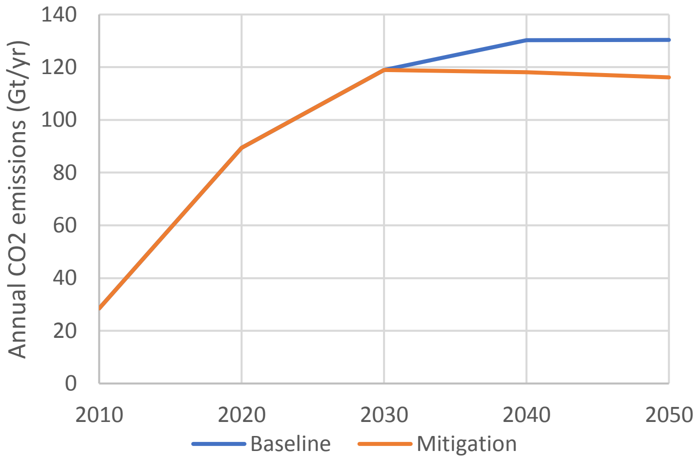

Figure 58. Annual carbon dioxide emissions associated with the production of methanol in China between 2010 and 2050 for the baseline and mitigation cases.

Table 6 The cumulative change in environmental impacts for methanol production between 2010 and 2050 under the mitigation case, relative to the baseline case.

Impacts	Methanol
ADP elements	-10%
ADP fossil	-5%
AP	-7%
EP	-10%
FAETP	-9%
GWP	-8%
HTP	-9%
MAETP	-9%
ODP	7%
POCP	-1%
TETP	-10%
PED	-5%

5.3 Olefins pathways

Overall, 9 feedstock and technology options were input to the model, detailed in Table 7. According to the market analysis in Section 2 and the publicly available literature, the initial stock was characterised with naphtha and coal-based technologies[52] as well as including the new coal-based olefins which are expected to become online by 2020. A decommissioning profile was assumed considering that half of the stock would retire in 2040 and a third of the initial stock would remain in 2050.

Table 7 Summary of the technologies selected for the production of olefins

Feedstock	Description	Acronym
Ethane	Ethylene, from ethane cracking	Cracking
Natural gas	Ethylene/propylene, from MTO, from natural gas	MTO_NaturalGas
Naphtha	Ethylene/propylene, from naphtha cracking	Cracking
Biomass	Ethylene/propylene, from MTO, from biomass	MTO_Biomass
Electrolysis: solar	Ethylene/propylene, from MTO, from solar electricity	MTO_solar
Electrolysis: wind	Ethylene/propylene, from MTO, from wind electricity	MTO_Wind
Electrolysis: grid	Ethylene/propylene, from MTO, from grid electricity	MTO_conv_electricity
Coal	Ethylene/propylene, from MTO, from coal	MTO_Coal
Propane	Propylene, from propane cracking	Cracking

Figure 59 displays the technological mix projections for both the financial model without a CO_2 price and the social model with a CO_2 price. For the financial model,

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[52] Deutsche Bank Markets Research (2014). China's Coal to Olefins Industry. Available: http://www.fullertreacymoney.com/system/data/files/PDFs/2014/July/3rd/0900b8c088667819.pdf

coal becomes the dominant technology displacing naphtha-cracking. When a 2C-consistent carbon price is applied, the naphtha cracking routes are decommissioned, and replaced with lower emitting technologies based on ethane and propane cracking. The coal-based technologies which remain in the mix throughout the timeframe of the analysis correspond to the coal-to-olefins capacities already planned to be installed before 2020 [53].

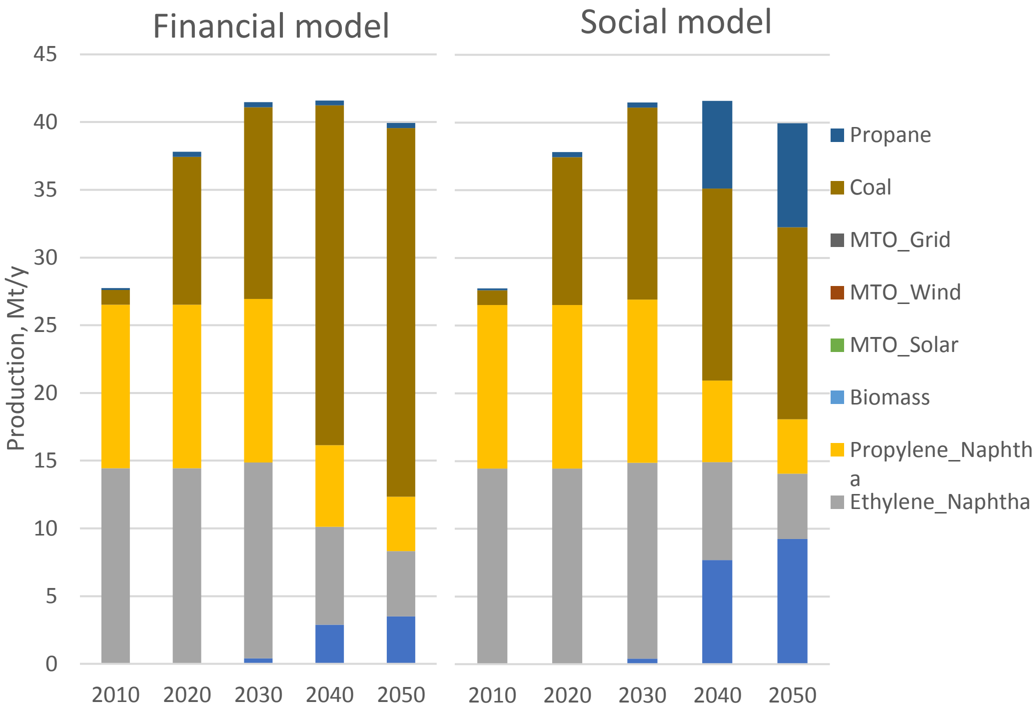

Figure 59 Projection of the production of olefins from the modelled technologies in China from the financial model without CO_2 price and the social model with CO_2 price.

The mitigation case is produced by running the financial model to determine the CO_2 price trajectory required to result in the same outcome as the socio-economically optimal sensitivity. This CO_2 price is shown in Table 8; the price differs in 2040 from the global MARKER CO_2 price in 2040, as it has to counteract the presence of such a cheap feedstock as coal.

Table 8 CO_2 price for mitigation policy

	2010	**2020**	**2030**	**2040**	**2050**
CO_2 price, USD / t	0	32	42	100	120

5.3.1 Environmental Impacts

Total annual CO_2 emissions associated with ethylene and propylene production in China are shown in Figure 60 for the baseline and mitigation case between 2010 and 2050. A gradual reduction in GHG emissions is seen in both baseline and mitigation

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[53] Deutsche Bank Markets Research (2014). China's Coal to Olefins Industry. Available: http://www.fullertreacymoney.com/system/data/files/PDFs/2014/July/3rd/0900b8c088667819.pdf

cases but the increase in production results in overall emissions rise until 2030. After this, the production rate plateaus but levelised emissions reductions (emissions per tonne of product) reduce further by 25 – 50% of the initial values. The average reduction in emissions between the baseline and mitigation case is 7% and 11% for ethylene and propylene respectively, as shown in Table 9. This table summarises the relative change in each environmental impact between the baseline and mitigation case up to 2050. Opportunities to mitigate the GWP of the olefins synthesis in China by around 10% would be associated to the relative abandon of coal in favour of lighter hydrocarbon feedstocks, whereas other environmental impacts are reduced much more.

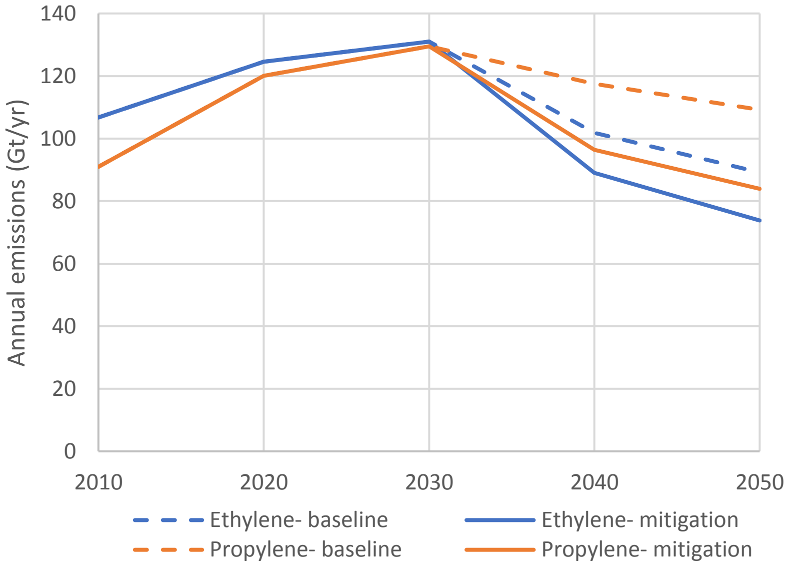

Figure 60. Annual carbon dioxide emissions associated with the production of ethylene and propylene in China between 2010 and 2050 for the baseline and mitigation cases.

Table 9 The cumulative change in environmental impacts for ethylene and propylene under the mitigation case, relative to the baseline case.

Environmental impact	Ethylene	Propylene
ADP elements	-30%	-29%
ADP fossil	-9%	-10%
AP	-18%	-22%
EP	-30%	-30%
FAETP	-26%	-28%
GWP	-7%	-11%
HTP	-26%	-28%
MAETP	-21%	-25%
ODP	2%	53%
POCP	-16%	-19%
TETP	-30%	-30%
PED	-9%	-11%

5.4 Ammonia pathways

The production profile for ammonia was estimated from the production of total nitrogen as described in Section 2, considering that the N-based fertilisers represent 86% of ammonia demand in China[54]. In the base year, the vast majority of ammonia production in China relies on coal[55], which was not included in the techno-economic and life cycle assessment studies. Consequently, it is assumed to be decommissioned over time and new investments are only possible for the alternative routes studied in Section 4. The 5 technologies available for ammonia production have been selected in Section 4. They are summarised in Table 10.

Table 10 Summary of the technologies modelled

Feedstock	**Route**
Natural gas	Ammonia synthesis from natural gas
Biomass	Ammonia synthesis from biomass [56]
Water (solar – electrolysis)	Ammonia synthesis from electrolysis and solar energy
Water (wind – electrolysis)	Ammonia synthesis from electrolysis and wind energy
Water (conv – electrolysis)	Ammonia synthesis from electrolysis and the conventional electricity

The petrochemical pathway in Figure 61 shows that investments in natural gas-based processes are favoured by the higher profitability compared to biomass until 2030. After 2030, biomass-based processes become more profitable due to the lower energy costs associated to the technology. Note that the competing coal-based route to ammonia has not been considered in this study.

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[54] Average between 2010 – 2014 values, source: USGS (2018). US Geological Survey Science Data Catalog [Online]. Available: https://data.usgs.gov/datacatalog/#fq=dataType%3A(collection%20OR%20non-collection)&q=*%3A* [Accessed 17/05/2018] USGS database, average between 2010 – 2014 values.

[55] Zhou, W., B. Zhu, Q. Li, T. Ma, S. Hu & C. Griffy-Brown (2010). CO2 emissions and mitigation potential in China's ammonia industry. Energy Policy 38:3701–3709. doi:10.1016/j.enpol.2010.02.048

[56] P. Tunå, C. Hulteberg & S. Ahlgren. (2014), Techno-economic assessment of non-fossil ammonia production. Environ. Prog. Sustainable Energy, 33: 1290-1297. doi:10.1002/ep.11886

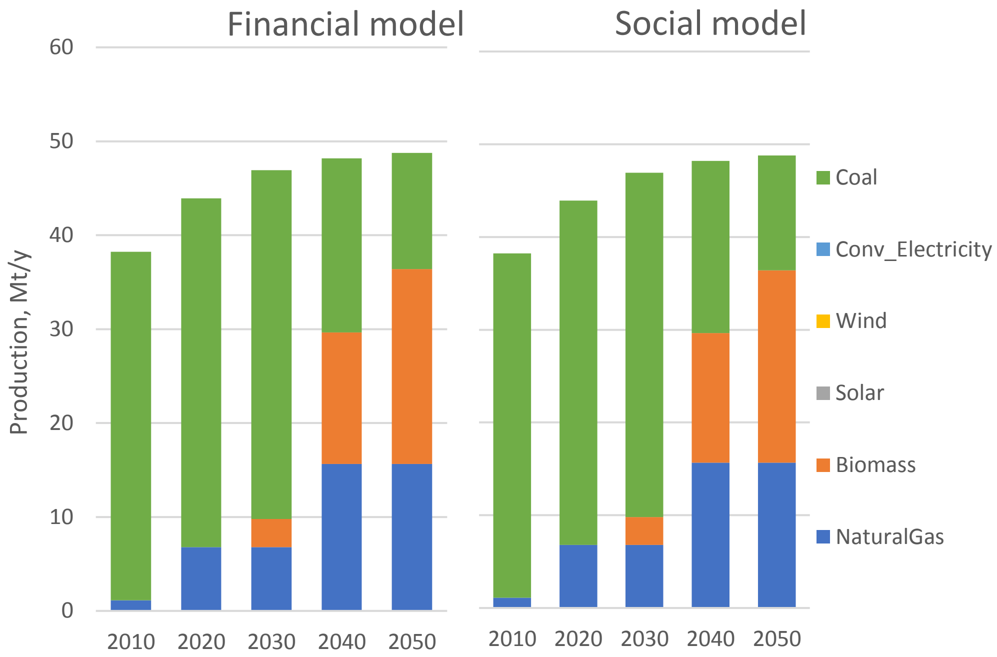

Figure 61 Projection of ammonia production from the modelled technologies in China from the financial model without CO_2 price (left) and the social model with CO_2 price (right)

When a CO_2 price is applied in the economic model, the social optimum coincides with the results from the financial model described above. This is due to the fact that the carbon price is not active until after 2020. Between 2020 and 2030, the lowest-emitting biomass route is more expensive because of higher capital costs. After 2030, biomass energy prices are sufficiently low to make this technology cost-competitive, with the addition of a CO_2 price making no difference to outcomes. For these reasons the pathway is close to the financial one.

Given that the baseline coincides with the social optimum, the mitigation case is not discussed here. In other words, the response of a profit-motivated actor mimics that of the least cost system under the influence of a global carbon price. In essence this means that no carbon price is required in China for ammonia production route choices to follow an identical pathway as appears desirable from a social decision maker's point of view. However, it is important to note that this result is strongly influenced by the lack of a coal-based ammonia production technology within this study.

5.4.1 Environmental Impacts

Table 11 summarises the cumulative impacts for ammonia production up to 2050. However, given that there was no variation between baseline and mitigation cases, no change occurs. Note, the impact associated to the initial stock of technologies was not included for lack of data, consequently these impacts are likely to be an underestimate.

Table 11 Cumulative environmental impacts for ammonia production

Environmental impacts	**Ammonia**
ADP elements (kg Sb eq)	1,760,000

ADP fossil (MJ eq)	24,200,000,000,000
AP (kg SO_2 eq)	8,540,000,000
EP (kg PO_4 eq)	621,000,000
FAETP (kg DCB eq)	168,000,000,000
GWP exc bio (kg CO_2 eq)	1,950,000,000,000
HTP (kg DCB eq)	634,000,000,000
MAETP (kg DCB eq)	768,000,000,000,000
ODP (kg R11 eq)	51,000
POCP (kg C_2H_4 eq)	629,000,000
TETP (kg DCB eq)	10,500,000,000
Primary Energy Demand (MJ)	37,900,000,000,000
GWP process (kg CO_2 eq)	361,000,000,000

5.5 Summary

This section has discussed scenarios of potential uptake of novel technologies in the manufacturing of methanol, ammonia and olefins in China.

Natural gas appears as a viable transitional option towards less CO_2-emitting technologies for methanol and ammonia production. The former, in particular, could switch from coal to natural gas, if the CO_2 price is sufficiently high. The second market shows that between 2020 and 2030, the lowest-emitting biomass route is more expensive because of higher capital costs. After 2030, biomass energy prices are sufficiently low to make this technology cost-competitive.

In the olefins market, opportunities to mitigate the GWP of the olefins synthesis in China by around 10% would be associated to the relative abandon of coal in favour of lighter hydrocarbon feedstocks. In doing so, other environmental impacts would be reduced even more. The technologies based on electrolysis still appear too expensive and do not appear in the sustainable petrochemical pathways.

6. Expert elicitations: sustainability challenges of the sector

Section 2 to Section 5 have focused on the analysis of demand, costs, environmental impacts and economics of petrochemical production options. In order to supplement these quantitative studies, this section elicits the perceptions of experts in the field to understand where the greatest potential and the greatest barriers to industrial progression lie.

The objective of the study was to explore the strengths and weaknesses of the previous quantitative results and to inform their analysis by synthesising the views of experts from industry, government and academia, to determine the environmental, economic, social and policy related barriers to further development of the petrochemical industry. In particular, questions were raised regarding opportunities and challenges related to improving sustainability in petrochemicals.

6.1 Interviews

Potential interviewees were shortlisted and agreed by the project group. Each was contacted and 6 were sought for interview. The objective of this study was not to develop a representative sample of stakeholder perceptions, but to provide an additional insight and validation or compliment to the previous quantitative economic and environmental studies. The interviews were intended to last for approximately 30 minutes and in reality varied from 20 - 45 minutes. Each interview was semi-structured, such that key questions were raised but adapted for suitability for each interview. The broad interview questions were the following:

1. *Generally, do you have any overarching thoughts of the way the petrochemical industry will change over the next 10, 20 or 30 years?*
2. *Do you predict any large-scale changes in demand for any of the following chemicals or derivatives? Methanol, olefins, ammonia.*
3. *Do you anticipate any other disruptions to markets of any of these products considered? What could they be? What might the potential causes and effects be?*
4. *What do you think will be the change in prices of these petrochemical commodities over the next 10, 20, 30 years?*
5. *Do you think the petrochemical sector will decarbonise? If so, how will it happen? Feedstocks? Processes? CCS or CCU?*
6. *What do you think will be the driver of petrochemical decarbonisation? e.g. carbon price/ regulation/ voluntary*
7. *What are the most promising decarbonising options for the industry?*

Three out of the six interviewees expressed the desire to remain anonymous in their contribution, thus all of the interviewees are presented this way. The interviewees consisted of: two from academia, one reader and one professor in the field of process engineering and environmental assessments; two from major international petrochemical companies (of director and division-lead position); and two from non-profit policy/technical advisory organisations with a focus on the petrochemical industry. The interviewees were from the UK, Spain, Germany and the US and all had experience internationally. Note that none specialised in Chinese petrochemical industry and whilst China was mentioned in most interviews, the results of these interviews should be considered to have a global perspective rather than relevant to a specific region.

6.2 Results

6.2.1 Demand projection

Global demand for petrochemicals is likely to continue to grow, in particular for methanol, but also ammonia and olefins. Demand is closely linked to population and economic growth, so growth in particular is expected in developing countries. Whilst CO_2 emissions may be decoupled from economic growth and demand growth, for example via increased renewable energy, other environmental impacts such as water footprint cannot and consequently there are likely to be other environmental barriers in the future with continued demand growth.

In particular methanol is expected by all interviewees to experience growth as it may be a key tool for decarbonisation in the future, as an intermediate product which may use low carbon feedstocks. Additionally, there is potential for its use as an energy carrier. Olefin production may increase significantly, but is dependent on regulation, in particular the impact of recycling regulation may change demand for virgin products. Ammonia demand may grow significantly in developing regions for fertiliser use, especially in India, China and Africa. The potential role of ammonia as an energy carrier could also increase demand significantly.

6.2.2 Price projections

In the shorter term, four interviewees suggest that petrochemical production will track demand and no material change in price will ensue. However in the longer term, prices are much less certain. Two opposing price drivers were discussed most frequently: the impact of reduced oil demand from transport; the impact of climate-related policy and regulation.

Five out of six interviewees mentioned the potential impact of reduced oil demand or fossil fuel demand in general. The growth in renewable electricity generation and the potential growth in electric vehicle uptake may significantly reduce demand for oil. This could result in increased availability of oil to the petrochemical industry, thus reducing the price. Given that petrochemical products typically represent the minority of products from a refinery, the majority being fuel products, this could spell a sea-change for refinery production business models. The impact is likely to be seen in terms of petrochemical prices, but also as a change to a heavier hydrocarbon feedstock will change processing needs. Given that oil can produce some petrochemicals than natural gas cannot, this could give rise to some far cheaper products (e.g. aromatics).

The US shale boom in the first decade of the 21st century created an oversupply of light hydrocarbons (e.g. ethane), resulting in a significant increase in light cracking for olefins. The projected decrease in oil price may turn the tide again. However, feedstock prices are highly variable across regions and so global price changes are multifaceted. For example, if shale is developed in China, this is likely to have a strong influence on the petrochemical industry.

Longer term, petrochemical price changes will be driven by political measures, either directly on the petrochemical industry or indirectly via others such as energy.

The development of the petrochemical industry in Middle East was mentioned as a potential driver of price changes by two interviewees, noting the current overcapacity of Europe and a possible increasing demand for local production in growing economies.

6.2.3 Drivers of change

Changes in the petrochemical industry will be governed by the cheapest feedstocks and processes. So far, the vast majority of effort from the industry has been in improved energy efficiency, given the cost-effectiveness on efficiency measures. However, there has been little drive towards deeper decarbonisation, due to the lack of regulatory mechanisms to support this. One interviewee suggested that less attention has been given to regulatory frameworks for petrochemicals than for the energy industry, so it is lagging behind. It was emphasised in all interviews that deep decarbonisation requires strong policy and regulatory frameworks to be realised.

There are a number of regulatory solutions that could help achieve this: the most common being a carbon price and/or an emissions performance standards. Lessons should be learnt from the experience of regional applications, for example the European Emissions Trading Scheme (ETS). In particular, managing prices by effective prediction of CO_2 volumes as emissions are reduced. However, there was emphasis on the need for global policies or regulation. The industry has high levels of international trade, creating the potential for 'carbon leakage', where regional carbon pricing may create incentives to import rather than produce products sustainably. National emissions performance standards may also be effective and views were put forward that appealing regulations are not technology-specific, but again much care must be taken to avoid the significant potential of carbon leakage, for example via border tariffs. There was broad support from all interviewees on policy measures to incentivise decarbonisation, but the need for a level playing field for all was emphasised.

