# On-board conversion of methanol to DME, a techno-economic evaluation

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# Abstract

This study examines the transition from marine diesel to alternative fuels in compression ignition (CI) engines using dimethyl ether (DME) and methanol (MeOH). Currently, dual fuel compression ignition (CI) engines require at least 30% diesel. However, using dimethyl ether (DME) enables the complete replacement of diesel. Due to DME's limited availability and gaseous state, on-board conversion of MeOH to DME is proposed. The Arklow Venture, with a 1740 kW CI diesel engine, serves as the reference vessel. Four DME-MeOH fuel scenarios were analyzed:

1. Direct Injection (DI) of pure DME.
2. DI of DME-crude (DME/MeOH/$H_2O$ mixture).
3. DI of DME-crude (30%) with Port Fuel Injection (PFI) of MeOH.
4. DI of MeOH and PFI of DME-crude (10%).

Cases 2-4, using DME-crude, simplify the conversion process as distillation of the DME product is not required. These cases achieve a higher net conversion efficiency (94.3%) compared to case 1 (90.9%). Total capital investments for cases 1-4 are 2.0, 1.2, 0.52, and 0.24 million EUR, respectively. Fuel-to-engine costs are 28.5, 25.5, 24.1, and 23.6 EUR/GJ. Case 3 is identified as the most viable option considering efficiency, cost, and retrofit maturity. While case 3 offers a feasible solution for completely replacing fossil diesel in CI engines, higher fuel costs compared to MeOH (22.4 EUR/GJ) and diesel (13.3 EUR/GJ) present a challenge without strict regulatory mandates.

# Contents

# 1 Introduction

Following the Paris Agreement, the derivative IMO targets aim at net-zero GHG emissions in maritime transport by 2050 compared to the 2008 baseline[1]. In Europe, the FuelEU maritime regulation strives for an 80% GHG intensity reduction[2]. With this in mind, methanol (MeOH) is considered a promising alternative fuel for marine applications, due to its low carbon content and potential to be produced from sustainable biogenic sources or renewable hydrogen and captured $CO_2$. Owing to the oxygen bound to its molecule, methanol also readily lowers the soot emissions from engines, and it can contribute to compliance with regulations of sulphur emission control areas.

Green Maritime Methanol (GMM) is a project series in the Netherlands in which sector-wide consortia investigate the feasibility of using methanol as a marine fuel. Its third iteration, GMM 3.0, was initiated to clarify several remaining challenges from the preceding two stages. This report discusses one of these challenges, namely the feasibility of utilizing on-board methanol to dimethyl ether (DME) conversion through a dehydration reactor. This option is interesting as DME is an excellent fuel for compression ignition engines. Where MeOH cannot fully replace diesel in a compression ignition engine, DME could. DME's properties allow it to be used as single fuel or in combination with methanol, as ignition source in a dual-fuel engine.

Methanol's disadvantages include, but are not limited to, a low lubricity, high corrosivity, lower heat of combustion (about 50% that of diesel), low flash point and a low cetane number. The latter makes methanol difficult to combust without an active ignition source (e.g., spark plug). Because DME has a very high cetane number, it can be used as the ignition fuel for methanol. Yet, DME also shares some of the disadvantages with methanol, such as a low lubricity and lower heat of combustion compared to diesel. How to treat these disadvantages, and how it affects the fuel options, is part of this report.

With an on-board MeOH to DME conversion plant, only methanol has to be bunkered; a fuel that is widely available in considerable quantities and has the potential for scale up when demand rises. DME, contrarily, is difficult to store and handle, since it is gaseous at standard temperature and pressure, making it unattractive to store in large quantities. GMM 3.0 aims at evaluating the on-board conversion of methanol to DME, thereby combining methanol's storage advantages with DME's added value for ease of ignition.

The main objective of this work was to determine the feasibility of a MeOH-to-DME plant based on a techno-economic assessment to determine the conversion plant sizing and costs. This assessment was done using the Aspen Plus and Aspen Process Economic Analyzer software. Four engine scenarios with DME as fuel were considered, where the DME is obtained from MeOH conversion requiring different conversion plants and accompanied costs.

[1] 2023 IMO strategy on reduction of ghg emissions from ships, https://www.imo.org/en/MediaCentre/PressBriefings/pages/Revised-GHG-reduction-strategy-for-global-shipping-adopted-.aspx

[2] Regulation (EU) 2023/1805, https://eur-lex.europa.eu/eli/reg/2023/1805/oj.

The following fuel scenarios were considered:

1. As close to 100% DME as possible
2. DME-crude (a mixture of 60% DME, 13% methanol, and 27% water by weight)
3. Port-injected methanol and direct-injected DME-crude
4. Direct-injected methanol and port-injected DME-crude

This report is organized as follows. Chapter 2 provides more details on the four fuel scenarios and the associated engine combustion processes. Outcomes of a literature survey on engine performance with DME/MeOH mixtures and associated costs for engine modification are included which was used for the selection of the four fuel cases and their fuel blend ratios. In Chapter 3, the process simulations that were set up for the different conversion scenarios are described including the mass and heat balances. In Chapter 4, the component sizing and plant costs of the different fuel scenarios are described. A breakdown of total equipment costs, the total capital investment and the normalized fuel costs are included as well as a sensitivity study assuming different MeOH and capital costs. This report closes with a summarizing discussion and conclusions in Chapter 5. In the discussion, the feasibility of each fuel case will be discussed based on the on-board plant costs as well as the needed engine modifications/retrofitting.

The Green Maritime Methanol project was supported by TKI Maritime and the Netherlands Ministry of Economic Affairs.

# 2 DME and MeOH fuel and combustion concepts

## 2.1 DME and MeOH fuel concepts

Methanol as a fuel for internal combustion engines is not a new idea. In fact, the fuel has been employed in automotive spark ignition engines for decades[3]. Yet, methanol is less suitable as a single fuel for compression ignition engine, owing to its high resistance to autoignition. This means that, to use methanol in CI engines for shipping applications, it must be combined with another fuel to improve the overall autoignition quality. This can be established either with a fuel blend injected through a single injection system, or via dual-fuel operation utilizing two separate injection systems. Both pathways are considered in this work.

From a methanol conversion plant, in the catalytic dehydration, a DME/MeOH/water stream is obtained, also referred to as DME-crude. Having a Cetane Number (CN) comparable to that of US specification diesel, such a mixture can already be applied in a CI engine[4,5]. Alternatively, the DME-crude can be further purified through distillation to obtain a pure DME stream for use as a single, primary fuel. DME has been shown to be an excellent fuel for CI engines, as fully calibrated and converted heavy-duty engines were already reported in literature[6].

To keep the DME consumption low, thus maintaining a low methanol-to-DME conversion rate, it is interesting to utilize methanol as the main fuel and only apply a small DME quantity as ignition source, i.e. the pilot injection. This can, again, be done in two ways. The methanol is injected into the intake manifold (port fuel injection, PFI) with a direct-injection (DI) DME pilot. Or, methanol is directly injected into the combustion chamber, and DME is fumigated into the intake port to initiate combustion.

From the preceding discussion, four fuel scenarios can be distilled, namely:

1. Using (close to) 100% DME after MeOH dehydration and consecutive DME purification for direct injection (DI) into the engine
2. Using the DME/MeOH/$H_2O$ mixture (DME-crude) from the MeOH dehydration reactor outlet without purification for direct injection into the engine cylinder
3. Using DME-crude as pilot fuel (DI) and MeOH as main fuel (PFI) in a dual-fuel system

[3] S. Verhelst, et al., *Methanol as a fuel for internal combustion engines*, Progress in Energy and Comb. Science, vol. 70, (2019), 43-88.
[4] S. Lee, D. Lopez Pintor, presentation given by Sandia National Labs to TNO on 27 March 2024 (unpublished work), *Potential of Ether-Based Ignition Improvers for Enabling (M)ethanol MCCI Combustion*, (2024).
[5] J. Ellis, B. Ramne, SPIRETH – End of Project Report, (2014).
[6] P. Soltic, et al., *The potential of dimethyl ether (DME) to meet current and future emissions standards in heavy-duty compression-ignition engines*, Fuel, vol. 355, (2024), 129357.

