PBL Netherlands Environmental
Assessment Agency

DECARBONISATION OPTIONS FOR LARGE VOLUME ORGANIC CHEMICALS PRODUCTION, LYONDELLBASELL ROTTERDAM

Charlotte Yong, Andrew Keys

18 January 2021

MIDDEN

Manufacturing Industry Decarbonisation Data Exchange Network

Decarbonisation options for Large Volume Organic Chemicals Production, LyondellBasell Rotterdam

The Hague, 2021
PBL publication number: 4533
TNO project no. 060.33956 / TNO 2020 P11920

Authors
Yong, C.M.F and Keys, A.

MIDDEN project coordination and responsibility
The MIDDEN project (Manufacturing Industry Decarbonisation Data Exchange Network) was initiated and is also coordinated and funded by PBL and ECN part of TNO (which is named TNO Energy Transition after 1-1-2020). The project aims to support industry, policymakers, analysts, and the energy sector in their common efforts to achieve deep decarbonisation. Correspondence regarding the project may be addressed to:
D. van Dam (PBL), Dick.vanDam@pbl.nl, or S. Gamboa Palacios (TNO), silvana.gamboa@tno.nl.

This publication is a joint publication by PBL and TNO Energy Transition and can be downloaded from: www.pbl.nl/en. Parts of this publication may be reproduced, providing the source is stated, in the form: *Yong, C. and Keys, A. (2021), Decarbonisation options for large volume organic chemicals production, LyondellBasell Rotterdam. PBL Netherlands Environmental Assessment Agency and TNO Energy Transition, The Hague*.

PBL Netherlands Environmental Assessment Agency is the national institute for strategic policy analysis in the fields of the environment, nature and spatial planning. PBL contributes to improving the quality of political and administrative decision-making by conducting outlook studies, analyses and evaluations in which an integrated approach is considered paramount. Policy relevance is the prime concern in all of PBL's studies. PBL conducts solicited and unsolicited research that is both independent and scientifically sound.

TNO Energy Transition has a twofold mission: to accelerate the energy transition and to strengthen the competitive position of the Netherlands. TNO conducts independent and internationally leading research and we stand for an agenda-setting, initiating and supporting role for government, industry and NGOs.

The report was offered for review to LyondellBasell but LyondellBasell did not comment on the content of the report. PBL and TNO remain responsible for the content. The decarbonisation options and parameters are explicitly not verified.

Contents

FINDINGS

Summary

LyondellBasell operates a total of three production sites and one deep-water terminal in the Port of Rotterdam. This report focuses on the Botlek and Maasvlakte sites only. The production sites have a diverse product portfolio as summarised below:

Table 1. Annual production capacity of products in the Maasvlakte and Botlek sites

Product	Annual Production Capacity (kt)
Maasvlakte	
Propylene Oxide (PO)	385
Styrene Monomer (SM)	864
Botlek	
Propylene Oxide (PO)	250
Propylene Glycol (PG)	80
Propylene Glycol Methyl Ether (PGME)	90
Tertbutyl Hydroperoxide (TBHP)	12
Methyl Tertiary Butyl Ether (MTBE)/ Ethyl Tertiary Butyl Ether (ETBE)	400
Gasoline Grade Tert-Butyl Alcohol (TBA)	589
Isobutylene	100
1,4 - Butanediol (BDO)	126
Allyl Alcohol (AA)	16
Methyl Propanediol (MPD)	20

These products are mainly used as intermediate chemicals, of which their derivatives are used for a wide range of applications, such as pharmaceutical products, paints and coatings, packaging materials and as gasoline additives. They are produced through six main chemical processes in Botlek and one main process in Maasvlakte.

The plant-wide integration allows optimised product flows across production processes and operating sites, as well as cascaded steam usage across process units. There is also a high integration between the production sites and the neighbouring utility companies, making scope 2 emissions (indirect emissions for generating electricity, external steam supply, etc.) an important source of emissions. The chemical processes are energy-intensive, primarily in the form of process steam consumption. The overall steam consumption amounts to around 8 PJ per year at each production site. The electricity consumption is calculated to be 0.5 and 0.9 PJ per year and waste fuel consumption are calculated to be 2.6 and 5 PJ per year, respectively, in Maasvlakte and in Botlek. The Maasvlakte and Botlek sites have reported scope 1 emissions (direct emissions of the production plant) of 13 and 327 kt CO_2 and calculated scope 1 and 2 emissions of 416 and 620 kt of CO_2, respectively, of which 88% are accounted for by steam, electricity and waste fuel consumption.

Several decarbonisation opportunities have been identified, in reducing both scope 1 and 2 emissions. The greatest potential is realised through decarbonising the high-temperature steam production. Applicable measures include the utilisation of electrode boilers, hydrogen combustion, (solid) biomass combustion, as well as through post-combustion carbon capture and storage. Other possible measures include integrated heat pumps in distillation columns. Usage of alternative low-carbon and/or bio-based feedstocks can provide a carbon reduction over the entire value chain, accountable as scope 3 emissions.

FULL RESULTS

Introduction

This report describes the current situation for the Large Volume Organic Chemicals (LVOC) production in the Netherlands and the options and preconditions for its decarbonisation. Specifically, for LyondellBasell. The study is part of the MIDDEN project (Manufacturing Industry Decarbonisation Data Exchange Network). The MIDDEN project aims to support industry, policymakers, analysts, and the energy sector in their common efforts to achieve deep decarbonisation. The MIDDEN project will update and elaborate further on options in the future, in close connection with the industry.

Scope

The Dutch Large Volume Organic Chemicals (LVOC) production is spread across multiple chemical companies and production sites. These are, for example, Shell Moerdijk, Shell Pernis and LyondellBasell.[1] The scope of this research will focus on the manufacturing of LVOC by LyondellBasell at its production sites, in Botlek and Maasvlakte.

The processes covered by this research are:

- Co-production of propylene oxide (PO) and styrene monomer (SM) (including ethylbenzene production through benzene alkylation process)
- Co-production of propylene oxide (PO) and tert butyl alcohol (TBA) (including isomerisation of n-butane)
- Propylene glycol (PG) production through the hydrolysis of propylene oxide (PO)
- Production of propylene glycol methyl ether (PGME) from propylene oxide (PO)
- Production of 1,4-butanediol (BDO), allyl alcohol & methyl propanediol (MPD) from propylene oxide (PO)
- Production of isobutylene through dehydration of tert butyl alcohol (TBA)
- Production of methyl tertiary-butyl ether (MTBE)/ ethyl tertiary butyl ether (ETBE) from isobutylene and methanol/ethanol

Products offered by LyondellBasell's production sites at Botlek and Maasvlakte are:

- Propylene Oxide (PO)
- Propylene Glycol (PG)
- Propylene Glycol Methyl Ether (PGME)
- Tertbutyl Hydroperoxide (TBHP)
- Methyl Tertiary-Butyl Ether (MTBE)
- Ethyl Tertiary Butyl Ether (ETBE)
- Styrene Monomer (SM)
- Gasoline Grade Tert-Butyl Alcohol (TBA)
- Isobutylene
- Butanediol (BDO)
- Allyl Alcohol (AA)
- Methyl Propanediol (MPD)

The main options for decarbonisation include:

- *Fuel Substitution* - electrode boiler, hydrogen combustion, (solid) biomass combustion
- *CO_2 Capture and Storage or Re-Use* – post combustion CO_2 capture

---

[1] The corresponding MIDDEN reports can be found on https://www.pbl.nl/en/publications/decarbonisation-options-for-large-volume-organic-chemicals-production-shell-moerdijk and https://www.pbl.nl/en/publications/decarbonisation-options-for-large-volume-organic-chemical-production-shell-pernis.

- *Use of Residual Energy* – Circular Steam Project, integrated heat pump in distillation columns
- *Feedstock Substitution* – sustainable alternatives for ethylene, propylene and methanol.

Reading guide

Section 1 provides a general introduction to LyondellBasell's operations in the Netherlands and more specifically, its operations in Botlek and Maasvlakte. Section 2 describes the current situation and processes present at LyondellBasell's Botlek and Maasvlakte sites. Section 3 describes the relevant feedstocks and products of these processes, while options for decarbonisation are systematically evaluated in Section 4. The feasibility of and requirements for those decarbonisation options are discussed in Section 5.

1 LyondellBasell in the Netherlands

1.1 LyondellBasell in the Netherlands

LyondellBasell is one of the largest chemical companies in the world, with saleable products including chemicals, polymers, fuels, and technologies. As a multinational company, its operations are widespread across the globe with manufacturing facilities in America, Europe and Asia (LyondellBasell, 2020). In the Netherlands, LyondellBasell has in total of three manufacturing facilities and a deep-water terminal (i.e. Europoort Terminal). These operating facilities are all located within the Port of Rotterdam industrial cluster, as shown in Figure 1. Table 2 summarises the three manufacturing sites in terms of their economic impact, site area, employee number and the scope 1 CO_2 emissions (direct emissions of the production plant) as registered with the Dutch Emission Authority (Dutch Emissions Authority, 2020).

Figure 1 Locations of LyondellBasell’s operating sites in Maasvlakte, Europoort, Botlek and Moerdijk, relative to the City of Rotterdam (LyondellBasell, 2014)

Table 2 Site-specific information in terms of site area, employee number, economic impact and CO_2 emissions on scope 1 basis (Dutch Emissions Authority, 2020; LyondellBasell, 2020; LyondellBasell, 2020; LyondellBasell, 2020)

Site	Registered Name	Site Area (‘$10^3 m^2$)	Employee Number	Economic Impact (million EUR)[2]	CO_2 Emissions (kt)
Botlek	Lyondell Chemie Nederland B.V.	480	435	289	327
Maasvlakte	Lyondell Bayer Manufacturing Maasvlakte VOF	600	260	289	13
Moerdijk	Basell Benelux B.V.	340	146	45	11

LyondellBasell’s reported emissions only account for 2% of the overall scope 1 emissions from the Dutch chemical industry. However, these emission figures only include the scope 1 emissions, hence there is a significant underestimation of the total CO_2 emissions across the product value chains. LyondellBasell’s strategic location at the Port of Rotterdam industrial cluster allows material and utility sharing between the neighbouring companies, through steam and product pipelines. Many of the required utilities (i.e. steam and electricity) and materials are not produced on-site. Hence, its scope 2 emissions (indirect emissions for generating electricity, external steam supply, etc.) and scope 3 emissions (other indirect emissions that occur in the value chain) are significant.

This research focuses only on the Botlek and Maasvlakte production sites. The scoping is made based on the sites’ economic impacts, which are substantially larger than the Moerdijk site. The two sites are described further in the following subsections.

1.2 Maasvlakte Site

The Maasvlakte production site started its operations in 2003 and is a joint venture between LyondellBasell and Covestro (formerly called Bayer MaterialScience). The two companies each own 50 per cent of the plant and its production, with LyondellBasell acting as the operator. The site houses other different functional buildings such as storage park, laboratory, office building and maintenance workshops. In addition, there are also on-site rail track and truck terminal and a deep-sea harbour (LyondellBasell, 2020). The location of the production site within the Maasvlakte region is as shown in Figure 2.

The Maasvlakte site has only two main end-products – propylene oxide (PO) and styrene monomer (SM), produced using its proprietary PO/SM technology. The PO/SM plant is also currently the largest in the world. Table 3 shows the two products manufactured at the Maasvlakte site and their respective annual production capacity. It is also noted in (Chemical Technology, n.d.), a large portion of LyondellBasell’s share of PO is used to supply feedstock to the butanediol (BDO) plant at the Botlek site.

---

[2] Estimate includes yearly total for goods & services purchased and employee pay and benefits, excluding raw materials purchased (basis 2016). This is converted from USD to EUR based on an average exchange rate of 1.11 EUR/USD in 2016.

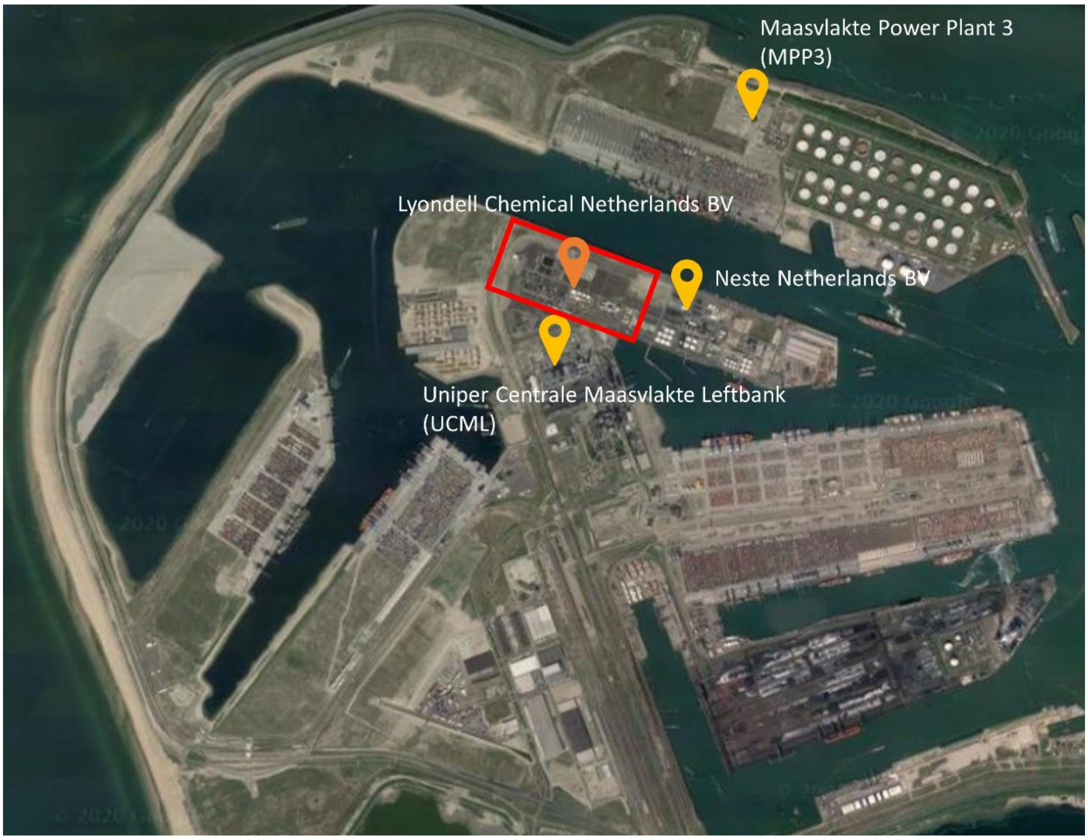

Figure 2 LyondellBasell's Maasvlakte site within the Maasvlakte region. Image is sourced and adapted from Google Maps.

Table 3 Products manufactured at the Maasvlakte site and their respective annual production capacity in kilotonnes, as estimated based on (Port of Rotterdam, 2016; Tebodin, 2017)

Product	Annual Production Capacity (kt)
Propylene Oxide (PO)	385
Styrene Monomer (SM)	864

1.3 Botlek Site

This production site has the longest history out of all LyondellBasell's operations in the Netherlands. Located in Botlek, Rotterdam, it has an independent harbour and site-owned train and truck terminal. It is also linked to the Maasvlakte production site by two 7 km pipelines (LyondellBasell, 2020). Figure 3 shows the location of the production within the Botlek region, as well as relative to a few important stakeholders of LyondellBasell's operations within the Rotterdam region, i.e. WKC Air Products and Eurogen C.V.

Figure 3 LyondellBasell’s Botlek site relative to other relevant industrial sites within the Botlek region. Image is sourced and adapted from Google Maps.

The facility was first built in 1972, producing propylene oxide (PO) and tert-butyl alcohol (TBA) through its proprietary PO/TBA technology. The site has since expanded in 1980 to also produce C4 (i.e. isobutylene), propylene glycol (PG), propylene glycol methyl ether (PGME), methyl tertiary-butyl ether (MTBE) and ethyl tertiary butyl ether (ETBE). In 2002, it became equipped with the world’s largest 1,4-butanediol (BDO) plant. The most recent expansion was in 2015, which saw an increase in butane isomerisation capacity and the addition of two on-site steam boilers (LyondellBasell, 2020). Figure 3 shows the whole suite of products produced in the Botlek production site (Port of Rotterdam, 2016). Some of the products are intermediate or by-products of the main production processes. At the same time, some are used as input materials for the other processes. The material relationships between the different processes are further described in 2.2 and as illustrated in Figure 7.

Table 4 The suite of products manufactured at the Botlek site and their respective annual production capacity in kilotonnes (Port of Rotterdam, 2016)

Product	Annual Production Capacity (kt)
Propylene Oxide (PO)	250
Propylene Glycol (PG)	80
Propylene Glycol Methyl Ether (PGME)	90
Tertbutyl Hydroperoxide (TBHP)	12
Methyl Tertiary Butyl Ether (MTBE)/ Ethyl Tertiary Butyl Ether (ETBE)	400
Gasoline Grade Tert-Butyl Alcohol (TBA)	589
Isobutylene	100
1,4 - Butanediol (BDO)	126
Allyl Alcohol (AA)	16
Methyl Propanediol (MPD)	20

2 Current Processes & Operations at LyondellBasell

LyondellBasell produces a wide suite of chemical products through in total seven chemical processes. The Maasvlakte site has only one main chemical production process – the propylene oxide/styrene monomer (PO/SM) co-production process. On the other hand, the Botlek site has a total of six main chemical processes.

This chapter will elaborate on the main chemical processes present in both production sites in Maasvlakte and Botlek. The elaboration includes a process description of the processes, as well as their respective energy and material flows. Besides, the main external utilities supplied to LyondellBasell are identified and described. On an important note, the current process information is gathered from public sources, and is not verified by LyondellBasell.

2.1 Current Processes and Operations at Maasvlakte Site

2.1.1 Current Processes

LyondellBasell's Maasvlakte operation site produces only two main products: propylene oxide (PO) and styrene monomer (SM) through its proprietary PO/SM co-production technology. The process utilises the ethylbenzene (EB) produced on-site through the benzene alkylation process between benzene and ethylene. The high-level material flow is as illustrated in Figure 4, while the two processes are separately described the later sub-sections.

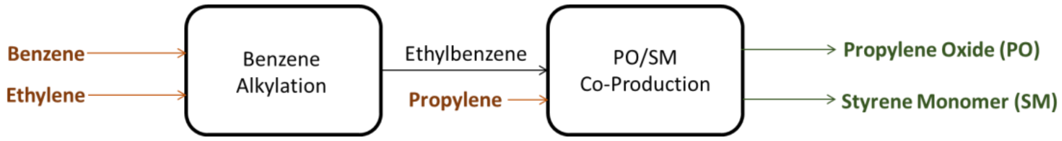

Figure 4 High level material flow in the benzene alkylation and PO/SM co-production processes

2.1.1.1. Benzene Alkylation Process

The benzene alkylation process utilises liquid benzene and gaseous ethylene as the raw input materials. It can be further differentiated into three main successive reaction steps: alkylation, ethylbenzene (EB) purification and transalkylation. The process is schematically illustrated in

Figure 5. Unless stated otherwise, the process is further elaborated based on (Tebodin, 2017), where a detailed process description and process flow diagram can be found.

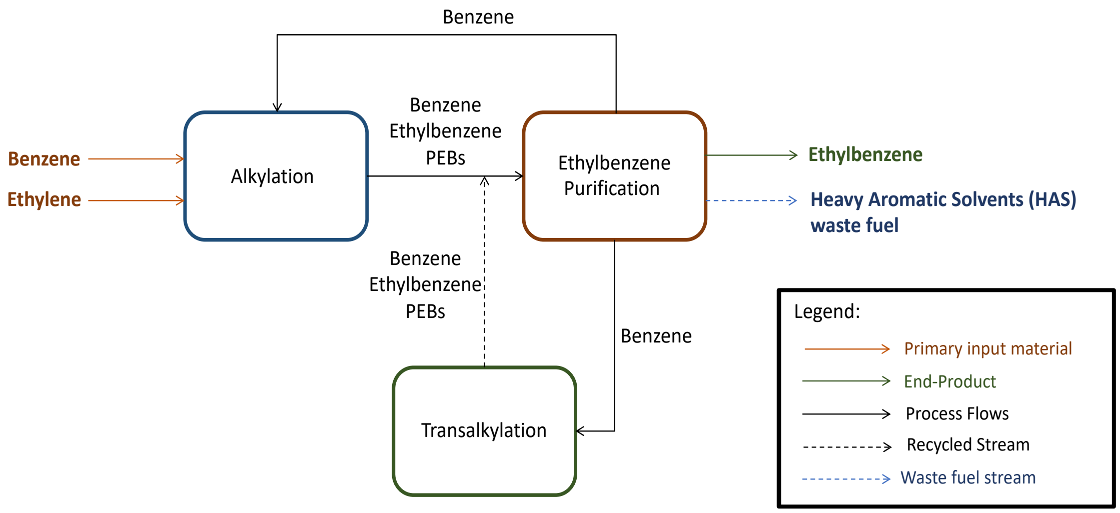

Figure 5 Simplified process flow diagram of the benzene alkylation process

Alkylation
Alkylation is an exothermic reaction between ethylene and benzene into ethylbenzene. In addition, some of the ethylene further react with (di)ethylbenzene to form polyethylbenzenes (PEBs). The liquid phase reaction takes place in two serially-connected reactors at a temperature range between 200°C to 250°C and pressure of 26 to 28 bar(g), in the presence of zeolite catalyst. The alkylation process can be described using the main reaction formulas below:

1) $C_6H_6(Benzene) + C_2(Ethylene) \Longrightarrow C_8H_{10}(Ethylbenzene) \qquad \Delta H = -113kJ/mol$
2) $C_8H_{10}(Ethylbenzene) + C_2(Ethylene) \Longrightarrow C_6H_4(C_2H_5)_2\ (Diethylbenzene) \qquad \Delta H = -113kJ/mol$
3) $C_6H_4(C_2H_5)_2\ (Dithylenzene) + C_2(Ethylene) \Longrightarrow C_6H_3(C_2H_5)_3\ (Triethylbenzene) \qquad \Delta H = -113kJ/mol$

Ethylbenzene (EB) Purification
The effluent from the alkylation unit are then fed into a succession of three distillation columns. The Benzene Column allows the recovery of excess benzene, which is sent to the alkylation unit and the transalkylation unit. The desired product, EB, is recovered from the EB column and later used as input material for the PO/SM co-production process. An EB/PEB stream is recovered from the PEB Column and sent to the transalkylation unit. The bottom product, the heavy aromatic solvent (HAS) stream, is instead exported as fuel.