The potential pace of change in decarbonisation of the petrochemical industry was mentioned in two interviews. On one side, the petrochemical industry was suggested to be potentially slow given its capital-intensive infrastructure, with plants being utilised for 40 years. On the other side, another interviewee suggested the industry could change quickly due to the flexibility of processes, feedstocks and decarbonisation options.

6.2.4 How to decarbonise

A number of options were discussed across the interviews regarding the most effective routes for decarbonisation. In fact, every interviewee touched on each of these options for decarbonisation:

- Increasing process efficiency
- Decarbonising fuel sources
- Bio-based feedstocks
- Low carbon hydrogen
- CCS
- Technology innovation

Efficiency increases will provide marginal gains in industrial decarbonisation, although the petrochemical industry is already highly efficient in many cases, given that this has long been a focus of attention. Small gains in efficiency may be counteracted by growth in global demand, so overall decarbonisation from efficiency gains is unlikely. There is always a cost incentive to increase efficiency, however deeper decarbonisation requires more incentive.

A unique challenge to the petrochemical industry is the need to decarbonise heat. It is an energy intensive industry, but low carbon heat is difficult to achieve. For example, electrification of heat is relatively inefficient and also places strain on electricity grids. Additionally, the use of renewable energy sources will increase the demand on rare metals, which adds another environmental burden to the decarbonisation routes. Small-scale nuclear that provides both electricity and heat could be an efficient low carbon option in the future if cost-competitive. It should be noted that public perception of the incorporation of nuclear energy into industrial production is likely to be a barrier to uptake.

The impact of low carbon methanol production was discussed frequently, in particular the methanol-to-olefins route. Methanol may be derived from low carbon sources, bio-based or from electrolytic hydrogen, and can be a base chemical for many other products. Currently, methanol-to-olefins (MTO) it is not cost-effective, besides in China with cheap coal. However, methanol could provide great flexibility in the future with the availability of cheaper low carbon feedstocks.

Bio-based feedstocks represents an opportunity to decarbonise the petrochemical industry. Sugar cane was mentioned as an efficient petrochemical feedstock, due to the potential to utilise the juice for feedstock and the cane for process fuel. Ethylene production from bioethanol was suggested by one to be the most promising route, which is already operational in Brazil, given the large bio-resource. BECCS (bioenergy with CCS) has the potential for use in the petrochemical industry, with biomass gasification to hydrogen for feedstock and sequestration of the carbon dioxide.

However, all interviewees suggested that there were significant barriers to large-scale bio-based process development. There are many competing applications for bio-based feedstocks and it is debatable which is most appropriate/efficient. In particular, barriers to the greater use of bio-based feedstocks were:

- Many bio-feedstocks are not molecularly similar to petrochemical products, resulting in high energy intensity and consequently high cost/low efficiency.
- Competition with the energy sector for bio-feedstocks currently favours the energy sector. Biofuels are often incentivised, but bio-chemicals are typically not, creating a financial disparity.
- Competition for bio-feedstocks with food systems should be avoided to prevent adverse impacts in areas with high levels of poverty.
- Cracking of bio-feedstocks will likely give different ratios of co-products which could affect the relative price, for example between ethylene and propylene
- One interviewee suggested bio-based routes will be significantly more expensive than other decarbonisation options, such as hydrogen production and CCS.
- With a projected increase in bio-based feedstocks for industry and energy, water impacts, land use changes and other environmental impacts may be significant and must be managed carefully in order to prevent shifting from one environmental impact to another.

Using hydrogen as a feedstock from a low carbon source may represent a good opportunity, in particular for methanol and ammonia production. Hydrogen may be derived via gasification of low carbon feedstocks or via electrolysis using low carbon electricity. However, currently these are neither cost-effective nor environmentally beneficial for many supply chains. These technologies mainly focus on meeting climate change targets, which indeed provide instrumental opportunities, however this narrow dimension might create bigger problems as these technologies are highly energy intensive, rely on high resource intensive energy sources (e.g. solar and wind installations), would create a higher water demand as well as intensifying land use change.

Another important point is that costs are highly heterogeneous across different regions. The use of excess renewable electricity, as power-to-gas, could generate cheaper hydrogen at times when electricity is cheap. However, this is dependent on the management of the power system: there may not be a reliable source. Additionally, if electricity system flexibility is managed well, this will be a relatively minor resource.

Most of the interviewees thought that fossil fuel prices would decrease, presenting an opportunity for CCS to become much more cost-effective compared to other decarbonisation options. Perceptions of the likelihood of CCS use becoming widespread in the petrochemical industry were mixed. There were suggestions it may be more effective in other industries, such as power or cement. However, the use of CCS with ammonia could be the attractive. Nevertheless, there are barriers in terms of long-distance transport and regional storage of CO_2. The link between enabling CCS and incentives such as carbon pricing is clear. A roll-out of CCS in the power sector (or other) may decrease infrastructural costs significantly and propagate its use in the petrochemical sector.

Recycling and the use of waste resources were suggested by four interviewees as having high potential to help minimise the impact of petrochemicals. Greater recycling lowers the usage of feedstock and increases energy efficiency, but represents a handling and separations challenge, as well as cost. The low recycling rate of polymers and solvents was remarked, partially due to difficulties and inefficiencies in some recycling routes, e.g. olefins and some polymers. As an example, current efforts towards increasing recycling of polymers in Europe was mentioned. Reusing polymers, mainly in composite materials, was identified as a key opportunity to reduce environmental impacts. An additional opportunity for waste utilisation is the use of natural gas from associated oil wells that may otherwise be flared.

Broadly, there was a view that the petrochemical industry will remain more dependent on fossil fuels, or more difficult to negate, than the energy sectors. This is perhaps most evident in the rapid decarbonisation of many nation's electricity mixes. Innovation from conventional processes was mentioned a number of times in relation to decarbonisation, although less so than the above-mentioned options. Options mentioned were progress in catalysis to increase efficiencies and reduce energy intensities, in particular for MTO processes, methane pyrolysis to produce solid carbon and negate the need for CCS, oxidative coupling of methane and alternative ammonia production methods. Whilst these processes were mentioned, emphasis on the greatest opportunities for decarbonisation was placed on low carbon feedstocks and the supply of decarbonised heat.

6.3 Summary

The semi-structured expert interviews are synthesised into a number of key points below.

- Global demand is likely to increase, especially for methanol as it may be increasingly used as an intermediary for low carbon petrochemical production.
- The price of oil may decrease in the longer term, which could lead to a shift in feedstock for the petrochemical industry to heavier hydrocarbon processes.
- All interviewees agree that much attention has already been given to maximising the efficiency of petrochemical processes. However, deeper decarbonisation requires an additional cost incentive.
- In order to achieve decarbonisation through regulatory change, any regulations must:
    - Ensure a level playing field across the industry
    - Be globally applicable or ensure the negation of ‘carbon leakage’

- There are many promising decarbonisation options, including the use of bio-based or renewable feedstocks and the use of innovative catalytic processes. However, there is clearly no silver bullet and each option exhibits multiple disadvantages or barriers, relating to cost, resource availability or in the case of bio-based feedstocks, creating competition with other critical industries such as food.

Overall, this study has highlighted some key issues faced by the petrochemical sector in the future. However, to add value to such a project in the future, the following recommendations are made:

- The interviews could take place at the start of the project in order to inform the inputs to the quantitative study. For example, the inclusion of decarbonisation processes or policy frameworks would be valuable.
- A larger sample of interviewees would be desirable. Given the large regional differences in the petrochemical industry, a focus on representativeness of stakeholders across different regions would yield a more nuanced analysis, especially with respect to key regions such as China.

7. Conclusions

This study has covered a wide range of aspects that bear upon aspects of sustainability in petrochemical industries. The study has included a market assessment, demand projection, techno-economic and environmental life cycle assessment of a multitude of production routes and key end-uses, and financial and economic modelling of these options in the Chinese context. Finally it has reflected upon this analyses via expert elicitation on key opportunities and challenges for petrochemicals. Key points are drawn out for each petrochemical studied, and finally an overview of the methodology for future sustainability assessment studies is presented.

7.1 Methanol

Methanol has a huge range of potential downstream products via methanol-to-olefins, and use as a fuel. Furthermore it is a relatively transportable product, implying the continuation of a healthy global marketplace. With respect to demand, the market study highlighted the rapid growth of methanol production, particularly in China. Methanol may be an intermediate product to a wide variety of end-uses as well as a fuel and, if produced effectively, could drive the decarbonisation of the industry. There is broad agreement from the market analysis and expert elicitations that demand for methanol is likely to increase substantially. The choice of production process is mainly driven by the price of the primary feedstock. Historically this has largely been natural gas, though coal-based processes have gained momentum in China due to the availability of favourably-priced coal.

A key alternative route to produce methanol, via the catalytic hydrogenation of CO_2, revolves entirely around more sustainable means of producing hydrogen. This hydrogen can be produced via a range of methods including biomass and coal gasification, steam methane reforming, or electrolysis based on various sources of electricity. Each of these routes to hydrogen has very different economic and environmental characteristics. At present, electrolysis-based routes, which are arguably superior in terms of potentially abating CO_2 emissions, are energy intensive and face very high capital costs. The energy intensity results in higher non-climate-related environmental impacts. Additionally, from a life cycle perspective these processes use large quantities of grid electricity (e.g. in equipment and process manufacturing), which results in slightly higher-than-expected GHG emissions for the Chinese case study (with high coal fuel mix). The decarbonisation of grid electricity, for example via the incorporation of CCS with thermal generation or renewables, would enable further decarbonisation of these options. However currently, while electrolysis capital cost remains high and the relative benefit is modest, the main competitors for hydrogen production are coal/biomass gasification and steam methane reforming.

In China, where production of methanol is expected to continue to grow rapidly, coal-based processes are dominating due to the low cost of coal. The rapid investment in these processes within the last decade (and expected to continue at least until 2020), means that they are likely to be in place for a considerable length of time. This implies a technology lock-in effect, which proves to be extremely important for methanol in China. This is because if a global 2C-consistent CO_2 price were imposed on the industry, natural gas feedstock would become more economically attractive, but may struggle to enter the market because of the coal-based stock already in place. The sustainability credentials of methanol are much improved by a switch from coal to gas, but progress is likely to be slow as incumbent coal-based processes will prove difficult to dislodge.

7.2 Olefins

Olefins are a key intermediate to the production of a huge range of goods that underpin daily life and economic activity. Ethylene and propylene are used primarily to manufacture plastics, while butadiene is used to create a variety of rubbers. As manufacturing of such goods has moved from Europe and North America to East Asia, so has demand for olefins. The dynamics of this market are further complicated by natural gas liquid (NGL) production providing a cheap feedstock in some regions, e.g. in the USA associated with shale gas and in the Middle East. This cheap feedstock means the cracking of lighter hydrocarbons becomes more economically attractive. Similarly, due to the low cost and high availability of coal in China, a large increase in coal-to-olefin processes has occurred in the last decade.

While naphtha cracking has historically been the processes of choice for olefin production, as stated above both lighter NGLs and coal have gained market share more recently. Methanol-to-olefins (MTO) is the key alternative process investigated in this study, as it may benefit from a clean source of methanol with improved sustainability credentials. From an environmental perspective, coal-to-olefins exhibits significantly higher emissions across all categories. Biomass and wind-sourced MTO routes showed potential to decrease emissions, though the higher efficiency conventional cracking routes were also seen to be competitive when based on lighter NGLs.

When considered in the context of a case study for China, naphtha cracking complemented with coal-to-olefins was seen to be the incumbent technology. Where a carbon price was imposed, there was a shift towards cracking of lighter hydrocarbons, as opposed to the more environmentally-sustainable options of MTO based on biomass or wind power. This reflects the high costs of these relatively immature options. Additionally, the stakeholder interviews revealed the wide-spread view that crude oil demand reduction associated with transport fuels may lower feedstock costs and shift olefin production towards heavier hydrocarbons again in the medium-term future.

7.3 Ammonia

Ammonia demand is largely driven by fertiliser demand, which in turn is driven by demand for cereal crops. Natural gas is the key feedstock for ammonia production worldwide, driving production towards the cheapest source of that gas. At the same time, food security issues incentivise local fertiliser production, leading to a tension between these drivers. Increasingly, the cost of the primary feedstock is the key issue, leading to production at otherwise stranded sources of natural gas, or where there is cheap coal in the case of China.

This study investigated the conventional natural gas route, three electrolysis driven routes, and one relying on the gasification of biomass. Overall the biomass-based route was found to be the most environmentally attractive, followed by electrolysis based on wind power. However, the suitability of biomass as a resource for ammonia, or more broadly, petrochemical production was contested in the stakeholder interviews, given its limited resource, potential to compete in resource with food systems and potential better suitability for other applications such as energy. For ammonia in particular, the importance of considering a range of environmental metrics instead of only climate change related impacts is particularly apparent, where a natural gas-based process outperforms even a solar based process across many impact categories, though not global warming potential.

When considering the economics of the process options for China, as energy prices evolve from 2010 to 2050, production switches initially towards natural gas-based processes, and then towards biomass based processes. This trend was apparent even when no CO_2 price was imposed. Furthermore, the addition of a CO_2 price did not change this trend. No electrolysis-based routes were selected in the financial modelling, reflecting the high prices of these relatively immature technologies.

7.4 Decarbonisation options

First and foremost, the use of coal-based feedstocks typically has the highest environmental impacts for all petrochemicals studied, in particular with respect to global warming potential: all other options for feedstocks and processes perform significantly better with the exception of coal-based electrolysis routes.

There are many promising options for petrochemical production which may provide decarbonisation, including the use of bio-based or renewable feedstocks and the use of innovative catalytic processes. However, there is clearly no silver bullet and each option exhibits multiple disadvantages or barriers, relating to cost, resource availability or in the case of bio-based feedstocks, creating competition with other critical industries such as food.

Using hydrogen as a feedstock from a low carbon source may represent a good opportunity for decarbonisation via gasification of low carbon feedstocks or via electrolysis using low carbon electricity. However, currently these are not cost-effective. Additionally, while these technologies may help to meet climate change targets, other environmental impacts are significantly higher given high energy intensities of the process, as well as water usage, land-use change and metal resource depletions.

Bio-based feedstocks perform very well in the environmental assessment of this study, but is a highly contested approach from the stakeholder elicitations. There are many competing applications/industries for bio-based feedstocks and it is debatable which is most appropriate/efficient for a limited resource. Many bio-feedstocks are not molecularly similar to petrochemical products, resulting in high energy intensity and consequently high cost/low efficiency. Competition with the energy sector for bio-feedstocks currently favours the energy sector, whilst competition for bio-feedstocks with food systems should be avoided to prevent adverse impacts in areas with high levels of poverty. With a projected increase in bio-based feedstocks for industry and energy, water impacts, land use changes and other environmental impacts may be significant and must be managed carefully in order to prevent shifting from one environmental impact to another.

A unique challenge to the petrochemical industry is the need to decarbonise heat. It is an energy intensive industry, but whilst there are many options for low carbon electricity, low carbon heat is difficult to achieve. For example, electrification of heat is relatively inefficient and also places additional strain on electricity grids. Additionally, the use of renewable energy sources will increase the demand on rare metals, which adds another environmental burden to the decarbonisation routes.

The implementation of carbon capture and storage (CCS) or utilisation (CCU) has some potential for the petrochemical commodities and clearly CCS with thermal power generation plants would greatly assist in lowering the emissions associated with electricity usage, but great care must be taken to account for the life cycle of any products produced here.

- Carbon dioxide may be utilised as a feedstock for methanol production. However, there are many end-uses for methanol and the carbon that forms methanol is likely to be released eventually as CO_2 after end-use. Consequently, it is vital that this is accounted for and is not just assumed to be stored indefinitely.
- CCS may also be used as part of the syngas production to make ammonia. However, most ammonia is used to produce urea which uses carbon dioxide and is again released at end-use phase, limited potential for emission avoidance.
- Depending on waste management option, the production of olefins may be a promising route for utilisation of CO_2, via methanol to olefins. However, the end-of-life of the plastic produced must be managed effectively to ensure emissions are minimised.

7.5 How to decarbonise: Technology and policy

The petrochemical industry may remain more dependent on fossil fuels than the energy sectors, given the high efficiencies in using fossil feedstocks and requirement for high-grade heat. However, a decarbonised energy sector, in particular in the provision of electricity and heat, would naturally help to decarbonise the industry. Whilst there has been continual effort to lower environmental impacts through improved efficiencies of petrochemical production, deep decarbonisation requires strong policy and regulatory frameworks to be realised.

Petrochemical production based on low carbon routes such as electrolysis face significant economic barriers. Thus they do not appear in the modelled sustainable petrochemical pathways for China produced herein. A CO_2 price does not promote electrolysis options even when they are supplied by renewable energy as they show marginal improvements in greenhouse gas performance on a life cycle basis. This outcome may change under alternative scenarios however: for example a decarbonised electricity grid would result in better performance of all electrolysis options (including solar and wind electrolyser). Additionally, the outcome might be altered if better information were available on how the cost of electrolysers may change if the technology is scaled up.

Carbon pricing is likely to lead to increased gas use in petrochemicals in China, for example for methanol and ammonia production. For ammonia production, biomass-based routes also were seen to be competitive in the longer term.

The most popular policy options amongst the stakeholders interviewed were carbon prices and emissions performance standards. However, the global nature of trade for petrochemicals necessitates the application of global policies or regulation. High levels of international trade creates the potential for 'carbon leakage', where regional carbon pricing may create incentives to import rather than produce products sustainably. National emissions performance standards may also be effective and stakeholder views suggest that non-technology-specific regulations are most appealing to industry. However again much care must be taken to avoid the significant potential of carbon leakage, for example via border tariffs. Additionally, the need for a level playing field was highlighted particularly by industrial stakeholders.

Technology lock-in from investments in coal-based petrochemical production are a significant barrier to improving sustainability in China. In the short to medium-term capacity investments in methanol and ammonia petrochemical production in China are focused on coal as a feedstock. The resulting plant has a lifetime of at least 25 years and probably closer to 40 years, meaning that very significant amounts of this capacity will still be present in the Chinese petrochemical production matrix towards 2050. Therefore, even under the influence of a 2C-consistent CO_2 price, the environmental sustainability of these petrochemicals over the first half of this century looks challenging.

In summary, there exists a great challenge with respect to decarbonisation of petrochemicals with high regional variability in costs, feedstocks and processes, contributing to strong global trade. With ever-increasing demand, the implementation of emissions policy is vital to meet climate targets, but must be implemented with great care to avoid creating market perversions and replacing one environmental impact (e.g. climate change) with another.

7.6 Recommendations for further work

There exists great challenges to decarbonise the petrochemical industry under changing demand and meeting cost expectations. The enabling of low carbon routes must be realised by a combination of improved efficiencies and closing the gap in costs between these and the mature fossil fuel options. Improved efficiencies may be achieved by

- Process innovation, e.g. through catalysis
- Identification of suitable bio-based feedstocks which require lower energy intensity for conversion
- A low-environmental-and-economic impact source of hydrogen

There is a need to identify how much emissions may be minimised by for each petrochemical, in order to assess potential decarbonisation targets. This study estimated environmental impacts based on a case study region of China, which has high carbon intensity of electricity, as well as other infrastructural resources. Consequently, the routes may exhibit significantly lower emissions if the case study region were different (i.e. where low carbon electricity and/or heat were available). An identification of a 'best case scenario' with respect to emissions may help to drive targets and further research to improve the sustainability of the industry.

In relation to improvements of the methodology tested in this report, a number of recommendations are made here. Given the broad range of assessments included in this study, a deeper and more insightful analysis would be achieved if the focus was on a smaller set of products, e.g. olefins or methanol. This would enable more time to synthesise and compare results with other studies. A revised scope of assessments may include

- Techno-economic, LCA and social impact characterisation of process options, feedstocks and decarbonisation methods.
- Comparative analysis between process routes across a chosen sub-set of the UN Sustainable Development Goals.
- A larger set of stakeholder interviews to strengthen and elicit the key challenges associated with the future petrochemical industry. Allow time to iterate and incorporate the findings of the expert elicitations into the other sections of analysis
- Identify key opportunities and barriers to petrochemical industrial development with respect to processes, feedstocks and policies.

Finally, this study has taken the view that social benefit can be maximised by minimising the cost of petrochemical production (after emissions costs are internalised), but future studies would benefit from a more nuanced and disaggregated view on social sustainability, including quantitative and qualitative measures of the social aspects of sustainability.

Appendix

The appendix of this report is structured in the same sections as the main body of the report, namely: market assessment; process engineering characterisation; environmental assessment; and petrochemical pathways.

A1 Market assessment

A1.1 Demand projections

The following figures show the demand per capita of butadiene, ethylene, methanol, propylene and ammonia as a function of the GDP per capita (total demand and total GDP have been employed for the regression of ammonia).