4. Using MeOH as main fuel (DI) with DME-crude (PFI) in a dual-fuel system also referred to as the Gane Fuel strategy[7].

Each fuel option relates to a specific combustion regime and engine layout; aspects that are discussed in more detail in the next section. Furthermore, each fuel option also brings about a specific layout for the conversion plant. This is further elucidated in Chapter 3 (see also Figure 3.2). Finally, in Chapter 4, the component sizes and costs are determined for each conversion plant layout to facilitate a comparison.

The authors acknowledge that the fuel options selected in this work are not an exhaustive list of possibilities. Nor are they necessarily the best options from engine efficiency and emissions point-of-view. These fuel options were selected to facilitate a retrofit solution for the maritime market on short notice, to replace fossil diesel and to maintain operation with a single bunker fuel. While adaptations to the engine system are required for all four options, they are limited to engine auxiliary systems; modifications to the base engine block, cylinder head and piston are in principle not required. Moreover, the four options treated here all allow to switch back to diesel-only operation: a fallback scenario for ship operators.

Two fuel options were left out of the assessment, for which some justification is in order:

1. Pure methanol operation using spark ignition, either via (low-pressure) DI or PFI
2. Dual-fuel operation with (high-pressure) DI of both methanol and DME

Obviously, the first alternative would make a techno-economic assessment of a MeOH-DME conversion plant obsolete, as DME is no longer needed in the fuel mix. But there are additional reasons to disregard this option for shipping applications. First, the fallback scenario to pure diesel operation will become unavailable since the cylinder head must be equipped with spark plugs. With regard to fuel availability, this could well be a showstopper for vessel operators. Second, running in SI mode necessitates extensive redesign of the base engine, in particular the piston, to lower the compression ratio and optimize the bowl shape.

The second alternative, a dual-fuel engine with DI of both MeOH and DME, is also considered a viable option for marine applications. Wärtsilä and MAN both have modified compression ignition engines for methanol-diesel DI dual-fuel operation[8,9]. However, these fuel injection technologies are not widely available, challenging to package in existing cylinder heads for bores smaller than roughly 20 cm, and generally more difficult to retrofit than a PFI-DI option. This option is therefore considered a viable option for new engines, rather than retrofit.

[7] R. Rezaei, SAE Powertrains, Fuels & Lubricants Digital Summit, 2021, *Gane Fuel - Introduction of an Innovative, Carbon-Neutral and Low Emission Fuel for HD CI Engines*.
[8] https://www.wartsila.com/marine/products/engines-and-generating-sets/wartsila-32-methanol-engine, accessed 23 July 2024.
[9] https://www.man-es.com/marine/products/two-stroke-engines/man-b-w-me-lgim, accessed 23 July 2024.

## 2.2 Engine and combustion considerations

To determine the fuel compositions for each of the four selected options, a literature review was conducted to find typical values for the:

a. Achievable blend compositions, i.e., methanol, water and DME fractions
b. Achievable engine efficiencies and emission levels
c. Impact on engine hardware

These values serve as key input to the simulations, as these values directly affect the required size of the plant's components. The blend composition is particularly relevant, as it determines the amount of DME that must be produced from methanol. In turn, this determines for a large part the sizing and costs of the conversion plant. The engine thermal efficiency and emissions also directly impact the total cost of operation, as these govern the fuel consumption and the need for aftertreatment. Last, the extent of engine hardware modifications affect the total cost of the retrofit solution.

Note that the fuel injection strategies in cases 1-4 are linked to a specific combustion process, as shown in Figure 2.1. And since the applied combustion process has consequences for the achievable blends, efficiencies, raw emissions and the engine hardware impact, the specifics are discussed here in more detail. The first two concepts use a single, direct injection (DI) fuel system, whereas 3 and 4 are dual-fuel concepts, utilizing both port fuel injection (PFI) and DI systems. This obviously implies that for a retrofit package with concepts 3 and 4, an additional fuel system must be installed.

While all fuel/combustion concepts rely on autoignition and can in principle be operated with high compression ratios, concept 3 is somewhat different due to its premixed (MeOH with air) nature, which may cause engine knock issues at high load. Ultimately, this limits the achievable methanol percentage in the fuel mix to 70% in case 3 (more MeOH is favorable as less MeOH has to be converted). The burn rates in concepts 1, 2, and 4 are controlled by the mixing rate imposed by the DI fuel injection event, making them inherently insusceptible to knocking. Hence, while concept 4 also utilizes PFI, the premixed fraction is only a few percent of the total fuel consumption, since DME serves as the ignition fluid. The total fraction of methanol in case 4 can therefore be much higher than in concept 3.

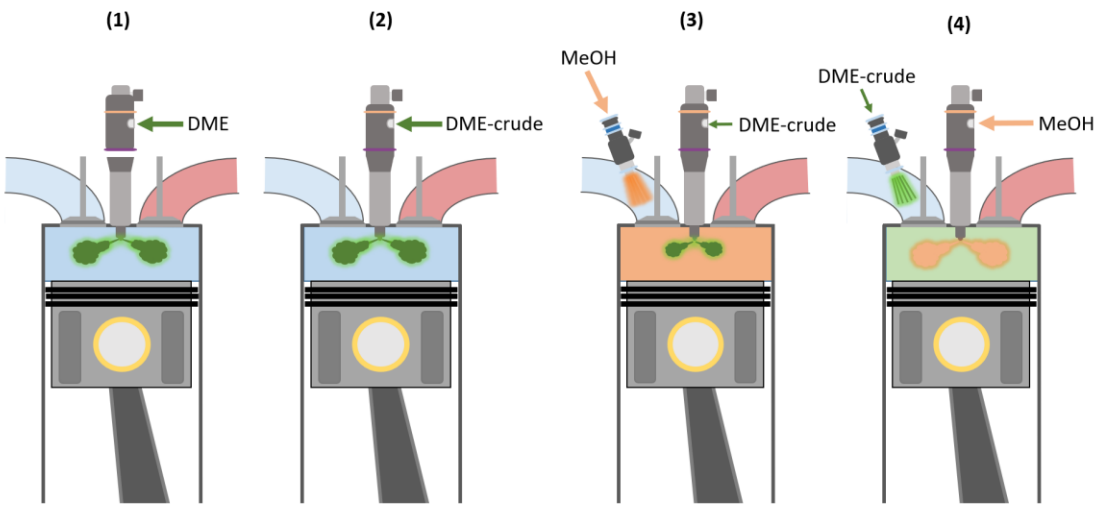


Figure 2.1: Overview of the four considered fuel injection strategies and their related combustion processes.

On the low end of the load range, the methanol percentage in the blend is again limited for concept 3 due to partial burn or even misfires. In such cases, the DME-crude amount must be increased to maintain stable combustion. Concepts 1, 2 and 4 are apparently less delimited in the usable methanol percentages, while there are other limits to consider. In the remainder of this section, particular advantages, and challenges of DME and methanol as engine fuels are addressed.

**(1) DI of (near) 100% DME**

DME is an excellent fuel for compression ignition engines owing to its tendency to autoignite. The Cetane Number (CN), a standard measure for a fuel's ignition delay in a CI engine, of DME is about 60 compared to a CN of (at least) 51 for EN590 specification diesel. Therefore, DME can be used in typical CI engines similarly as with regular diesel fuel. However, modifications are necessary to the fuel system. Due to DME's lower heat of combustion compared to diesel, a larger fuel flow is required. To accommodate this, a larger fuel pump and injectors must be installed. Furthermore, DME is has a low lubricity. This means that it can damage standard engine components under normal operation. Compatible O-rings and seals should be used in order to avoid lifetime-limiting issues. Because of its low lubricity, a lubricity enhancer is preferred to protect pump and injector to excessive wear. An oil-lubricated pump (as opposed to fuel lubrication) may be considered as an additional measure against pump wear. Last, the DME is supplied at elevated pressure from the day tank. Fortunately, this is very similar to the well-established LPG technology available on the market.