Transalkylation
Transalkylation reaction is a heat-neutral reaction between PEBs and benzene to form EB. The reaction takes place at around 215 °C and 22 bar(g), in the presence of zeolite catalyst. The effluent from the transalkylation unit containing unreacted benzene and PEBs is again recycled and purified through the distillation columns. The transalkylation process can be described using the main reaction equations below:

1) $C_6H_5(C_2H_5)_2\ (Diethylenzene) + C_2H_6(Benzene)\ =\ 2\ C_6H_5(C_2H_5)\ (Ethylbenzene)$
2) $C_6H_5(C_2H_5)_3\ (Dithylenzene) + C_2H_6(Benzene)\ =\ 3\ C_6H_5(C_2H_5)\ (Ethylbenzene)$

Material and Energy Flows for Benzene Alkylation Process
Table 5 summarises the material and energy flows for the benzene alkylation process. They are based on the Badger EBMax process described in (Hydrocarbon Processing, 2010), which matches closely with the process described above. The exothermic benzene alkylation process also produces steam of lower quality, which is assumed to be recovered and used in

the PO/SM co-production process. Value ranges for the benzene and ethylene input are sourced from (Falcke, et al., 2018), where the input amount shall differ based on the purity of the input streams. Benzene and ethylene are purchased from steam cracking facilities within the region and are transported through ship and pipeline (CE Delft, 2012). The HAS product, together with other waste fuels from the PO/SM co-production process, are exported as waste fuels to external parties.

Table 5 Material and energy flows for the benzene alkylation unit

Material/Energy	Unit	Value (range)	Reference
Input			
Benzene	t/t of EB	0.739 (0.735 - 0.746)	(Hydrocarbon Processing, 2010; Falcke, et al., 2018)
Ethylene	t/t of EB	0.265 (0.254 - 0.265)	(Hydrocarbon Processing, 2010; Falcke, et al., 2018)
High-Pressure Steam	GJ/t of EB	2.98	(Hydrocarbon Processing, 2010), using conversion factor of 3042MJ/t[3]
Output			
Low (LP)-to-Medium-Pressure (MP) Steam	GJ/t of EB	3.8	(Hydrocarbon Processing, 2010), using conversion factor of 2743 MJ/t[4]
Heavy Aromatic Solvents (HAS)	kg/t of EB	3 - 5.6	(Falcke, et al., 2018)

2.1.1.2. Propylene Oxide (PO)/ Styrene Monomer (SM) Co-Production Process

The PO/SM co-production process utilises the ethylbenzene produced in the Benzene Alkylation unit as the primary feedstock. Other raw input materials include propylene and hydrogen. The PO/SM can be further divided into seven main successive production units as shown in Figure 6. Unless stated otherwise, the process is further elaborated based on (Tebodin, 2017), where a detailed process description and process flow diagrams can be found.

---

[3] This assumes that the steam is provided at a pressure level of 50 bar(g) and 340 °C (Sluis, 2014)

[4] This assumes that the steam is provided at a saturated pressure level of 4.5 bar(g) (Tebodin, 2017)

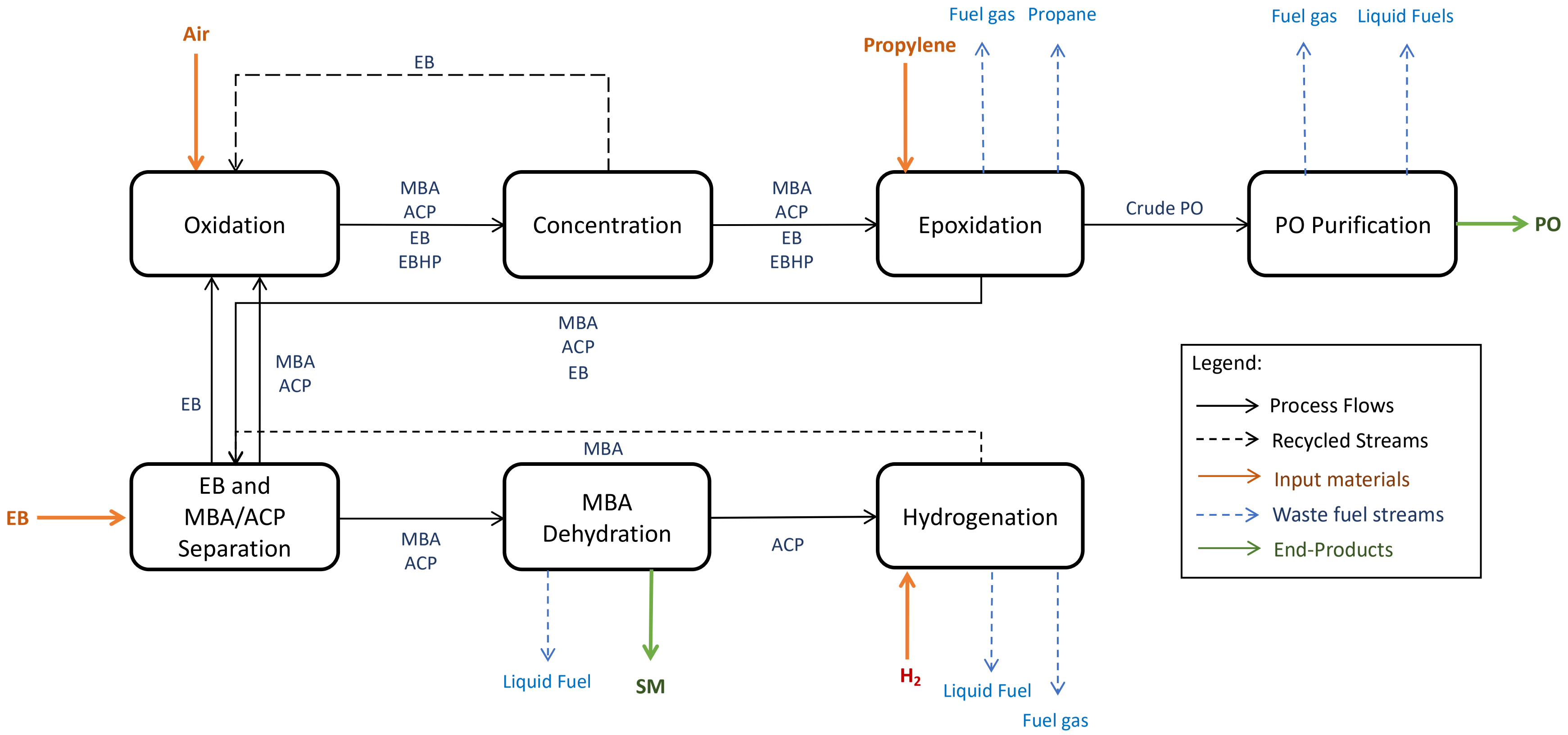

Figure 6 - Process flow diagram of the PO/SM co-production (adapted from Figure 12 in (Tebodin, 2017)

Oxidation

Oxidation is the first chemical reaction step of the PO/SM process. Ethylbenzene (EB) is oxidised into ethylbenzene hydroperoxide (EBHP), methylbenzyl alcohol (MBA) and acetophenone (ACP). The input material, EB, is fed from the EB and MBA & ACP separation unit. The oxidation reaction takes place within two oxidation reactors that are connected in series, at an operating temperature of around 148 °C and operating pressure of 2.4 to 2.7 bar(g). The air, which contains oxygen necessary for the reaction, is brought to the operating pressure with an electric compressor and fed into the reactors through spargers. The chemical reactions are as described using the reaction equations below.

Main exothermic reactions:

1) $C_8H_{10}\ (EB) + O_2 \Longrightarrow C_8H_{10}O_2\ (EHBP) \qquad \Delta H = -101kJ/mol$
2) $C_8H_{10}\ (EB) + \frac{1}{2}O_2 \Longrightarrow C_8H_{10}O\ (MBA) \qquad \Delta H = -190kJ/mol$
3) $C_8H_{10}\ (EB) + O_2 \Longrightarrow C_8H_8O\ (ACP)\ +\ H_2O \qquad \Delta H = -390kJ/mol$

The final liquid product from the reactors is then fed to the concentration unit. On the other hand, the off-gas is cooled in the economiser where the residual EB is condensed, fractionated and recycled back to the oxidation reactors. The remaining non-condensable is scrubbed with a stream of MBA/ACP to recover EB, which the stream is then sent to the EB and MBA & ACP separation unit. A wastewater stream containing acids and peroxides are sent to a lye processing system.

Concentration

The objective of the concentration unit is to increase the EBHP content in the stream fed from the oxidation unit, from 8% to 35% by weight. The concentration process is conducted in two concentrators, which are connected in series and operated in a vacuum condition.

Epoxidation

The concentrated EBHP is reacted highly exothermically with propylene to form PO and ACP as the main products. At the same time, MBA and ACP are formed as the by-products, and later used in the styrene production unit. The epoxidation occurs in two epoxidation reactors that are connected in series, with operating temperature and pressure of around 93-110 °C and 41 bar(g), catalysed by molybdenum catalyst. The reactions are as follows:

1) $C_8H_{10}O_2\ (EBHP) + C_3H_6 \Longrightarrow C_3H_6O\ (PO)\ +\ C_8H_{10}O\ (MBA)\ \ \Delta H = -209kJ/mol$
2) $C_8H_{10}O_2\ (EBHP) \Longrightarrow C_8H_{10}O\ (MBA)\ \ + \frac{1}{2}O_2$
3) $C_8H_{10}O_2\ (EBHP) \Longrightarrow C_8H_8O\ (ACP)\ \ + H_2O$

Following the epoxidation reaction in the reactors, the epoxidate stream is sent for distillation. The distillation process produces streams of fuel gas and propane-by products, which are exported or sold as fuel. This also produces a crude PO stream and a bottom product containing EB/MBA and ACP. Besides, a liquid stream is also produced and sent for the caustic water wash treatment.

PO Purification

The crude PO is then upgraded to saleable product of a purity of 99.9%, through a series of six extractive distillation columns. A few heat integration points are set up to utilise the recovered heat from the extractant circulatory system. Low-pressure steam is also utilised in three of the distillation columns, in addition to the recovered heat. The distillation stage also produces a fuel gas stream and two liquid fuel streams.

EB and MBA/ACP Separation

The EB and MBA & ACP Separation unit is fed with three streams from the Epoxidation unit, Oxidation unit and the ACP Hydrogenation unit. The streams are subsequently distilled to separate the EB, higher hydrocarbons and other residues from the MBA/ACP stream. The EB is separated through vacuum distillation, sent for caustic treatment and eventually used as an input for the Oxidation unit, along with the fresh EB stream from the Benzene Alkylation unit. The final MBA/ACP stream is used as a feed for the MBA Dehydration and SM Purification unit. The separation process also produces salt-containing wastewater stream (referred internally as RFO-637) which is sent to AVR for incineration (CE Delft, 2012), as well as a glycolic fuel stream.

MBA Dehydration and SM Purification

The MBA in the final MBA/ACP stream fed from the EB and MBA/ACP separation unit is dehydrated to form styrene monomer (SM) in this unit. The MBA dehydration process is an endothermic reaction and takes place in the presence of a strong organic acid catalyst, the Para Toluene Sulfonic Acid (PTSA). The dehydrogenation takes place in two parallel reactors, at an operating temperature of 200 °C and pressure of 310 mbar(g). The main dehydration reaction and other side-reactions are as described by the chemical equations below:

1) $C_8H_{10}O\ (MBA) \Longrightarrow C_8H_8\ (Styrene)\ + H_2O \quad \Delta H = +146 kJ/kg$
2) $C_8H_{10}O(MBA) \Longrightarrow C_8H_{10}(EB) + Heavies$
3) $2C_8H_8\ (SM) \Longrightarrow C_{16}H_{16}\ (styrene\ dimer)$

The vapour effluent is fed to a lye and water wash treatment and a series of distillation steps. This results in a pure stream of SM, a separated stream of MBA/ACP sent to the ACP Dehydrogenation unit, as well as liquid fuel.

ACP Hydrogenation

The hydrogenation of ACP into MBA occurs over fixed catalyst beds of copper oxide. The reactors are connected in series, with operating conditions ranging from 16 to 21 mbar(g) and 49 to 62 °C. It is also fed with an equal amount of EB from the storage tank and the required hydrogen is fed through a pipeline, supplied by an external party. Prior to the main hydrogenation process, the MBA/ ACP from the MBA Dehydration and SM Purification unit is first sent to a fractionator to separate out the heavy hydrocarbons through vacuum distillation, to prevent catalyst poisoning. The bottom product is then cooled and exported as fuel. The exothermic chemical reaction between ACP and hydrogen is as described by the chemical equation below:

$$C_8H_8O\ (ACP) +\ H_2 \Longrightarrow C_8H_{10}O\ (MBA) \quad \Delta H = -50 kJ/mol$$

Other side reactions include:

1) $C_8H_8\ (SM)\ +\ H_2 \Longrightarrow C_8H_{10}\ (EB)$
2) $C_8H_8O\ (MBA)\ +\ 2H_2 \Longrightarrow C_8H_{10}\ (EB) + H_2O$

The hydrogenate from the reactors is then sent to a flash drum to remove the waste gas. The remaining hydrogenate is recycled to the EB and MBA/ACP Separation unit.

Material and Energy Flows for the PO/SM Co-Production Process

Table 6 summarises the energy and material flows for the PO/SM co-production process. The required ethylbenzene is produced on-site through the benzene alkylation process. Propylene is sourced from steam cracking facilities and is transported through ship and pipeline (CE

Delft, 2012), while hydrogen is sourced via pipeline from Air Liquide (de Kruif, 2004). A number of waste fuel streams are identified, which the energy content is approximated based on indicative amount provided in (LyondellBasell, 2007) for the year 2006. The heavy liquid fuel output also includes the HAS stream from the benzene alkylation process. The glycolic fuel, heavy liquid fuel and vapour gas streams are sent to the UCML CHP plant as replacement fuel, while the propane stream is sold to the regular fuel market (CE Delft, 2012). On the other hand, the RFO-637 is sent to AVR Rozenburg as combustible fuel for the incineration of the caustic wastewater (CWW). The processes generally produce around 220 kt of CWW per year (LyondellBasell, 2007).

Table 6 Material and energy flows for the PO/SM co-production process

Material/Energy	Unit	Value (range)	Reference
Input			
Ethylbenzene	t/t of SM	1.15 (1.1-1.2)	(Falcke, et al., 2018)
Propylene	t/t of SM	0.33	Approximated based on propylene: PO stoichiometric ratio of 1:1
Hydrogen	kg/t of SM	4.17	Approximated based on maximum annual required quantity indicated in (Tebodin, 2017)
Electricity	GJ/t of SM	0.6 (0.576 – 0.72)	(Falcke, et al., 2018)
Steam (net input)	GJ/t of SM	5.89	see footnote[5]
Output			
Propylene Oxide (PO)	t/t of SM	0.45	(Tebodin, 2017)
Glycolic Fuel	GJ/t of SM	0.57	(LyondellBasell, 2007); conversion factor of 41 GJ/t
Heavy Liquid Fuel	GJ/t of SM	1.43	Including HAS stream from benzene alkylation process; (LyondellBasell, 2007); conversion factor of 41 GJ/t
Vapour Gas	GJ/t of SM	0.55	(LyondellBasell, 2007); conversion factor of 45.2 GJ/t
Propane	GJ/t of SM	0.42	(LyondellBasell, 2007); conversion factor of 45.2 GJ/t
Other Combustible Stream (RFO-637)	t/t of SM	0.03	(LyondellBasell, 2007)

2.1.2 Annual Material & Energy Consumption and CO_2 Emissions

2.1.2.1. Annual Material & Energy Consumption & Waste Fuel Production

Table 7 and Table 8 shows an estimation of the annual material and energy consumption for both the benzene alkylation and PO/SM co-production process. The figures are estimated based on the SM production capacity of 864 kt and the energy consumption values (on per unit tonne of product basis) indicated in Table 5 and Table 6.

---

[5] Net steam input for the PO/SM Co-production refers to net steam input from external utility company(ies). This assumes a gross steam input of 11.16 GJ/t SM (value range between 11.16 and 14.04 GJ/t of SM (Hydrocarbon Processing, 2010)), as well as utilisation of recovered heat from benzene alkylation process and PO/SM process, with an amount of 4.19 (Hydrocarbon Processing, 2010) and 1.08 (Falcke, et al., 2018) GJ/t of SM, respectively.

Table 7 Annual material usage for the PO/SM co-production process

Input Material	Annual Input (kt/year)
Benzene	730
Ethylene	260
Propylene	280
Hydrogen	4

Table 8 Annual energy usage for the PO/SM co-production process

Steam (PJ/year)	Electricity (PJ/year)	Total (PJ/year)
7.9	0.5	8.4

The amount of waste streams is estimated based on the statistics provided for 2006 in (LyondellBasell, 2007) and the (expected) increased in the original production capacity by 35% (Tebodin, 2017). These also provide valuable fuel streams if the production site withdraws its dependency on the external utility companies. The RFO-637 stream is used as combustible fuel stream for caustic wastewater incineration.

Table 9 Estimated amount of waste fuel streams from Maasvlakte site

	Annual amount (t/year)	Energy Content (PJ/year)
Propane	8000	0.36
Glycolic Fuel	12000	0.49
Heavy Liquid Fuel (RFO-635)	30100	1.23
Fuel Gas	10500	0.48
Other Combustible Stream (RFO-637)	40300	PM

2.1.2.2. Supply of Utilities

The main utilities required for the production of PO and SM through benzene alkylation and PO/SM co-production processes are electricity and medium-to-high pressure steam. These are exclusively sourced from the neighbouring utility sites, namely the Utility Centre Maasvlakte Leftbank (UCML) and Maasvlakte Power Plant 3 (MPP3). These two utility sites are owned by Uniper (formerly known as E.ON Benelux).

UCML was established in 2003 and consists of a gas-fired CHP (gas turbine equipped with a heat recovery steam generator (HRSG)) and direct-fired boilers (European Environment Agency, 2020; Sluis, 2014). It was primarily set up to produce processing steam for LyondellBasell’s Maasvlakte site and is connected to Maasvlakte site through a 25kV electricity cable (Energiekamer). Rated at 70 MW electricity output and 375 t/hour steam output (Uniper, n.d.), UCML also provides utilities to NesteOil and LNG GATE Terminal (Clingendael International Energy Programme (CIEP), 2017). MPP3, recently commissioned in 2017, is a coal and biomass (maximum of 30%) co-combustion power plant rated at 1070 MW. Besides, the new plant also produces steam and cooling water for nearby businesses, including LyondellBasell (Port of Rotterdam, 2018; Santen & Boere, 2016).

An integrated steam system of four steam pressure levels[6] is established at the Maasvlakte site to enable cascaded use of steam. For example, the high pressure (HP) steam condensate from one process is connected to the medium pressure (MP) steam system for use in other processes (Tebodin, 2017). The utility sites receive waste fuel streams, namely the glycolic fuel, fuel gas and heavy fuel from LyondellBasell's Maasvlakte site as replacement fuel (CE Delft, 2012; Port of Rotterdam, 2018). Nevertheless, the exact proportion of the steam and electricity sourced from the two different sites, as well as the proportion of the fuel streams received by them, are not known from public sources.

2.1.2.3. Annual CO_2 Emissions

Figure 6 shows the annual CO_2 emissions for the Maasvlakte production site. Scope 1 emissions refer to their reported emissions for the year 2019 (Dutch Emissions Authority, 2020). As there are no on-site steam boilers or furnaces, the scope 1 emissions could likely be attributed to the flaring, catalytic converter and thermal combustor systems (Tebodin, 2017).

The exact proportions of steam supply from UCML and MPP3, as well as their respective steam and electricity emission factors are not known. Therefore, the scope 2 emissions are estimated based on a gas-fired CHP electrical and steam thermal efficiency of 36% and 49%[7], respectively. This hence refers to electricity and steam emission factors of 85.4 and 52.8 kg/GJ, respectively, as determined based attribution method suggested in (European Commission, 2018) (See Appendix for the attribution formula).

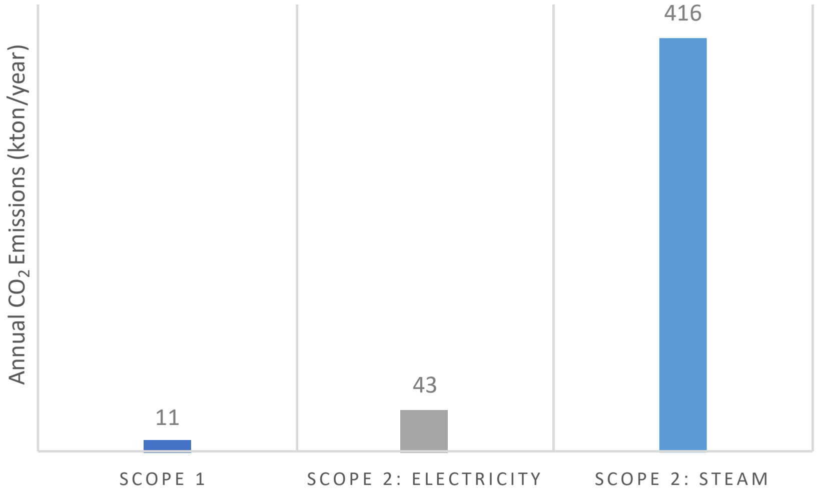

Figure 6 Estimated annual scope 1 and 2 emissions for the Maasvlakte site

2.1.2.4. Wastewater Treatment

The production processes in Maasvlakte produces a significant amount of caustic wastewater (CWW). This CWW is first treated and then sent for further processing, i.e. incineration. The incineration was performed at AVR Rozenburg[8] (IndustriePerspectief, n.d.), which received

---

[6] The four steam pressure levels are HP (50 bar(g)), MP (20 bar(g)), LP (4.5 bar(g)), and LLP(2.5 bar(g)).

[7] Based on reference efficiencies for a 45MW$_e$ GT in (Cogeneration Observatory and Dissemination Europe (CODE2), 2014).

[8] The waste treatment contract between LyondellBasell (Maasvlakte) and AVR is said to have expired in 2019.

approximately 220 kt of CWW from the Maasvlakte site through pipeline, as well as combustible waste streams from Maasvlakte and Botlek sites (Tebodin, 2017). The CWW, which contains a large amount of salt, was incinerated using the combustible waste streams and a significant amount of primary fuels (e.g. natural gas, oil), raising the temperature of the flue gas to a temperature of over 1200°C (CE Delft, 2012; Tebodin, 2017). The produced steam from the incineration was then used by AVR Rozenburg to produce electricity (fed to the grid) and processing steam for other industrial consumers (Tebodin, 2017). An energy savings and carbon reduction project, namely Circular Steam Project, is planned to begin operation in 2020 to process the CWW alternatively and in-house, as further described in 4.3.1.