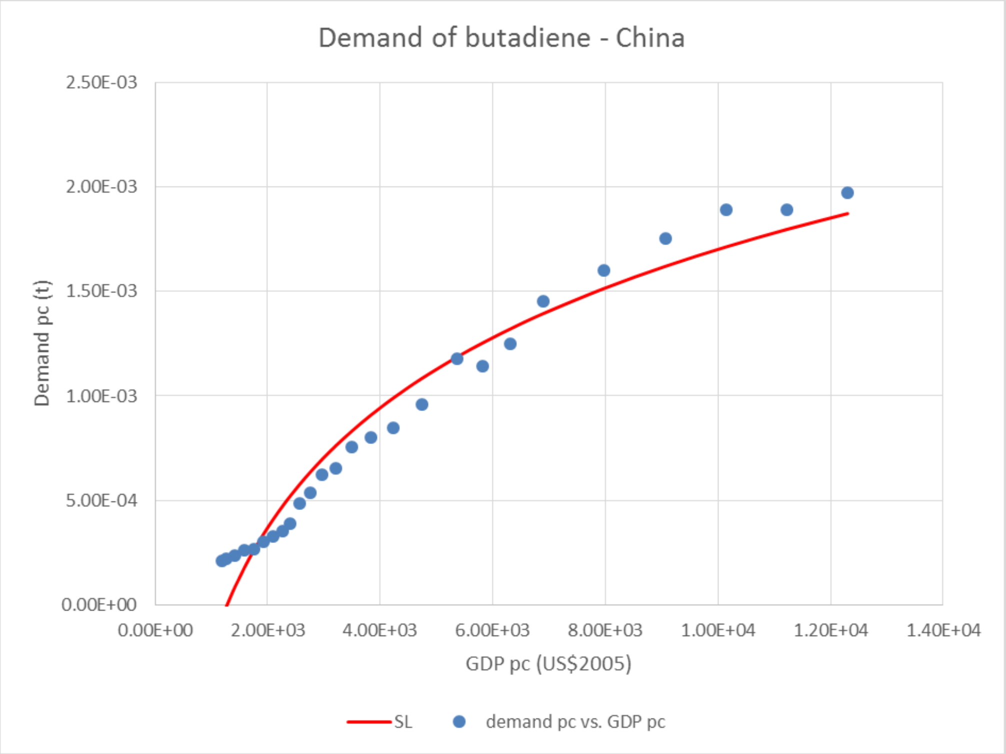

Figure A62 Demand per capita (t) of butadiene against GDP per capita (US$ 2005) – China

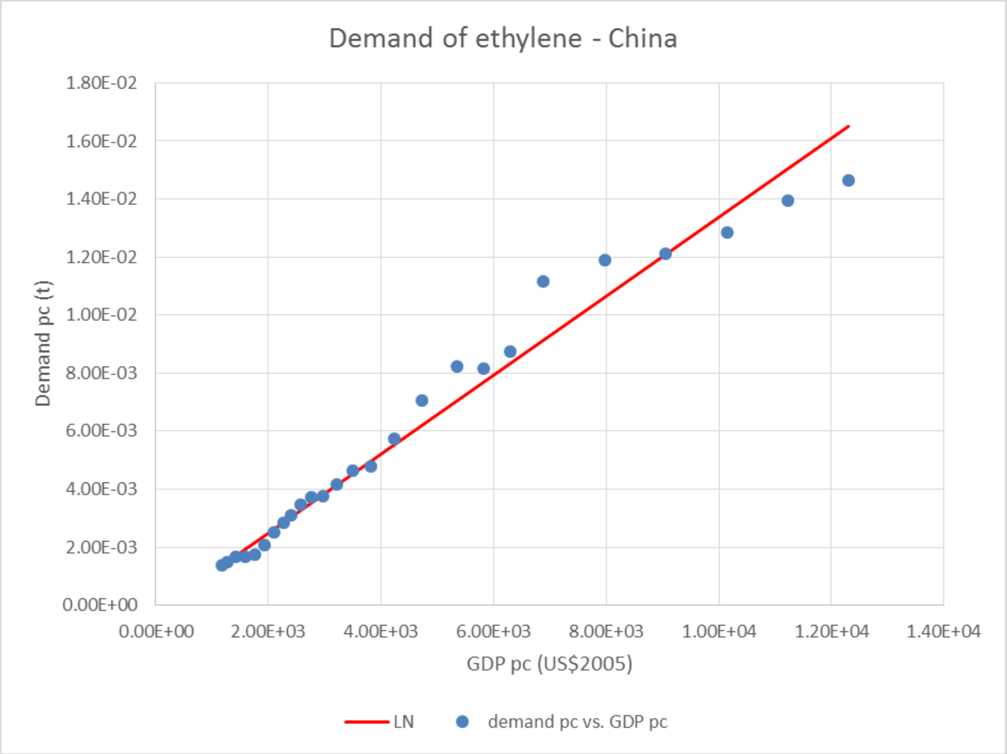

Figure A63 Demand per capita (t) of ethylene against GDP per capita (US$ 2005) - China

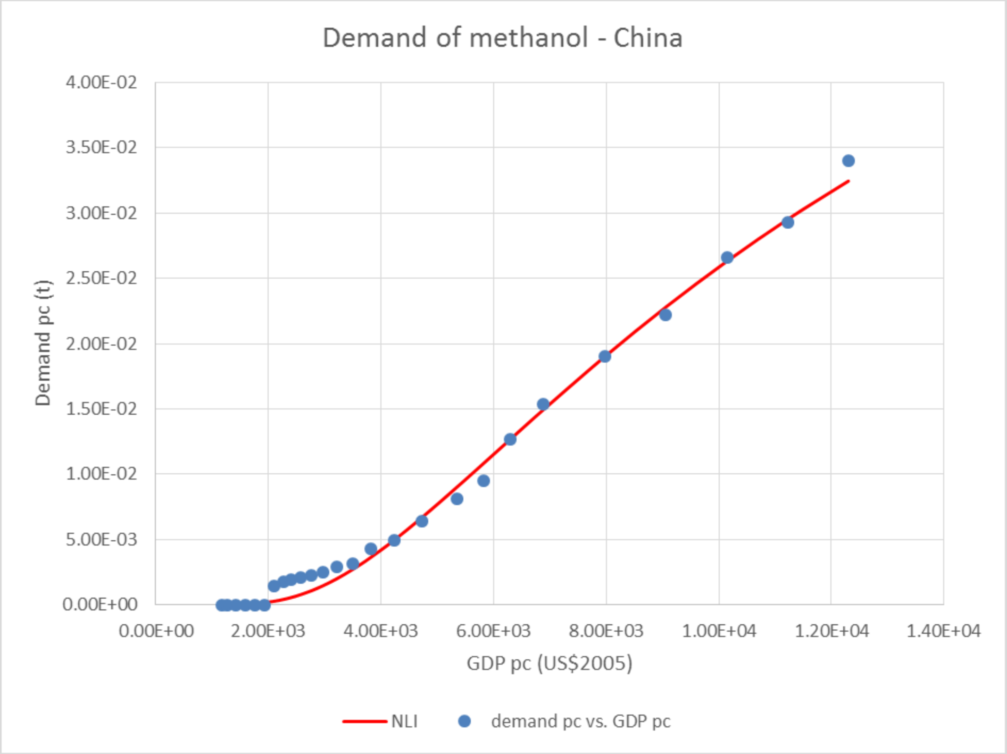

Figure A64 Demand per capita (t) of methanol against GDP per capita (US$ 2005) – China

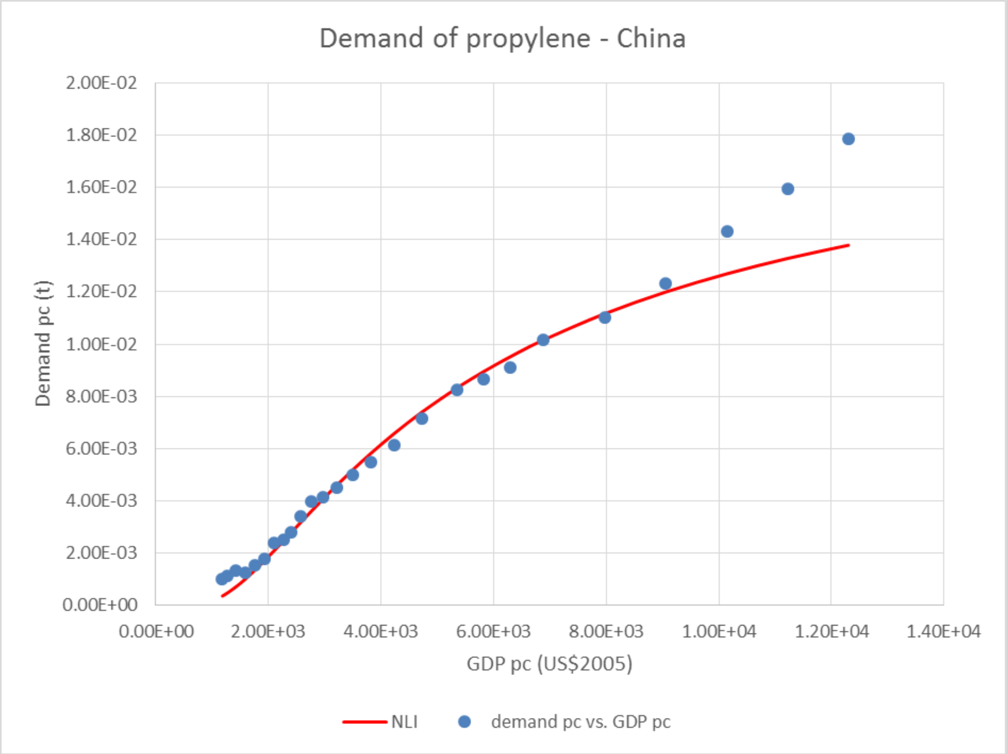

Figure A65 Demand per capita (t) of propylene against GDP per capita (US$ 2005) - China

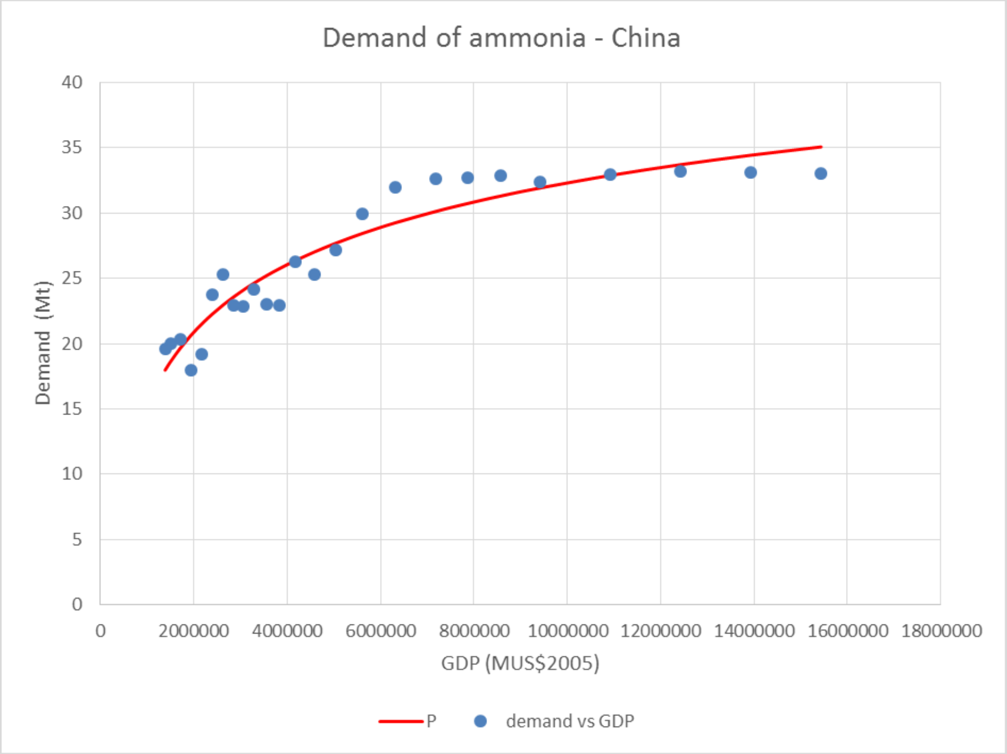

Figure A66 Demand (Mt) of ammonia against GDP (M US$ 2005) – China

A2 Process engineering characterisation additional information

A2.1 Conventional methanol synthesis

This process is assessed based on the following KPIs as given below. The primary differences between the processes is as follows:

- For Amirkhas, energy requirements are higher due to an extra reactor. The produced syngas is mixed with oxygen in an oxygen blown reformer. This process allows one to minimise carbon dioxide production and completely consume the methane. For Pérez-Fortes et al. only data regarding electricity consumption is available.
- For Pérez-Fortes et al., capital and operating cost are considerably higher due to the location of the plant. Raw material, product and electricity prices in EU are higher than in Saudi Arabia and Central America. Overall, raw material and utilities cost are strongly influenced by region.

Key Performance Indicator	Pellegrini et al.[57]	Pérez-Fortes et al.[58]	Amirkhas[59]
Scale	1,700,000 t/y	440,000 t/y	1,790,600 t/y
Energy requirements	-	-	-
Heat duty	2.89 GJ/t_{MeOH}	-	7.55 GJ/ t_{MeOH}
Cooling duty	-	-	-
Electricity duty	2.55 GJ/ t_{MeOH}	0.53 GJ/ t_{MeOH}	0.38 GJ/ t_{MeOH}
Input of other raw materials	0.612 t_{CH4}/ t_{MeOH}	0.64 t_{CH4}/ t_{MeOH}	0.019 t_{CH4}/ t_{MeOH}
	0.69 t_{H2O}/ t_{MeOH}	90 t_{H2O}/ t_{MeOH}	0.423 t_{O2}/ t_{MeOH}
Capital costs	382 €/ t_{MeOH}	845 €/ t_{MeOH}	395 €/ t_{MeOH}
Operating costs	38 €/ t_{MeOH}	400 €/ t_{MeOH}	210 €/ t_{MeOH}
Catalyst	Cu-containing catalyst	Cu/ZnO/Al_2O_3	-
Raw material and utilities cost			
Methanol (€/ t)	175	400	275
Methane (€/ t)	30	53	74
Electricity (€/ MWh)	26	85.6	36
Oxygen (€/ t)	-	-	51
Cooling Water (€/ t)	0.27	0.3	0.17
Plant location and prices	Saudi Arabia	Europe	Trinidad & Tobago

Table A12 KPIs for the conventional methanol process

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[57] L.A. Pellegrini, G. Soave, S. Gamba & S. Langè (2011). Economic analysis of a combined energy–methanol production plant. *Applied energy* 88.12: 4891-4897.

[58] M. Pérez-Fortes, J. C. Schöneberger, A. Boulamanti &E. Tzimas (2016). Methanol synthesis using captured CO 2 as raw material: techno-economic and environmental assessment. .*Applied Energy* 161 (2016): 718-732.

[59] E. Amirkhas, R. Bedi, S. Harley & T. Lango (2006). Methanol production in Trinidad & Tobago. *University of California, Davis* (2006). www.rajwantbedi.com/dg1_final.pdf.

A2.2 Alternative methanol synthesis

A detailed mass and energy balance are presented in the following table:

Stream	Phase	Mass flowrate (t/yr)	Composition (% molar)					Temp. (°C)	Pressure (bar)
			CO2	H2O	H2	CH4O	CO		
CO_2	Liquid	1,480,000	1	0	0	0	0	10	60
H_2	Gas	201,912	0	0	1	0	0	85	30
S1	Gas	6,176,000	0.13	0	0.78	0	0.09	26.85	72
S2	Gas	686,056	0.13	0	0.78	0	0.09	26.85	72
S3	Mixed	992,000	0.15	0.5	0	0.34	0.01	25.6	10
S4	Mixed	992,000	0.15	0.5	0	0.34	0.01	16.42	1.2
S5	Gas	1,544,000	0.25	0	0.75	0	0	-48.12	30
S6	Gas	7,856,000	0.13	0.02	0.75	0.02	0.08	231.19	46.75
S7	Gas	7,856,000	0.15	0	0.78	0	0.07	210	75
S8	Gas	220,500.6	0.88	0	0.03	0.04	0.05	16.85	1.22
S9	Liquid	775,299.8	0.02	0.58	0	0.4	0	16.85	1.22
S10	Mixed	775,299.8	0.02	0.58	0	0.4	0	80	1.1
S11	Gas	524,335.1	0.03	0.27	0	0.7	0	78.69	1
S12	Liquid	251,684.6	0	1	0	0	0	99.65	1
S13	Mixed	7,856,000	0.13	0.03	0.75	0.02	0.07	35	73.4
S14	Vapour	6,864,000	0.13	0	0.79	0	0.08	26.85	72
S15	Liquid	992,000	0.14	0.5	0.01	0.34	0.01	26.85	72
S16	Vapour	6,176,000	0.13	0	0.79	0	0.08	36.29	78
S17	Vapour	7,856,000	0.15	0	0.78	0	0.07	20.85	30
S18	Vapour	523,615.1	0.03	0.27	0	0.7	0	95.69	1.2
S19	Mixed	523,615.1	0.03	0.27	0	0.7	0	40	1
S20	Vapour	28,333.21	0.73	0.02	0	0.25	0	40	1
MeOH	Liquid	495,281.9	0.01	0.28	0	0.71	0	40	1

Table A13 Breakdown of the methanol PFD

This process is assessed based on the following KPIs as given below. In this comparison, hydrogen is purchased from a hypothetical renewable hydrogen supplier, thus cost related to alkaline water electrolysis are not considered.

The first case considered (A), utilises purchased H_2 from a hypothetical renewable hydrogen supplier. The operating cost of the plant are compared with an option which utilises (B) hydrogen from conventional sources (steam methane reforming and coal gasification). In the last case (C), renewable hydrogen is produced through alkaline water electrolysis, thus utilities, capital and operational cost for the added equipment are included in the evaluation.

a. Purchased renewable hydrogen (not produced)

Key Performance Indicator	ACUTEC project[94]	Pérez-Fortes Mar et al.[Error! Bookmark not defined.]
Scale	400,000 t/yr	440,000 t/yr
Whole Process CO_2 efficiency	99.60%	93.90%
Total energy requirements	2.5 GJ/$t_{methanol}$	5.3 GJ/$t_{methanol}$
Heat duty	1.00 GJ/$t_{methanol}$	1.6 GJ/$t_{methanol}$
Cooling duty	1.45 GJ/$t_{methanol}$	3.1 GJ/$t_{methanol}$
Electricity duty	0.05	0.6 GJ/$t_{methanol}$
Avoided CO_2 emissions	4.52-4.98 $t_{CO2}/t_{methanol}$	-
Amount of utilised CO_2	3.98 $t_{CO2}/t_{methanol}$	1.460 $t_{CO2}/t_{methanol}$
Input of other raw materials	0.5 $t_{H2}/t_{methanol}$	0.2 $t_{H2}/t_{methanol}$
Quantity of by-products	2.18×10^{-4} $t_{H2O}/t_{methanol}$ 3.34×10^{-6} $t_{CO}/t_{methanol}$	0.569 $t_{H2O}/t_{methanol}$ -
Capital costs & operating costs	500 €/$t_{methanol}$ 755 €/$t_{methanol}$	451 €/$t_{methanol}$ 665 €/$t_{methanol}$
Levelised production cost	3015 €/$t_{methanol}$	-
TRL (CCU vs. conventional)	5-6 vs. 9	5-6 vs. 9
Risk - impurities in inlet	High	High
Catalyst	$Cu/ZnO/Al_2O_3$	$Cu/ZnO/Al_2O_3$
Catalyst loading per product yield	9.2×10^{-5} $t_{cat}/t_{methanol}$	1.01×10^{-4} $t_{cat}/t_{methanol}$
Raw material and utilities		
hydrogen (€/t)	1,934.00	3,090
carbon dioxide	0	0
methanol (€/t)	350	400
cooling water (€/t)	-	0.03
electricity (€/MWh)	-	104.6
catalyst (€/t)	93,350.00	95,240

Table A14 KPIs for methanol process

b. Comparison between conventional and renewable hydrogen

In the case of hydrogen purchase, instead of production, different sources can be considered. Conventional hydrogen is produced through methane steam reforming or coal gasification; renewable hydrogen can be produced through a wide range of technologies. From these, alkaline water electrolysis has the highest TRL. Different sources for the raw material, and thus different prices, only influence operational cost. In the following table, operational cost and unit cost for hydrogen are compared with the industrial benchmark methanol production.

	Conventional methanol	Conventional H_2		Renewable H_2		
Hydrogen source	SMR	SMR	Coal Gasification	Alkaline water electrolysis		
Source	Pérez-Fortes et al.Error! Bookmark not defined.	DOE[60]	DOEError! Bookmark not defined.	Pérez-Fortes et al. Error! Bookmark not defined.	DOEError! Bookmark not defined.	ACUTEC project
Scale (t/yr)	440,000	440,000	440,000	440,000	440,000	400,000
OPEX (M€/yr)	401	473	276	668	795	1882
Hydrogen cost (€/t)	2100	2100	1100	3090	3500	

Table A15 Operational cost & H_2 cost for different hydrogen sources and comparison with industrial benchmark methanol production

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[60] Department of Energy, The H2A Central Production Model 3.0. Results are documented in the Current and Future H2A v3 case studies for Central Hydrogen Production from Grid Electrolysis which can be found at http://www.hydrogen.energy.gov/h2a_prod_studies.html.

c. Renewable hydrogen production through alkaline water electrolysis

Key Performance Indicator	ACUTEC project	A)	B)	C)	D)
Scale (t/yr)	400,000	122,760	58,740	66,330	57,750
Whole Process CO_2 efficiency	99.60%	81.6%	81.4%	88.3%	100%
Total energy requirements (GJ/$t_{methanol}$)	43	50.95	52.26	48.21	51.68
Heat duty	1.00	18.77	18.69	18.74	18.76
Cooling duty	1.45	-	-	-	-
Electricity duty	40.55$^{\text{Error! Bookmark not defined.}}$	32.18	33.57	29.47	32.91
Avoided CO_2 emissions (t_{CO2}/$t_{methanol}$)	4.52-4.98	-	-	-	-
Amount of utilised CO_2 (t_{CO2}/$t_{methanol}$)	3.98	1.39	2.90	2.57	2.95
Input of other raw materials					
H_2O (t_{H2O}/$t_{methanol}$)	-	1.70	1.71	1.72	1.72
H_2 (t_{H2}/$t_{methanol}$)	0.5	-	-	-	-
Quantity of by-products					
H_2O (t_{H2O}/$t_{methanol}$)	2.18×10^{-4}	0.57	0.57	0.57	0.57
CO (t_{CO}/$t_{methanol}$)	3.34×10^{-6}	-	-	-	-
H_2 (t_{H2}/$t_{methanol}$)		1.49	1.50	1.50	1.51
Capital costs & operating costs	1742 1892	2559 292	1730 286	3078 252	3241 260
Levelised production cost	3015 €/$t_{methanol}$	-	-	-	-
TRL (CCU vs. conventional)	5-6 vs. 9	5-6 vs. 9	5-6 vs. 9	5-6 vs. 9	5-6 vs. 9
Risk - impurities in inlet	High	High	High	High	High
Catalyst	$Cu/ZnO/Al_2O_3$	$Cu/ZnO/Al_2O_3$			
Catalyst loading per product yield (t_{cat}/$t_{methanol}$)	9.2×10^{-5}	1.14×10^{-4}	2.38×10^{-4}	2.11×10^{-4}	2.42×10^{-4}
Raw material and utilities cost					
water (€/t)	4	-	-	-	-
carbon dioxide (€/t)	0	42.00	20.00	22.63	19.67
methanol (€/t)	350	821.64	600.77	858.30	932.96
catalyst (€/t)	93,350	-	-	-	-
electricity (€/MWh)	-	off-peak renewable: 26.24 (500 MW, for 5h), 1.75 (100 MW, for 12 h); fossil: 64.47			
Location	EU	U.K.			