Since DME contains oxygen in its molecular structure, it has a low sooting tendency in diffusive combustion, as well as low emissions of carbon monoxide (CO) and unburned hydrocarbons (UHC). Contrarily, similar thermal efficiency and NOx emissions can be expected as the same combustion process is applied as in conventional diesel operation.

**(2) DI of DME-crude**

DME-crude consists of 60% DME, 17% methanol and 23% water by mass. This fuel shares most of its advantages and challenges with pure DME. Still, the heat of combustion is even lower, due to the methanol and water content, so pump and injector need to be sized slightly larger still. The thermal efficiency is again similar to diesel operation, due to the similarities in the combustion process. Since methanol and water have a high latent heat, and thus extract large amounts of heat upon evaporation, lower NOx emissions may be expected. More certain are the lower emissions of soot, UHC and CO given the presence of fuel-bound oxygen.

**(3) Dual fuel with MeOH PFI and DME DI**

Conventional dual-fuel operation is well established in CI engines. In most cases, diesel is used as the pilot fuel, while the main fuel can be picked from several options such as natural gas, E85 or methanol. Literature indicates a typical range of 70 ± 10% for the MeOH percentage in the fuel blend (see Table 2.1). Furthermore, higher thermal efficiency is possible, mainly in the mid load range, due to faster premixed burn rates as compared to diffusion combustion in the standard diesel engines. At lower loads, the thermal efficiency and MeOH blend fraction are limited due to partial burn of the fuel-air mixture. At high load, limitations mainly occur due to the occurrence of knock. Thus, overall, a similar thermal efficiency as in conventional diesel combustion can be anticipated. Soot and NOx emissions are generally lower, because of the largely premixed nature of the process. On the other hand, premixed combustion gives rise to elevated emissions of UHC, CO and, in case of alcohol fuels, also aldehydes.

Table 2.1: Typical blend composition, efficiency, and emissions levels, and required engine hardware modifications per fuel strategy.

| Concept | Blend composition | Efficiency/emissions | Engine hardware | Ref. |
|---|---|---|---|---|
| 1: DME (DI) | 100 wt.% DME | Efficiency similar to diesel<br>Lower soot, CO and UHC<br>Similar NOx as diesel | Larger pump and injectors<br>O-ring and seals<br>Pressurized lines<br>Lubricity enhancer | [10] |
| 2: DME-crude (DI) | 60 wt.% DME<br>17 wt.% MeOH<br>23 wt.% $H_2O$ | Efficiency similar to diesel<br>Lower soot, CO and UHC | Larger pump and injectors<br>O-ring and seals<br>Pressurized lines<br>Lubricity enhancer | [11,12] |
| 3: MeOH (PFI)<br>DME-crude (DI) | 70±10 wt.% MeOH<br>30±10 wt.% DME-crude | Higher efficiency possible<br>Lower soot and NOx<br>More CO, UHC and aldehydes | Port fuel injection system<br>O-ring and seals<br>Pressurized lines<br>Lubricity enhancer | [13] |
| 4: MeOH (DI)<br>DME-crude (PFI) | 5 wt.% DME-crude<br>95 wt.% MeOH | Efficiency similar to diesel<br>Lower soot and NOx | Larger pump and injectors<br>Port fuel injection, system<br>O-ring and seals<br>Pressurized lines<br>Lubricity enhancer | [14] |

**(4) Dual-fuel with MeOH DI and DME-crude PFI, a.k.a. Gane Fuel strategy**

The Gane Fuel strategy[14] is characterized by a small port injected DME quantity that burns in a premixed process, subsequently serving as the ignition source for methanol. Methanol, being the main fuel, is directly injected into the combustion chamber under high pressure and burns in a diffusion flame. So, while concept 4 shares the PFI-DI system configuration with concept 3, the PFI quantity is much lower, the DI quantity higher, and the main combustion regime is a mixing-controlled process instead of premixed. The DME contribution by weight is reported by Gane Fuel to be about 5%; a number that might vary with load and speed but not much. Thermal efficiency is similar to diesel combustion. Some efficiency points are lost because of the lower energetic content, giving rise to longer injection events. However, internal cooling due to methanol's high latent heat compensates this by lowering the heat transfer losses.

**Notes on the retrofit costs**

Retrofitting a vessel to operation on methanol and/or DME knows many aspects, and the costs associated with this conversion are complex and will vary. Here, focus is directed to the engine conversion, including its fuel system, piping and tank(s), and an attempt is made for a generic estimation of the retrofit costs. Only retrofits from a base diesel engine to a methanol-diesel dual-fuel engine are seen in literature. The best-known example is the Stena Germanica, of which the project retrofit costs were 450 €/kW[15], where kW relates to

[10] P. Soltic, et al., *The potential of dimethyl ether (DME) to meet current and future emissions standards in heavy-duty compression-ignition engines*, Fuel, vol. 355, (2024), 129357.
[11] J. Ellis, B. Ramne, SPIRETH – End of Project Report, (2014).
[12] S. Lee, D. Lopez Pintor, presentation given by Sandia National Labs to TNO on 27 March 2024 (unpublished work), *Potential of Ether-Based Ignition Improvers for Enabling (M)ethanol MCCI Combustion*, (2024).
[13] J. Dierickx, et al., *Retrofitting a high-speed marine engine to dual-fuel methanol-diesel operation: A comparison of multiple and single point methanol port injection*, Fuel Communications, vol. 7, (2021), 100010.
[14] R. Rezaei, et al., *Gane Fuel – Introduction of an Innovative, Carbon-Neutral and Low Emission Fuel for HD CI Engines*, SAE Technical Paper 2021-01-1198, (2021).
[15] https://www.methanol.org/wp-content/uploads/2016/07/Updates-from-Stena-Germanica-Per-Stefenson.pdf, accessed 31 July 2024.

the engine's peak power output. These costs included all parts and modifications to the engine, fuel system, piping and tanks, as well as an inert gas system. It was estimated that future conversions could be done at 350 €/kW. Taking more real-world examples into account, sustainable-ships.org arrives at a 250-550 €/kW range[16]. This results in an investment of €435.000 to €957.000 considering an engine with a 1740 kW power rating. However, these estimates best describe fuel option 3, and proper estimates for the other fuel options are lacking due to their novelty.

## 2.3 Conventions

For the study the following conventions are used:

- Units in METCBAR, being metric units with °C, bar, kW, and 1 (metric) ton being 1000 kg.
- Pressures are absolute pressures unless explicitly stated otherwise, e.g., bar(g).
- Gas volume is defined in $m_n^3$ at STP conditions. Since 1982, STP has been defined as a temperature of 273.15 K (0 °C, 32 °F) and an absolute pressure of 100 kPa [ISO 13443].
- LHV values of marine diesel (42.8 GJ/ton), MeOH (20.1 GJ/ton), DME (28.9 GJ/ton) and DME-crude (20.6 GJ/ton) were used.

[16] State of methanol as Marine Fuel, A techno-economic assessment for the use of methanol as marine fuel, version 2023-07-27, www.sustainable-ships.org.

# 3 Conversion plant technical evaluation

## 3.1 Introduction

This chapter describes the technical design and evaluation of a MeOH to DME conversion plant. In this scenario one bunkering fuel, MeOH, is present which is converted (completely or partially) into DME. In this way only one fuel has to be bunkered and the DME will act as either the main fuel or pilot fuel, depending on the considered case. The technical and economic evaluations consider the conversion of MeOH into DME (mixtures) but do not consider the engine performance with the different fuels. For the technical evaluation, the performance of the 4 processes was assessed by means of the net energy efficiency (from the total heat and mass balance).