2.2 Current Processes and Operations at Botlek Site

2.2.1 Current Processes

LyondellBasell's Botlek production site produces a wide range of chemical products (see Table 4). The production facility started with the propylene oxide/tert butyl alcohol (PO/TBA) co-production process in 1972 and has since then expanded to incorporate five other main production processes. These other chemical processes utilise the PO and TBA as their input materials to subsequently produce saleable end products or input material for another process (Chemical Technology, n.d.; LyondellBasell, 2007). The material relationships of the different chemical processes at the Botlek production site are illustrated in Figure 7. To further explain, part of the PO produced from the PO/TBA process is utilised as input materials for other chemical processes on-site, producing propylene glycol (PG), propylene glycol methyl ether (PGME), as well as in the Butanediol (BDO) process. The remaining PO is sold as final products to external parties. The TBA is either further purified and sold as gasoline grade TBA or further processed into isobutylene, the precursor chemical for the on-site production of methyl tertiary-butyl ether (MTBE) and ethyl tertiary butyl ether (ETBE). The co-product, tertbutyl hydroperoxide (TBHP), is purified into saleable end-product at a much lower capacity of around 12kt annually.

The six main chemical processes to be described in this subchapter are as follows:

2.2.1.1. Propylene oxide/tert butyl alcohol (PO/TBA) co-production (including the isomerisation of n-butane)
2.2.1.2. Production of propylene glycol (PG)
2.2.1.3. Production of propylene glycol methyl ether (PGME)
2.2.1.4. Production of isobutylene
2.2.1.5. Production of methyl tertiary butyl ether (MTBE) and ethyl tertiary butyl ether (ETBE)
2.2.1.6. Production of 1,4-butanediol (1,4-BDO), allyl alcohol & methyl propanediol (MPD)

Associated with the PO/TBA process are the TBHP purification process and the TBA purification process. The TBHP purification process utilises part of the effluent stream from the PO/TBA process to produce a concentrated TBHP solution. The TBA purification process instead purifies the crude TBA into gasoline grade TBA. The processes adopted for the TBHP purification and TBA purification in LyondellBasell's operation is however not known, hence not further described in this report.

The material and energy flows for the individual processes are included in their respective subsections. Additionally, the overall annual material and energy consumption, as well as waste fuel production are further detailed in 2.2.2.1.

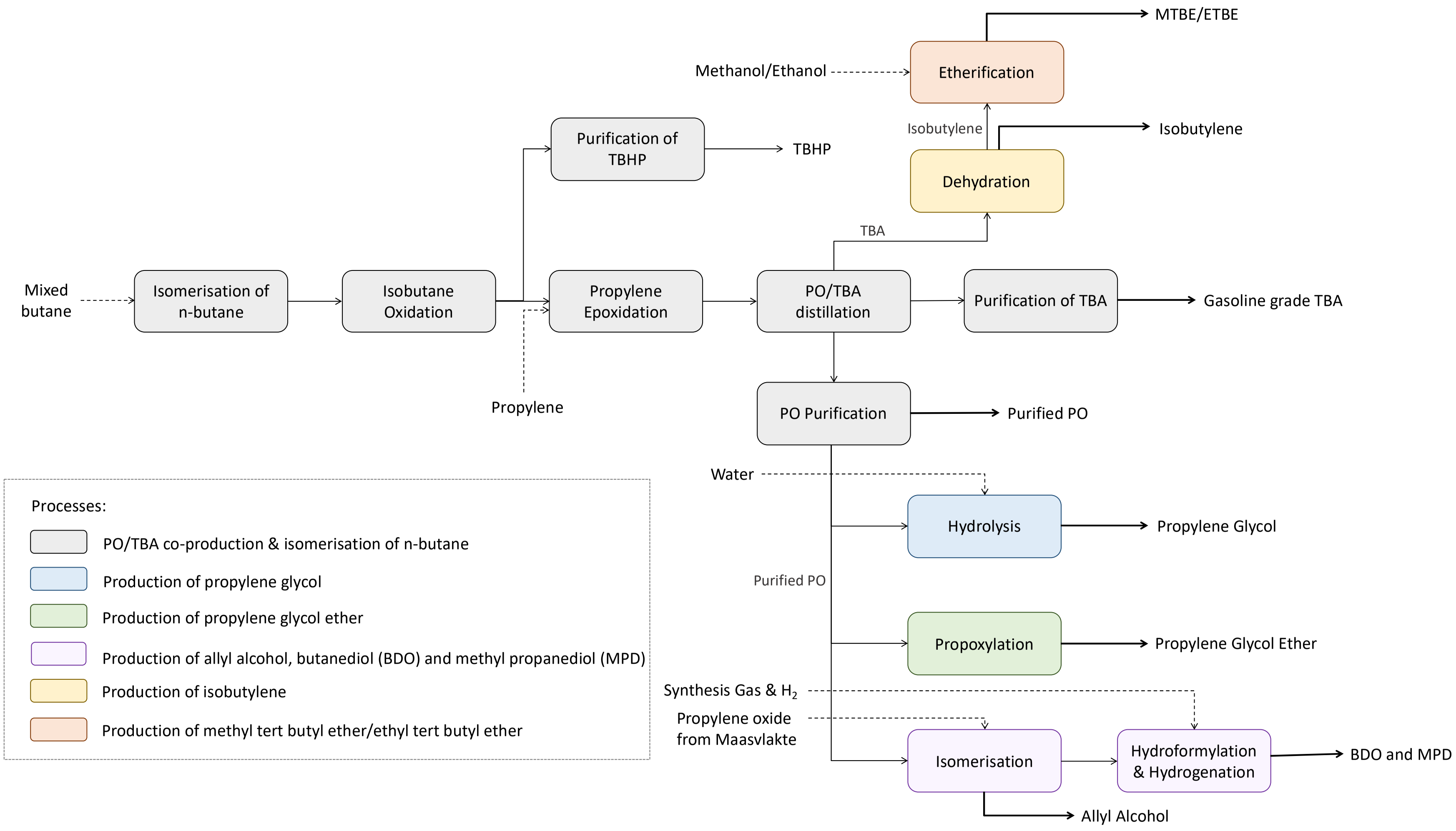

Figure 7 Material flows of the chemical processes at the Botlek production site (adapted from (LyondellBasell, 2007))

2.2.1.1. Propylene Oxide/Tert Butyl Alcohol (PO/TBA) Co-Production Process

The co-production process produces PO and TBA as the main co-products, as well as tert butyl hydroperoxide (TBHP) as the by-product. The process utilises propylene and isobutane as the main raw input materials. The isobutane feedstock is obtained from LyondellBasell's on-site butane isomerisation facility, which isomerises mixed butane stream into isobutane (LyondellBasell, 2007). The isomerisation process is further described later.

The PO/TBA co-production process can be further differentiated into two main successive units, the Isobutane Oxidation unit and the Propylene Epoxidation unit. The processing units are schematically presented in Figure 8 and further described in the following paragraphs based on (Ghanta, Fahey, Busch, & Subramaniam, 2013) unless stated otherwise. This process description is said to be reflecting LyondellBasell's conventional PO/TBA process in the United States.

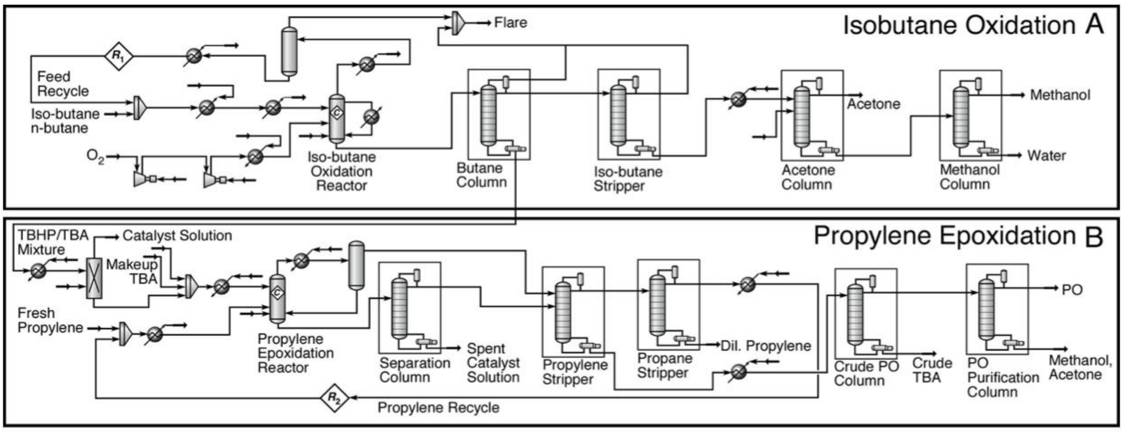

Figure 8 Process flow of the PO/TBA co-production process (Ghanta, Fahey, Busch, & Subramaniam, 2013)

Isobutane Oxidation

This stage involves the exothermic oxidation reaction between isobutane and oxygen to form TBHP and the major co-product, TBA. The TBHP and the TBA will then be fed to the second unit, propylene epoxidation, of which TBHP will further react with propylene to form propylene oxide. The oxidation occurs in a non-catalytic liquid phase in six parallelly-arranged continuous stirred tank reactors (CSTR), with typical conditions of 3 MPa and 135 °C. The reaction has an average residence time of 10 hours. The oxygen concentration in the liquid is kept below 4-7 mol%. The chemical reactions forming TBHP and TBA can be described with the chemical equations below (Ghanta, 2008):

1) $C_4H_{10}\ (Isobutane)\ +\ O_2 \Rightarrow C_4H_{10}O_2\ (TBHP) \qquad \Delta H = -251.5\ kJ/mol$

2) $C_4H_{10}(Isobutane)\ +\ \frac{1}{2}\ O_2 \Rightarrow C_4H_{10}O\ (TBA) \qquad \Delta H = -208.5\ kJ/mol$

The exothermic reaction also vaporises part of the mixture, which is partially condensed to recover the isobutane back to the reactors. The liquid fraction of the reactors, containing both unreacted reactants and products, are sent to a series of distillation columns where TBA and TBHP are recovered from other by-products. Cooling water is used in the condensers in all the distillation columns.

Propylene Epoxidation
TBHP formed in the Isobutane Oxidation unit is reacted with propylene in four parallelly-arranged stirred tank reactors to form propylene oxide and TBA. The epoxidation reaction occurs over a residence time of 2 hours, with operating conditions of 3.5 MPa and 121 °C, in the presence of a homogeneous molybdenum-based catalyst. The exothermic epoxidation reaction can be described using the chemical equation below (Ghanta, 2008):

$$C_3H_6\ (Propylene)\ +\ C_4H_{10}O_2\ (TBHP)\ \Rightarrow C_3H_6O\ (PO)\ +\ C_4H_{10}O\ (TBA)$$

Following the epoxidation reaction, the liquid effluent is sent to a series of distillation column where PO and crude TBA are separated out from the remaining mixture. The distillation stages also allow the catalyst solution and unreacted propylene to be recovered, while crude PO is further purified in the presence of octane as an extractive agent (LyondellBasell, 2007; U.S. Patent No. 5,133,839, 1992). Referring to Figure 8, the Separation Column, Propane Stripper and PO Purification Column are chilled with normal cooling water, while Propylene Stripper and Crude PO Column are cooled with chilled water.

Isomerisation of n-Butane

The butane isomerisation process serves to isomerise straight-chain n-butane into isobutane. The isobutane is then used as the input material for the PO/TBA co-production process. As indicated in (Staatscourant, 2012), LyondellBasell has an isomerisation capacity of 80 tonnes per hour. There are several different process configurations, differing in ways such as the type of catalyst utilised (i.e. zeolite or chloride-promoted), reaction temperatures, separator equipment used (i.e. separation based on boiling points or molecular size). These variations can be found described in (Coker, 2007; Siemens AG, 2016; Barthe, Chaugny, Roudier, & Delgado Sancho, 2015; Robinson & Hsu, 2017). Nonetheless, the exact process configuration utilised in the Botlek site is not known.

In general, the mixed-butane feedstock is first dried and then fed to the isomerisation reactors. The operating conditions differ depending on the type of catalyst used. Hydrogen gas is also added to inhibit the formation of olefins/carbon deposits (Barthe, Chaugny, Roudier, & Delgado Sancho, 2015; Robinson & Hsu, 2017). Following the isomerisation process, the light ends are fractionated and exported as fuel gas or sent to a recovery unit. Depending on the process configuration, the remaining stream, which contains unconverted n-butane, may or may not be sent to an additional separation column to recycle the unreacted n-butane (Barthe, Chaugny, Roudier, & Delgado Sancho, 2015). The recycling of unconverted n-butane shall lead to a yield between 95-98%, or otherwise, an 80% conversion rate (Barthe, Chaugny, Roudier, & Delgado Sancho, 2015).

Material and Energy Flows for PO/TBA Co-Production Process & Isomerisation of n-Butane

This section elaborates on the energy and material flows for the PO/TBA co-production process, as well as the n-butane isomerisation process, as shown in Table 10 and Table 11. The isobutane feedstock is provided by the on-site butane isomerisation capacity, which utilises mixed butane stream obtained from an external party (Staatscourant, 2012). The propylene feedstock is supplied from steam cracking installations through ship and pipeline (CE Delft, 2012), while the oxygen is supplied by Air Products.

As noted in the butane isomerisation process description above, the exact process configuration used by LyondellBasell is not known. A wide range of utility requirements is provided for the isomerisation of C4-C6 feedstock in (Barthe, Chaugny, Roudier, & Delgado Sancho, 2015), covering a spectrum of possible process configurations. The utility requirements shall differ based on the catalyst technology used, the separation method and the recycling process(es) involved. The mixed butane feed input is calculated based on an assumed yield of 95%. The annual mixed butane feedstock (see Table 17) is calculated assuming all isobutane required for the PO/TBA process is provided by the isomerisation unit.

Table 10 Material and energy flows of the PO/TBA process

Material/Energy	Unit	Value	Reference
Input			
Isobutane	t/t of PO	1.94	Approximated based on isobutane conversion efficiency of 100%, TBHP molar selectivity (based on isobutane consumption) of 53.4% and TBHP conversion rate of 98% and PO molar selectivity (based on TBHP consumption) of 98.5% (Ghanta, Fahey, Busch, & Subramaniam, 2013)
Propylene	t/t of PO	0.72	Approximated based on conversion efficiency and molar selectivity of 100%, and propylene: PO stochiometric ratio of 1:1 (Ghanta, Fahey, Busch, & Subramaniam, 2013)
Oxygen	t/t of PO	0.79	Approximated based on TBHP:O_2 and TBA:O_2 stochiometric ratio of 1:1 and 1:0.5
Electricity	GJ/t of PO	2.77	(Ghanta, Fahey, Busch, & Subramaniam, 2013)
Steam	GJ/t of PO	17.58	Approximated based on steam input parameter provided in (Ghanta, Fahey, Busch, & Subramaniam, 2013)[9] and conversion factor of 3042 MJ/t[10]

Table 11: Material and energy flows of the butane isomerisation process

Material/Energy	Unit	Value (range)	Reference
Input			
Mixed butane	t/t of isobutane	1.05	Approximated based on assumed yield of 95% (Barthe, Chaugny, Roudier, & Delgado Sancho, 2015)
Electricity	GJ/t of isobutane	0.09 (0.07-0.108)	(Barthe, Chaugny, Roudier, & Delgado Sancho, 2015)
Steam	GJ/t of isobutane	1.37 (0.91-1.83)	Approximated based on steam input parameter provided in (Barthe, Chaugny, Roudier, & Delgado Sancho, 2015)[11] and conversion factor of 3042 MJ/t[10]

2.2.1.2. Production of Propylene Glycol (PG)

The production of propylene glycol (PG) utilises the propylene oxide (PO) produced on-site through the PO/TBA co-production process, as the main input material. PG is produced through the direct hydrolysis of PO with water. The process flow is schematically represented in Figure 9, consisting of the hydrolysis reactors, dehydration columns and distillation

---

[9] Steam input of 5.78 t/t of PO (Ghanta, Fahey, Busch, & Subramaniam, 2013).

[10] This assumes that the steam is provided at a pressure level of 50 bar(g) and 340 °C (Sluis, 2014).

[11] Steam input range of 0.3 – 0.6 t/t of isobutane (Barthe, Chaugny, Roudier, & Delgado Sancho, 2015).

columns. The process is further described in the following paragraphs, primarily based on (Sullivan, 2012) unless stated otherwise.

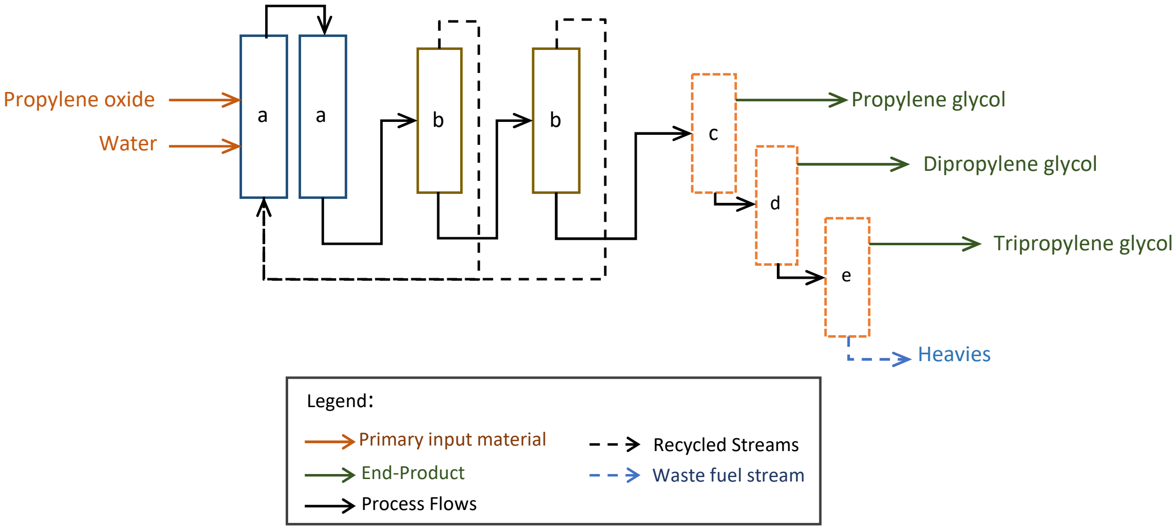

Figure 9 Process flow diagram in producing PG through the hydrolysis of PO. a) Hydrolysis reactors; b) Dehydration columns; c – e) Vacuum distillation columns (as adapted from (Sullivan, 2012)).

PO and water are fed into the two serially-arranged reactors at a molar ratio of 1:15, where the hydrolysis occurs without the presence of a catalyst. The excessive amount of water limits the formation of dipropylene glycol (DPG) and tripropylene glycol (TPG) (Martin & Murphy, 2000). The initial operating conditions are at 125 °C and approximately 2 MPa, of which the reactor temperature rises to 190 °C due to the exothermic reaction. The hydrolysis reaction can be described with chemical equations (Valbert, Zajacek, & Orenbuch, 1993) below:

$$C_3H_6O\ (PO) + H_2O \Rightarrow C_3H_8O_2\ (PG) \qquad \Delta H = -351\ kJ/mol$$

The reaction effluent generally consists of PG, DPG and TPG in the ratio of 100:10:1 (Sullivan, 2012), which shall vary depending on the propylene oxide to water ratio. Following the reaction, the liquid effluent is first fed to dehydration columns. Water is stripped off from the effluent and is recycled back to the reactors. The remaining stream is fed to a series of vacuum distillation columns, where PG, DPG and TPG are separated from each other. The heavy residues, consisting of heavier glycols, can be used as fuel (Martin & Murphy, 2000).

Material and Energy Flows for PG Production

Table 12 summarises the material and energy flows for the production of PG, on per unit tonne of PG basis, as sourced from (Dunn, et al., 2015). The numbers provided in the literature are as modelled by the authors using Aspen Plus with Peng-Robin thermodynamic property method. 90% of the steam consumption is consumed by the distillation columns.

Table 12 Material and energy flows for the production of PG

Material/Energy	Unit	Value	Reference
Input			
Propylene Oxide (PO)	t/t of PG	1.10	(Dunn, et al., 2015), which assumed conversion rate to PG of 89%
Electricity	GJ/t of PG	0.11	(Dunn, et al., 2015)
Steam	GJ/t of PG	9.28	Approximated based on primary fuel input in (Dunn, et al., 2015) using boiler efficiency of 80%[12]

2.2.1.3. Production of Propylene Glycol Methyl Ether (PGME)

Propylene glycol methyl ether (PGME) is synthesised through the propoxylation reaction between methanol and propylene oxide (PO) (LyondellBasell, 2017; LyondellBasell, 2007). The PO is manufactured on-site through the PO/TBA process. The reaction occurs in a closed system, at operating conditions of 94 to 180 °C and 26 bar (Munn, et al., 2006). Various types of acid and alkali-based catalysts can be used (Trent, 2001). The reaction is exothermic with the heat of reaction ranging between -80 to -100 kJ/ mol (Barnicki, 2017). The reaction also produces by-products including dipropylene glycol methyl ether (DPGME), tripropylene glycol methyl ether (TPGME), and other heavier ethers (Barnicki, 2017; Trent, 2001). It is noted that 2-methoxy-1-propanol will also form, which can be recovered and converted into PGME (Munn, et al., 2006). The main reaction is described with the chemical equation as follows:

$$C_3H_6O\ (PO) + CH_3OH \Longrightarrow C_4H_{10}O_2\ (PGME)$$

The reactor effluent is then fed to a series of distillation columns. The excess methanol is recovered and recycled to the reactor from the first column. The remaining effluent is then further distilled into different ether streams (Munn, et al., 2006; Barnicki, 2017). The bottom product, containing the catalyst solution, is recycled and reused or incinerated (Munn, et al., 2006; Falcke, et al., 2018).

Material and Energy Flows for PGME Production

Table 13 summarises the material and energy flows for the production of PGME, on per unit tonne of PGME basis. The energy inputs are as approximated in (Sutter, 2007) for the production of ethylene glycol methyl ether (EGME), based on a large chemical production plant in Germany. The EGME is formed from the reaction between ethylene oxide and ethanol. Nevertheless, it is assumed that the energy input values are applicable for the production of PGME, as the two processes shares a similar process flow and differ from each other within a relatively narrow range of operating conditions (Barnicki, 2017).

---

[12] As assumed in (Dunn, et al., 2015).

Table 13 Material and energy flows for the production of PGME

Material/Energy	Unit	Value	Reference
Input			
Propylene Oxide (PO)	t/t of PGME	0.76	approximated based on conversion efficiency of 100% and molar selectivity of 85% (Barnicki, 2017)
Methanol	t/t of PGME	0.42	approximated based on PGME: methanol stoichiometric ratio of 1:1, conversion efficiency of 100% and molar selectivity of 85%
Electricity	GJ/t of PGME	1.2	(Sutter, 2007)
Steam	GJ/t of PGME	1.6	approximated from primary fuel input provided in (Sutter, 2007) with assumed natural gas boiler efficiency of 80%

2.2.1.4. Production of Isobutylene

The production of isobutylene at LyondellBasell's Botlek site is through the dehydration process of tert butyl alcohol (TBA). The TBA is formed from the PO/TBA co-production process, as described in 2.2.1.1. The produced isobutylene is then used as the input material to produce methyl tertiary-butyl ether (MTBE) and ethyl tertiary butyl ether (ETBE) through etherification process (as described in 0) or sold as a final product.