Table A16 KPIs for MeOH process, data from the ACUTEC and Mignard et al. (A-D)

From this table, it is apparent that the key differences between A) to D) are:

- Option A, use of conventional electrolysis, with variable amounts of electricity available during off-peak time (base case).
- Option B, as in A, but with a constant supply of electricity during off-peak period.

- Option C, as in B, with the use of pressurised electrolysis to save energy.
- Option D, as in B, but with the use of a fuel cell plant to reduce electricity of fossil origin.

And key differences between Mignard et al. and the ACUTEC project:

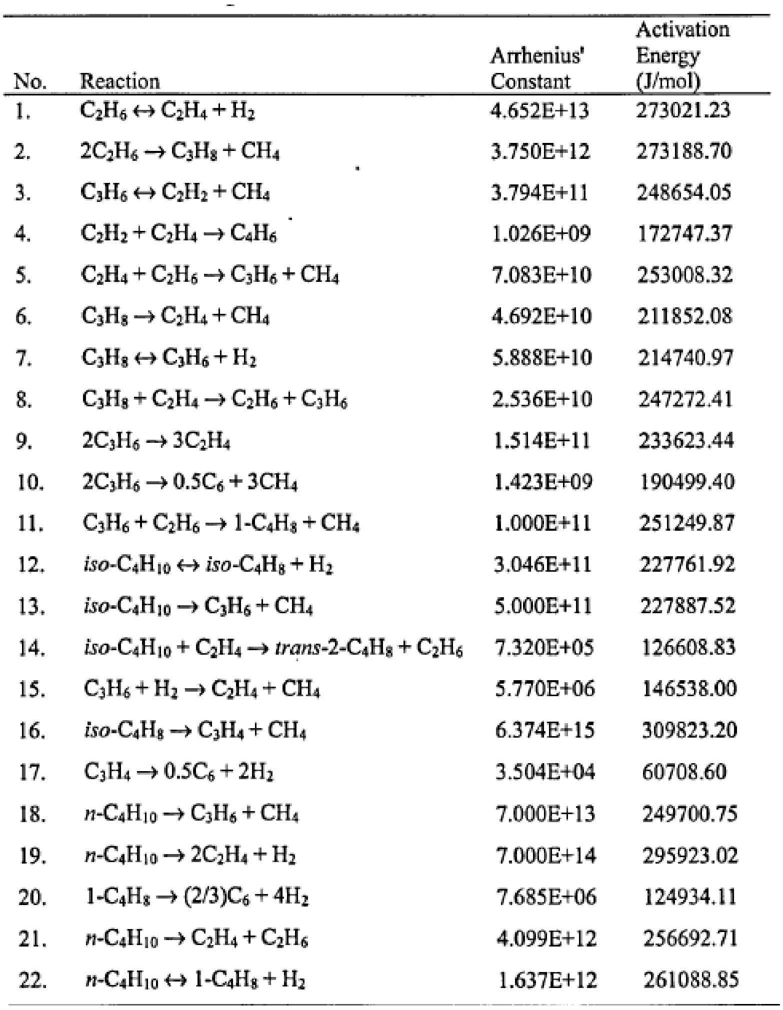
- For Mignard et al. utilities, capital and operational cost for the carbon dioxide separation are considered. CAPEX for carbon dioxide recovery is 6-12% of the total. In the ACUTEC project, CO_2 separation costs are not included.
- In the ACUTEC project, utilities for the electrolyser and carbon dioxide compression are taken from Van-Dal et al.[61] (on which the project was based), because not available elsewhere.
- For Mignard et al. the cost of CO_2 is based on total production cost. For the ACUTEC project, carbon dioxide is free.
- In the ACUTEC project, the methanol price is based on the market. For Mignard et al. the minimum selling price to set NPV to zero over a 15 year period (with a minimum accepted rate of return MARR) on initial investment of 10% was considered.

A2.3 Ethane and propane cracking

Typical reactions (Froment, 1992) in the reactor are listed below. Note that the actual reactions taking place depend on the particular hydrocarbons in the feedstock (e.g. ethane, propane, butane and their relative proportions).

---

[61] É. Simões, V. Dal & C. Bouallou (2013). Design and simulation of a methanol production plant from CO2 hydrogenation. Journal of Cleaner Production, 57, 38-45, https://doi.org/10.1016/j.jclepro.2013.06.008.



No.	Reaction	Arrhenius' Constant	Activation Energy (J/mol)
1.	$C_2H_6 \leftrightarrow C_2H_4 + H_2$	4.652E+13	273021.23
2.	$2C_2H_6 \rightarrow C_3H_8 + CH_4$	3.750E+12	273188.70
3.	$C_3H_6 \leftrightarrow C_2H_2 + CH_4$	3.794E+11	248654.05
4.	$C_2H_2 + C_2H_4 \rightarrow C_4H_6$	1.026E+09	172747.37
5.	$C_2H_4 + C_2H_6 \rightarrow C_3H_6 + CH_4$	7.083E+10	253008.32
6.	$C_3H_8 \rightarrow C_2H_4 + CH_4$	4.692E+10	211852.08
7.	$C_3H_8 \leftrightarrow C_3H_6 + H_2$	5.888E+10	214740.97
8.	$C_3H_8 + C_2H_4 \rightarrow C_2H_6 + C_3H_6$	2.536E+10	247272.41
9.	$2C_3H_6 \rightarrow 3C_2H_4$	1.514E+11	233623.44
10.	$2C_3H_6 \rightarrow 0.5C_6 + 3CH_4$	1.423E+09	190499.40
11.	$C_3H_6 + C_2H_6 \rightarrow 1\text{-}C_4H_8 + CH_4$	1.000E+11	251249.87
12.	$iso\text{-}C_4H_{10} \leftrightarrow iso\text{-}C_4H_8 + H_2$	3.046E+11	227761.92
13.	$iso\text{-}C_4H_{10} \rightarrow C_3H_6 + CH_4$	5.000E+11	227887.52
14.	$iso\text{-}C_4H_{10} + C_2H_4 \rightarrow trans\text{-}2\text{-}C_4H_8 + C_2H_6$	7.320E+05	126608.83
15.	$C_3H_6 + H_2 \rightarrow C_2H_4 + CH_4$	5.770E+06	146538.00
16.	$iso\text{-}C_4H_8 \rightarrow C_3H_4 + CH_4$	6.374E+15	309823.20
17.	$C_3H_4 \rightarrow 0.5C_6 + 2H_2$	3.504E+04	60708.60
18.	$n\text{-}C_4H_{10} \rightarrow C_3H_6 + CH_4$	7.000E+13	249700.75
19.	$n\text{-}C_4H_{10} \rightarrow 2C_2H_4 + H_2$	7.000E+14	295923.02
20.	$1\text{-}C_4H_8 \rightarrow (2/3)C_6 + 4H_2$	7.685E+06	124934.11
21.	$n\text{-}C_4H_{10} \rightarrow C_2H_4 + C_2H_6$	4.099E+12	256692.71
22.	$n\text{-}C_4H_{10} \leftrightarrow 1\text{-}C_4H_8 + H_2$	1.637E+12	261088.85

Table A17 Typical reactions

For the purposes of this study, it is important to capture the key material and energy inputs to produce a particular product slate; these will then be used to develop a baseline life cycle analysis.

Material and energy balances

A number of different data sets are compared to generate the input and output data for the processes. The following base case data are from a PhD thesis at Imperial College (2009)[62]. This used a base case with the key variables as follows.

---

[62] K.Y. Cheung. (2009). Site-wide and supply chain optimisation for continuous chemical processes. PhD Thesis, Imperial College London .

Variable name	Value
Ethane feed flowrate (kg/s)	15.76
Steam feed flowrate (kg/s)	8
Reactor heat flux (J/m2s)	40,000
Number of tubes	10
Tube length (m)	60
Tube diameter (m)	0.1
Ethylene production rate (kg/s)	8.98
C3+ flowrate (kg/s)	4.3
Demethaniser condenser duty (MW)	9.1
Demethaniser reboiler duty (MW)	5.5
Deethaniser condenser duty (MW)	3.1
Deethaniser reboiler duty (MW)	2.9
C2 splitter condenser duty (MW)	8.0
C2 splitter reboiler duty (MW)	6.2

Table A18 Data set 1 material and energy balances

These data are combined with data set 2 below to generate estimates of the material and energy inputs required to produce a unit of olefin product (or process a unit amount of feedstock). The cryogenic cooling duties are converted to power requirements using coefficients of performance. This provides useful information on the range of potential compositions exiting the furnace reactor.

Component	Mole fraction (base case)	Mole fraction (optimised case)
H_2	0.3030	0.2821
CH_4	0.2125	0.1865
C_2H_4	0.3339	0.3117
C_2H_6	0.0733	0.1224
C_3H_6	0.0329	0.0482
C_3H_8	0.0091	0.0222

Table A19 Data set 2, reactor output compositions, sourced from the thesis of M. Yan (2000)[63]

Data set 3, presented below, is sourced from the thesis of Borralho (IST, 2013)[64], provides data on a process primarily fed with propane rather than ethane. It also provides useful energy consumption data. The furnace reactor input and outputs are detailed in the table below.

Component	Inlet mass composition (%)	Outlet mass composition (%)
CH_4	0	16.7
C_2H_6	2.6	2.5
C_2H_4	0	29.0
C_2H_2	0	0.3
C_3H_8	74.9	8.3
C_3H_6	0	11.7
1-C_4H_8	0	0.3
1-3-C_4H_6	0	2.1
H_2	0	1.5
C_6H_6	0	5.2
H_2O	22.5	22.5

Table A20 Furnace reactor input and outputs, d*ata set 3 from modelling of an ethylene plant*

For an 850 ktpa process (ethylene basis), it is possible to determine compressor train duties following quenching of 40 MW, and refrigeration cycle duties of 31 MW.

Data set 4 draws on the work of Ghanta et al. (2014)[65], and provides an overall comparison of energy and material requirements. The key performance measures they derive are an overall yield of ethane to ethylene of 56.4%, fuel requirements of 13.7 MJ/kg ethylene, and power requirements of 0.2 MJ/kg ethylene.

Data Set 5 is sourced from the work of Patel (2003)[66], provides further energy and material balance data. Particularly pertinent are the yield and energy consumption data below.

---

[63] M. Yan (2000). Simulation and optimization of an ethylene plant. MS Thesis, Texas Tech University, USA.

[64] F.J.O. Borralho (2013). ‚Detailed Modelling and Optimisation of an Ethylene Plant. IST Lisbon, Portugal.

[65] M. Ghanta, D. Fahey & B. Subramaniam (2014). Environmental, “Environmental impacts of ethylene production from diverse feedstocks and energy sources.”, Appl Petrochem Res, 4:167–179.

[66] M. Patel (2003). Cumulative energy demand (CED) and cumulative CO_2 emissions for products of the organic chemical industry. Energy 28, 721–740.

Component	Yields (kg product/t feedstock		
	Naptha feed	Gas oil feed	Light hydrocarbon feed
Ethylene	299	252	568
Propylene	174	157	106
C4 products	106	108	58
Fuel oil	36	150	5
Pyrolysis gasoline and aromatics	237	219	55
Methane	130	101	177
Hydrogen and losses	18	13	31

Table A21 Data set 5 yield data

Reference		Process energy (GJ/t reference)		
		Naptha feed	Gas oil feed	Light hydrocarbon feed
1 t feed	Fuels	6.0	6.9	7.8
	Power	0.1	0.1	0.1
1 t Ethylene	Fuels	20.1	27.4	13.7
	Power	0.3	0.4	0.2

Table A22 Data set 5 energy consumption data

Data set 6 below shows benchmark data from operating units in Iran from S. Gowharifar et al. (2013)[67]. This provides operational data for a range of plants, including the yield and energy data below.

	Bandar Imam (BIPC) Olefins	Tabriz Olefins
Plant feed rate	108.7 t/hr	42.8 t/hr
Ethylene production	52.7 t/hr	15.7 t/hr
Propylene production	16.7 t/hr	6.6 t/hr
Fuel consumption	1113 GJ/hr	416 GJ/hr
Steam consumption	608 GJ/hr	73 GJ/hr
Power consumption	66 GJ/hr	46 GJ/hr

Table A23 Data set 6 benchmark operating data

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[67] S. Gowharifar, B. Sepehrian, G. Nasiri, A. Khoshgard & M. Momenifar (2013). Benchmarking, Standard Setting and Energy Conservation of Olefin Plants in Iran. Proceedings of the 2013 International Conference on Environment, Energy, Ecosystems and Development.

Data set 7 was produced by Ren et al. (2008)[68] and compares the steam cracking and MTO processes. This estimates a range of 10-15 GJ/t ethylene of energy use for ethylene production and 9-14 GJ/t product when all high value products (olefins) are counted. A yield of 80% of ethylene and 84% of high value products is reported.

Data set 8 is a Technip data sheet[69] which shows improvement of power consumption over time to 550 kWh/t ethylene.

Taking the data sets presented above together, and applying basic process analysis methods to them, the following quantities are estimated.

Case 1 Ethane cracking				
Basis	**1**	**t**	**ethane input**	
Inputs	lower bound	upper bound	unit	
water	0.3	0.9	t	
fuel (natural gas)	6	9	GJ	
power	1.5	2.5	GJ	
outputs	lower bound	upper bound	unit	
olefins	0.75	0.85	t	
other non-fuel HC (balance)	0.1	0.06	t	(for allocation or system boundary expansion, one may assume energy based credit at 45 GJ/t)
Case 2 Propane cracking				
Basis	**1**	**t**	**propane input**	
Inputs	lower bound	upper bound	Unit	
water	0.3	0.9	T	
fuel (natural gas)	6	9	GJ	
power	1.5	2.5	GJ	
outputs	lower bound	upper bound	Unit	
olefins	0.6	0.72	T	
other non-fuel HC (balance)	0.15	0.1	T	(for allocation or system boundary expansion, one may assume energy based credit at 45 GJ/t)

---

[68] T. Ren, M.K. Patel & K. Blok (2008). Steam cracking and methane to olefins: Energy use, CO_2 emissions and production costs. Energy 33 (2008) 817–833.

[69] Technip (2013). Ethylene Production.

[69]http://www.technip.com/sites/default/files/technip/publications/attachments/Ethylene_September_2013_Web_0.pdf

Table A24 Overall balances for cracking processes

A2.4 Methanol-to-olefins process

Material and energy balances

A number of data sets were used, detailed as follows: Data set 1 from Ren et al. (2008)[68] provide data for the UOP and ExxonMobil processes as follows:

Performance measure	UOP Process	ExxonMobil Process
Ethylene yield (t/t MeOH)	0.18	0.10
Total high value chemicals yield (t/t MeOH)	0.43	0.42
Total energy requirement (GJ/t ethylene)	13	25

Table A25 Data set 1 UOP and ExxonMobil processes

Data set 2 from Jasper and El-Halwagi (2015)[70], provide an overall yield table for methanol to olefins (MTO) and methanol to propylene (MTP).

Process	Methanol in (ktpa)	Propylene out (ktpa)	Ethylene out (ktpa)	Gasoline out (ktpa)
MTO	1560	386	214	-
MTP	1825	568		157

Table A26 Data set 2 overall yield for MTO

Data set 3 is from Salkuyeh and Adams II (2015)[71] and provides outlet stream composition data from the MTO reactor following water and methanol removal.

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[70] S. Jasper & M.M. El-Halwagi (2015). A Techno-Economic Comparison between Two Methanol-to-Propylene Processes. Processes, 3, 684-698.

[71] Y. K. Salkuyeh & T.Thomas A. Adams II (2015). Co-Production of Olefins, Fuels, and Electricity from Conventional Pipeline Gas and Shale Gas with Near-ZeroCO2 Emissions. Part II: Economic Performance. Energies, 8, 3762-3774; doi:10.3390/en8053762.

Species	Mole Percent
H_2O	0.4%
H_2	6.8%
CO_2	3.0%
CH_4	1.2%
MeOH	0.0%
C_2H_4	38.7%
C_2H_6	0.7%
C_3H_6	37.6%
C_3H_8	0.4%
C_4H_8	9.7%
C_5H_{10}	1.5%
DGA	0.0%
Total	100.0%

Table A27 Data set 3 Outlet stream composition for MTO

Data set 4 is from Funk et al. (2013)[72] who provide a range of results for different process conditions which indicate light olefins carbon yields of 85+% and propylene/ethylene ratios of 1.2 to 1.8. Data set 5 is sourced from McGregor (2014)[73] and indicates a yield of 1 t of olefins for every 2.6 t of methanol feed. Data set 6 is from Tian et al. (2015)[74] who analyse data from a commercial unit in China which has a light olefins selectivity of 80% and a new process at demonstration scale which has a selectivity of 85.7%. Taking data sets 1 to 6 together, the following quantities may be derived.

Alternative MTO process (UOP)				
inputs	1	t	methanol	
	2.331034	GJ	heat	
	1.017241	GJ	power	
outputs				
	0.17931	t	ethylene	
	0.227586	t	propylene	
	0.02069	t	other HC	(for allocation or system boundary expansion, one may assume energy based credit at 45 GJ/t)
	0.406897	t	total olefins	

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[72] G.A. Funk, D. Myers & B. Vora (2014). A different game plan", Hydrocarbon Engineering, Dec 2013.

[73] McGregor, J, "Methanol to Olefins: A Pillar of Capacity Additions in China, but does MTO have a Role in India?", IOCL Conclave, February 7, 2014.

[74] P. Tian, Y. Wei, M. Ye & Z. Liu (2015)., Methanol to Olefins (MTO): From Fundamentals to Commercialization.", ACS Catal. 5, 1922−1938.

Table A28 MTO process (UOP) characteristics

Process economics

Capital costs

Steam cracking process

The capital costs have been collected from a range of references including Cutler (2013)[75]; Petrochemical Update (2016)[76], Chemical Engineering online (2015)[77] and Seddon (2015)[78]. They give rise to the figure below.

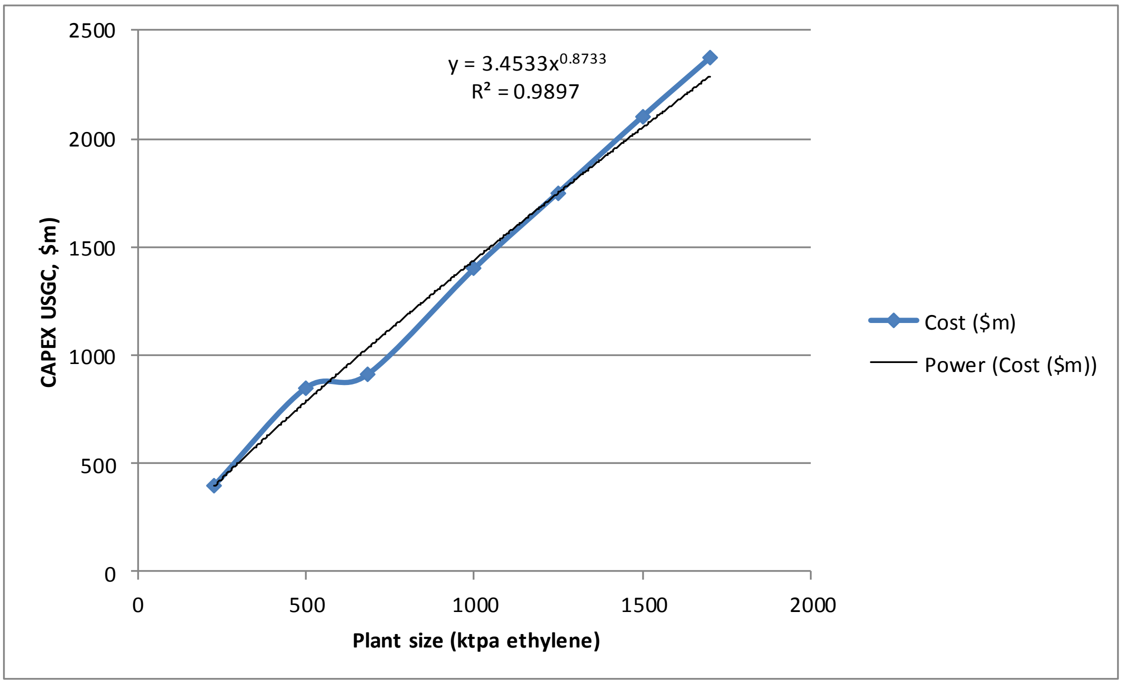

Figure A67 Capital cost regression for steam cracking process

This provides a correlation of Cost ($m) = 3.4533PC$^{0.8733}$ where PC is the plant capacity in ktpa. Using 1000 ktpa as our base case, we establish a capital cost of $1439m. Assuming an economic life of 25 years and a discount rate of 10%. This gives an equivalent annual capital cost of 158.6 m$, or a cost per tonne of ethylene of $158.6. For the fixed operating costs, in line with the recommendation of Sinnott (2005)[79], assume 10% of CAPEX.

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[75] J. Cutler (2013). Ethylene plants and shale gas: world scale vs regional sized ethylene plants. Penn State Shale Webinar, June, 2013.

[76] Petrochemical Update (2016). Infographic: US ethane cracker construction costs rise 1-2% year on year. April, 2016.

[77] Chemical Engineering online (2015). Ethylene production via cracking of ethane-propane. November, 2015.

[78] D. Seddon (2015). Chemical economics - cracking operations. January, 2015. www.duncanseddon.com/docs/pdf/steam-cracking-operations-forum-docs.pdf

[79] R.K. Sinnott (2005). Coulson & Richardson's Chemical Engineering, Volume 6, Fourth Edition, Chemical Engineering Design. Elsevier, Oxford, UK.

MTO process

For MTO, the price data is somewhat scarcer. Based on the data available from McGregor (2014)[80], IHS (2003)[81], Platts (2015)[82], and PWC (2012)[83], the figure below was derived.