## 3.2 Use case

For this assignment, the Arklow Venture was selected as the ship to be hypothetically converted to a DME/MeOH propelled vessel. This Arklow Venture is a 3000 GT ship for dry bulk trade, with a mean diesel consumption of 250 kg/h (1400 kW with max. 1740 kW)[17]. It contains a 1740 kW MaK6M25 main engine with two auxiliary 154 kW generators and a 66 kW emergency generator. It was built in 2017, IMO: 9772589. The ship's history shows that each charter duration is quite different, but falls within the range of 10-200 h. It has a settling tank and day tank both 7m$^3$ and a 93m$^3$ fuel bunker for diesel oil, which would be enough for about 13 days of sailing assuming the mean fuel consumption.


Figure 3.1: The Arklow Venture.

For the DME fuel cases, a day tank for DME / or mixtures for 24 h operation was assumed, which would be a 12 m$^3$ tank for DME. This requires continuous production of the DME fuel to

[17] A. de Jager, memo, Analyse vaargegevens 3000GT ARKLOW VENTURE, 02-03-2022.

keep the tank close-to-full. In case the conversion plant is not operational, the ship can then still sail for 24 h. By sizing the plant to the fuel consumption, this keeps the conversion plant small and limits the costs. It was also assumed that the current installed diesel tank will be used for MeOH as diesel will no longer be required for these scenarios. As a consequence the range on a full tank will be shorter than for diesel, because of the lower volumetric energy density of MeOH.

## 3.3 MeOH conversion plants

Based on the required mean 1400 kW output, the required fuel flows were calculated for the different cases as listed in Table 3.1, based on the recommendations of Table 2.1. The DME-crude here was determined based on the thermodynamic equilibrium in the dehydration reactor at an outlet of 369 °C resulting in a 60 wt.% DME, 17 wt.% MeOH and 23 wt.% $H_2O$. Total mass flows were then based on the equivalent lower heating values, keeping the feed LHV power to the engine equal for all scenarios. For case 3, it is assumed that 30% of energy is supplied by DME-crude. In case 4, 10% of the energy is supplied by the DME-crude via PFI, higher amounts could lead to premature autoignition and excessive compression work. It is important to note that the engine fuel efficiency was assumed equal for all the DME/MeOH cases when compared to the diesel performance (case 0).

Table 3.1: Fuel flows calculated for the different fuel cases.

| Fuel case | Description | DI | PFI | MeOH to conv plant | Fuel to engine |
|---|---|---|---|---|---|
| | | [kg/h] | [kg/h] | [kg/h] | [kW] |
| 0 | Diesel reference | 273 Diesel | | | 3246 |
| 1 | DME | 410 DME | | 570 | 3246 |
| 2 | DME-crude | 567 DME-crude | | 567 | 3246 |
| 3 | Dual fuel (DI of DME-crude) | 170 DME-crude | 407 MeOH | 170 | 3246 |
| 4 | Fumi / GANE (PFI of DME-crude) | 523 MeOH | 57 DME-crude | 57 | 3246 |

The simplified process flow diagrams (PFDs) of the MeOH-to-DME conversion plants can be found in Figure 3.2. In the conversion plant of case 1, the MeOH is pumped and pressurized from the MeOH bunker to a heat exchanger followed by an evaporator to bring the MeOH into the gas phase. MeOH conversion through catalytic dehydration then takes place in the adiabatic reactor filled with catalyst in which the DME-MeOH-$H_2O$ (DME-crude) mixture is formed according to the equilibrium reaction. As pure DME is required in this case 1, the DME-crude is distilled in a distillation unit to provide pure DME to be stored in a day tank for usage in the engine. The pure MeOH from the distillation can be recycled back to the dehydration reactor. Finally, the pure water also obtained in the distillation can be discarded.

Case 2 is similar to case 1 but much simpler as the DME-crude does not have to be distilled and no recycle is required. Same holds for cases 3 and 4, which are identical to case 2, only a smaller MeOH stream has to be processed.

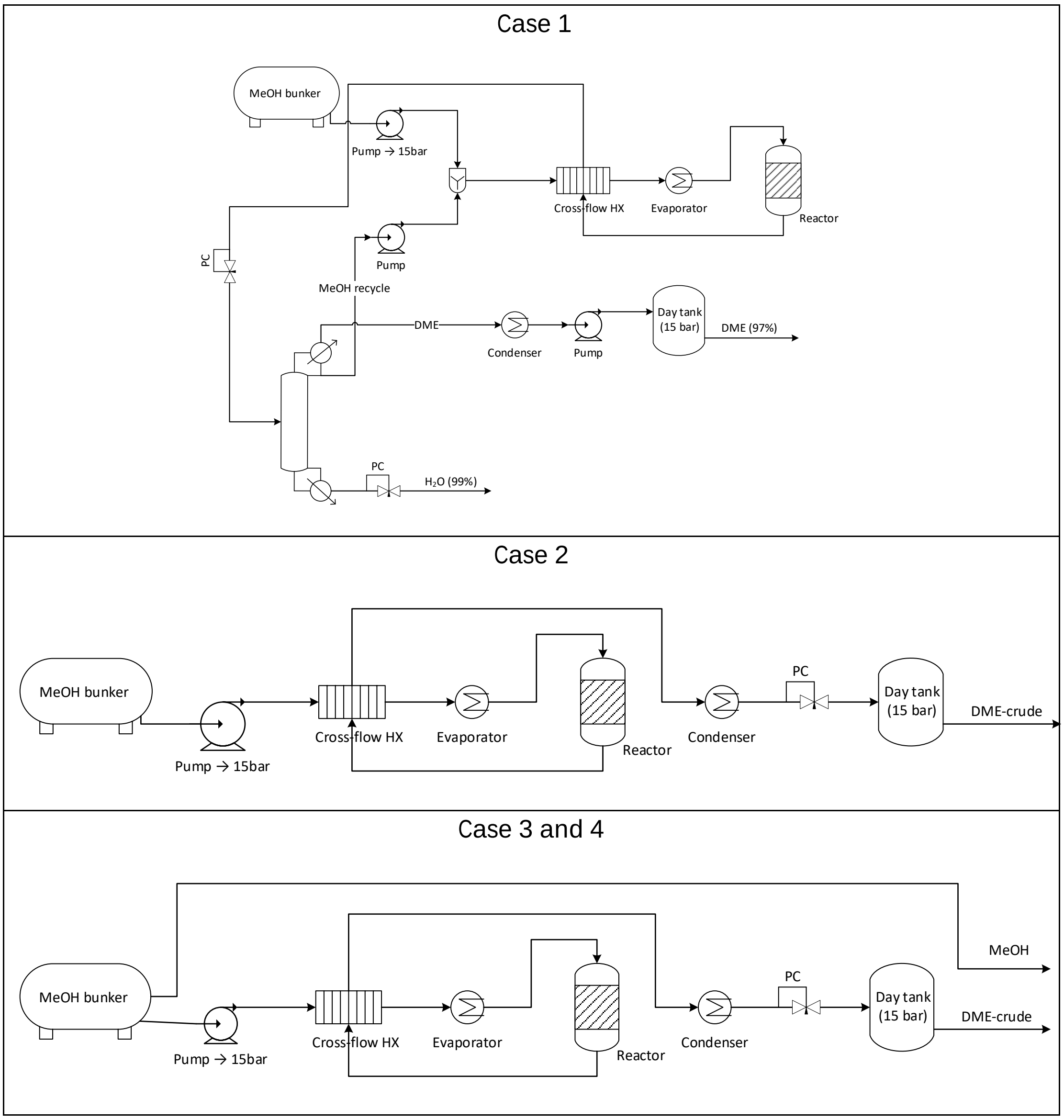


Figure 3.2: Process flow diagrams of fuel cases 1-4.

# 3.4 Process modelling specifications

Table 3.2 shows all the specifications/settings and assumptions taken in the Aspen Plus process simulations for all the unit installations that are part of the conversion plant. Included are also feed and product stream specifications.