The dehydration process can be carried out in the liquid or vapour phase (with a temperature between 260 and 370 °C), while the latter requires higher-cost equipment and more energy. In addition, different types of catalyst and an azeotroping agent may be used, depending on the process design (Weissermel & Arpe, 2003; Europe Patent No. EP0712824A1, 1996). The process described below is a liquid phase dehydration reaction, based on a European patent assigned to ARCO Chemical Technology, L.P. (currently known as LyondellBasell) (Europe Patent No. EP0712824A1, 1996) unless stated otherwise.

The TBA is dehydrated into isobutylene and water endothermically, in the presence of para toluene sulfonic acid (PTSA) catalyst. The dehydrator is operated at a temperature of 160 °C and pressure of approximately 14 bar (IHS Markit, 2013). The reversible reaction can be described with the chemical equation (Honkela, Ouni, & Krause, 2004) as follows:

$$C_4H_{10}O\ (TBA)\ \rightleftharpoons\ C_4H_8\ (Isobutylene)\ +\ H_2O \qquad \Delta H\ =\ 26-34\ kJ/mol$$

Following that, the stream is sent to the separation zone for further phase separation. The cooled reaction mixture consists of three phases, a vapour stream, an organic-rich layer and a water-rich layer. The vapour stream, made up of 96.4% of isobutylene, is separated from the liquid condensate as the final product. The organic-rich condensate is recycled back to the dehydrator, while the water-rich layer is removed as a wastewater stream.

Material and Energy Flows for Isobutylene Production

Table 14 summarises the material and energy flows for the production of isobutylene, on per unit tonne of isobutylene basis. The energy consumption data is sourced from (Lassacher, Fazeni-Fraisl, & Lindorfer, 2018). The process assessed in (Lassacher, Fazeni-Fraisl, &

Lindorfer, 2018) has however assumed the use of a zeolite-based catalyst with phosphoric acid, instead of a PTSA catalyst.

Table 14: Material and energy flows for the production of isobutylene

Material/Energy	Unit	Value	Reference
Input			
Tert butyl alcohol (TBA)	t/t of isobutylene	1.43	Approximated with conversion efficiency of 98% and stream purity of 94.5% (Europe Patent No. EP0712824A1, 1996)
Electricity	GJ/t of isobutylene	0.22	(Lassacher, Fazeni-Fraisl, & Lindorfer, 2018)
Steam	GJ/t of isobutylene	14.21	(Lassacher, Fazeni-Fraisl, & Lindorfer, 2018); equivalent to 5.1 tonnes of steam at 13.79 bar

2.2.1.5. Production of Methyl Tertiary Butyl Ether (MTBE) and Ethyl Tertiary Butyl Ether (ETBE)

LyondellBasell's Botlek site has a total annual production capacity of 400 kt for both methyl tertiary butyl ether (MTBE) and ethyl tertiary butyl ether (ETBE), though the proportions of the two products are not known (Port of Rotterdam, 2016). The production processes of MTBE and ETBE are similar in terms of the reaction process (Domingues, Pinheiro, & Oliveira, 2017; Weissermel & Arpe, 2003) and only require slight configuration modifications (Barthe, Chaugny, Roudier, & Delgado Sancho, 2015), as further explained below. MTBE is produced through the etherification process between isobutylene and methanol, while ETBE forms from the reaction between isobutylene and ethanol.

Part of the required isobutylene is sourced from the on-site isobutylene production unit (as described in 0), which has an annual capacity of 100 kt. The remaining input is expected to be supplemented by external party. The methanol and ethanol are sourced from external parties. In addition, bio-based ethanol is also used to produce bio-ETBE, of which the capacity is not known. The etherification process described below is generally applicable for the MTBE production process, primarily based on (Barthe, Chaugny, Roudier, & Delgado Sancho, 2015) unless stated otherwise.

MTBE production

The process configuration may either involve two reactors in a so-called conventional process (Figure 10) or combination of a reactor and a reactive distillation column in a so-called reactive distillation process (Figure 11), prior to further distillation. In both process configurations, the etherification reaction between methanol and isobutylene is catalysed using an acidic ion exchange resin catalyst and operated under the pressure of 14 bar(g) and a temperature range of 45-90 °C (Hydrocarbon Processing, 2010; Barthe, Chaugny, Roudier, & Delgado Sancho, 2015). The etherification reaction can be described with the chemical equation (Zhang, Hidajat, & Raj, 2001) below:

$$C_4H_8\ (Isobutylene) + CH_3OH\ (methanol) \rightleftharpoons C_5H_{12}O\ \ (MTBE) \qquad \Delta H = -37.3\ kJ/mol$$

The effluent is then fed into either a reactive distillation column or a second reactor, allowing a second-time reaction to take place, maximising the conversion rate to over 99%. In the process where reactive distillation column is used, the ether stream is recovered as the bottom product from the reactive distillation column. Whereas in the conventional process, the effluent is fed to the debutaniser for MTBE recovery. Subsequently, the effluent from either the distillation column or the debutaniser is fed to a water wash column where methanol readily dissolves in the water solvent and the raffinate is removed. The resulting methanol-water mixture is then distilled, and the recovered methanol stream is recycled back to the first reactor. The use of pervaporation membrane as a separation method is also noted in (Weissermel & Arpe, 2003).

The process employed at LyondellBasell's Botlek site is likely to be a conventional process, where adiabatic fixed bed reactors are used (Hamid & Ali, 2004). It is also mentioned in (Europe Patent No. EP0671394A1, 1995), that the reaction occurs in the presence of a sulfonic acid catalyst, under operating conditions of 50 °C and 14 bar.

ETBE production

It is noted in (Barthe, Chaugny, Roudier, & Delgado Sancho, 2015) that the MTBE unit may be used to produce ETBE with minor modifications. The modifications include increasing the bottom temperature in the catalytic column, adjusting the temperatures in ethanol/water column and increasing the capacity of the column and cooler.

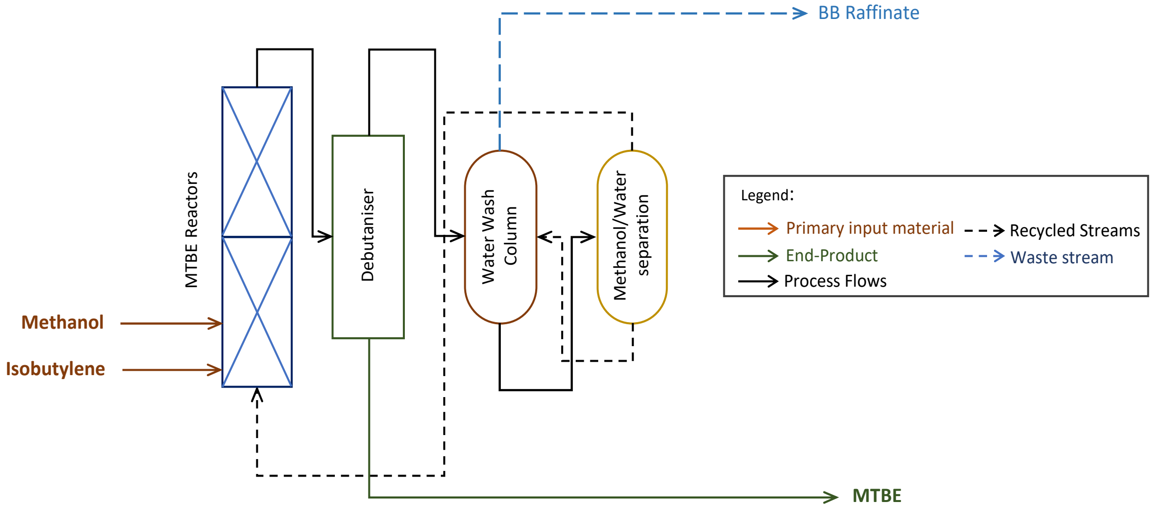

Figure 10 A simplified process flow diagram, adapted from an Uhde (Edeleanu) MTBE process utilising two serially connected reactors shown in (Hydrocarbon Processing, 2010)

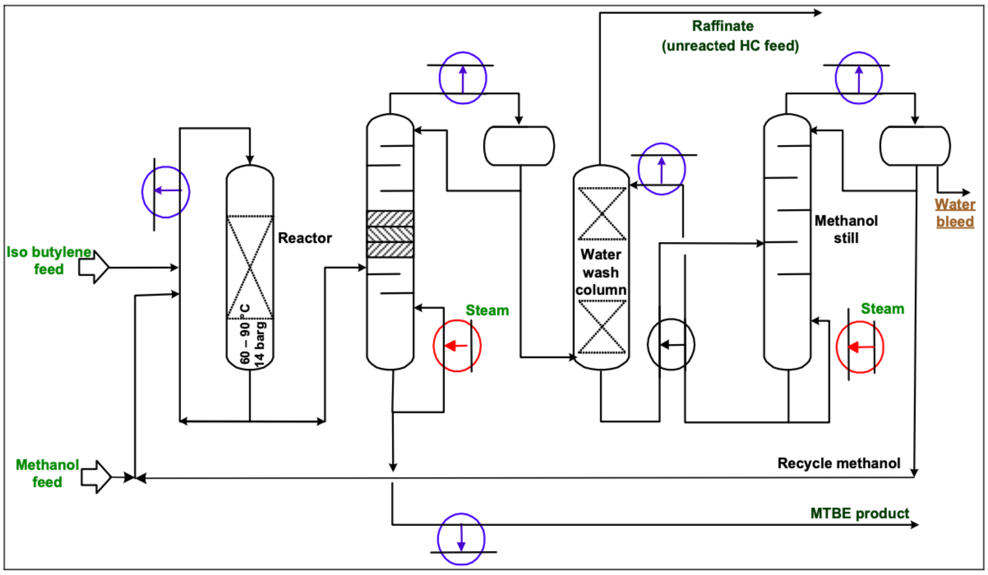

Figure 11 Process flow diagram of a simplified MTBE plant utilising reactive distillation column. Taken from Figure 2.16 in (Barthe, Chaugny, Roudier, & Delgado Sancho, 2015)

Material and Energy Flows for the ETBE/MTBE Production

Table 15 summarises the material and energy flows for the production of MTBE/ETBE, on per unit tonne of product basis. The ETBE process is likely to require a higher amount of processing heat content than a MTBE process.

Table 15 Material and energy flows for the production of MTBE/ETBE

Material/Energy	Unit	Value (range)	Reference
Input			
Isobutylene	t/t of MTBE	0.65	approximated with conversion efficiency of 99% (Barthe, Chaugny, Roudier, & Delgado Sancho, 2015) and molar selectivity of 99.5% (Hydrocarbon Processing, 2010)
Methanol	t/t of MTBE	0.36	approximated based on MTBE: methanol stoichiometric ratio of 1:1
Isobutylene	t/t of ETBE	0.45	approximated with conversion efficiency of 99% (Barthe, Chaugny, Roudier, & Delgado Sancho, 2015) and molar selectivity of 99.5% (Hydrocarbon Processing, 2010)
Ethanol	t/t of ETBE	0.56	approximated based on ETBE: ethanol stoichiometric ratio of 1:1
Electricity	GJ/t of MTBE	0.06 (0.04-0.07)	(Barthe, Chaugny, Roudier, & Delgado Sancho, 2015)
Steam	GJ/t of MTBE	4.3 (2.9-5.7)	Approximated based on steam input parameter provided in (Barthe, Chaugny, Roudier, & Delgado Sancho, 2015) [13] and conversion factor of 2863 MJ/t[14]

---

[13] Equivalent to 1.5 t (range between 1-2 t) of steam input per tonne of MTBE (Barthe, Chaugny, Roudier, & Delgado Sancho, 2015)

[14] Assumes that the steam is provided at a pressure level of 20 bar(g) and 235 °C (Sluis, 2014)

2.2.1.6. Production of 1,4-Butanediol (BDO), Allyl Alcohol & Methyl Propanediol (MPD)

The production of 1,4-Butanediol (BDO) utilises the propylene oxide (PO) produced on-site or from the Maasvlakte site (Chemical Technology, n.d.), in addition to other input materials such as syngas and hydrogen supplied by Air Products. The BDO production also yields saleable by-products such as allyl alcohol and methyl propanediol (MPD, an isomer of BDO). While several alternative routes are available in producing the different products, the BDO production route from PO, which together yields allyl alcohol and MPD, provides the highest economic feasibility by utilising self-produced PO as raw material (Raytheon Engineers & Constructors, 1998). The production technology is originally developed by a Japanese chemical manufacturer, Kuraray (Independent Commodity Intelligence Services (ICIS), 2010).

The BDO production involves two main units, namely the allyl alcohol unit and the BDO unit. The overall BDO yield is at around 77 mol% of propylene oxide (PE International, 2013). The process flow is as illustrated in Figure 12 and described in the following paragraphs. The process description is based primarily on (Raytheon Engineers & Constructors, 1998) unless stated otherwise.

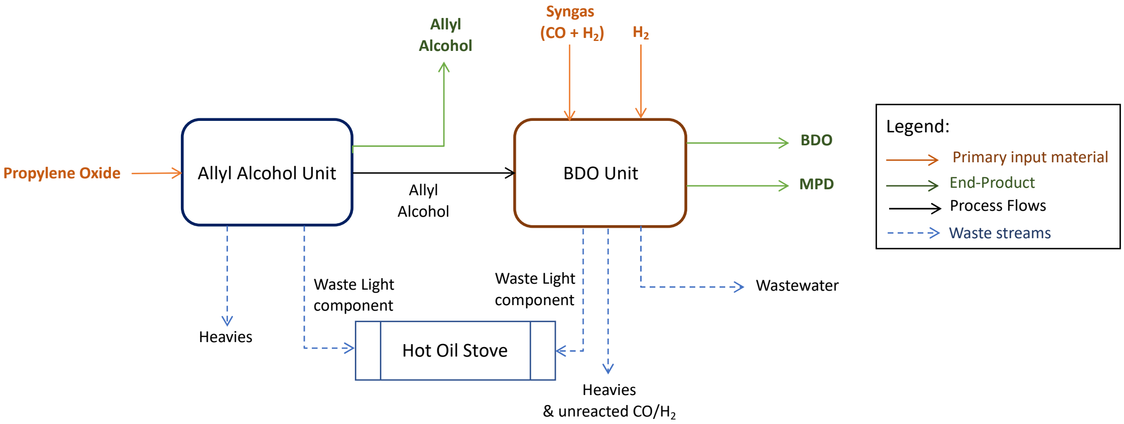

Figure 12 Process flow diagram of the production of BDO, allyl alcohol & MPD (Raytheon Engineers & Constructors, 1998)

Allyl alcohol unit

PO is isomerised into allyl alcohol in this unit, in the presence of hot oil/metallic catalyst slurry. The slurry phase (alternatively a gas-phase) reaction is performed under the temperature of 300 °C and pressure of 1 bar (PE International, 2013). The isomerisation process can be described with the chemical equation as follows:

$$CH_3CHCH_2O\ (PO) \Longrightarrow CH_2 = CHCH_2OH\ (Allyl\ Alcohol)$$

The reactor effluent is then fed to a multistage distillation zone. The unreacted PO stream is recycled back to the reactor and the lighter fraction is removed and used as waste fuel in the on-site hot oil stove. The final product, allyl alcohol is distilled out from the remaining stream. Additionally, the catalyst, of which the active surface may be contaminated with heavy by-products, is constantly regenerated. Acetone and thermal oil are distilled out and reused in the catalyst regeneration process. The remaining stream, containing heavy substances and contaminated catalyst is removed and exported to third parties as fuel.

Butanediol (BDO) unit
The allyl alcohol formed in the allyl alcohol unit is further converted into BDO through two chemical reactions, hydroformylation and hydrogenation. The allyl alcohol is first fed into the hydroformylation reactor, which in reaction with synthesis gas (carbon monoxide (CO)/hydrogen (H_2) mixture) forms hydroxy-butyraldehyde (HBA). The reaction is likely to take place in the presence of a Rhodium-based catalyst dissolved in toluene solvent, with operating conditions of 3 bar and 60 °C (PE International, 2013). Alternatively, other types of catalyst, temperature and pressure ranges between 20-100°C and 1.4-41 bar may be used (U.S. Patent No. US20170144953A1, 2017). The reaction effluent is later sent to the extraction zone, with water acting as the extractive agent. The toluene/catalyst mixture is recycled back to the reactor, while the remaining product-containing aqueous solution is fed to the hydrogenation reactor, after being stripped off of carbon monoxide. The hydroformylation reaction is as described with the chemical equation below:

$$CH_2 = CHCH_2OH\ (Allyl\ Alcohol)\ +\ CO + H_2\ \Longrightarrow C_4H_8O_2\ (HBA)$$

Following the extraction, the aqueous solution, containing HBA, is fed to the hydrogenation reactor. The reaction between HBA and hydrogen forms BDO, as well as MPD as a by-product. The hydrogenation is likely to occur over a reaction temperature of 150 °C and pressure of 35 bar, in the presence of Raney Nickel catalyst (PE International, 2013). Alternatively, other types of catalyst, temperature and pressure ranges between 60-200 °C and 14-103 bar may be used (U.S. Patent No. US20170144953A1, 2017). Following the reaction, the catalyst is then removed from the reaction effluent by passing through a filter and an ion exchanger. The main hydrogenation reaction is as described with the chemical equation below:

$$C_4H_8O_2\ (HBA)\ + H_2\ \Longrightarrow\ C_4H_{10}O_2\ (BDO\ or\ MPD)$$

The remaining effluent, containing BDO and MPD, is then sent for further distillation, where purified streams of BDO and MPD are obtained. The remaining distillation fractions include a fraction of light component compounds, recovered as fuel for the on-site hot oil stove. In addition, heavies and unreacted CO and H_2 are removed and exported as waste fuel to external parties and the wastewater stream is sent for biological wastewater treatment.

Material Flows for the BDO, Allyl Alcohol & MPD Production

Table 16 summarises the material flows for the production process, on per unit tonne of BDO or MPD basis. Regrettably, there is no public information on the electricity and steam consumption.

Table 16 Material flows for the BDO process

Material/Energy	Unit	Value	Reference
Input			
Propylene Oxide (PO)	t/t of BDO	0.84	approximated with conversion yield of 77 mol% of PO (PE International, 2013)
Carbon Monoxide (CO)	t/t of BDO or MPD	0.31	approximated based on CO:BDO stoichiometric ratio of 1:1
Hydrogen (H_2)	t/t of BDO or MPD	0.04	approximated based on H_2:BDO stoichiometric ratio of 2:1

2.2.2 Annual Material & Energy Consumption and CO_2 Emissions

2.2.2.1. Annual Material & Energy Consumption and Waste Fuel Production

Table 17 shows an estimation of the annual material consumption for the different processes in the Botlek production site. The figures are estimated based on the production capacities listed in Table 4 and the material consumption values (on per unit tonne of product basis) indicated in their respective material and energy balance tables.

Table 17 Yearly material consumption (kt/year) for the different processes at the Botlek production site

Input Material	Process	Estimated annual Input (kt/year)
Propylene	PO/TBA co-production	180
Mixed Butane	PO/TBA co-production	510
Oxygen	PO/TBA co-production	200
Propylene Oxide (PO)	Production of PG	90
	Production of PGME	70
	Production of BDO, allyl alcohol, MPD	80
Methanol	Production of PGME	40
	Production of MTBE/ETBE*	145
TBA	Production of isobutylene	140
Isobutylene	Production of MTBE/ETBE	260
Carbon Monoxide (CO)**	Production of BDO, allyl alcohol, MPD	40
Hydrogen (H_2)**	Production of BDO, allyl alcohol, MPD	5
	Total	**1760**

* *assumed production of MTBE only.*

** *material consumption approximated based on the production capacities of both BDO and MPD.*

Figure 13 shows an estimation of the annual energy usage for the different processes at the Botlek production site. The figures are estimated based on the production capacities listed in Table 3 and the energy consumption values (on per unit tonne of product basis) indicated in their respective material and energy flows tables. Processes such as BDO production, TBHP purification and TBA purification are excluded as the information is not available.

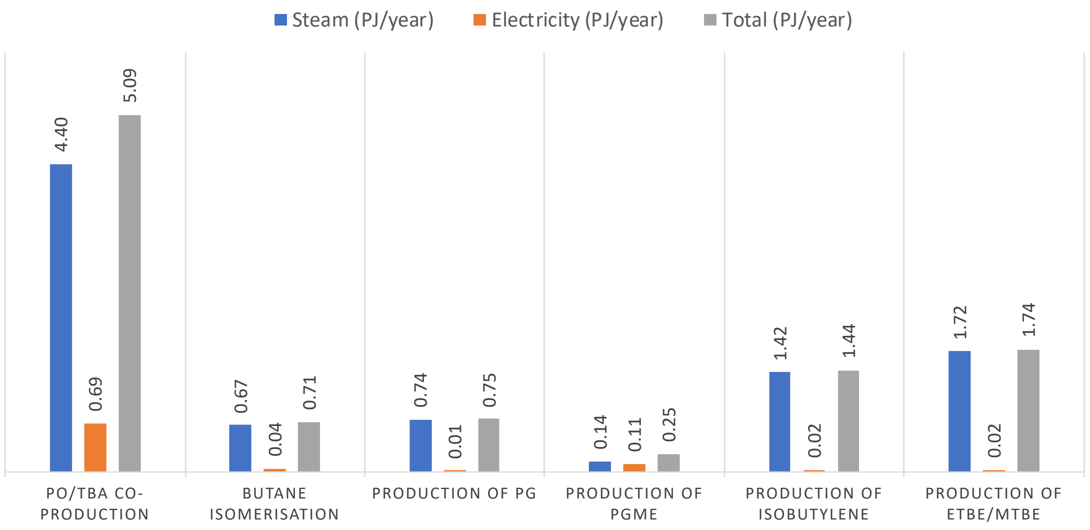

Figure 13 Annual energy consumption for the individual processes at the Botlek site

Nevertheless, these figures shall be an overestimation of the overall energy consumption as it is expected that there is a cascaded use of steam throughout the production complex. To get a better indication of the overall steam usage, the EU-ETS free carbon certificate allocation of 506 kt (Dutch Emissions Authority (NEA), 2020), for the year 2013, is used as a reference estimation for the steam consumption. This corresponds to an 8.04 PJ of steam (or other measurable heat) consumption (Table 18).[15] Without further verification from LyondellBasell, it is here assumed that the 2013 allocation reflects more or less the actual steam usage for the production site, as a whole. Notwithstanding, the expansion of isobutane isomerisation capacity in 2015 may have increased the total steam consumption slightly but is negligible (~2%).