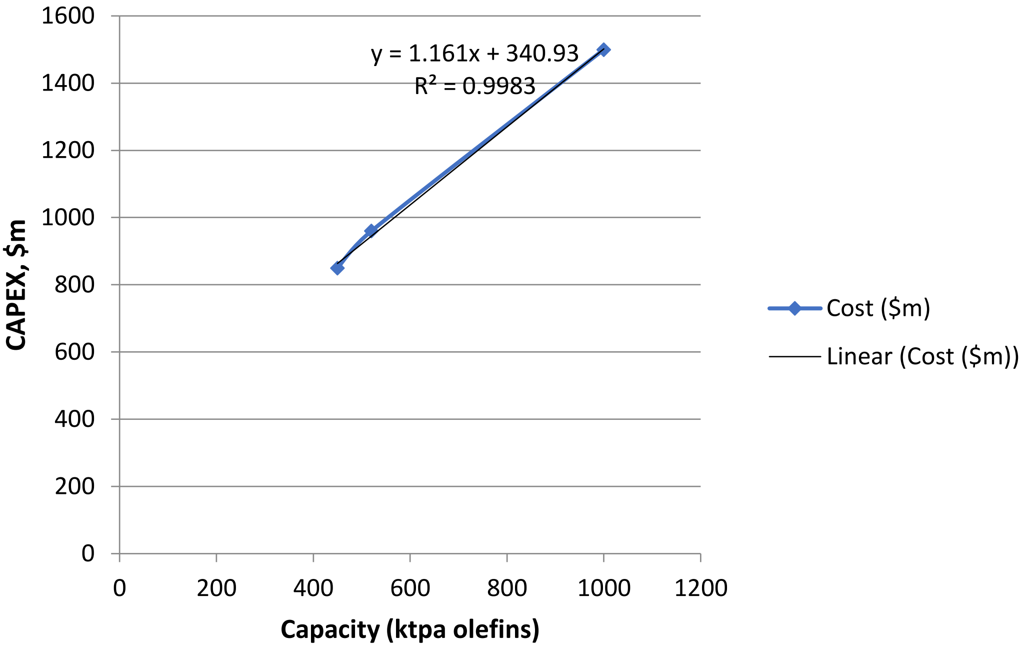

Figure A68 Capital cost regression for MTO process

This gives rise to the following equation for CAPEX y = = 1.161x + 340.93. For a 1000 ktpa olefins plant, a CAPEX of $1500m is expected. This is marginally higher than that steam cracker because of the front end. This translates to $165.3/t olefins.

Deployment

Steam cracking is a mature technology, with approximately 175 mtpa ethylene production and 125 mtpa propylene globally, and deployment dispersed globally. In contrast, MTO process technology is in its infancy, with significant deployments in China (as part of "coal-to-olefins", CTO) technology. There are approximately 20 projects underway or operating and around 8 mtpa capacity is available as of 2016 and 10 mtpa expected by the end of 2017[84]. Globally, around 3-4mtpa olefins

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[80] L. McGregor (2014).Methanol to Olefins: A Pillar of Capacity Additions in China, but does MTO have a Role in India? IOCL Conclave, February 7, 2014.

[81] HIS Markit, PEP Review 2001-11, UOP Methanol to Olefins, 2003.

[82] Platts (2015). China's olefins future shaped by economics and environmental concerns. February, 2015.s

[83] Booz & Company (2012).&, Future of chemicals VIII: Rebalancing global feedstock disruptions with "on-purpose" technologies. https://www.strategyand.pwc.com/media/file/Future-of-chemicals-VIII_Rebalancing-global-feedstock-disruptions-with-on-purpose-technologies.pdf.pdf

[84] M. Eramo (201). Global Ethylene Market Outlook: Low Cost Feedstocks Fuel The Next Wave Of Investments In North America and China. Chemical Insights IHS Chemical. Inaugural Ethylene Forum. Available: http://media.corporate-ir.net/media_files/IROL/11/110877/05_Global_Ethylene_Market_Outlook_Eramo.pdf.)

are produced by MTO processes with purchased methanol rather than CTO, which produces around 13 mtpa[85].

Renewable inputs

Both processes could in principle be driven by renewable energy inputs. Fuel gas for heat substituted by bio-methane or bio-SNG or renewable hydrogen and power provided by renewable sources. Methanol for the MTO process can be produced from:

- Renewable hydrogen and CO_2 from air capture
- Biomass or waste through gasification and methanol synthesis

Ethylene can also be produced by dehydration of bio-ethanol[86].

A2.5 Conventional ammonia process

Key performance indicator (KPI)

Key Performance Indicator	Bartels[87]	Appl M.[88] (SMR)	Appl M.Error! Bookmark not defined. (Coal)
Scale (t/yr)	726'000	600'000	600'000
Total energy requirements (GJ/t_{NH3})	39	28.5	48
Heat duty	-	27.1	-
Cooling duty	-	-	-
Electricity duty	-	1.4	-
Input of raw materials			
CH4 (t_{CH4}/t_{NH3})	1.00	1.00	2.78
Quantity of by-products			
CO2 (t_{CO2}/t_{NH3})	3.1	3.10	7.52
Capital costs & Operating costs (€/t_{NH4})	840.96 -	456.80 114.68	913.60 139.56
Raw material and utilities cost			
methane (€/t)	-	155.95	-
Coal (€/t)	-	-	45.645828
ammonia (€/t)	453.78	191.86	191.86
catalyst (€/t)	Variable	3.3 €/tNH3	-
electricity (€/MWh)	-	-	-

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[85] M. Alvarado (2016).The changing face of the global methanol industry. Insight IHS Chemical Bulletin, Issue 3. http://www.methanol.org/wp-content/uploads/2016/07/IHS-ChemicalBulletin-Issue3-Alvarado-Jun16.pdf

[86] IEA-ETSAP and IRENA (2013). Production of Bio-ethyleneTechnology Brief. https://www.irena.org/DocumentDownloads/Publications/IRENA-ETSAP%20Tech%20Brief%20I13%20Production_of_Bio-ethylene.pdf

[87] J.R. Bartels (2008). A feasibility study of implementing an Ammonia Economy. Graduate ThesisTheses and Dissertations. Paper 11132.

[88] M. Appl (1999). Ammonia principles and industrial practice. Weinheim,Wiley-VCH. ISBN 3-527-29593-3

Location	USA	Europe	Europe

Table A29 KPIs for the conventional ammonia process

The key differences between the projects outlined above are:

- Appl M. consider two different ways of producing hydrogen, through steam methane reforming (SMR) or through coal gasification.
- Capital cost and raw material cost differences are due to different publication year. Bartels utilise 2008 ammonia price, where Appl. uses values from 1998. Capital cost differences are due to different construction year and CAPEX evaluation methods.
- Values for electricity cost where not published on both papers.
- Mass balances were not published by Bartels, values are calculated from a reference publication by Ramezan and Stiegel[89].

Catalyst		
SMR	Desulphurisation (gas)	MoOx/CoOx
	Desulphurisation (solid)	ZnO
	Primary steam reformer	Ni-based
	Secondary steam reformer	Ni-based
	High temperature shift reaction	FeCr2O3
	Low temperature shift reaction	Cu/ZnO
Ammonia	Haber-Bosch synloop	FeOx-based

Table A30 Catalyst used for ammonia production

A2.6 Low carbon ammonia production

Key performance indicator (KPI)

The following key performance indicators are available for ammonia production.

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[89] G. Stiegel, J. Gary, & M.Ramezan (2006). Hydrogen from coal gasification: An economical pathway to a sustainable energy future. International Journal of Coal Geology 65.3 (2006): 173-190.

Key Performance Indicator	Matzen et al.[90]	Mueller-Langer et al[91]
Scale (t/yr)	400,833	400,833
Total energy requirements (GJ/t_{NH3})	55.70	43.28
Heat duty	43.94	9.10
Cooling duty	11.76	11.66
Electricity duty	-	22.52
Input of raw materials		
Air (t_{air}/t_{NH3})	1.09	1.09
from which N2 (t_{N2}/t_{NH3})	0.84	0.84
Water (t_{water}/t_{NH3})	1.63	1.63
from which H_2 (t_{H2}/t_{NH3})	0.18	0.18
Quantity of by-products		
O_2 (t_{O2}/t_{NH3})	1.70	1.70
Capital cost (€/t_{NH3})	435	1087 – 877 - 627
Operating cost (€/t_{NH3})	652	Variable, see **Error! Reference source not found.**
Raw material and utilities cost		
Catalyst type	FeOx-based	FeOx-based
ammonia (€/t)	528.40	528.40
water (€/t)	-	2.26
electricity (€/MWh)	58.50	Variable, see **Error! Reference source not found.**
Location	USA	EU

Table A31 KPIs for the sustainable ammonia process

Matzen et al. published a fully integrated ammonia synthesis production with ASU for the generation of nitrogen and wind powered alkaline water hydrolysis. Mueller-Langer et al. only worked on the hydrogen production with different sources of electricity, thus values for Haber-Bosch synloop and ASU are taken from Matzen et al. and updated with for energy prices.

The three different values of CAPEX in Mueller-Langer et al. are due to different evaluation of electrolyser cost. Since the published paper was working on a small-scale hydrogen production, in order to produce the needed amount of raw material for the production of ammonia, the electrolyser needed to be scaled accordingly. The first value corresponds to the CAPEX for small-scale electrolyser multiplied by the number of unit needed to produce the required amount of H_2. The second value is obtained with the following scaling law published by Mignard et al.**Error! Bookmark not defined.**; Dutton et al. and Wendt et al.: $C_{el} = 200P + 16000P^{0.60625}$ (C investment

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[90] M. Matzen, M. Alhajji, & Y. Demirel. (2015). Technoeconomics and sustainability of renewable methanol and ammonia productions using wind power-based hydrogen. *J Adv Chem Eng* 5.128 (2015): 2.

[91] F. Mueller-Langer, E. Tzimas, M. Kaltschmitt, & S. Peteves. (2007). Techno-economic assessment of hydrogen production processes for the hydrogen economy for the short and medium term. ."International Journal of Hydrogen Energy 32.16 (2007): 3797-3810.

cost in £, P capacity (kW), correlation valid up to 500 MW). The last CAPEX corresponds to the electrolyser cost per kW (€/kW) used by Matzen et al.

Electrolyser capital cost per kW		
Wendt et al. 1998	Matzen et al. 2014	Mueller-Langer et al. 2007
31,318	278	767

Table A32 Comparison of electrolyser capital costs

As can be seen in the table, the CAPEX cost per kW of electrolyser varies considerably between different authors. Main reason for the difference is assumed to be year of publication and thus technology level (newer electrolysers are more efficient and cheaper).

Mueller-Langer et al. uses conventional & renewable electricity, in both cases energy is bought not produced. Information on operational costs as function of electricity price and thus source are given in the following table. Electricity prices are taken from the annual report on renewable energy costs published by the International Renewable Energy Agency (IRENA)[92]. Matzen et al. only utilise wind electricity.

Electricity source	Electricity cost range (€/MWh)		OPEX (€/t_{NH3})	
Wind offshore	90.58	150.97	698.18	1119.58
Wind onshore	52.84	90.58	434.80	698.18
Solar thermal	35.34	94.24	312.69	723.70
PV	67.94	150.97	540.15	1119.58
Hydro small-scale	22.65	45.29	224.10	382.13
Hydro large-scale	7.55	37.74	118.76	329.45
Geothermal	23.56	53.01	230.49	435.99
Non-renewable	28.23	35.00	263.04	310.31

Table A33 Electricity cost for different sources and corresponding OPEX

A2.7 Urea production

Conventional urea is synthesised through the ammonia stripping urea manufacture process (Snamprogetti process) and the CO_2 stripping urea manufacturing process licensed by Stamicarbon (Stamicarbon 2014), together they represent 75% of the urea production technology market share[93].

Detailed mass and energy balance are presented in the following table:

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[92] IRENA (2015). Renewable Power Generation Costs in 2014. Bonn, Germany: International Renewable Energy Agency.

[93] M. Baker (2012). Overview of Industrial Urea Markets: Applications and Opportunities. TFI Fertilizer Technology and Outlook Conference, Philadelphia, PA, US..

Stream	Phase	Mass flowrate (t/yr)	Composition (% molar)					Temp. (°C)	Pressure (bar)
			UREA	CARB	CO_2	NH_3	H_2O		
S01	Liquid	378,078	0	0	0	1	0	34	157
S02	Mixed	1,976,456	0.008	0.092	0.24	0.6	0.06	91.87	60
S03	Mixed	1,976,456	0.01	0.32	0.13	0.45	0.09	167	138
S04	Mixed	1,976,000	0.21	0.15	0.06	0.29	0.29	183	138
S05	Vapour	135,965	0	0	0.46	0.5	0.04	183	138
S06	Liquid	1,840,488	0.23	0.17	0.02	0.26	0.32	183	138
S07	Vapour	514,210	0	0	1	0	0	100	60
S08	Vapour	1,019,472	0	0	0.45	0.52	0.03	159.53	60
S09	Liquid	1,392,000	0.35	0.15	0.02	0.03	0.45	129.98	60
S10	Liquid	1,335,224	0.27	0	0.12	0.26	0.35	72.4	138
S11	Liquid	468,800	0	0	0.27	0.56	0.17	72.4	138
S12	Liquid	866,424	0.5	0	0	0	0.5	72.4	138
S13	Liquid	468,800	0	0.6	0	0.03	0.37	72.4	138
S15	Vapour	25,858	0	0	0.99	0.005	0.005	81.88	138
S17	Liquid	578,908	0	0.6	0.04	0.03	0.33	125.72	138

Table A34 Breakdown of the urea PFD

Key performance indicator (KPI)

This process is assessed based on the following KPIs as given below.

Key Performance Indicator	ACUTEC[94]Error! Bookmark not defined. project	IGSAS[95] project	Chauhan Mukesh[96]
Scale (t/yr)	660,000	274,000	386,000
Whole Process CO_2 efficiency	80%	-	-
Energy requirements (GJ/t_{urea})	2.83	37.91	2.40
Heat duty (GJ/t_{urea})	2.35	37.60	-
Cooling duty (GJ/t_{urea})	0.48	-	-
Electricity duty (GJ/t_{urea})	-	0.31	-
Avoided CO_2 emissions (t_{CO2}/t_{urea})	0.77	-	-
Amount of utilised CO_2 (t_{CO2}/t_{urea})	0.77	0.77	1.33
Input of other raw materials (t/t_{urea})			
NH4 synthesis: fuel oil	-	0.18	-
naphtha	-	0.43	-
refinery gas	-	0.26	-
Urea synthesis: NH_4	0.57	0.58	0.51
Quantity of by-products (t/t_{urea})			
NH4 (excess from NH_4 synthesis)	-	0.33	-
H_2O	0.3	0.3	0.3
Capital costs	87	929.36	2.16
operating costs (t/t_{urea})	252	291.03	2.92
Levelised production cost (t/t_{urea})	287	-	-
TRL (CCU vs. conventional)	9 vs. 9	9 vs. 9	9 vs. 9
Risk - impurities in inlet	Low	-	-
Catalyst	-	-	-
Catalyst loading per product yield	Not applicable	Not applicable	Not applicable
Raw material and utilities cost			
fuel oil (€/t)	-	102.38	-
naphtha (€/t)	-	121.86	-
refinery gas (€/t)	-	105.30	-
carbon dioxide (€/t)	0	by-product from NH4 synthesis	0
ammonia (€/t)	-	185 (selling price)	148.49
urea (€/t)		242.50	311.84
electricity (€/MWh)	-	58.50	-

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[94] ACUTEC project delivered by Imperial College to the EC JRC

[95] V, Dimitri, &N. Craig (1972). Turkey-Igsas Ammonia-Urea Manufacturing Project. International Bank for reconstruction and development. International development association. http://documents.worldbank.org/curated/en/876201468121489428/pdf/multi-page.pdf

[96] CHAUHAN, MUKESH M. "UREA PROJECT REPORT." M.M. Chauhan. (2017). Urea Project Report. IV Chemical M.S. University Baroda. Available: https://kupdf.com/download/urea-project-report_58fe9212dc0d602f6d959e7c_pdf

Location	EU	Turkey	India

Table A35 KPIs for urea process

The primary differences between the projects investigated is as follows:

- In the IGSAS project, capital and operational cost for the ammonia are considered; in the other two cases, ammonia is bought as raw material. Thus, capital cost is much higher than in the other two cases. Moreover, this project was developed in 1972, cost of equipment may vary considerably due to advance in technology. Only inflation was considered to update the costs.
- For Chauhan Mukesh, both CAPEX and OPEX are extremely low. The purchased cost of equipment (PCE) and capex amount to €0.255 M and €0.834 M respectively; the ratio was (CAPEX/PCE) 3.3.
- In the ACUTEC project, PCE was €8.45 M, based on CEPCI methodology the calculated CAPEX was €166 M; and a CAPEX/PCE ratio of 19.6. Thus, location can be a source of the difference in PCEs, and different evaluation method for CAPEX. For operational costs discrepancies, location, therefore raw materials and utilities, can be assumed as the source of the difference. Missing data on raw material and utility cost do not allow to draw conclusions.
- In the IGSAS project, the ammonia produced is higher than the one utilised to synthesise urea. The extra ammonia is sold. Here there is the possibility to boost urea production in the case of extra carbon dioxide available.
- In the IGSAS project, ammonia is synthesised through naphtha, fuel oil and refinery gas. Modern production is based on natural gas.

A3 Environmental assessment additional information

A3.1 Feedstocks and processes considered for environmental assessment

Error! Reference source not found. below outlines the feedstocks and routes considered for each environmental assessment, each given a specific case study identifier.

#ID	Product	Feedstock	Processes
1	Ethylene	Ethane	Ethylene, from ethane cracking
2	Ethylene/propylene	Natural gas	Ethylene/propylene, from MTO, from natural gas synthesis
3	Ethylene	Naphtha	Ethylene, from naphtha cracking
4	Propylene	Naphtha	Propylene, from naphtha cracking
5	Ethylene/propylene	Biomass	Ethylene/propylene, from MTO, from biomass gasification
6	Ethylene/propylene	Electrolysis: solar	Ethylene/propylene, from MTO, from solar electrolysis
7	Ethylene/propylene	Electrolysis: wind	Ethylene/propylene, from MTO, from wind electrolysis
8	Ethylene/propylene	Electrolysis: grid	Ethylene/propylene, from MTO, from grid electrolysis
9	Ethylene/propylene	Coal	Ethylene/propylene, from MTO, from coal gasification
10	Propylene	Propane	Propylene, from propane cracking
11	Polypropylene	Propane	Polypropylene, from propylene, from propane cracking
12	Polypropylene	Natural gas	Polypropylene, from propylene, from MTO, from natural gas synthesis

13	Polypropylene	Biomass	Polypropylene, from propylene, from MTO, from biomass gasification
14	Polypropylene	Electrolysis: solar	Polypropylene, from propylene, from MTO, from solar electrolysis
15	Polypropylene	Electrolysis: wind	Polypropylene, from propylene, from MTO, from wind electrolysis
16	Polypropylene	Electrolysis: grid	Polypropylene, from propylene, from MTO, from grid electrolysis
17	Polypropylene	Coal	Polypropylene, from propylene, from MTO, from coal gasification
18	HDPE	Ethane	HDPE, from ethylene, from ethane cracking
19	HDPE	Natural gas	HDPE, from ethylene, from MTO, from natural gas synthesis
20	HDPE	Biomass	HDPE, from ethylene, from MTO, from biomass gasification
21	HDPE	Electrolysis: solar	HDPE, from ethylene, from MTO, from solar electrolysis
22	HDPE	Electrolysis: wind	HDPE, from ethylene, from MTO, from wind electrolysis
23	HDPE	Electrolysis: grid	HDPE, from ethylene, from MTO, from grid electrolysis
24	HDPE	Coal	HDPE, from ethylene, from MTO, from coal gasification
25	Methanol	Natural gas	Methanol, from natural gas synthesis
26	Methanol	Biomass	Methanol, from biomass gasification
27	Methanol	Electrolysis: solar	Methanol, from catalytic hydrogenation, from solar electrolysis
28	Methanol	Electrolysis: wind	Methanol, from catalytic hydrogenation, from wind electrolysis
29	Methanol	Electrolysis: grid	Methanol, from catalytic hydrogenation, from grid electrolysis
30	Methanol	Coal	Methanol, from coal gasification
31	DME	Natural gas	DME, from methanol, from natural synthesis
32	DME	Biomass	DME, from methanol, from catalytic hydrogenation, from biomass gasification
33	DME	Electrolysis: solar	DME, from methanol, from catalytic hydrogenation, from solar electrolysis
34	DME	Electrolysis: wind	DME, from methanol, from catalytic hydrogenation, from wind electrolysis
35	DME	Electrolysis: grid	DME, from methanol, from catalytic hydrogenation, from grid electrolysis
36	DME	Coal	DME, from methanol, from coal gasification
37	Ammonia	Natural gas	Ammonia, from natural gas synthesis
38	Ammonia	Biomass	Ammonia, from biomass gasification
39	Ammonia	Electrolysis: solar	Ammonia, from solar electrolysis
40	Ammonia	Electrolysis: wind	Ammonia, from wind electrolysis
41	Ammonia	Electrolysis: grid	Ammonia, from grid electrolysis
42	Urea N fertliser	Natural gas	Urea N fertliser, from natural gas synthesis
43	Urea N fertliser	Biomass	Urea N fertliser, from biomass gasification
44	Urea N fertliser	Electrolysis: solar	Urea N fertliser, from solar electrolysis
45	Urea N fertliser	Electrolysis: wind	Urea N fertliser, from wind electrolysis
46	Urea N fertliser	Electrolysis: grid	Urea N fertliser, from grid electrolysis
47	Urea-formaldehyde resin	Natural gas	Urea-formaldehyde resin, from ammonia and methanol, from natural gas synthesis
48	Urea-formaldehyde resin	Biomass	Urea-formaldehyde resin, from ammonia and methanol, from biomass gasification
49	Urea-formaldehyde resin	Electrolysis: solar	Urea-formaldehyde resin, from ammonia and methanol, from catalytic hydrogenation with solar electrolysis
50	Urea-formaldehyde resin	Electrolysis: wind	Urea-formaldehyde resin, from ammonia and methanol, from catalytic hydrogenation with wind electrolysis
51	Urea-formaldehyde resin	Electrolysis: grid	Urea-formaldehyde resin, from ammonia and methanol, from catalytic hydrogenation with grid electrolysis

Table A36 List of case study product-feedstock combinations

A3.2 Inventory tables

The inventory associated with each set of production processes is given below.