Overall GLOBAL property method chosen was the Predictive Redlich-Kwong-Soave equation of state (PRSK). In the modelling of the process, pressure drops and heat losses to the environment have been neglected.

Table 3.2: Specifications for process modelling.

| Unit/Stream name | Function | Settings / assumptions |
|---|---|---|
| MeOH | Feed stream | 100 vol.% MeOH is assumed as feed |
| Pump1 | Compression fresh MeOH to 15 bar | 15 bar (no efficiency specified) |
| Pump2 | Compression recycled MeOH to 15 bar if applies (i.e., Case1) | 15 bar (no efficiency specified) |
| MX1 | Mix fresh MeOH and recycled MeOH from distillation columns (is applies, i.e., Case1) | 0 bar, vapor-liquid as valid phases, max. iterations 30 with tolerance 0.0001 |
| HX1 | Heat exchange between hot stream out of dehydration reactor (≈ 332 °C) and cold stream in (≈ 31 °C) | HeatX, countercurrent, shortcut, hot stream outlet temperature 124 °C, minimum temperature approach 20 °C |
| H1 | Finish heating up of the feed to the dehydration reactor | Heater, 228 °C, 0 bar (no ΔP), valid phases vapor-liquid |
| DMEREACT | Dehydration of MeOH to produce DME and $H_2O$ | RGibbs reactor, 0 bar (no ΔP), 0 heat duty (adiabatic), calculation option: calculate phase equilibrium and chemical equilibrium |
| V5 | Expansion of the DMEREACT product to the distillation pressure (5 bar) | Valve, adiabatic flash for specified outlet pressure (pressure changer), outlet pressure 5 bar, valid phases vapor-liquid, max. iterations 30 with error tolerance 0.0001 |
| DIST-$H_2O$ | Purification of the DME stream separating $H_2O$ from DME and MeOH by means of distillation | RadFrac distillation unit, calculation type is equilibrium, 18 number of stages, partial-vapor-liquid condenser, Kettle reboiler, valid phases vapor-liquid, convergence strongly non-ideal liquid, 1 mole reflux ration, 20000 Cal/sec reboiler duty, 0 free water reflux ratio, feed stream in stage 9, pressure drop 0, condenser temperature 40 °C<br><br>The objective of the purification is that the DME is purified (separated from the $H_2O$) and the discharged $H_2O$ has a purity of >99.9 wt. % so it could be possible to dump it. |
| $H_2O$ | Pure water from distillation | 99.9 wt% |
| H2 | Condensation of the DME stream. DME stream after distillation column is gaseous and it needs to be condensed in order to store it | Cooler, 0 bar (no ΔP), vapor fraction 0, valid phases vapor-liquid |
| PUMP3 | Compression DME stream to 15 bar | 15 bar (no efficiency specified) |
| H3 | Heating DME stream to the storage temperature | Heater, 40 °C, 0 bar (no ΔP), valid phases vapor-liquid |
| DAYTANK | Mimics the DME storage in a simplified way | Flash unit, 40 °C, 0 bar (no ΔP), valid phases vapor-liquid |
| DMEFINAL | Final DME product | 40 °C, 15 bar, 95.3 mol.% DME, 4.5 mol.% MeOH, $H_2O$ trace |

Design specifications (DS):

- For the Case 1 (100% DME) two design specifications are specified in the distillation column:
  - 1 → $H_2O$ purity → with this DS the content of MeOH in $H_2O$ (bottom product) is established. Assumption: MeOH mass fraction = 0.001. To achieve this DS, the reboiler duty is modified.
  - 2 → MeOH purity → with this DS the content of $H_2O$ in MeOH (top product) is established. Assumption: $H_2O$ mass fraction = 0.03. To achieve this DS, the reflux ratio is adapted.
- For all the cases feed amount is determined according to the specifications detailed in Table 3.1 where the assumptions of all the fuel cases are explained.

At specific composition, a mixture of DME/MeOH/water can demix to form two liquid phases. It was found that for the current choice for thermodynamic method and thermodynamic parameters the model cannot predict this demixing. This was therefore assessed separately, using the ternary liquid-liquid equilibrium from literature. Here is was found that the daytank the composition is sufficiently far from the conditions at which demixing would occur, so demixing in the tank is not expected.

## 3.5 Process modelling results

The process models are set up for Case 1 (100% DME) and Case 2 (DME-crude), which are the main processes. Cases 3 and 4 will simply be scaled down based on the results obtained for Case 2, because cases 2-4 all produce DME-crude only on a different scale.

<u>Sensitivity analysis</u>

DME is produced from MeOH trough dehydration (Eq.1). It is an exothermic reaction without variation of mole number, so it is not thermodynamically affected by reaction pressure whereas it is thermodynamically slightly favored at low temperature[18]. A sensitivity analysis of the DME reactor (methanol dehydration reactor) was performed in order to assess the impact of the temperature on the process performance in terms of the DME concentration as part of the DME, MeOH and $H_2O$ mixture (DME-crude). The sensitivity analysis is based only on the dehydration reactor using MeOH as feed. The result is shown in Figure 3.3 where it can be observed that the product will consist of ca. 60 wt.% DME, 15-30 wt.% MeOH balanced with $H_2O$.

| | |
|---|---|
| Eq. 1 $2CH_3OH \leftrightarrow CH_3OCH_3 + H_2O$ | $\Delta H^0 = -24\ kJ\ mol^{-1}$ |

[18] A. Brunetti, M. Migliori, D. Cozza, E. Catizzone, G. Giordano, G. Barbieri, Methanol Conversion to Dimethyl Ether in Catalytic Zeolite Membrane Reactors, ACS Susta.in. Chem. Eng. 8 (2020) 10471–10479. https://doi.org/10.1021/acssuschemeng.0c02557.

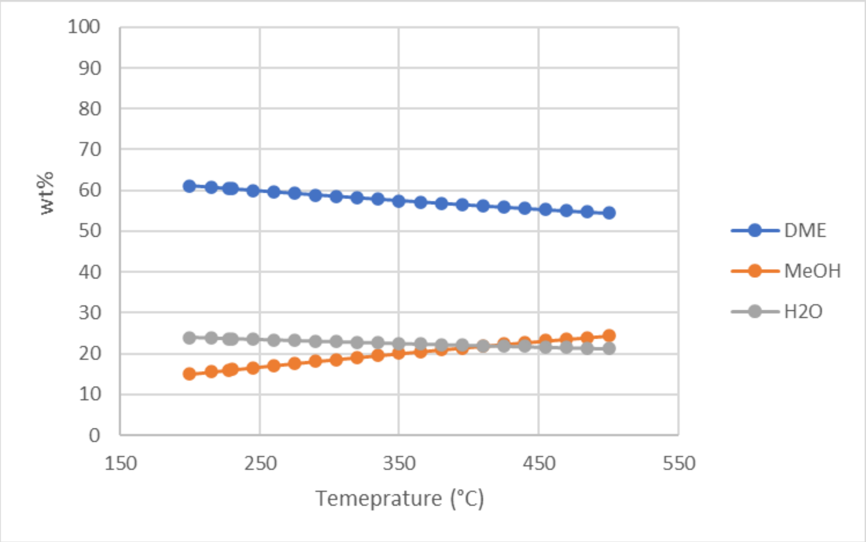


Figure 3.3: Sensitivity analysis on the effect of temperature on product composition in the MeOH dehydration reactor.

**<u>CASE 1 – 100% DME</u>**

In the first case, the use of (close to) 100% DME after MeOH dehydration and consecutive DME purification for direct injection (DI) into the engine is considered. The flowsheet for this case without considering heat integration is shown in Figure 3.4. First, the reactants (fresh MeOH and recycled MeOH) are pumped to the operating pressure (15 bar), mixed and then heated to the operating temperature (228 °C). Operating pressure and temperature were chosen based on previous experiences at TNO. The product goes to a distillation column where the DME rich stream is separated from the unreacted MeOH and $H_2O$.