Table 18 Estimated steam and electricity consumption for the Botlek Site

Steam (PJ/year)	Electricity (PJ/year)	Total (PJ/year)
8.0	0.9 [16]	8.9

The estimated amount of waste fuel streams produced from Botlek's operations are based on its 2005 statistics in (LyondellBasell, 2007) for streams that are being exported (see Table 19). "Others" stream refers to the residual fuel (oil/gas) that has been consistently burnt on-site prior to the installation of the new steam boilers. The amount is estimated based on the site's scope 1 emissions in the year 2005 of 131 kt and averaged emission factor and lower heating value (LHV) of residual fuel oil and chemical waste gas. The energy content for other fuel streams are calculated based on LHV listed in Table 31.

---

[15] The free carbon certificate allocation is determined based on the "heat benchmarking", which assumes that the steam is provided by a natural gas boiler of 90% conversion efficiency, while also considering historical consumption and correction factors (European Union, 2015). The heat (i.e. steam) usage is back-calculated using simplistic assumption that the free allocation reflects directly the actual steam usage, with no correction factors applied, as such: $\frac{506\ kton\ CO2}{56.6\ kton\ CO2/PJ} * 90\%$. 506 kt CO_2 corresponds to the carbon certification allocation, 56.6 kt CO_2/PJ corresponds to the emission factor of natural gas, and 90% is the assumed conversion efficiency of a natural gas boiler.

[16] Excluding the BDO production, TBHP purification and TBA purification processes

Table 19 Estimated amount of waste fuel streams

	Annual amount (tonne/year)	Energy Content (PJ)
A fuel	38500	1.58
Fuel gas	20300	0.92
Pentane	6800	0.31
Propane	7100	0.32
Others	43500	1.87

2.2.2.2. Supply of Utilities

In 2016, LyondellBasell's Botlek site began operating two on-site steam boilers of 115 MW_{th} capacity, fuelled mainly by natural gas and other waste gases, with a small fraction by liquid waste fuels (European Environment Agency, 2020). Additionally, it is noted that hot oil stoves are used on-site, utilising waste thermal oil as input (Raytheon Engineers & Constructors, 1998). LyondellBasell also obtains its electricity and steam needs from external utility sites, namely WKC Air Products and Eurogen C.V. Rotterdam Rozenburg.

WKC Air Products is a combined-cycle gas turbine (CCGT) combined heat and power (CHP) plant co-owned by Air Products and Electrabel. It is rated at 96 MW_{elec} and 225 tonnes of steam output per hour (Jagger, 2000; Port of Rotterdam, 2016). The CHP plant supplies steam to LyondellBasell, while the produced electricity is self-consumed by Air Products and fed to the electricity grid. In addition, LyondellBasell is supplied with steam and electricity from Eurogen C.V. Rotterdam Rozenburg. It is a CHP facility consisting of two gas-fired plants co-owned by Huntsman, LyondellBasell, ENECO and Air Liquide; and has an electricity and steam capacity of 88 MW_{elec} and 270 tonnes of output per hour (Kreijkes, 2015). The external utility facilities also receive the waste fuel streams produced by LyondellBasell Botlek (CE Delft, 2012).

LyondellBasell's steam supply is currently provided jointly by its own steam generation and external supply, as suggested by its scope 1 emissions. Nevertheless, it is estimated that the production site is capable of being self-sufficient, following the installation of the two 115 MW_{th} steam boilers. The generally high scope 1 emissions prior to year 2016 suggested the presence of existing boilers (i.e. hot oil stoves (Raytheon Engineers & Constructors, 1998)) for on-site steam generation, corresponding to around 1.5 PJ[17] of steam output. In addition to this, the new boilers shall allow a total steam production of 7 PJ, running at 97% capacity. Hence, it can be concluded that the pre-2015 boilers (i.e. hot oil stoves) and new boilers would in theory capable to cover all of the steam requirements. Both the Eurogen C.V. Rotterdam Rozenburg and WKC Air Products have been in operation since 1994 and 2002 (Port of Rotterdam, 2010; Port of Rotterdam, 2006). Given the average lifetime of an industrial CHP is typically in the range of 15-30 years, the retirement of the two utility sites is assumed to be realised in the upcoming decade. Transitioning into being self-sufficient can be viewed as a logical choice in this case. These assumptions have, however, not been verified by LyondellBasell.

---

[17] Estimated based on estimated amount of fuel burnt on-site (see Table 19) and conversion efficiency of 79.5% (average between steam boiler efficiencies for fuel oil and waste gas)

2.2.2.3. Annual CO_2 Emissions

The reported scope 1 emissions for the year 2019 is 322 kt (Dutch Emissions Authority, 2020), attributable to its on-site steam generation and other operations such as flaring, which is assumed negligible. The remaining steam-related emissions falls within the scope 2 emissions, with steam being supplied from external utility companies. However, there is no public data on the amount of steam supplied by external utility sites, hence the scope 2 steam-related emissions are not quantified.

The scope 2 electricity emissions[16] are quantified based on a gas-fired CHP with electrical and steam thermal efficiency of 36% and 49%, respectively. The electricity emission factor is 85.4 kg/GJ, determined based attribution method suggested in (European Commission, 2018) (See Appendix for the attribution formula).

The steam-related emissions are quantified based on the assumption the steam is supplied by the on-site boilers and stoves (without external steam supply), utilising both the residual fuel streams (see Table 19) and natural gas as fuel input. The LHVs and the emission factor of the different fuel type are listed in Table 31 and Table 32. The boiler efficiencies are 85%, 84% and 75% for natural gas, fuel oil and recovered gas, respectively.

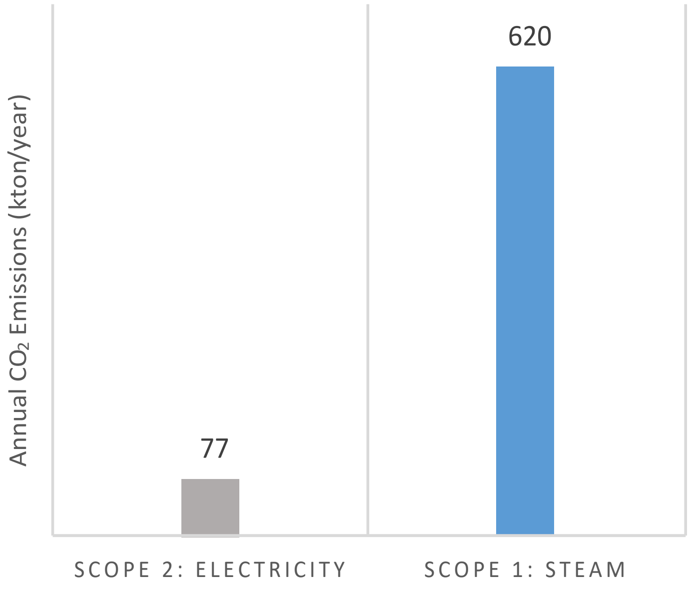

Figure 14 Estimated annual emissions for the Botlek site

3 Feedstocks, Products and Applications

LyondellBasell produces a wide range of products at the Botlek and Maasvlakte sites (see Table 3 and Table 4 for the production capacities). These products are mainly intermediate chemicals, which are used to produce a wide range of every-day applications further down their value chains. The final products are, for example, cosmetic products, food packaging, seat cushions and textiles. Products such as ETBE, MTBE and TBA may be used as an end-product, as a gasoline oxygenate. The optimised product flows throughout the production complexes minimise the raw material requirements from external parties. Particularly, propylene oxide produced on-site which is used as input material for three other chemical processes. Nonetheless, some processes are supplemented with materials supplied from external parties, such as benzene, ethylene, and propylene. These are transported to the site via pipelines (from the neighbouring industrial sites), and ships in some cases. Specific details of where each raw material comes from is given in the previous chapter.

The following sub-chapter 3.1 details the feedstocks required for the chemical processes, that are supplied by external parties. Sub-chapter 3.2 details the products produced at the two production sites.

3.1 Feedstocks

This sub-chapter discusses the main feedstocks utilised in the chemical processes. Specifically, the ones supplied by external parties. An overview of the feedstocks discussed further in this sub-chapter and their associated processes are provided in Table 20. Carbon monoxide (CO) and hydrogen (H_2) are not further described as the consumption is negligible. They are also further detailed in (Cioli & Schure, in preparation).

Table 20 Overview of feedstocks discussed in sub-chapter 3.1

Feedstock	Process(es)
Benzene	- Benzene alkylation (Maasvlakte)
Ethylene	- Benzene alkylation (Maasvlakte)
Propylene	- PO/SM co-production (Maasvlakte) - PO/TBA co-production (Botlek)
Butane	- Isomerisation of n-butane (Botlek)
Methanol	- Production of PGME (Botlek) - Production of MTBE (Botlek)
Ethanol	- Production of ETBE (Botlek)

3.1.1 Benzene

Benzene (C_6H_6) is an aromatic hydrocarbon. The compound exists as a clear, colourless liquid with a gasoline-like odour. It is also highly flammable, with a flashpoint of -18°C, and has a density lower than water (National Center for Biotechnology Information, 2020). Benzene is most often used in the manufacturing of ethylbenzene (50% of total usage) and cumene (20% of total usage). The production of the compound primarily occurs via steam cracking of naphtha and other liquid feeds, and the catalytic reforming of naphtha (The Essential Chemical Industry, 2016). A detailed section on benzene and its production via steam cracking are also included in (Wong & van Dril, 2020).

The benzene market is forecasted to expand in the future, contributed by the demand growth of the benzene derivatives such as styrene polymers and ethylbenzene. Increasing demand for styrene polymers for many end-uses, such as textile, packaging etc. is expected, particularly within the Asia Pacific region, coinciding with the economic development in the emerging markets (Modor Intelligence, 2020).

3.1.2 Ethylene

Ethylene exists as a colourless gas with sweet odour and taste. Being the most manufactured chemical globally (by weight), ethylene is used as the building block for a wide range of applications, with derivatives including polyethylene and ethylene oxide. The most common production route for ethylene is through steam cracking of natural gas and crude oil (The Essential Chemical Industry, 2017). A detailed section on ethylene and its production via steam cracking is included in (Wong & van Dril, 2020).

Global demand for ethylene is expected to grow faster than the average world gross domestic product (GDP), over the next five years. This is mainly driven by the growth of polyethylene-based consumables, polyethylene terephthalate (PET) products, as well as polyvinyl chloride (PVC) for construction and pipe applications, particularly in the Chinese market (IHS Markit, 2020).

3.1.3 Propylene

Propylene is a colourless, highly flammable gas. It is the second-most commonly manufactured chemical building block for a wide range of applications through derivatives such as polypropylene and propylene oxide. The main production methods are the steam cracking of naphtha and catalytic cracking of gas oil. Nevertheless, due to the growing demand, an increasing amount of propylene is currently produced through on-purpose propylene (OPP) processes, such as catalytic cracking of propane, the MTO (Methanol-To-Olefins) process and the reaction between ethene and butenes (The Essential Chemical Industry, 2017). A detailed section on propylene and its production via steam cracking and catalytic cracker feed distillation is included in (Wong & van Dril, 2020; Block & van Dril, 2020).

The consumption of propylene is expected to grow in the coming years, fuelled by the economic growth of the emerging countries. The dominant outlet for propylene shall continue to be polypropylene with its share expected to expand further. Regional demand growth of other propylene derivatives (e.g. propylene oxide, cumene) are also forecasted (IHS Markit, 2019). The market trends and prices are discussed in greater detail in (Block & van Dril, 2020).

3.1.4 Butane

Butane, specifically n-butane, is a highly flammable hydrocarbon, exists in gaseous form at room temperature and atmospheric pressure. It has a wide range of applications - as a gasoline blend or as a finished product, such as refrigerant and liquified petroleum gas

(LPG). Additionally, it is used as a raw material for the production of synthetic rubber. Butane is primarily recovered from natural gas processing and refinery operations (i.e. steam cracking and catalytic reforming) (National Center for Biotechnology Information, 2020).

The increasing demand for LPG is expected to raise the consumption of butane over the next few years (Mordor Intelligence, 2020). Particularly for industrial use purposes, as a fuel for heating solutions or power generation. The largest regional growth is forecasted to come from the Asia Pacific region, with the largest consumption coming from China and India. In the Asia Pacific, the demand for butane as a transport fuel is increasing due to the growing transport activities and increasing demand for cleaner fuel in countries such as China and Japan.

3.1.5 Methanol

Methanol exists as a colourless liquid with an alcoholic odour. It is a common commercial chemical for a variety of applications (i.e. solvents, antifreeze, fuel additives) and for the manufacturing of different chemicals (i.e. ETBE and PGME) (National Center for Biotechnology Information, 2020). Methanol is typically manufactured from synthesis gas (a mixture of carbon monoxide and hydrogen). The synthesis gas can be derived from oil and natural gas, as well as from "green" or renewable sources, such as biomass (The Essential Chemical Industry, 2017). Other production methods include through the fermentation of biogas and methanol synthesis process. The manufacturing of (bio-)methanol is further discussed in (Khandelwal & van Dril, 2020).

The methanol consumption is expected to rise, particularly in the Asia Pacific region, driven by the increasing demand for methanol-based fuel. On the contrary, health risk exposure may also hinder the market growth. A healthy demand growth of its formaldehyde derivative, widely used in the construction, automotive, and personal care industry, is also expected (Mordor Intelligence, 2020). A more detailed discussion on methanol can be found in (Block & van Dril, 2020; Khandelwal & van Dril, 2020).

3.1.6 Ethanol

Ethanol, or ethyl alcohol, is commonly found in alcoholic beverages and household items such as in cleaning and personal care products. It may also be used as a chemical building block for the production of ETBE and various plastic materials (National Center for Biotechnology Information, 2020). Ethanol is most commonly produced through the fermentation of sugar crops (i.e. sugar cane, corn). This production process is further detailed in (Khandelwal & van Dril, 2020).

Strong growth is expected of ethanol consumption, driven by the biofuel demand as well as its use in beer production and food processing. This, however, may be hampered by the increasing penetration of hybrid electric vehicles and awareness of the adverse effect of alcohol consumption. The strongest surge is expected from the North American region, which sees more stringent regulations in reducing the use of fossil fuel (Mordor Intelligence, 2020). Further details on ethanol can also be found in (Khandelwal & van Dril, 2020).

3.2 Products and Applications

The following describes the main products manufactured by LyondellBasell, at the Botlek and Maasvlakte site. Tertbutyl Hydroperoxide (TBHP), methyl propanediol (MPD) and allyl alcohol are not further discussed in the sub-chapter, as their production volume is less significant

(<20 kt/year). As noted in the previous chapter, some of the products are used as input material for other processes on-site.

3.2.1 Propylene Oxide (PO)

Propylene oxide (PO) is a highly flammable, volatile, colourless liquid. The compound is also soluble in water and miscible with other organic solvents. PO is an intermediate chemical for a wide variety of downstream products. Up to 60% of the manufactured PO is consumed in polyurethane production (ICIS Chemical Business, 2018). Polyurethane is used to produce products such as rigid forms for thermal insulation, mattresses, seat cushion etc. Around 25-30% of the PO consumption can be attributed to the production of propylene glycol. The remaining is used to produce glycol ethers, BDO and other chemical derivatives (ICIS Chemical Business, 2018).

PO is synthetically made on an industrial scale through a number of possible production routes. For example, through the PO/SM co-production and PO/TBA co-production processes, employed by LyondellBasell. The oldest production method is the chlorine method, which utilizes a high amount of chlorine and is highly polluting (ICIS Chemical Business, 2018). PO is manufactured through the dehydrochlorination of propylene chlorohydrin, which is formed through the reaction between chlorine, propylene and water. Recent production development includes the method based on cumene as an oxygen carrier (POC), as well as the hydrogen peroxide to propylene oxide (HPPO) method (Sumitomo Chemical Co., Ltd., 2019). The total PO capacity within the Netherlands is around 1100 kt. The other two major players are Ellba (Shell and BASF) and Shell, with an annual production capacity of 250 and 210 kt, respectively.

Significant demand growth is expected for PO, driven by the increasing consumption of its polyurethane derivatives (Market Reports World, 2020). High demand for polyurethane is expected from the European automotive industry, as well as the construction industry in Europe and the Asia Pacific. Particularly, the infrastructure development in the Asia Pacific shall propel the market growth.

3.2.2 Styrene Monomer (SM)

Styrene monomer appears as a colourless to dark liquid and has a sweet odour (National Center for Biotechnology Information, 2020). Styrene is predominantly used in the manufacturing of polystyrene – the fourth most common polymer manufactured. Its other derivatives include styrenic resins such as acrylonitrile butadiene styrene (ABS), styrene butadiene latex (SBL), styrene butadiene rubber (SBR) and styrene acrylonitrile (SAN) (Falcke, et al., 2018).

Styrene is mainly produced through the dehydrogenation of ethylbenzene. The other major process being the PO/SM co-production employed by LyondellBasell. The other two styrene producers in the Netherlands are Shell (990 kt SM; PO/SM co-production process) and Trinseo (250 kt SM; dehydrogenation of ethylbenzene). This chemical product is also discussed in (Wong & van Dril, 2020).

Some sources have forecasted the styrene market to grow over the next few years, driven by the demand for polystyrene for packaging applications, particularly in the growing consumer electronics industry (Mordor Intelligence, 2020). Asia Pacific is forecasted to be the dominant market, specifically China, which may also see increasing demand in other consumer industries, i.e. food and beverages (Mordor Intelligence, 2020). Recycled styrene has gained a lot of traction, whereby companies are developing styrene recycling techniques

(PR Newswire, 2020). Nevertheless, some sources are sceptical about the increasing health and environmental concerns of styrene usage and have suggested a declining demand for styrene (PR Newswire, 2020).

3.2.3 Gasoline Grade Tert-Butyl Alcohol (TBA)

Tert-butyl alcohol, or known as tert-butanol, is a colourless oily liquid with an alcoholic odour. It is used as intermediate chemicals in the production of other high-volume chemicals. For example, isobutylene, which is subsequently used to produce MTBE/ETBE (LyondellBasell, 2020). It can also be used as a solvent for paints & coatings applications or as an octane booster in gasoline. TBA may be co-produced with propylene oxide, as described in 2.2.1.1, or otherwise, through the acid-catalysed hydration of isobutylene (Chemical Book, 2020).

Rising demand for TBA for the paints and coatings applications, is expected from the emerging economics, stemming from the rapid growth in construction and infrastructure sectors. Increasing disposable income would also raise the demand for cars, in turn, increasing the consumption of TBA-based paints and solvents. Its consumption in the food & beverage and pharmaceutical segments will also rise. The regulations on the volatile organic compound (VOC) emissions may hamper the growth, at the same time, stimulating the development of bio-based, eco-friendly variants (TMR Research, 2020).

3.2.4 Propylene Glycol (PG)

Propylene glycol, also known as 1, 2-propanediol, is a clear and colourless liquid, and absorbs water readily (i.e. hygroscopic) (National Center for Biotechnology Information, 2020). It is generally recognized as safe for use in food and has a wide range of industrial and pharmaceutical applications. It is widely used as a basic chemical in the production of unsaturated polyester resin, as a lubricant or heat-transfer fluid. Other uses include humectant for tobacco, and as a solvent for food and pharmaceutical products.

Rising demand for PG is expected from both the developed and developing economies. Its derivative, unsaturated polyester resin, is forecasted to be the main driving force, due to its growing application in the construction and infrastructure industry. Particularly, in developing countries with increasing infrastructure investments. The growth in the transport industry is also expected in stimulating the PG market growth, increasing its application as aircraft deicing fluid, automotive coolants, and hydraulic & brake fluids (Markets and Markets, 2020).

3.2.5 Propylene Glycol Methyl Ether (PGME)

Propylene Glycol Methyl Ether, also known as 1-Methoxy-2-propanol exists as a colourless liquid, with a weak pleasant odour. It is often used in the manufacturing of lacquers and paints, as it is a good solvent for celluloses, acrylics, dyes, inks and stains. Its other usage includes antifreeze material of the cooling system and heavy-duty engines, as well as used in cleaning formulations for household and industrial cleaning products (National Center for Biotechnology Information, 2020).

The increasing demand of biodegradable, eco-friendly solvent may drive the growth of the PGME market in Europe, following the stringent EU regulations which demand the use of volatile organic compound (VOC) solvents in industrial and coatings applications. The PGME market growth in the Asia Pacific region is expected to be driven by the rapid development in the construction and transport sector. This would lead to higher paints and coatings consumption, where PGME is often used as a solvent. Other than that, the growth of the electronics industry would also fuel the demand of PGME, mainly for the use of metal degreasing and equipment cleansing (Transparency Market Research, 2020).

3.2.6 1,4 - Butanediol (BDO)

1,4–butanediol exists as a colourless oily and almost odourless liquid. It is mainly used as an intermediate chemical for the production of tetrahydrofuran (THF) and polybutylene terephthalate (PBT). It is also used in the manufacturing of gamma-butyrolactone and polyurethane elastomers (Sampat, 2011). There are a wide variety of production methods available. The most prevalent one being the Reppe process from acetylene and formaldehyde. Other processes include the butadiene-acetic acid process, BDO from maleic anhydride and dichlorobutene process, as described in (Sampat, 2011). Production method to produce bio-based BDO has also been developed, through the fermentation of glucose (Intratec Solutions, 2018).

The BDO market is expected to grow strongly, due to the growing demand for polybutylene terephthalate (PBT). PBT is used to produce various end-user applications in the lightweight automotive industry and the electronics industry (Mordor Intelligence, 2020). These two industries are expected to grow significantly in the Asia Pacific region, specifically China and India (Mordor Intelligence, 2020). Other expected demand growth comes from the growing use of spandex in the textile industry (Market Research Future, 2020). The shifting preference for sustainable products may also escalate the production and consumption of bio-based BDO (Market Research Future, 2020).

3.2.7 Isobutylene

Isobutylene exists as a colourless gas form with a faint petroleum-like odour. The compound is alternatively called 2-methylpropene or isobutene. It has a broad range of usages, such as a chemical building block for the production of synthetic rubber and various plastics, but is primarily used in the production of MTBE/ETBE (National Center for Biotechnology Information, 2020; Fact.MR, 2020). Isobutylene is most commonly produced through the catalytic dehydrogenation of isobutane. Other production methods include the dehydration of tert butyl alcohol (TBA) and separation from refinery streams by reaction with sulfonic acid (LUMITOS AG, 2020).

The rapid growth of demand is expected for isobutylene, mainly driven by the increasing consumption in the production of MTBE/ETBE due to the rapid expansion of the fuel industry. It is also increasingly consumed in the production of antioxidants, fragrances, and gas odorization products (Fact.MR, 2020).