Methanol

Methanol, from natural gas, 1 kg		
Heat, district or industrial, natural gas	5.18	MJ
Transport, pipeline, onshore, long distance, natural gas	0.998	tkm
Natural gas, processed, for olefins production, at plant	0.62	kg
Electricity, medium voltage	0.029	MJ
Transport, freight, lorry	0.010	tkm
Transport, freight train	0.010	tkm
Process-specific burden, sanitary landfill	0.0005	kg
Methanol, from coal, 1 kg		
Water, deionised, from tap water, at user	5.91	kg
Hard coal	1.72	kg
Natural gas, from medium pressure network, at service station	0.01	kg
Fly ash and scrubber sludge waste	-0.027	kg
Inert waste, for final disposal	-0.090	kg
Wastewater, average	-3.25	m3
Methanol, from catalytic hydrogenation, 1 kg		
Cooling energy, from natural gas	1.45	MJ
Heat, natural gas	1	MJ
Hydrogen	0.5	kg
Electricity, medium voltage	0.05	MJ
Aluminium oxide catalyst	9.20E-05	kg
Spent oxychlor catalyst waste	-9.20E-05	kg
Methanol, from biomass, 1 kg		
Synthetic gas, from biomass	7.1255	m3
Electricity, medium voltage	0.9963	MJ
Water, deionised, from tap water, at user	0.85	kg
Aluminium oxide catalyst	0.00024	kg
Copper oxide catalyst	9.00E-05	kg
Zinc, for catalyst	3.00E-05	kg
Nickel, 99.5%, for catalyst	2.00E-05	kg
Molybdenum, for catalyst	1.00E-05	kg
Methanol production facility	3.70E-11	pcs.
Wastewater produced	-0.00532	m3

Table A37 Process inventory for methanol production via different routes

Olefins

Ethylene, from ethane cracking, 1 kg		
Heat, natural gas	9.38	MJ
Electricity, medium voltage	2.5	MJ
Ethane	1.25	kg
Water, deionised, from tap water, at user	0.1	kg
Heavier hydrocarbon production (for use as fuel)	-0.16	kg

Ethylene/ propylene, from methanol-to-olefins, 1 kg		
Heat, natural gas	10.24	MJ
Electricity, medium voltage	4.47	MJ
Methanol, at plant	4.39	kg
OUTPUTs		
propylene [allocatable product]	1	kg
ethylene, average [allocatable product]	0.79	kg
RER: propane/ butane, at refinery [fuels]	0.09	kg
Propylene, from propane cracking, 1 kg		
Heat, natural gas	11.36	MJ
Electricity, medium voltage	3.03	MJ
Propane	1.52	kg
Water, deionised, from tap water, at user	0.91	kg
Heavier hydrocarbon production (for use as fuel)	-0.19	kg

Table A38 Process inventory for olefin production via different routes

Ammonia

Ammonia, from natural gas, 1 kg		
Natural gas, high pressure	1.19	m3
Water	1.1	kg
Electricity, medium voltage	1.4	MJ
Heat, natural gas	0.027	MJ
Disposal, municipal solid waste, 22.9% water, to sanitary landfill	0.0002	kg
Nickel, 99.5%, catalyst	0.00035	kg
Solvents, organic, unspecified, at plant	3.0E-05	kg
Chemical plant, organics	4.0E-10	pcs.
Transport, freight, rail	0.00023	tkm
Transport, lorry >16t, fleet average	4.00E-05	tkm
Ammonia, from water electrolysis, 1 kg		
Electricity, medium voltage	22.52	MJ
Transport, coal freight, rail	0.000228	tkm
Cooling energy, natural gas	11.76	MJ
Transport, lorry >16t, fleet average	4.00E-05	tkm
Heat, natural gas	0.04394	MJ
Water, deionised, from tap water, at user	1.63	kg
Ammonia, from biomass gasification, 1 kg		
Disposal, municipal solid waste, 22.9% water, to sanitary landfill	0.0002	kg
Transport, lorry 20-28t, fleet average	3.80E-05	tkm
Electricity, medium voltage	0.252	MJ
Nickel, 99.5%, catalyst	0.00035	kg
Solvents, organic, unspecified, at plant	3.00E-07	kg
Natural gas, high pressure	2.37	MJ
Water, deionised, from tap water, at user	3.84	kg
Wood chips, mixed, u=120%, at forest	0.0037	m3
Wood chips, mixed, from industry, u=40%, at plant	0.0013	m3
Waste wood chips, mixed, from industry, u=40%, at plant	0.00080	m3
Water, ultrapure, at plant	0.31	kg

Sodium hydroxide, 50% in H2O, production mix, at plant	0.0017	kg
Sulphuric acid, at plant	0.0069	kg
Electricity, medium voltage, at grid	0.21	MJ
Transport, lorry 20-28t	0.087	tkm
Transport, freight, rail	0.0077	tkm
Disposal, wood ash mixture, pure, 0% water, to municipal incineration	0.0048	kg
Disposal, wood ash mixture, pure, 0% water, to sanitary landfill	0.0036	kg
Treatment, sewage, from residence, to wastewater treatment, class 2	0.00021	m3
Industrial furnace, natural gas	3.9E-09	pcs.
Synthetic gas plant	1.90E-09	pcs.

Table A39 Process inventory for ammonia production via different routes

End-use products

Polypropylene, from propylene, 1 kg		
Propylene, at plant	1.00	kg
Electricity, medium voltage	0.59	MJ
Electricity, at cogen, for natural gas turbine	0.54	MJ
Transport, pipeline	0.06	tkm
Heat, natural gas	0.019	m3
Petroleum refining, for olefins production, at plant	0.005	kg
Disposal, solid waste, unspecified, to municipal incineration	0.0021	kg
Transport, barge, residual fuel oil powered	0.00091	tkm
Water, potable	0.00061	m3
Transport, barge, diesel powered	0.00027	tkm
Transport, combination truck, diesel powered	0.00022	tkm
Transport, train, diesel powered	0.00014	tkm
Disposal, solid waste, unspecified, to sanitary landfill	0.00011	kg
Residual fuel oil, combusted in industrial boiler	4.34E-06	m3
HDPE, from ethylene, 1 kg		
Ethylene, at plant	0.99	kg
Electricity, cogenerated, at plant	0.79	MJ
Electricity, medium voltage	0.64	MJ
Transport, pipeline, onshore, petroleum	0.19	tkm
Heat, natural gas	0.036	m3
Water, potable	0.00068	m3
Disposal, solid waste, unspecified, to sanitary landfill	0.00036	kg
Disposal, solid waste, unspecified, to municipal incineration	0.00026	kg
Residual fuel oil, combusted in industrial boiler	6.01E-06	m3
Disposal, solid waste, unspecified, to waste-to-energy	4.00E-06	kg
Liquefied petroleum gas, combusted in industrial boiler	3.75E-08	m3
Urea, from ammonia, 1 kg		
Transport, coal freight, rail	0.61	tkm
Cooling, natural gas	0.49	MJ
Ammonia, steam reforming, liquid, at plant	0.58	kg
Chemical plant, organics	4.07E-10	pcs.
Transport, lorry >16t, fleet average	0.10	tkm
Heat, natural gas	2.39	MJ
Urea-formaldehyde resin, 1 kg		
Heat, natural gas	1.42	MJ
Transport, coal freight, rail	0.98	tkm
Hard coal, burned in industrial furnace 1-10MW	0.95	MJ
Heat, district or industrial, other than natural gas	0.69	MJ
Urea, as N, at regional storehouse	0.59	kg

Methanol, at plant	0.55	kg
Electricity, medium voltage	0.30	MJ
Transport, lorry >16t, fleet average	0.16	tkm
Disposal, catalyst base CH2O production, 0% water, to residual material landfill	0.023	kg
Chemical plant, organics	5.8E-10	pcs.
DME, from methanol, 1 kg		
Heat, natural gas	2	MJ
Methanol, at plant	1.46	kg
Electricity, medium voltage	1.20	MJ
Transport, coal freight, rail	0.88	tkm
Transport, lorry >16t, fleet average	0.15	tkm
Chemical plant, organics	4.0E-10	pcs.

Table A40 Process inventory for production of selected downstream petrochemical products

Additional assumptions

The study considers carbon dioxide emissions from fossil sources and biogenic sources. The GWP values presented in the results only include fossil source CO_2 emissions, to allow for the fact that the biogenic CO_2 emissions has included a drawdown of CO_2 from the atmosphere during its life cycle (i.e. any CO_2 emitted from a biogenic source was originally derived from CO_2 in the atmosphere and so is net-zero). The impact of including biogenic CO_2 in the study would cause many of the biomass-sourced options to become negative emissions: this is because the drawdown from agricultural cultivation is considered and the carbon is stored within the product. Given that the final fate of the embodied carbon is uncertain (i.e. whether it remains in the product indefinitely or is emitted to atmosphere after end-use), it is a conservative assumption to exclude biogenic emissions and so no negative emissions are allowed for.

The process routes that include catalytic hydrogenation utilise CO_2 that may have been derived from fossil fuels. This is taken as an input to the process but not as a negative emission: i.e. we do not assume that this CO_2 would have otherwise been emitted. Additionally, captured CO_2 is typically accredited to the upstream process that captures (e.g. at a power plant or industrial CCS facility) and excluding the negative emission ensures that we are not double-counting for this benefit. Again, this is a conservative assumption that if relaxed would cause negative emissions for these routes.

A3.3 Environmental impacts of end-uses of petrochemicals

Urea-formaldehyde resin

This section analyses the environmental performance of five routes to produce formaldehyde urea resin. First an overview of the results is described to then analyse the performance by impact. Finally, a hotspot analysis is carried out for representative routes.

Results

Figure A69 exhibits the environmental impacts of the resin production by five different routes. The results show similar trends as the ones found in ammonia and urea productions. The best option is the biomass gasification route with the lowest impact in 11 out of 12 categories. Alike the previous analyses, the worst option is the grid powered electrolytic route underperforming in all impact categories. Although the conventional route (from natural gas) outstands the solar powered electrolytic route in nine out of 12 impacts, both options dispute the third and fourth positions in many category, sometimes with variations as little as 2% (e.g. AP). The solar powered electrolytic route performs better in key impacts such as GWP and ADP fossil. Finally, wind power electrolytic route is the second best option.

Global warming potential (GWP)

CO_2 and methane emissions from the electricity mix and the natural gas supply chain are the main contributors of the high impacts associated with the grid powered electrolytic (26.2 kg CO_2 eq./kg resin) and the conventional (5.4 kg CO_2 eq./kg resin) routes. The biomass gasification route is the best option, with 2.8 kg CO_2 eq./kg resin. Finally, the wind and solar powered electrolytic routes are at the top position, with 25% and 67% higher GWP than the best option.

Abiotic resource depletion (ADP) fossil

The use of coal and natural gas are the main drivers of the depletion of fossil resources and the reason why biomass gasification and wind powered electrolytic routes show the best performance in this category. Both routes exhibit similar values with variations of just 3%. The conventional route doubles the best option, biomass gasification route (32 MJ/ kg resin), but the grid powered electrolytic route is still the worst option with impacts 5.7 times higher.

Primary energy demand (PED)

Although non-renewable energies dominate this impact, it is interesting to see how a larger use of renewable energies in high energy intensive processes deteriorate this impact. The electrolytic routes exhibit the highest PED when compared with the conventional and biomass gasification routes, which show up to 3.4 times lower PED than the electrolytic routes.

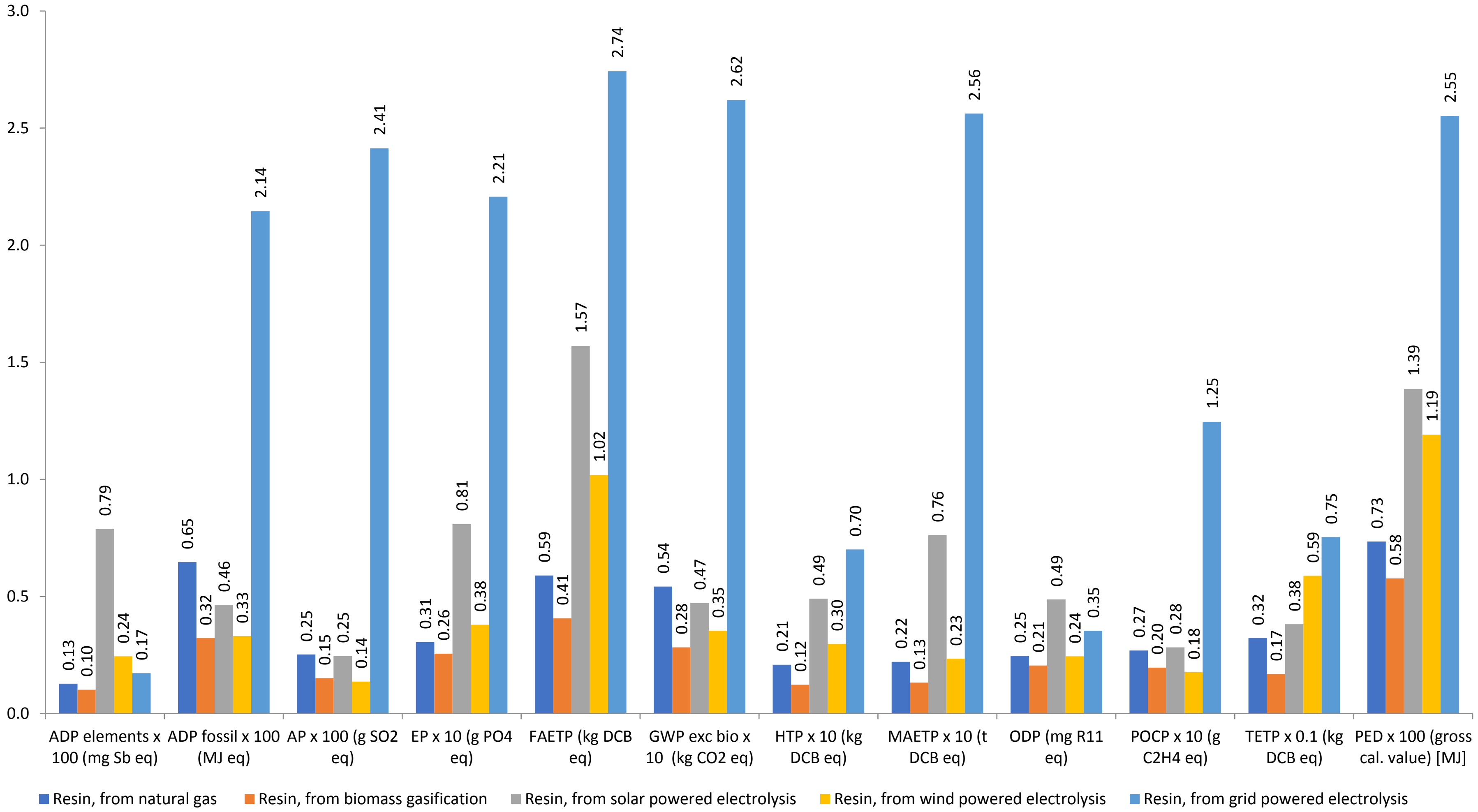

Figure A69 Comparison of the environmental Impacts of formaldehyde-resin production routes. Impacts are expressed per functional corresponding to 1 kg of resin

Hotspots

This section analyses the life cycle stage contribution of the conventional and solar powered-electrolytic routes of the resin production, to understand the influence of every stage in the environmental performance of the technologies.

The raw materials stage, referring to the production of methanol and urea, leads all the impact categories, while the process stage contributes less than 10% on average. The only important exceptions are seen in ADP elements and POCP, where its contribution is 27% and 20%, respectively. The reasons are the emission from the life cycle of the electricity mix, which is mainly coal-based.

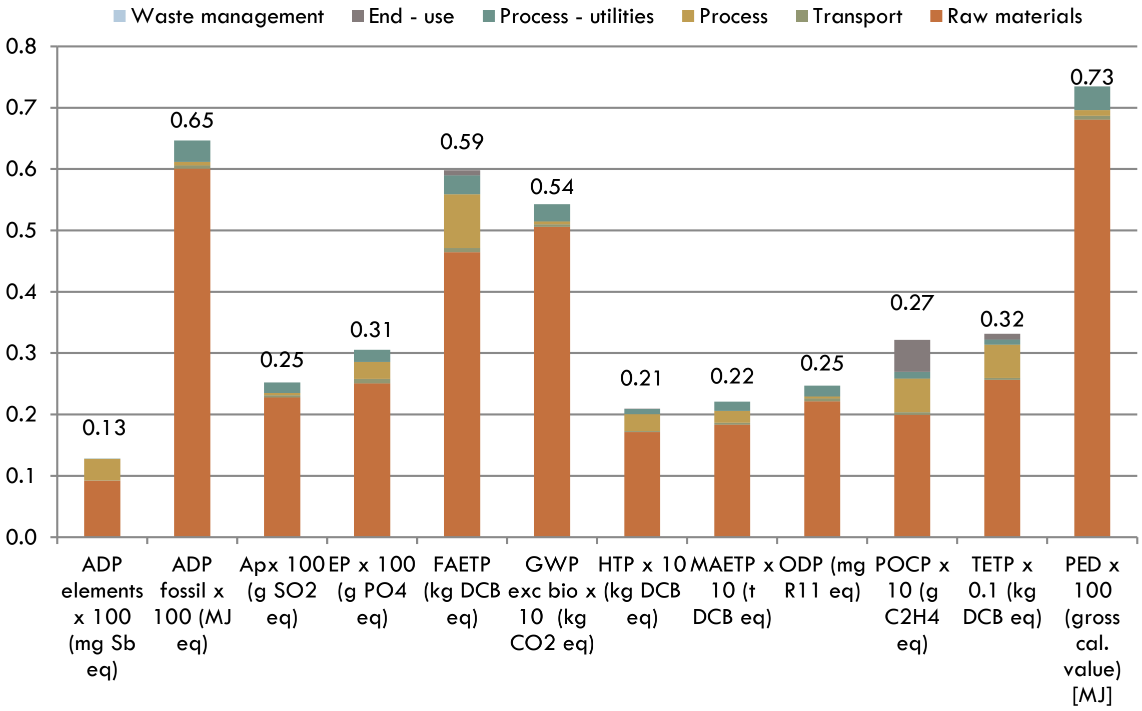

Figure A70 Environmental impacts and life cycle stage contribution of the resin production from natural gas

Although with different absolute values, the resin production from solar-powered electrolytic route does not show important differences in the stage contribution. All the impacts are again led by the raw materials stage.

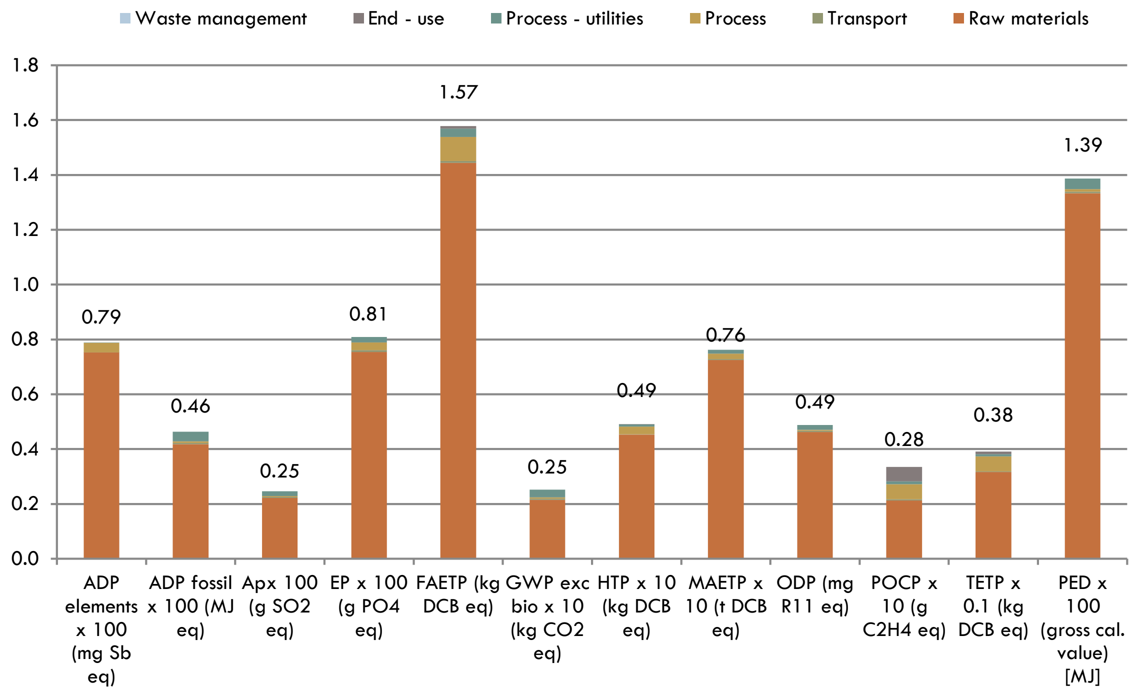

Figure A71 environmental impacts and life cycle stage contribution of the resin production from solar powered electrolysis

HDPE and Polypropylene

For the production of high density polyethylene and propylene, the emissions are very similar to those of the derivative feed sources, namely ethylene and propylene. Emissions vary typically by 10% per kg of product but the comparison of routes is entirely the same. Consequently, the hotspot analysis does not delve into detail on this, but see the sections on olefins for further information. The figures below show the results associated with 1 kg production of HDPE and polypropylene.