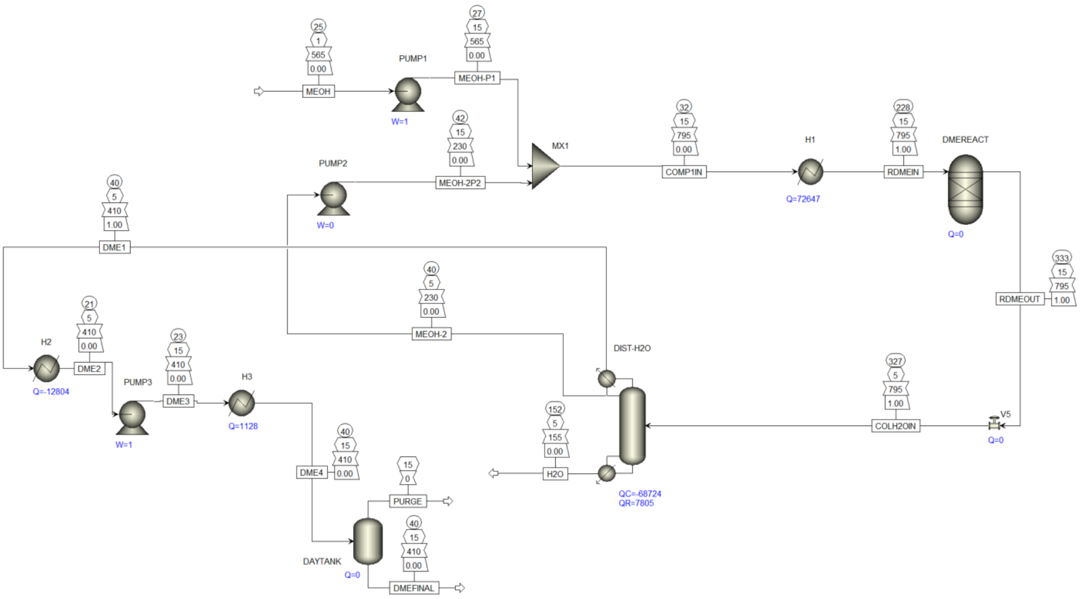


Figure 3.4: Flowsheet of Case 1 (100% DME) without heat integration.

The mass balance of this case without considering heat integration is shown in Table 3.3. The product from the reactor has a composition of around 20 wt.% $H_2O$, 14 wt.% MeOH and 65wt.% DME. After the distillation unit, a MeOH rich stream is recycled back to the reactor (around 30% of the product stream, mass based), the DME stream has a purity of 96.8 wt.% and having the $H_2O$ stream a purity of 99.9 wt.%. If a higher DME purity is desired, there is still room for optimization of the distillation column. However, this value was considered good enough for the purpose under study in this project.

Table 3.3: Mass balance of Case 1 (100% DME) without heat integration.

| | Units | Fresh MeOH | Reactor IN | Reactor OUT | Final DME | MeOH recycle | $H_2O$ |
|---|---|---|---|---|---|---|---|
| Molar Vapor Fraction | | 0.00 | 1.00 | 1.00 | 0.00 | 0.00 | 0.00 |
| Molar Liquid Fraction | | 1.00 | 0.00 | 0.00 | 1.00 | 1.00 | 1.00 |
| Temperature | C | 25.00 | 228.00 | 332.91 | 40.00 | 40.00 | 151.78 |
| Pressure | bar | 1.00 | 15.00 | 15.00 | 15.00 | 5.00 | 5.00 |
| **Mass Flows** | **kg/hr** | **565.00** | **794.81** | **794.81** | **410.00** | **229.82** | **155.00** |
| $H_2O$ | kg/hr | 0.00 | 6.89 | 162.03 | 0.30 | 6.89 | 154.84 |
| MEOH | kg/hr | 565.00 | 666.25 | 114.39 | 12.97 | 101.26 | 0.15 |
| DME | kg/hr | 0.00 | 121.67 | 518.39 | 396.73 | 121.66 | 0.00 |
| **Mass Fractions** | | | | | | | |
| $H_2O$ | | 0.00 | 0.01 | 0.20 | 0.00 | 0.03 | 1.00 |
| MEOH | | 1.00 | 0.84 | 0.14 | 0.03 | 0.44 | 0.00 |
| DME | | 0.00 | 0.15 | 0.65 | 0.97 | 0.53 | 0.00 |

Regarding the energy balance, the dehydration reactor runs adiabatic and therefore, there is no exchange of heat. However, there are still some heating and cooling requirements in the process. Regarding heating, three are the main requirements, the heating of the reactants (fresh MeOH and MeOH recycle) to the operating temperature (304.16 kW), the duty of the reboiler in the distillation column (32.68 kW) and the heating of the final DME product after pumping it to the pressure of the daily tank (4.72 kW). On the other hand, there are two main cooling requirements, the first is the duty of the condenser in the distillation column (287.73 kW) and the second is the duty for liquefaction of the final DME product after the distillation column (53.61 kW). The T-Q curves of the process utilities are shown in Figure 3.5.

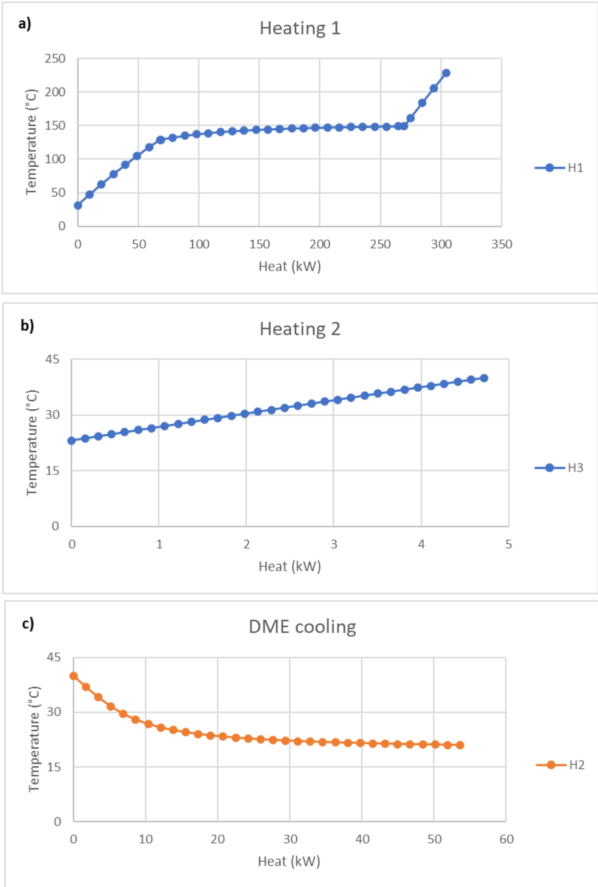


Figure 3.5: T-Q curve for heating utilities a) heating of reactants; b) heating of final DME and T-Q curve corresponding to the liquefaction of the final DME (c).

To avoid the external utilities as much as possible, a heat exchanger is placed in the process diagram to exchange heat between the reactants that will be heated and the product of the dehydration reactor that will be cooled down (Figure 3.6). The heat exchanged in this unit is 192.66 kW and the minimum temperature difference in the pinch point of the heat exchanger added ($\Delta T_{min}$) is around 20 °C. The T-Q curve of the new heat exchanger is shown in Figure 3.7. The external utilities cannot be completely avoided due to temperature limitations and therefore there is still a heating penalty of 179 kW as well as a cooling penalty of 179 kW that should be covered by external utilities. Nevertheless, the heating and cooling duties are around 48% less after the heat integration.