3.2.8 Methyl Tertiary-Butyl Ether (MTBE)/Ethyl Tertiary Butyl Ether (ETBE)

Both Methyl Tertiary-Butyl Ether and Ethyl Tertiary Butyl Ether exist as a colourless liquid. They are used as gasoline oxygenates, which helps to reduce automobile emissions and the formation of ozone. LyondellBasell produces bio-ETBE which may be used as biofuel that meets the European certification requirements. Particularly, gasoline containing bio-ETBE has over 66% lower greenhouse gas emissions than 100% fossil fuel-based gasoline (Sustainable Fuels, 2020).

Increasing demand for MTBE is expected from the Asia Pacific region, driven by the automotive gasoline demand. On the contrary, the use of MTBE in several developed countries (i.e. US, Japan and Europe) is banned due to toxic emissions concerns (Mordor Intelligence, 2020). Such concerns have stimulated investment in developing bio-based

MTBE or usage of alternative gasoline oxygenates, i.e. ethanol and ETBE (Merchant Research & Consulting, Ltd., 2020; Mordor Intelligence, 2020). A more in-depth discussion of MTBE can be found in (Block & van Dril, 2020). It is noted that ETBE is primarily used in Western Europe and with increasing demand from the Japan market. It is preferred as a fuel additive than ethanol and also generates lower carbon emissions than MTBE (Merchant Research & Consulting, Ltd., 2020).

4 Options for Decarbonisation

The analysis performed on LyondellBasell’s current operations at the Maasvlakte and Botlek production sites has shown that the annual energy consumption is significant. The energy consumption is also the major contributor to LyondellBasell’s CO_2 emissions (on scope 1 and 2 basis). Based on own estimations, around 90% (for Botlek site) and 94% (for Maasvlakte site) of the consumed energy are for heating purposes, supplied in the form of processing steam. The remaining can be attributed to their electricity consumption.

This chapter proposes and discusses a number of decarbonisation options that are applicable for decarbonising LyondellBasell’s operations at the two production sites. These can be further put into four broad categories, as shown by the overview provided in Table 21. While some products may be produced through alternative process(es), possible carbon reduction or energy savings opportunities that involves process replacement using different types of feedstock are not considered, given that the complexes are optimised in their product flows. The use of drop-in feedstock substitutes are considered.

Table 21 Overview of the proposed decarbonisation options

Category	Decarbonisation Options
Fuel Substitution for Steam Production	Electrode Boiler
	Hydrogen Combustion
	(Solid) Biomass Combustion
CO_2 Capture and Storage or Re-Use	Post Combustion Carbon Capture and Storage
Use of Residual Energy	Circular Steam Project
	Integrated Heat Pump in Distillation Columns
Feedstock Substitution	Low-Carbon/Bio-based Ethylene
	Low-Carbon/Bio-based Propylene
	Low-Carbon/Bio-based Methanol
	Low-Carbon/Bio-based Benzene

The different options are described in their respective sub-chapters, detailing their technological concepts and application, as well as applicable technical and economic parameters (investment cost, operation & maintenance costs etc.).

4.1 Fuel Substitution for Steam Production

4.1.1 Electrode Boiler

Several power-to-heat (PtH) technologies have been developed to address various industrial heating needs. These range from low-temperature heat pump to electric furnaces for the use in petrochemical cracking and metal industries at a temperature up to 3000°C (Schure & Semeijn, 2020; Berenschot, 2017). Technologies that are commonly applicable for high temperature (between 250 to 350°C) steam generation are limited to electric boilers and electrode boilers (Marsidi, 2018). Electric boiler technology, which works with a resistance heating principle, is capable for heating gases to a temperature up to 600°C. It has, however, a relatively small capacity, up to 5 MWe (Berenschot, 2017). Such low capacity is significantly lower than the two steam boilers currently employed in the Botlek site, which both have a thermal output of 115 MW, while the annual steam demand in the Maasvlakte site ranges up to 8 PJ. As such, electric boiler is likely not suitable as a possible option. On the other hand, the maximum capacity of a single electrode boiler is significantly larger than an electric boiler, reaching up to 70 MWe (Berenschot, 2017; Marsidi, 2018), or even 90 MWe (Element Energy; Jacob, 2018).

The commercially available electrode boiler is capable of producing saturated steam of up to 350°C (Berenschot, 2017; Marsidi, 2018). Its operating principles rely on the conductive and resistive properties of water to carry electric current and to generate steam. To further explain, the electricity flows through the electrodes generate an electric field which causes the water molecules to move at high speed, which in turn generates heat for steam production (Altenergy, 2020). The electrode boiler technology is said to have achieved a technological readiness level of 9 (Berenschot, 2017). The following tables are summaries of the technical and economical parameters for the electrode boiler technology.

Table 22 Technical parameters for the electrode boiler technology

Parameter	Unit	Value	References
Full load hours	hour/year	8500 - 8760	(Berenschot, 2017)
Efficiency	%	95 – 99.9	(Berenschot, 2017; Marsidi, 2018)
Technical Lifetime	Years	15	(Element Energy; Jacob, 2018)
Carbon Abatement Potential	%	100; if green electricity is used	

Table 23 Economic parameters for electrode boilers

Parameter	Unit	Value	References
Investment Cost[18] *Reference capacity: 70MW$_e$*	€$_{2018}$/kW$_e$	75.4 – 123.3	(Planbureau voor de Leefomgeving (PBL), 2020; Element Energy; Jacob, 2018)
Fixed O&M Cost	€$_{2018}$/kW$_e$/year	1.4 – 47	(Planbureau voor de Leefomgeving (PBL), 2020; Element Energy; Jacob, 2018)
Variable O&M Cost	€$_{2018}$/MWh	0 - 0.2	(Planbureau voor de Leefomgeving (PBL), 2020; Element Energy; Jacob, 2018)
Fuel Cost	-	electricity price	

4.1.2 Hydrogen Combustion

Hydrogen-based combustion is one of the promising options in decarbonising high-temperature heat production. Hydrogen (H_2) combustion can readily replace steam production from gas-fired steam boilers or other fossil fuel-based CHP facilities without requiring much modification to the main process configurations. Additional investment is,

---

[18] Refers to the total boiler installed cost (TIC). The cost range is re-estimated based on original reference capacities in (Planbureau voor de Leefomgeving (PBL), 2020; Element Energy; Jacob, 2018), using a scale factor of 0.7

however, needed for boiler retrofitting at the Botlek site or a new boiler installation at the Botlek/Maasvlakte site.

Hydrogen boiler technology for steam generation is said to have achieved a TRL of 9 (Hart, et al., 2015). The boiler capacity is quoted between 5 to 50 MW through market consultation (Navigant, 2019), possibly reaching up to 200 MW (Element Energy; Jacob, 2018). On the other hand, the existing natural gas-fired steam boilers employed at the Botlek site may be retrofitted, reducing the investment costs. Retrofitting is required due to the different combustion characteristics between hydrogen and natural gas combustion, leading to challenges such as changes in heat transfer characteristics, increased NO_x emissions and changes in flue gas composition. The TRL for burner retrofitting is currently at TRL 7 and is projected to reach commercial readiness by around 2025 (Durusut, et al., 2019). Co-burning of hydrogen with another gaseous mix (i.e. natural gas, furnace gas) could also be performed with the hydrogen boiler.

The following tables summarise the technical and economic parameters the retrofitting of a natural gas boiler. There is limited literature available for hydrogen combustion and what is available generally refers to the cost of retrofitting an existing gas boiler. Thus, the cost of a new boiler system is not included. However, the cost of a new boiler specially for hydrogen combustion is thought to be comparable to that of a natural gas equivalent. The technical lifetime of the retrofitted boiler is constrained by the remaining lifetime of the existing combustor. The variable O&M cost is dependent on the amount of fuel usage and the fuel cost. The fuel cost differs according to the hydrogen sources and is further discussed in the following sub-section.

Table 24 Technical parameters for a retrofitted boiler

Parameter	Unit	Value (Range)	References
Full load hours	hour/year	7500 – 8760	(Navigant, 2019)
Efficiency	%	90	(Hart, et al., 2015; Navigant, 2019)
Technical Lifetime	Years	25	(Hart, et al., 2015)

Table 25 Economic parameters for a retrofitted boiler

Parameter	Unit	Value (Range)	References
Retrofitted Hydrogen Boiler			
Investment Cost [19] *Reference Capacity: 50 MW_{th}*	$€_{2018}/kW_{th}$	89 – 250	(Navigant, 2019) (VNP, 2018)
Fixed O&M Cost	$€_{2018}/kW_{th}/year$	4 – 60	(E4Tech, 2015) (Navigant, 2019)

4.1.2.1. Hydrogen Source: Blue and Green Hydrogen

The hydrogen feedstock may be produced on-site or sourced from external production site, which requires additional investments for a new production facility or possibly the construction of a new pipeline connection. Hydrogen can be produced from fossil-based (i.e. natural gas, coal) and renewable-based (i.e. biomass, renewable electricity) energy, through a wide variety of production routes. Nonetheless, the decarbonisation potential of a

---

[19] The investment cost in (Navigant, 2019) is re-estimated based on the original reference capacity and using a scale factor of 0.7. This yields the lower limit of 89 $€/kW_{th}$. The upper limit refers to (VNP, 2018).

hydrogen-based steam production varies greatly, depending on the primary energy input and the chosen production technology. Hydrogen can be further categorised into three “colour” categories, namely grey, blue and green hydrogen, based on the carbon emissions of the production routes. Only blue and green hydrogen have carbon abatement potential, whereby blue hydrogen involves the use of carbon capture and storage and green hydrogen is produced using carbon-neutral feedstock or fuel/electricity.

One of the possible near carbon-neutral hydrogen sources is from the blue hydrogen production. The H-Vision project is a large-scale blue hydrogen project kickstarted for the Port of Rotterdam industrial cluster (Deltalinqs, 2019). The project is ambitioned to start its operations in late 2025 and running at full capacity in 2030. The H-Vision is touted as the near-term decarbonisation option and the infrastructure built will pave the way to transitioning into green hydrogen usage in the future. The blue hydrogen produced from H-Vision would be mainly used to power industrial processes in refineries and power plant (Deltalinqs, 2019). The current preferred technology, high-pressure Auto Thermal Reforming (ATR), offers advantages in terms of economies of scale and operational flexibility over the other technologies. Hydrogen will be produced as the energy carrier by reforming both the high-caloric natural gas and residual gases from the industrial processes. Nonetheless, carbon capture & storage is required in coupling with the ATR. The project will take advantage of the PORTHOS project, storing the captured CO_2 under the North Sea. The PORTHOS project is briefly described in 4.2.2. In addition, an additional gas network is expected to be installed to allow the flow of flue gases from industrial production facilities to the blue hydrogen production plants, as well as to feed the hydrogen gas to the industrial facilities. The coupling of ATR and CCS results in a reduced emission factor of 0.028 tCO_2/MWh of H_2 (Deltalinqs, 2019).

The H-Vision project does not only offer a near carbon-neutral fuel for LyondellBasell’s operations but also offers an alternative use of the unavoidable residual fuel gas produced from the industrial processes. The maximum scope, which assumes participation of LyondellBasell and a number of additional users in comparison to the reference scope defined in (Deltalinqs, 2019), expects an installed hydrogen production capacity of 3820 MW and 1000 MW of hydrogen storage in a salt cavern. The reference scope allows a maximum curb on reduction of 3 Mt of CO_2, with carbon mitigation cost ranges between 86 and 146 € per tonne of CO_2 (Deltalinqs, 2019), depending on the macroeconomic scenarios assumed.

Alternatively, hydrogen may be purchased from large scale, off-site green hydrogen production. Green hydrogen is generally produced through water electrolysis process, by which carbon-neutral, renewable electricity is used to separate water molecules into hydrogen and oxygen in a 1:8 weight ratio, allowing a 100% CO_2 reduction. This production route also avoids the use of fossil fuel, in comparison to the blue hydrogen which utilises natural gas as the main feedstock. A cost analysis was conducted (Navigant, 2019), with a concluded range of green hydrogen price between 3000 to 8000 €/tonne of H_2. The high uncertainty is mainly due to the wide range of investment costs determined through both literature review and market consultation. Other cost components included in the cost analysis are energy costs (€30 – 70/MWh), OPEX (3 – 5% of CAPEX) and oxygen selling price (13 – 40 €/tonne of O_2). It is, however, projected that the levelized cost of hydrogen would decrease rapidly in the next decades, reaching parity with the production cost of blue hydrogen. A recent report from Hydrogen Council (Hydrogen Council, 2020) projected that the cost of green hydrogen could drop to about 850 - 1280 €/t[20] in optimal regions, and 1700 – 2560 €/t under average conditions. Such cost improvement is driven by strong reductions in electrolyser CAPEX, through the deployment of about 70 GW of electrolyser capacity worldwide. This would see the CAPEX of electrolysers falling from around 1360 to

---

[20] Assuming an exchange rate of 0.85 EUR/USD.

340 €/kW. Similar projections trend is forecasted by IRENA (IRENA, 2018), though the reduction is less rapid with production cost ranges between 1490 to 2770 €/t.

4.1.3 (Solid) Biomass Combustion

Biomass may also be used as a carbon-neutral replacement fuel, allowing complete decarbonisation. This is provided that the sourced biomass adheres to the sustainability criteria in accordance with the EU Directive (European Commission, 2017). There is a wide variety of biomass technologies applicable for heating applications, using biomass in solid, liquid and gas forms, as detailed in (Planbureau voor de Leefomgeving (PBL), 2020). As reported in (Phillips & Flach, 2019), the majority of the biomass usage in industrial furnaces or boilers are woody biomass, such as wood chips or pellets. The wood chips may be sourced domestically or imported from agricultural and forestry residues, as well as from industrial residues (i.e. sawdust and wood scrap from wood processing industry). Wood pellets can be sourced domestically but are primarily imported from abroad with the United States as the main supplier (Phillips & Flach, 2019).

The following consider the use of solid biomass boilers at the Botlek and Maasvlakte sites as an alternative steam generation system. Facilities such as biomass storage system, flue gas cleaning etc. may be needed, in addition to the boiler. The following tables provide a summary of the techno-economic parameters for an industrial wood pellet steam boiler.

Table 26 Technical parameters for an industrial wood pellet steam boiler

Parameter	Unit	Value	References
Full load hours	hour/year	8500	(Uslu, 2018; Planbureau voor de Leefomgeving (PBL), 2020)
Efficiency	%	90	(Uslu, 2018; Planbureau voor de Leefomgeving (PBL), 2020)
Technological Readiness Level (TRL)	-	9	(Uslu, 2018)
Technical Lifetime	Years	12 – 15	(Uslu, 2018; Planbureau voor de Leefomgeving (PBL), 2020)

Table 27 Economic parameters for an industrial wood pellet steam boiler

Parameter	Unit	Baseline Value (Range)	References
Investment Cost[21] *Reference Capacity: 50 MW* [22]	$€_{2018}$/kW$_{th}$	440 – 585	(Planbureau voor de Leefomgeving (PBL), 2020; Element Energy; Jacob, 2018)
Fixed O&M Cost	$€_{2018}$/kW$_{th}$	5.9 - 44	(Planbureau voor de Leefomgeving (PBL), 2020; Element Energy; Jacob, 2018)
Variable O&M Cost	$€_{2018}$/kWh$_{th}$	0.0008 – 0.0034	(Planbureau voor de Leefomgeving (PBL), 2020; Element Energy; Jacob, 2018)
Fuel Cost		Biomass cost	

---

[21] The cost range is re-estimated based on original reference capacities in (Element Energy; Jacob, 2018; Planbureau voor de Leefomgeving (PBL), 2020), using a scale factor of 0.7. The cost includes the relevant equipment costs (biomass handling system, flue gas cleaning etc.) and the construction costs

[22] It is noted in (Danish Energy Agency, 2020) that biomass boiler capacity ranging up to 200 – 300 MW is available for CHP. Typical industrial boiler is however around 20 MW, possibly up to 50 MW.

4.2 CO_2 Capture and Storage or Re-Use

Carbon capture and storage (CCS) allows the continued usage of fossil fuels in LyondellBasell's operations, whilst achieving deep decarbonisation. The implementation of CCS, however, requires a series of infrastructure to be developed, including carbon capture installation at the industrial sites, transport network (i.e. pipeline, truck or boat), subsequently the reuse of the captured carbon (e.g. in greenhouses) and/or permanent storage deep in geological formations. Currently, a CO_2 transport & storage project, PORTHOS, is being initiated as collective infrastructure for the Port of Rotterdam industrial cluster (Port of Rotterdam, EBN & Gasunie, 2020), as further detailed in the following sub-section.

There are three main categories of carbon capture technologies, namely post-combustion, pre-combustion and oxyfuel combustion (Leung, Caramanna, & Maroto-Valer, 2014). Carbon capture takes place after fuel combustion in a post-combustion process, removing CO_2 from the flue gas (Leung, Caramanna, & Maroto-Valer, 2014). For a pre-combustion process, primary fuel (i.e. coal, natural gas) is first converted into H_2 and CO_2 through processes such as gasification and steam reforming. The pure stream of CO_2 is then captured (Leung, Caramanna, & Maroto-Valer, 2014). A practical example is such as the H-Vision blue hydrogen project. Oxygen, instead of air, is used in the oxyfuel combustion process. This results in flue gas stream composed mainly of CO_2, water, particulates and SO_2. The particulates and SO_2 is separated out through conventional methods, while the pure stream of CO_2 is captured and stored. The technology however requires a large amount of oxygen from the energy-intensive air separation units (Leung, Caramanna, & Maroto-Valer, 2014). Adjustments are also required for the existing air-fired boilers, including the installation of specific burners, flue gas recycling duct and fan (Marcano, et al., 2011).

An analysis has been conducted by (Berghout, Kuramochi, Broek, & Faaij, 2015), investigating the cost-effectiveness of the different CCS configurations at the Botlek industrial site. The different configurations consider not only the three main types of capture technologies but also the possible industrial synergies between companies. Nonetheless, considering only the independent carbon-capturing effort by LyondellBasell, post-combustion carbon capture technology may be the most applicable, as it is the preferred option for retrofitting existing plants, as well as for gas-fired and oil-fired boilers (IEAGHG, 2007; Leung, Caramanna, & Maroto-Valer, 2014). The captured CO_2 can then make use of the PORTHOS project, to be transported and stored under the North Sea or re-used.

4.2.1 Post-Combustion Carbon Capture

Post-combustion carbon capture technologies may be further differentiated based on the CO_2 separation methods. For example, adsorption, absorption and membrane separation methods (Leung, Caramanna, & Maroto-Valer, 2014). The chemical absorption technology based on monoethanolamine (MEA) is suggested as the most promising separation method, achieving a capture efficiency of 90 % (Wang, Zhao, Otto, Robinius, & Stolten, 2017; Leung, Caramanna, & Maroto-Valer, 2014; Berghout, Kuramochi, Broek, & Faaij, 2015). Amine-based capturing technology also has a TRL of 9. The MEA sorbent is used to separate the CO_2 from the flue gas, which then regenerated through a stripping or regenerative process (Leung, Caramanna, & Maroto-Valer, 2014). Additional heat and electricity are required for the capturing process. Following the initial capturing, it is expected that the CO_2 stream is compressed to a pressure of 35 bar for it to be transported through the PORTHOS CO_2 grid (Planbureau voor de Leefomgeving (PBL), 2020). Table 28 and Table 29 provide a summary of the technical and economical parameters for the carbon capturing and compression process, leading up to the connection with PORTHOS network. The reference capturing technology is based on the 30% MEA absorption method.

Table 28 Technical parameters for post-combustion carbon capturing, purification and compression

Parameter	Unit	Value	References
Full load hours	hour/year	7350 – 8500	(Berghout, Kuramochi, Broek, & Faaij, 2015)
CO_2 Capture Efficiency	%	90	(Berghout, Kuramochi, Broek, & Faaij, 2015)
Technical Lifetime	Years	15 – 25	(Berghout, Kuramochi, Broek, & Faaij, 2015)
Regeneration heat required for carbon capturing	GJ_{LHV}/tCO_2	3.5 – 4.0[23]	(Berghout, Kuramochi, Broek, & Faaij, 2015)
Electricity for carbon capturing	GJ_e/tCO_2	0.1 – 0.3	(Berghout, Kuramochi, Broek, & Faaij, 2015)
Electricity for CO_2 compression	GJ_e/tCO_2	0.45	(Berghout, Kuramochi, Broek, & Faaij, 2015)

Table 29 Economic parameters for post-combustion carbon capturing, purification and compression

Parameter	Unit	Value	References
CAPEX *(Reference CO_2 Capture Capacity: 800 kt/year)*			
Stack Modification	$M€_{2018}$/stack	0.1	(Berghout, Kuramochi, Broek, & Faaij, 2015)
SCR/FGD[24] units	$€_{2018}/(tCO_2/year)$	26	(Berghout, Kuramochi, Broek, & Faaij, 2015)
CO2 Capturing Equipment	$€_{2018}/(tCO_2/year)$	79	(Berghout, Kuramochi, Broek, & Faaij, 2015)
CO2 treatment & compression	$€_{2018}/(tCO_2/year)$	12	(Berghout, Kuramochi, Broek, & Faaij, 2015)
OPEX			
Maintenance	-	3% of Total Plant Cost	(Berghout, Kuramochi, Broek, & Faaij, 2015)
Labour, Taxes & Insurance, Administration & Overhead	$€_{2018}/tCO_2$	2.45	(Berghout, Kuramochi, Broek, & Faaij, 2015)
Connection Cost[25]	$€_{2018}/tCO_2/year$	4.3	(Planbureau voor de Leefomgeving (PBL), 2020)
Others[26]	$€_{2018}/tCO_2$	2.7	(Berghout, Kuramochi, Broek, & Faaij, 2015)

---

[23] Lower carbon concentration, which is the case for oil or gas-fired systems, requires higher regeneration heat and electricity.

[24] SCR: Selective catalytic reduction; FGD: Flue gas desulphurisation

[25] Assumed 3km connection from the industrial site to the PORTHOS CO_2 grid

[26] Includes water usage and chemical costs (Berghout, Kuramochi, Broek, & Faaij, 2015)

4.2.2 PORTHOS Project

The Port of Rotterdam CO_2 Transport Hub and Offshore Storage (PORTHOS) project aims to set up a collective CO_2 transport and storage facility for the industrial companies in the Port of Rotterdam (Port of Rotterdam, EBN & Gasunie, 2020). The individual companies are expected to perform their carbon capturing, subsequently supplying to the main CO_2 grid running through the port area. The CO_2 will be compressed in a centralised station, before being transported to an offshore platform, through an offshore transport network. The compressed CO_2 will then be pumped into the porous sand reservoir, more than 3 km beneath the North Sea seabed. Additionally, the CO_2 grid may be connected to sites where CO_2 may be utilised (i.e. greenhouses). A final investment decision is expected in late 2021, with expected initial operations in late 2023. As described in 0, PORTHOS will also be one of the main components of the H-Vision project.