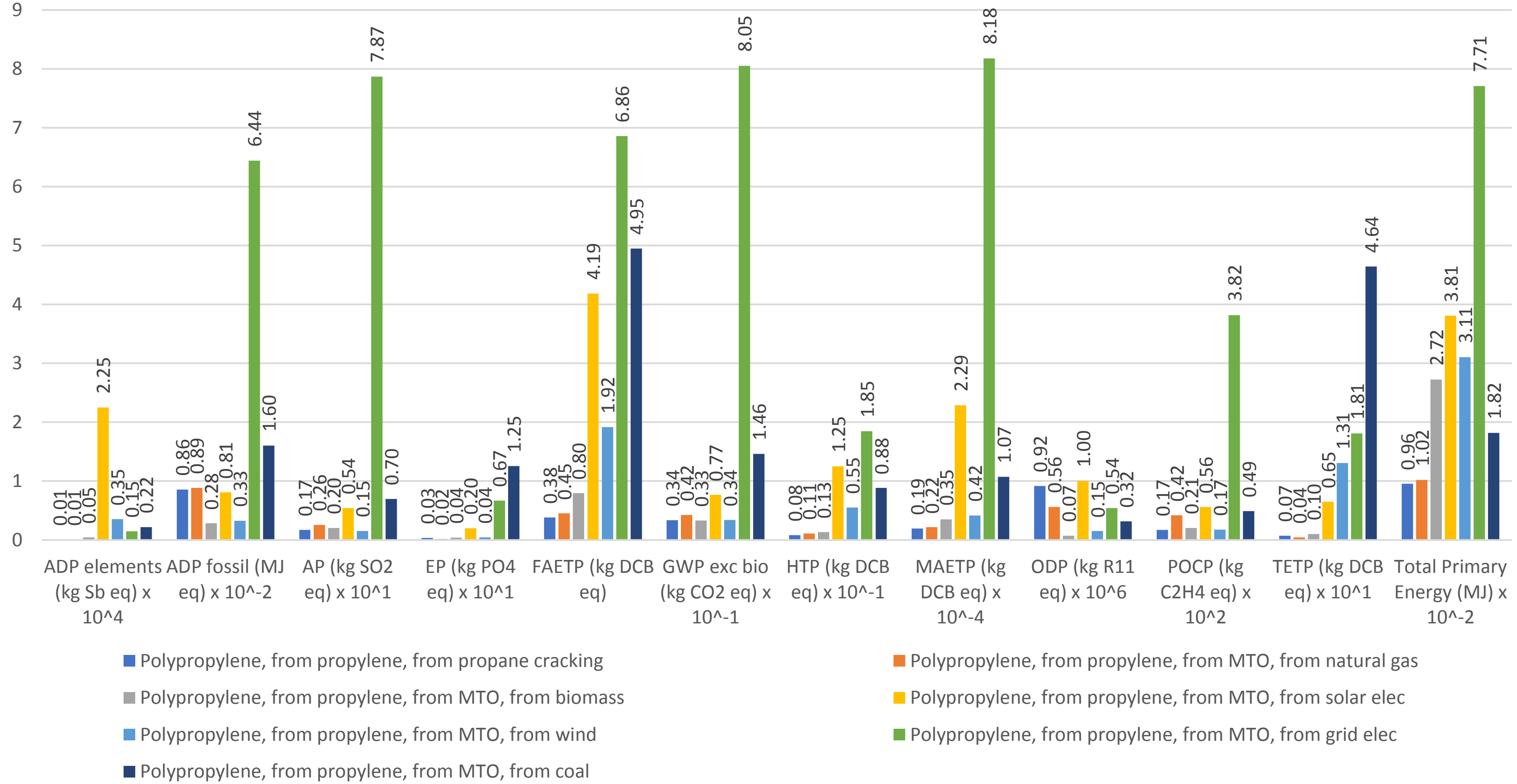

Figure A72 Environmental Impacts associated with different routes to 1 kg polypropylene production, allocated by mass

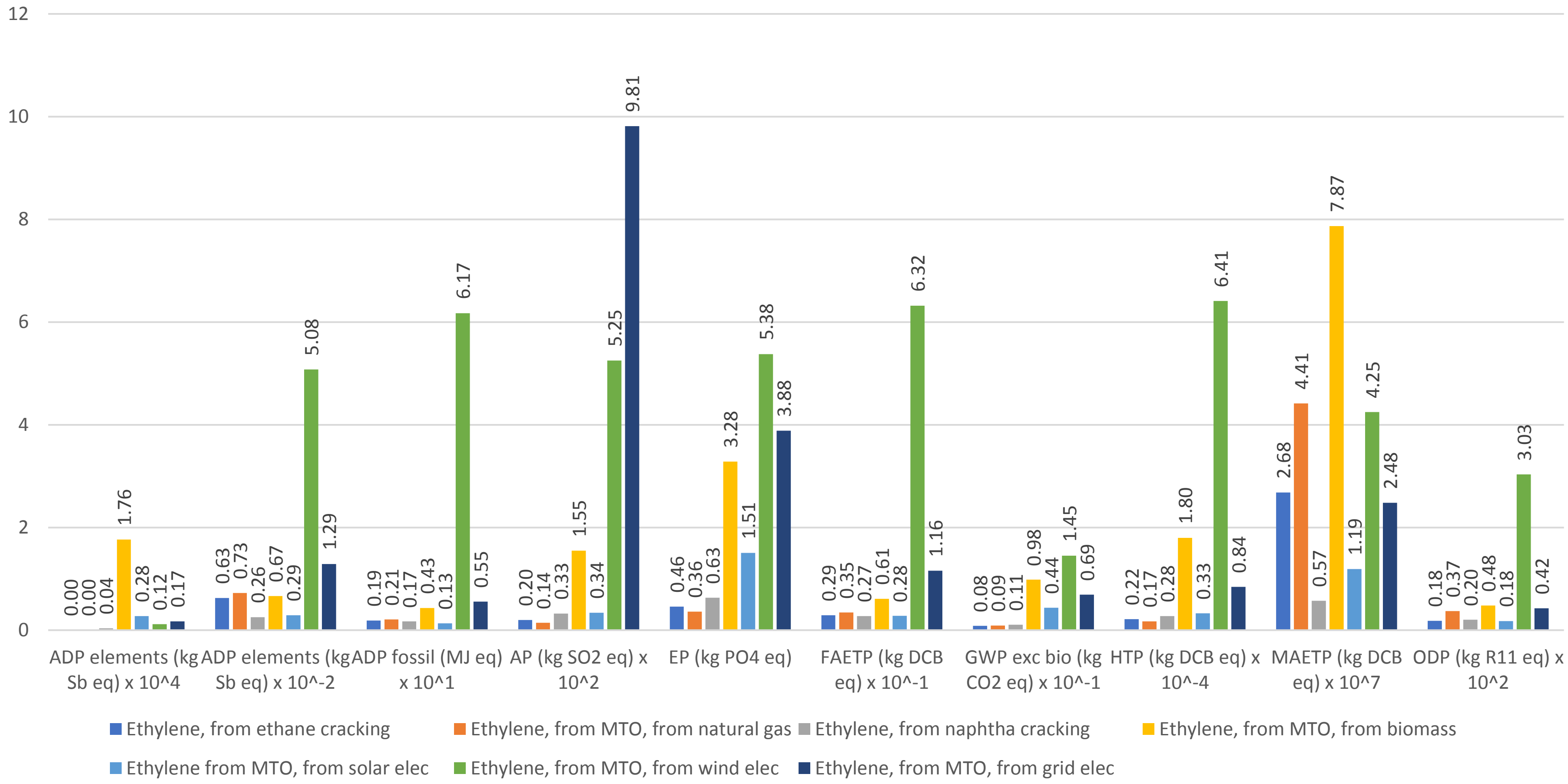

Figure A73 Environmental impacts associated with 1 kg of high density polyethylene production from different production routes, allocated by mass

DME

The environmental impacts of DME production using methanol manufactured from the six routes mentioned in Section 0. It is important to note that only methanol is produced from alternative routes while the production of DME itself follows the conventional options, which means the energy requirements are provided by the electric grid and natural gas (heating). Overall, the best option is the biomass gasification route with the lowest impact in seven out of 12 categories. Surprisingly, the second best options are the conventional route-using methanol produced from natural gas and the one using methanol from wind powered electrolysis. The worst option is again the methanol produced by grid powered electrolytic route with the highest impact in nine out of 12 categories. This route is closely followed by the production of DME from coal-based methanol, which shows the second worst performance. Following, a detailed analysis of each impact is discussed.

Global warming potential (GWP)

GWP ranges from 1.7 kg CO_2 eq./kg DME to 47.8 kg CO_2 eq./kg DME. The best options are the DME routes based on methanol produced by biomass gasification and wind-powered electrolysis. The worst option is the DME produced using methanol from the grid-powered electrolytic route. The second worst option is the route based on methanol from coal, which surprisingly shows 5.6 times lower impacts than the grid electrolytic route. The option based on methanol from solar powered electrolytic route shows 1.9 times higher impacts than the DME from conventional methanol (natural gas), which is 2.3 kg CO_2 eq./kg DME.

Abiotic resource depletion (ADP) fossil

As expected, DME produced from feedstock based on biomass gasification and renewable technologies (solar and wind) exhibit the lowest impacts, ranging from 16.8 MJ/ kg DME in the case of biomass to 48.1 MJ/ kg DME in the case of solar powered electrolysis. The highest ADP fossil is seen in the DME from grid powered electrolytic methanol with 22.6 times higher impact, mainly due to a high electricity demand provided by a coal-based grid. The DME manufactured using methanol from natural gas and coal routes show impacts 3.1 and 5.7 times higher than the best alternative.

Primary energy demand (PED)

Although non-renewable energies, the alternative routes show higher PED than the conventional routes - coal and natural gas. This is largely to the embodied energy as it is the case of biomass gasification (161 MJ/kg DME) and the high-energy intensive process as the electrolytic routes. Summarising, the large PED is found in the DME produced from methanol obtained by grid powered electrolysis (458 MJ/kg DME), followed by solar and wind powered electrolysers, with impact 2.5 and 2 times lowers than the similar grid powered technology. The best option is the DME manufactured from natural gas and coal-based methanol, with 59 and 107 MJ/kg DME, respectively.

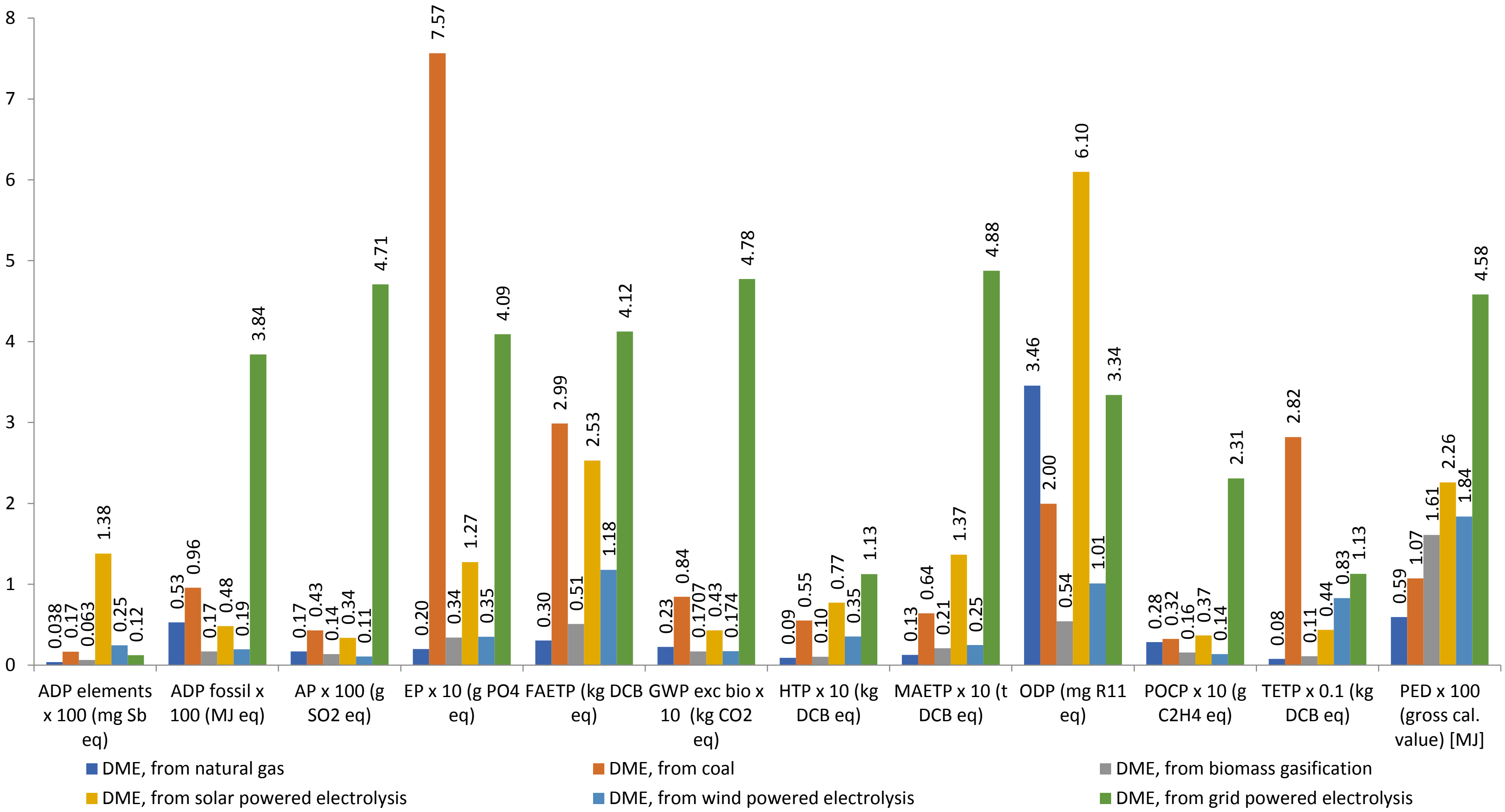

Figure A74 Comparison of the environmental Impacts of formaldehyde-resin production routes. Impacts are expressed per functional corresponding to 1 kg of DME

Hotspots

This section analyses the stage contribution in the environmental impacts of the three representative DME routes: methanol from natural gas, biomass gasification and solar powered electrolysis.

The figure below shows the life cycle stage contribution of the DME produced from methanol obtained by the conventional route (natural gas). Similar to ammonia, three stages lead the contribution to all the environmental impact categories. The largest contributor is the raw material stage, methanol, which leads nine out of 12 impacts categories, accounting for over 50% of the impacts. The process-utilities stage contributes to all the impact categories, however only by less than 10%. The only three exceptions are the ADP elements, HTP and TETP, where this stage contributes from 45% in the case of HTP to 93% in the case of ADP elements; emission from the production of organic solvents and less so by the electric supply mix.

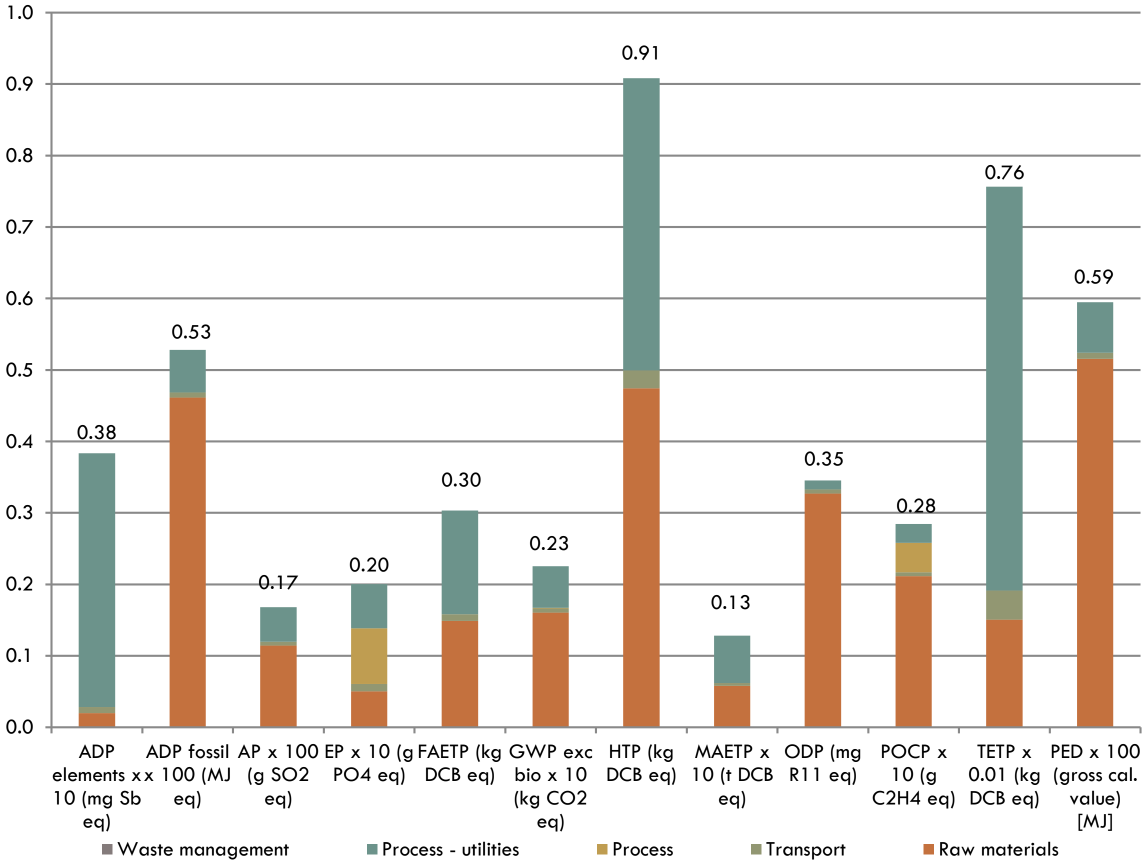

Figure A75 environmental impacts and life cycle stage contribution of the DME production from methanol manufactured by natural gas

As seen in Figure A76, three stages drive the environmental impacts of the DME produced from methanol from biomass gasification. Like the natural gas based route, the raw material stage contributes up to 98% across all the impacts. The process-utility stage has the highest contribution, up to 60%, in ADP elements, HTP and TETP, due to the life cycle of the organic solvents use in the production of the DME. The electricity supply mix has an important contribution, although less than 20%, in both process and process-utility stages.

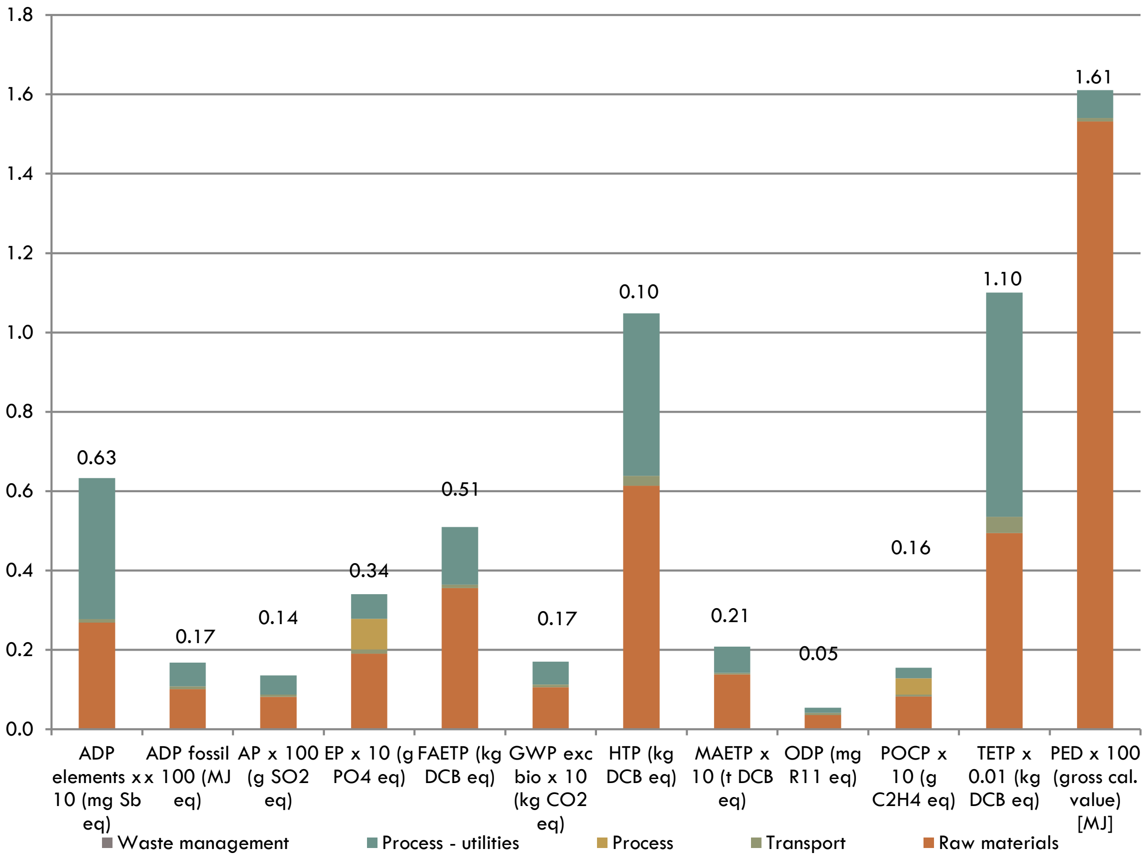

Figure A76 environmental impacts and life cycle stage contribution of the DME production from methanol manufactured by biomass gasification

As expected, the raw materials stage of methanol from solar electrolysis, dominates the environmental impacts (see Figure A77), mainly due to the impacts associated to the life cycle of the solar panels. It is important to note that although all the other stages are the same for all the DME routes, the source of methanol is the key to reduce the environmental burden of the DME.