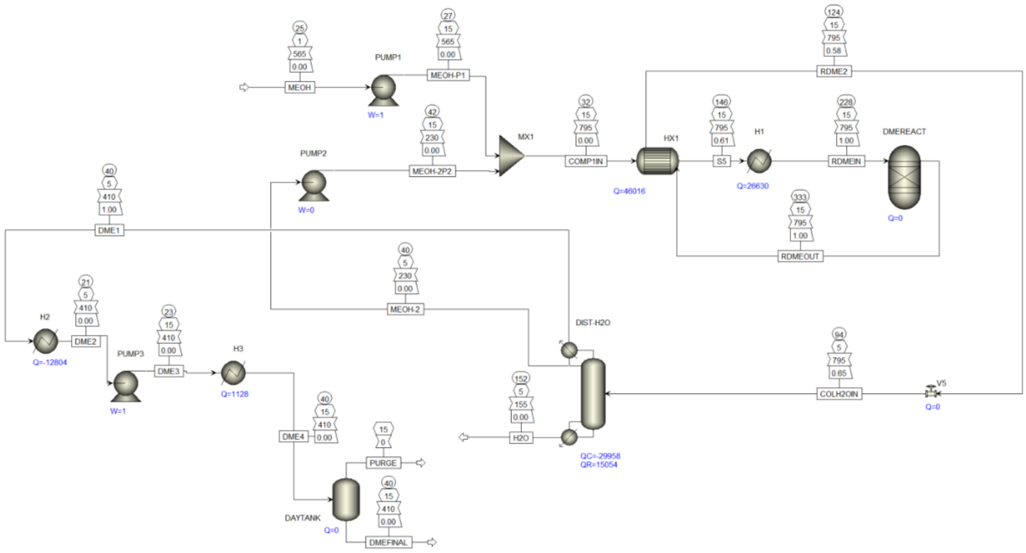


Figure 3.6: Flowsheet of Case 1 (100% DME) with heat integration.

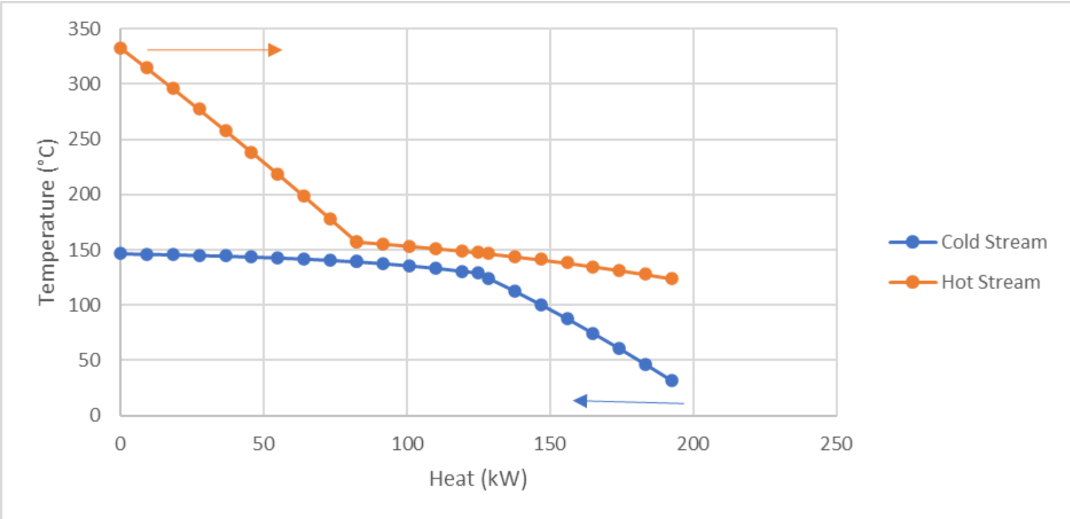


Figure 3.7: T-Q curve of the heat exchanger added for the case with heat integration.

## CASE 2 – DME-crude

For the second case, producing a DME-crude without purification for direct injection into the engine cylinder is explored. The flowsheet for this case is shown in Figure 3.8. MeOH is pumped and heated to the operating conditions (15 bar, 228 °C) which are the same as in the previous case. The product of the reaction is already the crude but needs to be cooled down to 40 °C to be stored in the daily tank prior to injection into the engine. During this cooling step the crude liquefies and so it is stored in a liquid phase. Storage pressure is assumed to be 15 bar, the same as the operating pressure.

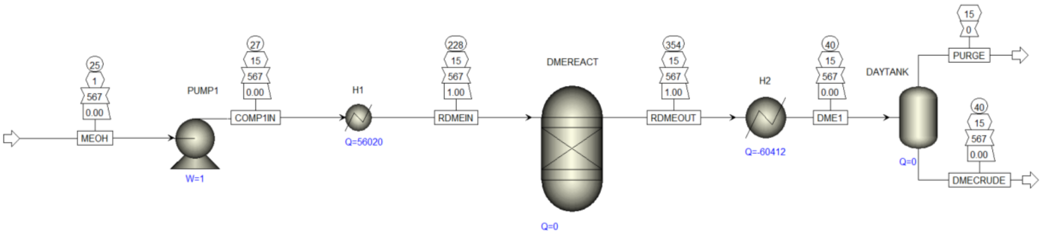


Figure 3.8: Flowsheet of Case 2 (DME-crude) without heat integration.

The mass balance without heat integration is shown in Table 3.4. It can be observed that the composition of the crude is 60 wt.% DME, 16 wt.% MeOH and 24 wt.% $H_2O$, which is similar the one reported for the OBATE fuel in the SPIRETH project where this concept was already developed[11].

Table 3.4: Mass balance of Case 2 (DME-crude) without heat integration.

| | Units | **Fresh MeOH** | **Reactor IN** | **Reactor OUT** | **DME-crude** |
|---|---|---|---|---|---|
| Molar Vapor Fraction | | 0.000 | 1.000 | 1.000 | 0.000 |
| Molar Liquid Fraction | | 1.000 | 0.000 | 0.000 | 1.000 |
| Temperature | C | 25.000 | 228.000 | 354.069 | 40.000 |
| Pressure | bar | 1.000 | 15.000 | 15.000 | 15.000 |
| **Mass Flows** | **kg/hr** | **567.000** | **567.000** | **567.000** | **567.000** |
| $H_2O$ | kg/hr | 0.000 | 0.000 | 133.915 | 133.915 |
| MEOH | kg/hr | 567.000 | 567.000 | 90.634 | 90.634 |
| DME | kg/hr | 0.000 | 0.000 | 342.451 | 342.451 |
| **Mass Fractions** | | | | | |
| $H_2O$ | | 0.000 | 0.000 | 0.236 | 0.236 |
| MEOH | | 1.000 | 1.000 | 0.160 | 0.160 |
| DME | | 0.000 | 0.000 | 0.604 | 0.604 |

Regarding the energy balance, the dehydration reactor runs adiabatic and therefore, there is no exchange of heat. However, there are still some heating and cooling requirements in the process. The first stands for the heating of the fresh MeOH to the reaction temperature (≈235 kW) and the second for the cooling of the product (≈253 kW). The T-Q are represented in Figure 3.9 a and b respectively.