The industrial companies supplying CO_2 to the collective PORTHOS infrastructure are expected to pay a processing tariff, inclusive of both storage and transport fees. The current estimate provided by PBL suggests a processing tariff of 60 €/tCO_2[27] (Planbureau voor de Leefomgeving (PBL), 2020). Contrarily, H-Vision feasibility study suggested a range between 17 to 30 €/tCO_2, calculated based on a report by EBN and Gasunie, and using TNO's in-house model (Deltalinqs, 2019).

4.3 Use of Residual Energy

4.3.1 Circular Steam Project

As mentioned in 2.1.2.4, the PO/SM co-production process produces an enormous amount of caustic wastewater (CWW). The CWW was previously incinerated in AVR Rozenburg. An energy savings cum carbon reduction project, Circular Steam Project, has recently been initiated, involving an investment worth 150 million Euro. According to (IndustriePerspectief, n.d.), this project aims to internally process the wastewater streams to generate reusable steam. 40 per cent of the wastewater streams will be biologically treated to produce biogas, which is used for steam production. The wastewater will then be cleaned using a Moving Bed Bio-Reactor (MBBR), followed by a dissolved air flotation step, before being discharged into the port. The remaining 60 per cent of the salt-containing wastewater streams will be incinerated at above 900˚C to produce steam. Such high temperature is expected to cause part of the salt to melt, which could then be collected as condensate. The remaining salt would remain as small, solid droplets in the flue gas, to be filtered out later. The salt can be used in the concrete and glass industries, upon government's permission. The resultant high-pressure steam will be reused in the production units. It is estimated that this project will allow an energy saving of 0.9 PJ annually and reduction of 140 kt of CO_2 emissions between the parties. It is unclear how this will impact the direct emissions of LyondellBasell, however, it is sure to reduce the indirect part. It also prevents an annual discharge of 11 million kg of salt into surface water.

4.3.2 Integrated Heat Pump in Distillation Column

Distillation columns play a large role in the chemical processes at the two production sites, which account for a significant proportion of the energy consumption. The distillation columns pose possible energy saving opportunities through the use of heat pump systems and heat integration. The technical potential of such interventions cannot be determined and

---

[27] Calculated based on occupancy rate of 70%.

there is a possibility that the technologies have already been employed to some extent. Nonetheless, the following provides a short introduction to the technologies.

Heat pump systems may be operated in conjunction with the distillation columns, mainly in two broad categories - the absorption heat pump and the mechanical heat pump (Jana, 2013). Heat pump systems allow up-gradation of heat from a low-temperature heat source for use in the high-temperature sink. The absorption heat pump system utilises a close loop refrigerant system, allowing heat to be transferred through the evaporation and condensation of the refrigerant. On the other hand, in a mechanical heat pump system, the vapour leaving the top of a distillation column is electrically compressed to a higher pressure and temperature, then is reused to heat the bottom liquid. Heat integrated distillation column (HIDiC) provides energy reduction opportunities through the use of both heat pump and heat integration between the stripper and rectifying sections. This provides better economic benefits to a heat pump-only system as it requires a lower compression ratio if there aren’t any other usage restrictions (Jana, 2013).

In the case of styrene separation, the capital cost of a HIDiC system is approximately 35% higher than that of a conventional system, however, an operating cost reduction of 83% owed to the lower operating pressure. A mechanical heat pump system alone, based on vapor recompression (VRC), yields a capital cost comparable to a HIDiC system and an operating cost reduction of 86%. VRC is marginally less expensive due to the use of simpler equipment, namely the use of only one heat exchanger as opposed to several (Harwardt & Marquardt, 2012). The equipment used in both systems is already widely implemented in industry (such as compressors and heat exchangers), however, the configurations themselves are less widely implemented.

(Jana, 2013) provides a detailed review of the heat pump assisted distillation column technologies, while (Bruinsma & Spoelstra, 2010) provides a short overview of other types of heat pump system (i.e. thermoacoustic heat pump). It is noted that in (Marina, Smeding, Zondag, & Wemmers, 2017), that heat pump technologies may potentially be used in the production of styrene, 1,4- butanediol, propylene oxide, propylene glycol and MTBE. However, the exact types of process considered in (Marina, Smeding, Zondag, & Wemmers, 2017) is not known.

4.4 Feedstock Substitution

It is suggested that throughout the cradle-to-grave value chains of propylene oxide and styrene monomer derivatives, the feedstock production is the most energy-intensive phase (CE Delft, 2012), contributing towards LyondellBasell’s scope 3 emissions. The carbon reduction in the feedstock production is often dependent on the decarbonisation effort of its suppliers, i.e. steam cracking facilities. The decarbonisation opportunities relevant for the conventional production of propylene, ethylene and benzene are discussed in detail in (Wong & van Dril, 2020).

On the other hand, feedstock produced through unconventional, low-carbon footprint route may be actively sought, effectively reducing LyondellBasell’s scope 3 emissions and/or overall emissions throughout the value chains. The use of alternative feedstocks in the PO/SM and PO/TBA co-production processes would have an implication for the other chemical processes that produce PO or TBA-based derivatives, such as reducing their scope 3 emissions and/or introducing bio-based fraction into the products. The use of bio-based feedstock may also allow a reduction in scope 1 emissions[28]. The current processes at the two production sites produce a significant amount of unavoidable waste fuel, a substantial source of fossil-based carbon emissions. With the use bio-based feedstock(s) in the production process(es), the waste fuel streams stemmed from incomplete chemical conversion shall contain a biomass fraction, where the magnitude depending on the amount and type of bio-based feedstock used. The subsequent burning of the (partially) bio-based waste fuel shall lead to lower accountable scope 1 emissions. The biomass fraction is considered carbon-neutral, provided that sustainability criteria set out for the EU-ETS is complied (European Commission, 2017).

In LyondellBasell's site in Wesseling, Germany, a joint project with Nestle is in operation which enables bio-based polyethylene and bio-based polypropylene production through the use of bio-based raw material such as waste and residual oils. The bio-based feedstocks can be flexibly inputted to in the pre-existing steam cracker. Thus far, the project has successfully produce several thousands of tonnes of bioplastics to be used for food packaging (Agro & Chemie, 2019). In the Botlek site, bioethanol is already being used in the production of ETBE (Sustainable Fuels, 2020). Table 30 summarises a selection of other alternative feedstocks that are relevant for the chemical processes at the Botlek and Maasvlakte production sites. More in-depth descriptions of these alternative feedstocks have been included in the other MIDDEN reports (i.e. (Wong & van Dril, 2020; Khandelwal & van Dril, 2020)), hence not repeated here. It is important to note that the list of alternative feedstocks is not exhaustive.

Table 30 Selection of alternative low carbon/bio-based feedstocks that are applicable for the LyondellBasell's chemical processes at the Botlek and Maasvlakte sites

Feedstock	Alternative
Ethylene	Ethylene via low carbon methanol-to-olefin (MTO) process. This process is able to directly convert methanol into ethylene (amongst other olefins) with only water as a by-product. This process has a TRL of 8-9 (DECHEMA, 2017) (Wong & van Dril, 2020).
	Bio-ethylene from the dehydration of bioethanol. This occurs over an alumina or silica-alumina catalyst at 300 °C in either a fixed or fluidized bed reactor. This process currently has a TRL level of 7-9 (DECHEMA, 2017) (Wong & van Dril, 2020).
Propylene	(Bio-)propylene via (bio-) low carbon methanol-to-propylene (MTP) process. This process follows the same principles as that of MTO. Bio-propylene is produced if bio-methanol being used, while low carbon methanol refers to methanol synthesized through the hydrogenation of captured fossil-based CO_2 (DECHEMA, 2017) (Wong & van Dril, 2020).
Methanol	Bio-methanol from the gasification of biomass. This process follows the same principles as of fossil-fuel based production, i.e. through the gasification of coal followed by steam reforming and methanol synthesis. Based on biomass, this process has a TRL level of 6-7. Another method is based on additional liquid CO_2 injection with the surplus of hydrogen produced in the process. The biogenic CO_2 (produced from biogas production) is reacted with hydrogen to produce bio-methanol using methanol synthesis (Khandelwal & van Dril, 2020) (DECHEMA, 2017).

---

[28] And/or scope 2 emissions, if fuel streams are exported to external utility companies where LyondellBasell receives its steam and/or electricity supply.

	Low carbon methanol produced from green H_2 and captured CO_2. This process is in principle the same as that of the conventional process but with hydrogen instead being produced via electrolysis with zero-carbon electricity (DECHEMA, 2017) (Wong & van Dril, 2020).
	Methanol has the potential to be produced from non-recyclable residual waste, including plastics. Residual waste can first be converted to syngas via gasification, and then subsequently converted into methanol. A project involving a consortium of companies in the Port of Rotterdam area aims to do this as an alternative to the incineration of waste streams in the area, both to reduce the resulting emissions and to close the loop of material and energy streams (Bomgardner, 2016).
Benzene	Benzene can be produced from biomass via several different processes. The most developed route is the gasification of biomass, followed by methanol synthesis and finally a methanol-to-aromatics (MTA) stage. This process converts methanol to a range of aromatic compounds (including benzene) using a zeolite catalyst at 370-540 °C and 20 to 25 bar. Benzene must then be separated from the other BTX components. This process has a TRL level of 6–7 (DECHEMA, 2017).
	Benzene produced via hydrogen-based methanol. This route is based on a combination of the low carbon methanol production process and the MTA process, both of which are described above. This process has a TRL level of 7 (DECHEMA, 2017).

5 Discussion

Several decarbonisation opportunities have been identified for LyondellBasell, specifically its Botlek and Maasvlakte production sites. Decarbonisation of steam production provides the greatest scope 1 and 2 emission reduction. On the other hand, the use of alternative feedstocks provides carbon mitigation opportunities throughout the value chains. The following qualitatively discusses the opportunities and barriers applicable to the decarbonisation options identified in Chapter 4. Notwithstanding, owing to their dependency on external utility companies (particularly Maasvlakte site), carbon reduction effort made by its steam/electricity suppliers would also effectively help to decarbonise LyondellBasell's operations by reducing its scope 2 emissions.

Electrode Boiler

The decarbonisation potential through electrode boiler application is heavily dependent on the fed electricity mix, considering scope 2 emissions. A net-zero steam production could only be achieved if the electricity input itself is CO_2-neutral. With this being said, it is likely that a wide-spread implementation of the technology is more promising after 2030 when a large penetration of renewable energy is expected within the electricity mix (Berenschot, 2017). Alternatively, while green electricity cannot be segregated or traced when fed into the national power grid, LyondellBasell may "green" its electricity supply by purchasing the Guarantee of Origin (GoO) certificates or through the arrangement of Power Purchasing Agreement (PPA), before the national power grid is fully decarbonised. An increasingly high electricity price may serve as a hindrance for a full electrification. Instead, a hybrid combination of electrode boiler and gas-fired technology may offer a better business case, whereby electrode boilers are used during the period of lower electricity prices (Berenschot, 2017).

Hydrogen Combustion

The hydrogen combustions options, through the use of green and/or blue hydrogen are also promising. Nonetheless, the blue H_2 production, as suggested by H-Vision, requires the use of CCS and natural gas, hence arguments against the CCS options (see below) are also relevant. The supply of green H_2 is, however, uncertain in the 2030s. The upscaling of green hydrogen production requires a much bigger penetration of renewables (i.e. wind and solar), which is currently not available. This, alongside the energy cost, should be considered when comparing green hydrogen combustion versus renewable electricity-based electric boilers. The efficiency of producing green hydrogen is logically much lower but there may be some cost arbitrage benefits possible given the possible flexibility of hydrogen production. The H-vision project also plans to import hydrogen from world regions with high green hydrogen potential from low cost electricity generation (such as Northern Africa) to serve its domestic and regional customers. On the other hand, the Blue H_2 production through the H-Vision is envisioned to start its first supply in 2026. The H-Vision project also involves the construction of a common H_2 distribution network, which shall facilitate the distribution of green H_2 in the long run. It is important to note that decarbonisation can only be realised through hydrogen combustion if blue H_2 or green H_2 is used. Similar to the CCS option, the supply security of blue or green H_2 is enhanced when there is a collective infrastructure effort (as offered by H-vision project) or an established trading hub and distribution network. Alternatively, self-production may be established on-site by electrolysis technologies such as Alkaline Electrolyser (AEL) or Proton Exchange Membrane (PEM), which are presently more expensive.

(Solid) Biomass Combustion

It is expected that increasing amount of wood chips and pellets have to be imported to meet the biomass demand (Phillips & Flach, 2019). Owing to LyondellBasell's strategic location in the Port of Rotterdam, the supply of woody biomass may be facilitated through the Port of Rotterdam. The Port of Rotterdam has a good shipping connection to Canada and the United States, the two main wood pellet suppliers. It also has extensive biomass handling facilities, making it an attractive biomass hub for the North-western European market (Port of Rotterdam, 2020). It is recognised that biomass plays a major role in a climate-neutral economy. Nonetheless, the use of biomass, particularly for energetic purpose is highly controversial. As of now, there is a limit of 25 PJ per year of biomass that can be co-fired in coal-fired power plants (IEA Bioenergy, 2018). On the other hand, biomass for renewable heat and CHP may be eligible for the Stimulation of Sustainable Energy Production (SDE+) scheme, if the sustainability criteria are met (Netherlands Enterprise Agency (RVO), 2020). The SER has recently called for the subsidy to be phased out for electricity and low-temperature applications, while high-temperature heat generation with fewer alternatives may be given the priorities (Sociaal-Economische Raad (SER), 2020). However, the availability of sustainable biomass is likely to be a constraint in the long run. In a recent report published by PBL, the expected biomass demand of the Netherlands cannot, in any perspective, be fulfilled by the national supply. Relative to the expected biomass availability of the EU in 2050, the Netherlands is expected to need between 0.6 – 6.5% of this. Other challenges concluded in the report include the long carbon payback time and the potential abuse of the wood pellet industry by the felling of natural forest and the pelletization of entire trees (Planbureau voor de Leefomgeving (PBL), 2020). It is also suggested that there shall be a cascaded and efficient use of biomass, with direct combustion of biomass being the least preferred usage. With this being said, the use of biomass for high-temperature steam generation may be a risky option, running into supply security issues and possibly a restricted use for energetic purposes, in the future.

CO_2 Capture and Storage or Re-Use

CO_2 capture and storage or re-use generally receives opposing public opinions on its role in driving the sustainable energy transition. A research conducted by (Whitmarsh, Xenias, & Jones, 2019) shows that CCS garnered the least support in the Netherlands, among four other surveyed countries. Major concerns include long-term storage risks, as well as it encourages the prolonged use of fossil fuels. In the case of LyondellBasell, the use of CCS shall sustain LyondellBasell's dependency on fossil fuel (i.e. natural gas) at least past 2050. On the policy front, the European Union (European Commission, 2020) and the Netherlands recognise the significant potential of CCS in achieving climate reduction goals. While onshore CCS projects are banned within the Netherlands, following the case of Barendrecht project (Lipponen, et al., 2017), offshore CCS and CCU (carbon capture and utilisation) projects are allowed and are actively pursued. For example, subsidy schemes are provided by the Netherlands Enterprise Agency (RVO) (Netherlands Enterprise Agency (RVO), 2020). Notwithstanding, the decarbonisation option requires large scale, preferably collective infrastructure, as offered by PORTHOS project. In the case of the PORTHOS project, it has recently been granted the Project of Common Interest (PCI) status by the European Union, as part of the umbrella project - CO2 TransPorts[29]. The PCI status allows potential EU subsidy to be granted to the PORTHOS project (PORTHOS, 2020). Such policy support has enhanced the implementation feasibility of the option. Nonetheless, the CCS option does not offer a complete carbon abatement without additional intervention(s), i.e. co-firing biomass (i.e. biogas) reach net-zero emissions or even negative emissions.

---

[29] The CO_2 TransPorts project aims to connect the neighbouring ports (i.e. Antwerp, Ghent) to the PORTHOS storage field, via a CO_2 pipeline.

Integrated Heat Pumps in Distillation Columns

The energy savings potential offered by the use of heat pumps in the distillation columns is not clear. It is possible that heat integration and/or heat pump measures are already in use. On the other hand, it is noted that there are existing steam recycling systems employed at the two complexes, where the steam of decreased quality from one processing unit is being passed down to another with a lower temperature steam requirement. Hence, further use of the heat pump system may affect the current cascading steam system or offer little energy savings improvements.

Feedstock Substitution

LyondellBasell’s scope 3 emissions are highly dependent on the decarbonisation opportunities taken up by the upstream feedstock production of its suppliers. The use of alternative low-carbon or bio-based feedstocks can contribute towards overall carbon mitigation. The current economics of those alternative production routes are less promising in comparison to the conventional production routes. For instance, the production cost of ethylene/propylene from low-carbon MTO process is double the production cost of a conventional steam cracking process (DECHEMA, 2017). The product quality implications from the use of those drop-in sustainable substitutes are also unclear. In addition to that, the lack of a mature supply chain for those sustainable alternatives is also an important barrier. Notwithstanding, the future availability of sustainable biomass sources is a concerning issue, as already noted in the discussion on (solid) biomass combustion. Another alternative is by using chemicals produced from residual waste, such as methanol produced from residual waste via gasification. This reduces the emissions that would arise from otherwise incinerating the waste.

References

Altenergy. (2020). *Electrode boilers*. Retrieved May 2020, from http://altenergy.lv/en/electrode-boilers-2/

Barnicki, S. D. (2017). Synthetic Organic Chemicals. In *Handbook of Industrial Chemistry and Biotechnology* (pp. 423-530). Springer International Publishing.

Barthe, P., Chaugny, M., Roudier, S., & Delgado Sancho, L. (2015). *Best Available Techniques (BAT) Reference Document for the Refining of Mineral Oil and Gas.*

Berenschot. (2017). *Electrification in the Dutch process industry.*

Berghout, N., Kuramochi, T., Broek, M., & Faaij, A. (2015). Techno-economic performance and spatial footprint of infrastructure configurations for large scale CO2 capture in industrial zones. A case study for the Rotterdam Botlek area (part A). *International Journal of Greenhouse Gas Control, 39*, 256-284.

Block, T., & van Dril, T. (in preparation). *Decarbonisation Options for Large Volume Organic Chemicals Production, Shell Pernis.*

Bruinsma, O., & Spoelstra, S. (2010). Heat pumps in distillation.

CE Delft. (2012). *The PO Production Chain and Possibilities for Energy Savings.*

Chemical Book. (2020). *tert-Butanol*. Retrieved August 2020, from https://www.chemicalbook.com/ChemicalProductProperty_EN_CB5206388.htm

Chemical Technology. (n.d.). *Rotterdam*. Retrieved March 2020, from Chemical Technology: https://www.chemicals-technology.com/projects/polyurethane-base-products-rotterdam/

Cioli, M., Schure, K., & Ramirez, A. (in preparation). *Decarbonisation Options for Industrial Gases Production.*

Clingendael International Energy Programme (CIEP). (2017). *Looking under the Hood of the Dutch Energy System.*

Cogeneration Observatory and Dissemination Europe (CODE2). (2014). *D5.1 - Final Cogeneration Roadmap Member State: The Netherlands.*

Coker, A. K. (2007). *Ludwig's Applied Process Design for Chemical and Petrochemical Plants.*

Danish Energy Agency. (2020). *Datasheet for industrial process heat.*

de Kruif, F. (2004, January 23). *Havenman Benders: Investeringen komen niet vanzelf*. Retrieved April 2020, from Nieuwsblad Transport: https://www.nieuwsbladtransport.nl/archief/2004/01/23/havenman-benders-investeringen-komen-niet-vanzelf/?gdpr=accept

DECHEMA. (2017). *Low Carbon Energy and Feedstock for the European Chemical Industry.*

Deltalinqs. (2019). *Blue hydrogen as accelerator and pioneer for energy transition in the industry.*

Domingues, L., Pinheiro, C., & Oliveira, N. (2017). Economic comparison of a reactive distillation-based process with the conventional process for the production of ethyl tert-butyl ether (ETBE). *Computers and Chemical Engineering, 100*, 9-26.

Dunn, J., Adom, F., Sather, N., Han, J., Snyder, S., He, C., . . . You, F. (2015). *Life-cycle Analysis of Bioproducts and Their Conventional Counterparts in GREET.*

Durusut, E., Mattos, A., Simon, R., Moore, I., Kiely, C., Yousid, S., . . . Giles, A. (2019). *Conversion of Industrial Heating Equipment to Hydrogen.*

Dutch Emissions Authority (NEA). (2020). *Overzicht toewijzing gratis emissierechten.* Retrieved from ttps://www.emissieautoriteit.nl/onderwerpen/toewijzing-ets/documenten/hulpdocument/2014/12/08/overzicht-toewijzing-gratis-emissierechten

Dutch Emissions Authority. (2020). *Emissiecijfers 2013-2019.*

Element Energy; Jacob. (2018). *Industrial Fuel Switching Market Engagement Study.*

Energiekamer. (n.d.). *Verzoek om een informele zienswijze namens Neste Oil Netherlands B.V. .*

European Commission. (2015). Commission Delegated Regulation (EU) 2015/2402 . *Official Journal of the European Union, L 333/54*.

European Commission. (2017). *Guidance Document: Biomass issues in the EU ETS.*

European Commission. (2018). *Annexes to the Commission Delegated Regulation determining transitional Union-wide rules for harmonised free allocation of emission allowances pursuant to Article 10a of Directive 2003/87/EC of the European Parliament and of the Council.*

European Commission. (2020). *Carbon Capture and Geological Storage*. Retrieved from https://ec.europa.eu/clima/policies/innovation-fund/ccs_en

European Environment Agency. (2020). *Plant-by-plant emissions (LCP) and information on derogations.* Retrieved 2020 April, from European Environment Agency: https://www.eea.europa.eu/data-and-maps/data/lcp-9/plant-by-plant-emissions-lcp

European Union. (2015). *EU ETS Handbook.*

Fact.MR. (2020). *Isobutylene Market Forecast, Trend, Analysis & Competition Tracking - Global Market Insights 2020 to 2030*. Retrieved August 2020, from https://www.factmr.com/report/3786/isobutylene-market

Falcke, H., Holbrook, S., Clenahan, I., Lopez Carretero, A., Sanalan, T., Brinkmann, T., . . . Delgado Sancho, L. (2018). *Best Available Techniques (BAT) Reference Document for the Production of Large Volume Organic Chemicals - Industrial Emissions Directive 2010/75/EU (Integrated Pollution Prevention and Control).*

Gaur, S., Mandimutsira, B., White, D., & Dubner, W. (2017). *U.S. Patent No. US20170144953A1.*

Ghanta, M. (2008). Modeling of the phase behavior of light (C2 & C3) olefins in liquid phase epoxidation systems and experimental determination of gas/liquid mass transfer coefficients.