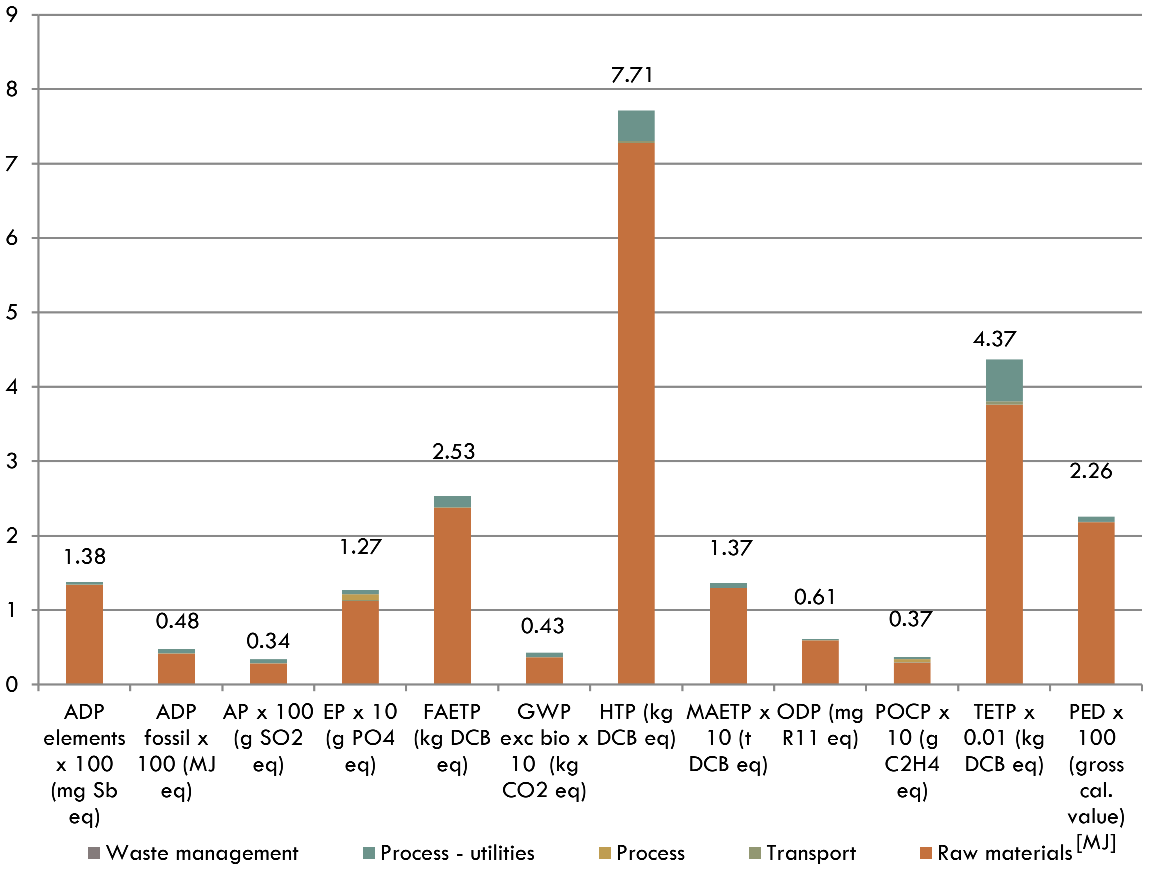

Figure A77 environmental impacts and life cycle stage contribution of the DME production from methanol manufactured by solar powered electrolysis

A3.4 Description of other environmental impacts for all petrochemicals

This section contains the remaining environmental impacts estimated in work package 3. Nine environmental impacts are discussed and showed in the following section.

Methanol processes

Abiotic resource depletion potential (ADP) elements

The conventional route of methanol from natural gas has the lowest impact on ADP elements, with 1.3 x 10^{-7} kg Sb eq./kg. Depletion of elemental resources such as rare earth metals result in higher impacts associated with renewable generators due to their use of elements such as silver and platinum in the construction of solar panels, wind turbines and ancillary equipment. In fact, the impacts associated with catalytic hydrogenation using wind and solar electricity are 100 and 700 times more (respectively) than methanol production from methane.

Acidification potential (AP)

Methanol from catalytic hydrogenation using wind powered electrolysis gives the lowest AP at 3.6 g SO_2 eq./kg, which is approximately half that of methanol from natural gas (7.8 g SO_2 eq./kg). Methanol from biomass also has lower impact, but coal and solar driven electrolysis results in high impacts of 20 and 25 g SO_2 eq./kg respectively. The manufacture of solar panel systems contributes via NOx and SO_2 emissions associated with steel, copper, aluminium, lead and silicon production.

Eutrophication potential (EP)

EP impacts are higher for all unconventional production routes and lowest for methanol from natural gas. Methanol from biomass gasification and wind electrolysis impacts are approximately 4 times higher than from natural gas, whereas methanol from coal is 150 times higher, at 51 g PO_4 eq./kg. The main contributors are NOx emissions from coal extraction, processing and combustion.

Freshwater aquatic ecotoxicity potential (FAETP), human toxicity potential (HTP), marine aquatic ecotoxicity potential (MAETP), and terrestrial ecotoxicity potential (TETP)

For each of the toxicity indicators, the conventional methanol from natural gas exhibits the lowest emissions, where biomass gasification is the second lowest. Catalytic hydrogenation from grid electrolysis has the largest impact of 3 out of 4 indicators, primarily due to the NOx and SOx emissions associated with electricity production, as well as the inefficiency of the process route. Methanol from coal also performs poorly and is the highest impact for terrestrial ecotoxicity, again due to waste treatment emissions of NOx and SOx and other chemicals.

Ozone depletion potential (ODP)

Ozone depletion potentials have a relatively minor variation across the options, with methanol from biomass representing the lowest value (2.5×10^{-8} kg R11 eq./kg) and catalytic hydrogenation from solar electrolysis representing the highest (4.1×10^{-7} kg R11 eq./kg). The main contributor appears to be due to the construction of PV cells using tetrafluoroethylene.

Photochemical ozone creation potential (POCP)

The lowest contributors to POCP impacts are from biomass and catalytic hydrogenation of wind, representing 39% and 30% of the impact of the conventional methanol from natural gas (1.4 g C_2H_4 eq./kg). By far the largest impact is from catalytic hydrogenation using grid electrolysis (15.3 g C_2H_4 eq./kg), whereas methanol from coal also has a significant impact (1.7 g C_2H_4). Emissions are mainly hydrocarbon emissions to atmosphere and due to the electricity supply mix.

Olefins production

Abiotic resource depletion potential (ADP) elements

The conventional methods perform best with respect to ADP elements, given the heavy metal requirements of the alternative options as described in the previous section. Propylene from propane and from MTO derived from natural gas have similar impacts at 5×10^{-7} kg Sb eq./kg.

Acidification potential (AP)

Grid electrolysis and MTO from coal exhibit the highest acidification impacts, with 0.6 and 0.05 g SO_2 eq./kg for ethylene, respectively. MTO from solar electrolysis also performs poorly due to the NOx and Sox emissions mentioned in the methanol section. Lowest impacts are from olefin production from biomass from wind electrolysis via MTO, at 0.01

and 0.014, respectively. In comparison, ethylene from ethane cracking exhibits emissions of 0.017 kg SO_2 eq./kg.

Eutrophication potential (EP)
For eutrophication, all alternative routes exhibit higher emissions than the conventional routes of ethane, propane and naphtha cracking. Ethylene from ethane cracking exhibits emissions of 1.8 g PO_4 eq./kg, whereas the electrolytic routes are between 1.7 and 30 times more impactful, due to phosphate and nitrous oxide emissions associated with electricity generation.

Freshwater aquatic ecotoxicity potential (FAETP), human toxicity potential (HTP), marine aquatic ecotoxicity potential (MAETP), terrestrial ecotoxicity potential (TETP)
In terms of the toxicity impacts, broadly the conventional routes from oil and gas sources are the least impactful, followed by MTO from biomass, with the electrolytic routes and coal sources presenting the highest results. Given the relative energy intensity of the MTO electrolytic routes, heavy metal release associated with solar panel, wind turbine and ancillary equipment production cause much of the toxicity impacts. Examples of key impacts are emissions from wastewater from the coal processing of nickel, copper and vanadium, contributing the majority of the freshwater toxicity impacts.

Ozone depletion potential (ODP)
Biomass and wind electrolysis routes have the lowest impacts associated with ODP, with 5.7×10^{-8} and 1.2×10^{-7} kg R11 eq./kg. ethane cracking and MTO from coal exhibited similar impacts, whereas the solar drive electrolytic option is the highest. The oil and gas derived routes have impacts chiefly associated with transport due to the assumed use of Halon as a fire retardant across some pipelines. Note that this is only applicable to some regions and it is not certain that this applies to China.

Photochemical ozone creation potential (POCP)
Lowest impacts of POCP are from wind electrolysis and ethane cracking at 1 and 1.1 gC_2H_4 eq./kg respectively. The biomass route is 20% higher, whereas the coal and solar electrolytic hydrogenation are 3-4 times greater, due to carbon monoxide, nitrogen and sulphur oxides arising from coal extraction and wastewater treatment. The highest impacts are from grid driven electrolysis, due to the coal fraction of the grid mix.

Ammonia production

Abiotic depletion potential (ADP) elements
In the case of ADP elements, the high amount of copper, gold and silver positioned the solar powered electrolytic route as the highest impact with 24. 6 mg Sb eq./kg NH_3; followed by wind powered electrolytic route (8.86 mg Sb eq./kg NH_3) and then by the grid powered route (5.4 mg Sb eq./kg NH_3). The biomass gasification and the conventional routes are the best options with 0.19 and 3.67 mg Sb eq./kg NH_3, respectively.

Acidification potential (AP)
Sulphur dioxide and to a lesser extent, nitrous oxides emissions lead this impact, mainly coming from the life cycle of the electricity generation and natural gas. The lower energy requirements or the avoidance of fossil-based energy are the reason for such low impacts

seen in biomass gasification (2.6 g SO_2 eq./kg NH_3), followed by the wind (3.9 g SO_2 eq./kg NH_3) and solar (6.9 g SO_2 eq./kg NH_3) powered electrolytic routes. The conventional route and the grid powered electrolytic routes show 6.3 and ~30 times higher impacts than the best option.

Eutrophication potential (EP)

EP ranges from 0.37 g PO_4 eq./kg NH_3 for the biomass gasification route to 6.9 g PO_4 eq./kg NH_3 for the grid powered electrolytic route. Similar to AP, the life cycle of the electricity generation and the natural gas use are the main sources of phosphate and nitrogen oxide emissions, which dominate this impact. The conventional route outperforms the solar powered electrolytic route with ~60% lower impacts.

Freshwater aquatic ecotoxicity potential (FAETP), human toxicity potential (HTP), marine aquatic ecotoxicity potential (MAETP), and terrestrial ecotoxicity potential (TETP)

HTP ranges from 0.12 kg DCB eq./kg NH_3 for biomass gasification route to 2.65 kg DCB eq./kg NH_3 for grid powered electrolytic route. The wind powered is the second best options, with 8.6 times higher impact than the biomass gasification route. It is interesting to note that the conventional route exhibits 26% and 1.07 times lower impact than the solar and grid powered electrolytic routes, respectively. The conventional route also outperforms the solar and grid powered electrolytic routes in MAETP and FAETP. This is due to emissions of beryllium, vanadium and nickel from the life cycle of the electricity generation.

Nevertheless TETP exhibits a similar trend as GWP, where biomass gasification displays the best performance (0.99 g DCB eq./kg NH_3) and the grid powered electrolytic route the worst (26 g DCB eq./kg NH_3). This is the only impact where wind powered electrolytic route performs 40% worse than the alternative solar powered one. The conventional route exhibits 16% lower impacts than the worst option.

Ozone depletion potential (ODP)

ODP varies from 0.03 mg R11 eq./kg NH_3 in the case of biomass gasification route to 0.28 mg R11 eq./kg NH_3 for the solar powered electrolytic route. This is due to the use of halon as retardant in the natural gas life cycle. The second best option is the conventional route with 0.09 mg R11 eq./kg NH_3. The other electrolytic routes exhibit impacts 25% (wind) and 15% (grid) lower ODP than the solar powered one.

Photochemical ozone creation potential (POCP)

POCP ranges from 0.2 to 4.1 g C_2H_4/kg NH_3. The lowest impact is found in biomass gasification route while the highest in the grid powered electrolytic route. Although the conventional route occupies the fourth position, its POCP is nearly 4 times lower. The natural gas and the electricity life cycles are the main contributor through sulphur dioxide, NVOC and methane emissions.

Urea

Abiotic depletion potential (ADP) elements

The large use of materials, in particular of metals such as copper, gold, silver and lead, positioned the renewables, solar and wind, powered electrolytic routes at the bottom, with

3.6 and 1.3 times higher impacts than the best option, biomass gasification route (4 mg Sb eq./kg urea).

Acidification potential (AP)

Emission of sulphur and nitrous oxides drives this impact, with the worst option found in the grid electrolytic route, followed by the conventional one. Nevertheless the best option is the biomass gasification with 96 g SO_4 eq./kg urea, the wind and solar powered electrolytic routes show very similar values, varying less than 3% when compare to the best.

Eutrophication potential

Interestingly, EP is the only category where all the routes show similar scores, with variations lower than 4%. This is mainly due to NO_3 emissions from the use phase, which is the same for all routes.

Freshwater aquatic ecotoxicity potential (FAETP), human toxicity potential (HTP), marine aquatic ecotoxicity potential (MAETP), and terrestrial ecotoxicity potential (TETP)

The large use of coal to provide the electricity requirement is the main reason of the poor performance of the grid powered electrolytic route, which has the highest impact across all toxicities. Although the wind powered electrolytic route is the second best option in almost all the toxicities except for FAETP, it is interesting to see that the conventional route closely follows it, with impacts such as HTP and MAETP only ~9% higher. The only exception is TETP, where the conventional route is nearly the worst, only overpassed by the grid powered electrolytic route. Finally, except for TETP, the solar powered electrolytic route is worse than the natural gas conventional route when toxicity related impacts are assessed, with up to 52% higher scores.

Ozone depletion potential (ODP)

Like ADP elements, the solar powered electrolytic route is the worst option for ODP. The use of halon as retardant in the natural gas supply chain drives this performance. In this impact, the conventional route outstands the so-called sustainable routes, with up to 60% lower impacts. The grid and wind powered electrolytic routes show similar impacts, 0.15 and 0.16 mg R11 eq./kg urea.

Photochemical ozone creation potential (POCP)

This impact exhibits the same trend as GW. Hence, the best option is the biomass gasification route, followed by wind and solar powered electrolytic routes, and then the conventional route. By far, the worst option is the grid electrolytic route because of sulphur dioxide, NVOC and methane emissions from the coal and natural gas life.

Urea-formaldehyde resin

Abiotic resource depletion (ADP) elements

The avoidance of metals such as copper, gold, silver and lead largely use in the equipment, structures and auxiliaries of renewable energy sources (e.g. solar), is the main reason of the strong performance of biomass gasification and the conventional routes. The wind and grid electrolytic routes exhibit impacts 69% and 1.38 times higher than the biomass gasification with 10 mg Sb eq./kg resin. Finally, the worst option is solar powered electrolytic route with a score 6.9 times higher than the best option.

Acidification potential (AP)

SO_2 and nitrous oxide emissions lead this impact, where the grid powered electrolytic route is the worst option with 241 g SO_4 eq./kg resin. Although by far, 16.6 times lower, the wind powered electrolyser and the biomass gasification routes are the best options across the impact, followed by the conventional and the wind powered electrolytic routes, which exhibit similar impacts with 25.2 and 24.5 g SO_4 eq./kg resin.

Eutrophication potential (EP)

As indicated in Figure 55, biomass gasification route is the best option with 2.5 g PO_4 eq./kg resin, followed by the conventional route from natural gas, with 20% higher impact. This is one of the few categories where the conventional route outperforms the renewable energy base electrolytic routes, which show 48% (wind) and 2 times (solar) higher scores.

Freshwater aquatic ecotoxicity potential (FAETP), human toxicity potential (HTP), marine aquatic ecotoxicity potential (MAETP), and terrestrial ecotoxicity potential (TETP)

Emissions of Beryllium, vanadium ad nickel drive the low performance of the grid powered electrolytic route, being the worst option across all the toxicities with impacts 3.5 to 18.4 times higher than the best option - biomass gasification route. It is interesting to note that the conventional route exhibits lower impacts compared to the wind and solar powered electrolytic routes.

Ozone depletion potential (ODP)

The use of Halon and R11 as retardants drive the poor performance of the solar powered electrolytic route, making ODP the only impact where this route is the worst across all the options, with 0.49 mg R11 eq./kg resin. Wind power electrolytic and conventional routes exhibit half of these impacts while the biomass gasification represents only 40%.

Photochemical ozone creation potential (POCP)

This impact ranges from 1.8 g C_2H_4 eq./kg resin in the case of wind powered electrolytic route to 12.5 g C_2H_4 eq./kg resin in the case of the grid powered electrolytic route. The conventional route positioned third with 2.7 g SO_4 eq./kg resin, closely followed by solar powered electrolytic route with 5% higher values. The main emissions are NVOC, SO_2 and methane.

DME

Abiotic resource depletion (ADP) elements

As seen in previous analyses, DME based on methanol produced by natural gas and biomass gasification routes are the best technology when ADP elements is considered, as they exhibit the lowest impact with 3.8 and 6.3 mg Sb eq./kg DME, respectively. The use of biomass and natural has help to avoid the extraction of rare elements, which is the main contributor in the case of technologies like solar and wind powered routes, with 138 and 25 mg Sb eq./kg DME, respectively. DME produced from methanol manufactured by coal and grid powered electrolyser routes show impacts 32% and 50% lower than products from wind-powered electrolytic route.

Acidification potential (AP)

This impact is the only category where the wind powered electrolytic products exhibit the best results (10.6 g SO_2 eq./kg DME). DME based on methanol produced by biomass gasification and by the conventional route show impacts 28% and 58% higher than the best option, respectively. The worst option, 44.3 times higher impacts, is the DME produced from grid powered electrolytic methanol due to SO_2 and nitrous oxide emissions coming from the coal based grid.

Eutrophication potential (EP)

Interestingly, both fossil fuel routes – natural gas and coal – occupy the top and the bottom of this impact category with the lowest EP at 2 g PO_4 eq./kg DME (natural gas) and the highest impact at 40.9 PO_4 eq./kg DME (coal). DME made from methanol produced by biomass gasification and wind powered electrolyser show similar scores, with impacts 70% and 76% higher than the best option, respectively.

Freshwater aquatic ecotoxicity potential (FAETP), human toxicity potential (HTP), marine aquatic ecotoxicity potential (MAETP), and terrestrial ecotoxicity potential (TETP)

When toxicity related impacts are assessed, DME produced from methanol manufactured by natural gas is the best option, closely followed by the biomass gasification route. The worst performance, up to 38 times higher than the best options, is found in DME based on methanol produced from grid powered electrolytic route, due to the emission coming from the life cycle of the electricity production. Coal and solar powered electrolytic routes show similar performance, except for TETP, where DME based on methanol from coal route is the worst across all routes.

Ozone depletion potential (ODP)

DME based on methanol produced by solar powered electrolytic route is the worst option with 6.1 mg R11 eq./kg DME. This is mainly due to emission from life cycle of solar panels. This is closely followed by the grid powered electrolytic and coal based routes, with impacts 43% and 45% lower. The best option is DME produced from methanol coming from biomass gasification with 0.54 mg R11 eq./kg DME.

Photochemical ozone creation potential (POCP)

DME manufactured from methanol obtained by the grid powered electrolytic route is by far the worst option with 23.1 g C_2H_4 eq./kg DME, corresponding to 9 times higher impacts. The other five routes show similar values, ranging from 1.4 g C_2H_4 eq./kg DME in the case of products made from wind-powered electrolytic routes to 3.7 g C_2H_4 eq./kg DME in the case of solar powered electrolytic products.

A3.5 Waste management options

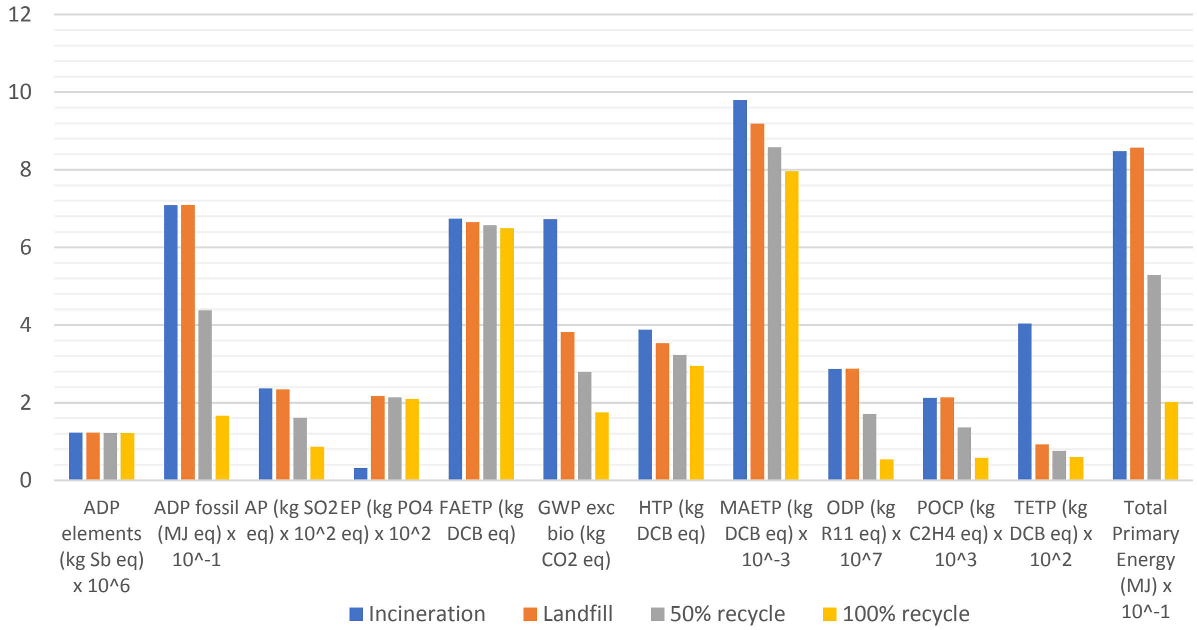

Figure A78 Life cycle environmental impacts associated with 1 kg HDPE pipe, for different end-of-life waste management options.

A3.6 Environmental assessment limitations

There were several limitations to this study, relating to data sources and the incorporation of transport and waste emissions. The study is limited in terms of the comprehensiveness and comparability of the data sources, as well as the regional applicability. Where possible, Chinese-relevant data sources were used but this was not the case in many instances. For instance, environmental impacts associated with Chinese natural gas production was not found, consequently an adapted Ecoinvent source was used that reflected the non-EU, non-North America, 'Rest-of-World' case. Additionally, there are some data gaps for some processes, particularly with respect to direct process emissions, transportation and waste management. The disaggregation of individual supply chain stage data was not possible for a number of conventional process routes, such as olefin production from naphtha cracking and ethane cracking.

Evaluating technology options to mitigate greenhouse gas emissions

IEA Greenhouse Gas R&D Programme

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