Ghanta, M., Fahey, D., Busch, D., & Subramaniam, B. (2013). Comparative Economic and Environmental Assessments of H2O2 -based and Tertiary Butyl Hydroperoxide-based Propylene Oxide Technologies. *ACS Sustainable Chemistry & Engineering*, 268-277.

Gupta, V. P. (1996). *Europe Patent No. EP0712824A1.*

Hamid, H., & Ali, M. (2004). *Handbook of MTBE and other gasoline oxygenates.* Marcel Dekker.

Hart, D., Howes, J., Lehner, F., Dodds, P., Hughes, N., Fais, B., . . . Crowther, M. (2015). *Scenarios for deployment of hydrogen in contributing to meeting carbon budgets and the 2050 target.*

Honkela, M., Ouni, T., & Krause, A. (2004). Thermodynamics and kinetics of the dehydration of tert-butyl alcohol. *Industrial and Engineering Chemistry Research, 43*(15), 4060-4065.

Hydrocarbon Processing. (2010). *Petrochemical Processes 2010.*

Hydrogen Council. (2020). *Path to hydrogen competitiveness: A cost perspective.*

ICIS Chemical Business. (2018). *2017-2018 Chemical Profiles.*

IEA Bioenergy. (2018). *The Netherlands - 2018 Update: Bioenergy policies and status of implementation.*

IEAGHG. (2007). CO2 Capture from Medium Scale Combustion Installations.

IHS Markit. (2013). *High Purity Isobutylene from tButanol by LyondellBasell Process.*

IHS Markit. (2019, November). *Propylene - Chemical Economics Handbook*. Retrieved August 2020, from https://ihsmarkit.com/products/propylene-chemical-economics-handbook.html

IHS Markit. (2020, February). *Ethylene - Chemical Economics Handbook*. Retrieved August 2020, from https://ihsmarkit.com/products/ethylene-chemical-economics-handbook.html

Independent Commodity Intelligence Services (ICIS). (2010). *Butanediol (BDO) Production and Manufacturing Process.*

IndustriePerspectief. (n.d.). *LyondellBasell Archieves - Utilities*. Retrieved August 2020, from utilities.nl: https://utilities.nl/tag/lyondellbasell/

Intratec Solutions. (2018, November 1). *Technology Profile: Bio-based Butanediol Production*. Retrieved August 2020, from https://www.chemengonline.com/bio-butanediol-production-glucose/

IRENA. (2018). *Hydrogen from renewable power: Technology outlook for the energy transition.*

Jagger, A. (2000). *Air Products, Electrabel plant to power Rotterdam BDO unit* . Retrieved from ICIS: ttps://www.icis.com/explore/resources/news/2000/12/20/129160/air-products-electrabel-plant-to-power-rotterdam-bdo-unit/

Jana, A. (2013). Advances in heat pump assisted distillation column: A review. *Energy Conversion and Management*.

Khandelwal, M., & van Dril, T. (2020). *Decarbonisation Options for the Dutch Biofuels Industry.*

Kreijkes, M. (2015). *Groningen–Rotterdam: Changing dynamics. The reduction of gas production in the Netherlands and the influence on the energy dependency of the Rotterdam industrial cluster.*

Lassacher, S., Fazeni-Fraisl, K., & Lindorfer, J. (2018). *Full Life Cycle Assessment report of fossil isobutene reference process according to ISO 14040/14044.*

Leonard, J. J., Sullivan, G., Piel, W., & Eilerts-De-Haan, H. (1995). *Europe Patent No. EP0671394A1.*

Leung, D. Y., Caramanna, G., & Maroto-Valer, M. (2014). An overview of current status of carbon dioxide capture and storage technologies. *Renewable and Sustainable Energy Reviews, 39*, 426-443.

Lipponen, J., McCulloch, S., Keeling, S., Stanley, T., Berghout, N., & Berly, T. (2017). The Politics of Large-scale CCS Deployment. *Energy Procedia, 114*, 7581-7595.

LUMITOS AG. (2020). *Isobutylene*. Retrieved August 2020, from chemeurope.com: https://www.chemeurope.com/en/encyclopedia/Isobutylene.html#_ref-1/

LyondellBasell. (2007). *Milieuverklaring Lyondell Chemie Nederland B.V. & Lyondell Bayer Manufacturing Maasvlakte VOF: Over het jaar 2006.*

LyondellBasell. (2014). *Botlek & Maasvlakte.*

LyondellBasell. (2017). *2017 Data Book.*

LyondellBasell. (2020). *Botlek Site Fact Sheet.*

LyondellBasell. (2020). *Corporate Profile.*

LyondellBasell. (2020). *Maasvlakte Fact Sheet.*

LyondellBasell. (2020). *Moerdijk Fact Sheet.*

LyondellBasell. (2020). *Tebol 93 Alcohol*. Retrieved 2020 August, from https://www.lyondellbasell.com/en/chemicals/p/Tebol-93-ALCOHOL/bcb19261-eb30-4316-a121-6c99106e5e61

Marcano, N., Recourt, P., Tsiava, R., Laurent, J., Lethier, S., Deveaux, M., . . . Quet, J. (2011). Oxycombustion at Lacq CCS Pilot Plant: Preliminary Analysis of Burner-Boiler Performance. *2nd Oxyfuel Combustion Conference (OCC2)*, (pp. 1-3).

Marina, A., Smeding, S., Zondag, H., & Wemmers, A. (2017). A Bottom-Up Approach for Determining the European Heat Pump Potential.

Market Reports World. (2020, June 4). *Global Propylene Oxide Market 2020- Industry Trend, Business Growth, Segmentation, Competitors, Revenue, Size, Share, Industry Analysis and Forecast Details for 2023*. Retrieved August 2020, from https://www.marketwatch.com/press-release/global-propylene-oxide-market-2020--industry-trend-business-growth-segmentation-competitors-revenue-size-share-industry-analysis-and-forecast-details-for-2023-2020-06-04

Market Research Future. (2020, August). *Global 1, 4-Butanediol Market Information- by Applications (PBT (PolyButylene Terephthalate), THF (Tetrahydrofuran), GBL (Gamma butyrolactone), Polyurethane and others) and Region - Forecast to 2022*. Retrieved August 2020, from https://www.marketresearchfuture.com/reports/butanediol-market-2326

Markets and Markets. (2020). *Propylene Glycol Market*. Retrieved August 2020, from https://www.marketsandmarkets.com/Market-Reports/propylene-glycol-market-264488864.html?gclid=Cj0KCQjws536BRDTARIsANeUZ59LR0BvHAGMDNCx2QS0BfBLzsMCRN-PqP68mE-onJAZX24KtuVpvKsaAvreEALw_wcB

Marsidi, M. (2018). *Electric Industrial Boiler.*

Martin, A., & Murphy, F. (2000). Glycols, Propylene Glycols. In *Kirk-Othmer Encyclopedia of Chemical Technology.* John Wiley & Sons, Inc.

Merchant Research & Consulting, Ltd. (2020, May). *Ethyl Tertiary Butyl Ether (ETBE): 2020 World Market Outlook and Forecast up to 2029*. Retrieved August 2020, from https://mcgroup.co.uk/researches/ethyl-tertiary-butyl-ether-etbe

Modor Intelligence. (2020). *Benzene Market - Growth, Trends, and Forecast (2020-2025)*. Retrieved August 2020, from https://www.mordorintelligence.com/industry-reports/benzene-market

Mordor Intelligence. (2020). *1,4-Butanediol Market - Growth, Trends, and Forecast (2020 - 2025)*. Retrieved August 2020, from https://www.mordorintelligence.com/industry-reports/1-4-butanediol-market

Mordor Intelligence. (2020). *Butane Market - Growth, Trends and Forecast (2020-2025)*. Retrieved August 2020, from https://www.mordorintelligence.com/industry-reports/butane-market

Mordor Intelligence. (2020). *Ethyl Alcohol (Ethanol) Market - Growth, Trends, and Forecasts (2020 - 2025)*. Retrieved August 2020, from https://www.mordorintelligence.com/industry-reports/ethyl-alcohol-market

Mordor Intelligence. (2020). *Methanol Market - Growth, Trends and Forecast (2020 - 2025)*. Retrieved August 2020, from https://www.mordorintelligence.com/industry-reports/methanol-market

Mordor Intelligence. (2020). *Methyl Tert Butyl Ether (MTBE) Market - Growth, Trends and Forecast (2020-2025)*. Retrieved August 2020, from https://www.mordorintelligence.com/industry-reports/methyl-tertiary-butyl-ether-mtbe-market

Mordor Intelligence. (2020). *Styrene Market - Growth, Trends, and Forecast (2020 - 2025)*. Retrieved August 2020, from https://www.mordorintelligence.com/industry-reports/styrene-market

Munn, S., Aschberger, K., Cosgrove, O., Pakalin, S., Paya-Perez, A., Schwarz-Schulz , B., & Vegro , S. (2006). *European Union Risk Assessment Report: 1-methoxypropan-2-ol (PGME) Part I-environment.*

National Center for Biotechnology Information. (2020). *PubChem Compound Summary for CID 1030, Propylene glycol*. Retrieved August 2020, from https://pubchem.ncbi.nlm.nih.gov/compound/Propylene-glycol

National Center for Biotechnology Information. (2020). *PubChem Compound Summary for CID 241, Benzene*. Retrieved August 2020, from https://pubchem.ncbi.nlm.nih.gov/compound/Benzene.

National Center for Biotechnology Information. (2020). *PubChem Compound Summary for CID 702, Ethanol*. Retrieved August 2020, from https://pubchem.ncbi.nlm.nih.gov/compound/Ethanol

National Center for Biotechnology Information. (2020). *PubChem Compound Summary for CID 7501, Styrene*. Retrieved August 2020, from https://pubchem.ncbi.nlm.nih.gov/compound/Styrene

National Center for Biotechnology Information. (2020). *PubChem Compound Summary for CID 7843, Butane*. Retrieved August 2020, from https://pubchem.ncbi.nlm.nih.gov/compound/Butane

National Center for Biotechnology Information. (2020). *PubChem Compound Summary for CID 7900, 1-Methoxy-2-propanol*. Retrieved from https://pubchem.ncbi.nlm.nih.gov/compound/1-Methoxy-2-propanol.

National Center for Biotechnology Information. (2020). *PubChem Compound Summary for CID 8255, Isobutylene*. Retrieved August 2020, from https://pubchem.ncbi.nlm.nih.gov/compound/Isobutylene

National Center for Biotechnology Information. (2020). *PubChem Compound Summary for CID 887, Methanol*. Retrieved August 2020, from https://pubchem.ncbi.nlm.nih.gov/compound/Methanol.

Navigant. (2019). *Verkenning uitbreiding SDE+ met industriële opties.*

Netherlands Enterprise Agency (RVO). (2019). *The Netherlands: list of fuels and standard* CO_2 *emission factors version of January 2019.*

Netherlands Enterprise Agency (RVO). (2020). *Carbon Capture, Utilization and Storage (CCUS)*. Retrieved from https://www.rvo.nl/onderwerpen/duurzaam-ondernemen/energie-en-milieu-innovaties/carbon-capture-utilisation-and-storage

Netherlands Enterprise Agency (RVO). (2020). *Sustainability criteria for solid biomass under the SDE+ scheme.* Retrieved July 2020, from https://english.rvo.nl/subsidies-programmes/sde/sustainability-criteria

PE International. (2013). *Process data set: Butanediol from propylene oxide; PO Oxirane; production mix, at producer; (en)*.

Petrochem. (n.d.). *Industrie bundelt krachten en spreidt risico's.*

Phillips, S., & Flach, B. (2019). *The Dutch Industrial Market for Biomass.*

Planbureau voor de Leefomgeving (PBL). (2020). *Beschikbaarheid en toepassingsmogelijkheden van duurzame biomassa. Verslag van een zoektocht naar gedeelde feiten en opvattingen. .*

Planbureau voor de Leefomgeving (PBL). (2020). *Conceptadvies SDE++ 2021 CO2 Afvang En-Opslag (CCS).*

Planbureau voor de Leefomgeving (PBL). (2020). *Conceptadvies SDE++ 2021 vebranding en vergassing van biomassa.*

Planbureau voor de Leefomgeving (PBL). (2020). *Eindadvies Basisbedragen SDE++ 2020.*

Port of Rotterdam. (2006). *Facts and Figures on Rotterdam's Oil and Chemical Industry.*

Port of Rotterdam. (2010). *Facts and Figures on the Rotterdam Energy Port and Petrochemical Cluster.*

Port of Rotterdam. (2016). *Facts and Figures on the Rotterdam Energy Port and Petrochemical Cluster.*

Port of Rotterdam. (2018, April 1). *Uniper's MPP3: pivot and catalyst for the biobased economy*. Retrieved from Port of Rotterdam: https://www.portofrotterdam.com/en/news-and-press-releases/unipers-mpp3-pivot-and-catalyst-for-the-biobased-economy

Port of Rotterdam. (2020). *Port of Rotterdam Becomes International Hydrogen Hub.*

Port of Rotterdam. (2020). *Port of Rotterdam, Biomass handling, storage and distribution.*

Port of Rotterdam, EBN & Gasunie. (2020). *Rotterdam CCUS - Project Porthos: CO2 transport and storage.*

PORTHOS. (2020). *Possible EU subsidy for international CO2 storage cooperation*. Retrieved July 2020, from https://www.porthosco2.nl/en/possible-eu-subsidy-for-international-co2-storage-cooperation/

PR Newswire. (2020, February 18). *Global Styrene/ Market Outlook on Size, Trends And 2020 Key Player Analysis Report*. Retrieved August 2020, from https://www.prnewswire.com/news-releases/global-styrene-market-outlook-on-size-trends-and-2020-key-player-analysis-report-

301006589.html#:~:text=The%20global%20styrene%20market%20reached,nearly%20%2434.1%20billion%20by%202023.&text=Styrene%20is%20primaril

Raytheon Engineers & Constructors. (1998). *Startnotitie voor de milieueffectrapportage voor de oprichting van een BDO-fabriek in de Botlek te Rotterdam door Lyondell Chemical Nederland, Ltd.*

Robinson, P., & Hsu, C. (2017). Petroleum and Its Products. In *Handbook of Industrial Chemistry and Biotechnology* (pp. 13-106).

Sampat, B. (2011). 1,4-Butanediol: A Techno-Commercial Profile. *Chemical Weekly*, 205-211.

Santen, S., & Boere, R. (2016, May 14). *Uniper MPP3 centrale essentieel voor verduurzaming*. Retrieved April 2020, from Energiepodium: https://energiepodium.nl/artikel/uniper-mpp3-centrale-essentieel-voor-verduurzaming

Schure, K., & Semeijn, V. (2020). *Decarbonisation options for the Dutch PVC industry.*

Siemens AG. (2016). *Refining Industry: Butamer Isomerisation Unit.*

Sluis, M. v. (2014). *Het nuttig aanwenden van de restwarmte uit het retourcondensaat van UCML in de regio Maasvlakte.*

Sociaal-Economische Raad (SER). (2020). *Biomassa in balans: Een duurzaamheidskader voor hoogwaardige inzet van biogrondstoffen.*

Staatscourant. (2012). *Aanmeldnotitie voor uitbreiding isomerisatiecapaciteit C4-fabriek Lyondell Chemie Nederland B.V., Theemsweg 14 te Rotterdam-Botlek, DCMR Milieudienst Rijnmond.*

Staffell, I. (2011). *The Energy and Fuel Data Sheet.*

Sullivan, C. (2012). Propanediols. In *Ullmann's Encyclopedia of Industrial Chemistry.* Wiley-VCH Verlag GmbH & Co. KGaA.

Sumitomo Chemical Co., Ltd. (2019). *Trends and Views in the Development of Technologies for Propylene Oxide Production.*

Sustainable Fuels. (2020, October 29). *In the news: LyondellBasell advances clean burning fuels*. Retrieved from https://www.sustainablefuels.eu/mediaroom/in-the-news-lyondellbasell-advances-clean-burning-fuels/

Sutter, J. (2007). *Life Cycle Inventories of Petrochemical Solvents.* Swiss Centre for Life Cycle Inventories.

Tebodin. (2017). *Milieueffectrapport POSM afval(water)verwerkingsproject Lyondell Chemie Nederland B.V. locatie Maasvlakte.*

Tebodin. (2017). *Veiligheidsrapport – Gesterde delen Lyondell Chemie Nederland B.V. locatie Maasvlakte Deel 0 en 1.*

The Essential Chemical Industry. (2016, October 18). *Benzene and methylbenzenes*. Retrieved August 2020, from https://www.essentialchemicalindustry.org/chemicals/benzene.html

The Essential Chemical Industry. (2017, July 4). *Ethene (Ethylene)*. Retrieved from https://www.essentialchemicalindustry.org/chemicals/ethene.html

The Essential Chemical Industry. (2017, February 17). *Methanol*. Retrieved August 2020, from https://www.essentialchemicalindustry.org/chemicals/methanol.html

The Essential Chemical Industry. (2017, January 26). *Propene (Propylene)*. Retrieved from https://www.essentialchemicalindustry.org/chemicals/propene.html

Thomas Shih, T., & Bryn Mawr, P. (1992). *U.S. Patent No. 5,133,839.*

TMR Research. (2020). *Tert-butanol Market (End-user - Paints & Coatings, Flavors & Fragrance, Pharmaceuticals) - Global Industry Analysis, Size, Share, Growth, Trends, and Forecast 2017 - 2025*. Retrieved August 2020, from https://www.tmrresearch.com/tert-butanol-market

Transparency Market Research. (2020). *Propylene Glycol Ether Market - Global Industry Analysis, Size, Share, Growth, Trends, and Forecast 2019 - 2027*. Retrieved August

2020, from https://www.transparencymarketresearch.com/propylene-glycol-ether-market.html

Trent, D. L. (2001). Propylene Oxide. In *Kirk-Othmer Encyclopedia of Chemical Technology* (pp. 8-10). John Wiley & Sons, Inc.

Uniper. (n.d.). *Our power plants in the Netherlands*. Retrieved April 2020, from Uniper: https://www.uniper.energy/power-generation/countries/netherlands

Uslu, A. (2018). *Biomss Steam Boiler for Industry > 5 MWth.*

Valbert, J., Zajacek, J., & Orenbuch, D. (1993). Propylene Oxide and Glycol. In *Encyclopedia of Chemical Processing and Design* (Vol. 45, pp. 88-127).

Wang, Y., Zhao, L., Otto, A., Robinius, M., & Stolten, D. (2017). A Review of Post-combustion CO_2 Capture Technologies from Coal-fired Power Plants. *Energy Procedia*, *114*, pp. 650-665.

Weissermel, K., & Arpe, H.-J. (2003). *Industrial Organic Chemistry.* Wiley.

Whitmarsh, L., Xenias, D., & Jones, C. (2019). Framing effects on public support for carbon capture and storage. *Palgrave Communications, 5*(1), 1-10.

Wong, L., & van Dril, T. (in preparation). *Decarbonisation Options for Large Volume Organic Chemicals Production, Shell Moerdijk.*

Zhang, Z., Hidajat, K., & Raj, A. (2001). Determination of Adsorption and Kinetic Parameters for Methyl tert-Butyl Ether Synthesis from tert-Butyl Alcohol and Methanol. *Journal of Catalysis, 200*(2), 209-221.

Appendix A: Calculations

Lower Heating Value (LHV) and Emission Factor by Fuel Type

Table 31 Lower heating value (LHV) by fuel type

Fuel type	Unit	Value	References
Natural Gas	GJ/Nm^3	0.03165	(Netherlands Enterprise Agency (RVO), 2019)
Residual Fuel Oil *(e.g. A fuel, glycolic fuel, heavy liquid fuel streams)*	GJ/t	41	(Netherlands Enterprise Agency (RVO), 2019)
Chemical Waste Gas *(e.g. propane, pentane and fuel gas streams)*	GJ/t	45.2	(Netherlands Enterprise Agency (RVO), 2019)
Wood Pellets	GJ/t	17	(Planbureau voor de Leefomgeving (PBL), 2020)
Hydrogen	GJ/t	120	(Staffell, 2011)

Table 32 Emission factor by fuel type

Fuel	Unit	Value	Reference
Natural Gas	kg/GJ	56.6	(Netherlands Enterprise Agency (RVO), 2019)
Residual Fuel Oil *(e.g. A fuel, glycolic fuel, heavy liquid fuel streams)*	kg/GJ	77.4	(Netherlands Enterprise Agency (RVO), 2019)
Waste Chemical Gas *(e.g. propane, pentane and fuel gas streams)*	kg/GJ	62.4	(Netherlands Enterprise Agency (RVO), 2019)

Combined Heat & Power (CHP) Emission Attribution Method

The steam and electricity emission factors ($EF_{CHP,heat}$ and $EF_{CHP,el}$, respectively) are determined based on attribution method suggested in (European Commission, 2018), with the adapted formulas as follows:

$$EF_{CHP,heat} = Em_{CHP} * A_{CHP,heat}/Q_{net}$$

$$EF_{CHP,el} = Em_{CHP} * A_{CHP,el}/EL_{net}$$

$\mathrm{EF}_{\mathrm{CHP,heat}}$ = Steam emission factor (kg/GJ)

$\mathrm{EF}_{\mathrm{CHP,el}}$ = Electricity emission factor (kg/GJ)

$A_{CHP,heat}$ = Attribution factor for heat (-)

$A_{CHP,el}$ = Attribution factor for electricity (-)

Q_{net} = net steam output (GJ)

EL_{net} = net electricity output (GJ)

Where Em_{CHP} , $A_{CHP,heat}$ *and* $A_{CHP,el}$ are calculated as follows:

$$Em_{CHP} \ = EF_i * F_i$$

$$A_{CHP,heat} = \frac{\eta_{heat}/\eta_{ref,heat}}{\eta_{heat}/\eta_{ref,heat} + \eta_{el}/\eta_{ref,el}}$$

$$A_{CHP,heat} = \frac{\eta_{el}/\eta_{ref,el}}{\eta_{heat}/\eta_{ref,heat} + \eta_{el}/\eta_{ref,el}}$$

Em_{CHP} = Emissions from the CHP (kg)

EF_{i} = Emission factor for the fuel type i (kg/GJ)

F_{i} = Fuel consumption (GJ)

η_{heat} = Thermal efficiency of the CHP (-)

η_{el} = Electrical efficiency of the CHP (-)

$\eta_{ref,heat}$ = Reference efficiency for steam production in a stand-alone boiler (85%) (European Commission, 2015)

$\eta_{ref,heat}$ = Reference efficiency of electricity production without cogeneration (52.5%) (European Commission, 2015)