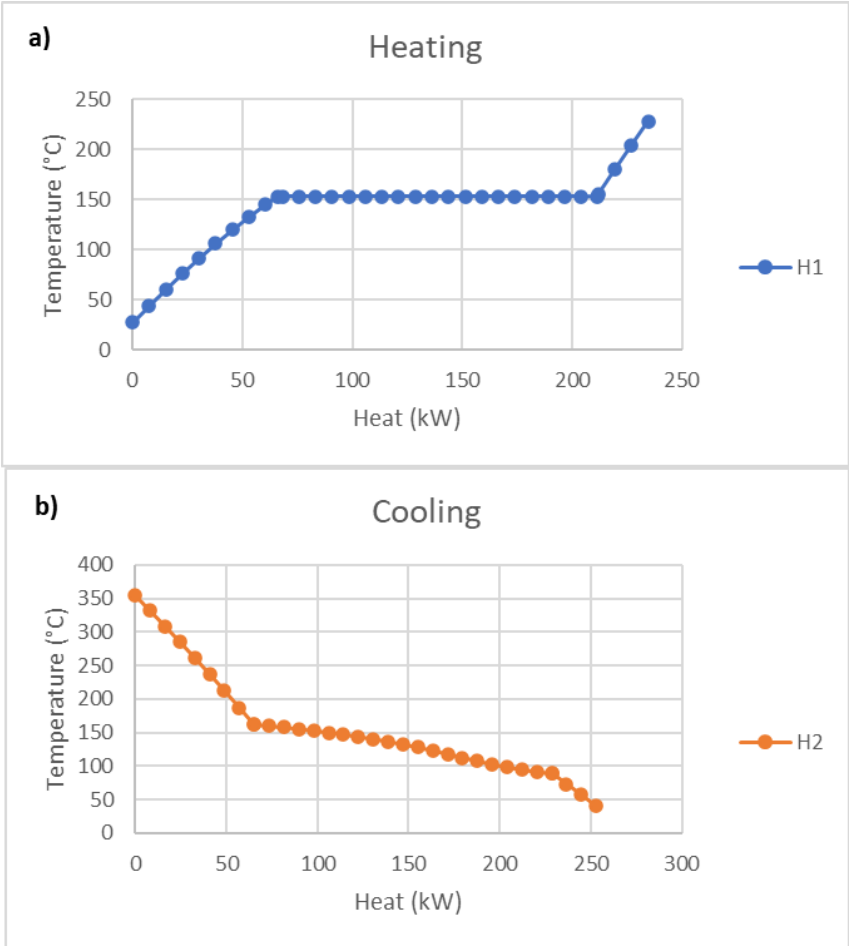


Figure 3.9: T-Q curves for fresh MeOH heating (a) and DME-crude cooling (b).

In order to avoid external utilities as much as possible, a heat integration is possible between the cold fresh MeOH and the hot DME-crude. Therefore, a heat exchanger was placed as can be seen in the flowsheet of Case 2 with heat integration (Figure 3.10). The minimum temperature difference in the pinch point of the heat exchanger ($\Delta T_{min}$) is around 20 °C and 122 kW is exchanged. The T-Q curve of the new heat exchanger is shown in Figure 3.11.

The cooling and heating utilities cannot be avoided completely with this heat integration due to temperature crossover limitations. Therefore, there is still a heating penalty (112 kW) which is around 52 % lower than in the case without integration and a cooling penalty (131 kW), around 48 % lower than before the integration.

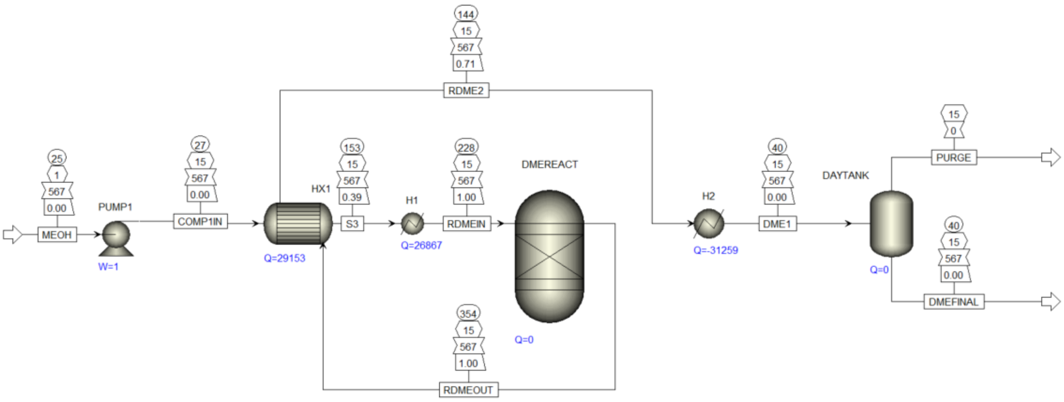


Figure 3.10: Flowsheet of Case 2 (DME-crude) with heat integration.

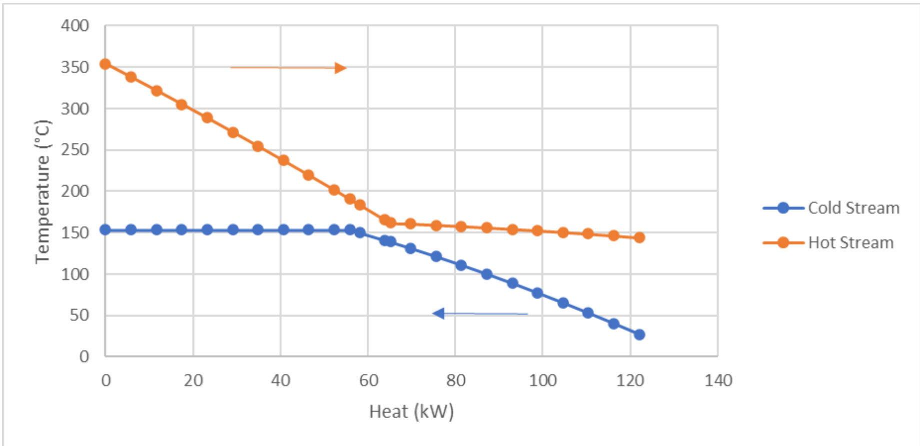


Figure 3.11: T-Q curve of the heat exchanger added for the case with heat integration.

<u>**Technical evaluation**</u>

A summary of the cases is shown in Table 3.5. The cases are compared in terms of heating and cooling requirements, power duty and net efficiency. It can be observed that the highest efficiency is obtained for the DME-crude (Case 2) as expected, since all the products of the reactions are used as fuel and no separation is done. In addition, the heating and cooling requirements in Case 2 are lower, making this case a promising one. The power duty is also lower.

Table 3.5: Comparison of the main cases in terms of heating and cooling requirements, power duty and net efficiency.

| | Heating duty (kW) | Cooling duty (kW) | Power duty (kW) | Net efficiency (%, LHV based) |
|---|---|---|---|---|
| Case 1 (100% DME) without HI | 341.56 | 341.34 | 2.22 | 81.7 |
| Case 1 (100% DME) with HI | 179.24 | 179.04 | 2.22 | 90.9 |
| Case 2 (DME-crude) without HI | 234.55 | 252.93 | 1.25 | 86.6 |
| Case 2 (DME-crude) with HI | 112.49 | 130.88 | 1.25 | 94.3 |

# 4 Conversion plant - Equipment sizing and economic evaluation

## 4.1 Introduction

This chapter discusses the results of the economic evaluation of the use cases. It discusses sizing and estimation of costs of the conversion plant, estimation of operating costs and the resulting total cost of fuel to the engine.

## 4.2 Starting points, methodology and key performance indicators

### 4.2.1 General

The methodology that was followed for this chapter is depicted in Figure 4.1. The development of the process model to establish the mass and energy balances for the process have been described in Chapter 3. The results from this are input for the equipment sizing and estimation of the operating expenses. The equipment costing is done using the software tool Aspen Process Economic Evaluator (APEA)[19]. Starting points for sizing of the individual components used are discussed in section 4.2.6.

The total capital investment (TCI) is then estimated using Lang factors (surcharges to the bare equipment costs), following the method of the American Association of Chemical Engineers[20]. The surcharge factors have been adapted so to account for the specific case of an on-board small package unit rather than a large chemical plant for which the factors are originally developed. This method was judged to be more accurate for small scale system than using APEA for obtaining the total capital investments.

The plant investments and operating costs are then combined in an economic model to arrive at the economic indicators. The operating cost and economic model based on the method of the American Association of Cost Engineers (AACE)[2], but with values adapted for this specific project. The adaptations mainly involved omitting costs for foundations,

[19] AspenTech. <www.asptentech.com> (2024).
[20] AACE. Conducting technical and economic evaluations as applied for the process and utility industries. TCM Framework: 3.2 - Asset Planning, 3.3. Report No. Investment Decision Making. AACE International Recommended Practice no 16R-90., (2003).

lowering costs for piping as for the more compact design (50% standard value), and omitting cost for site facilities and overhead.

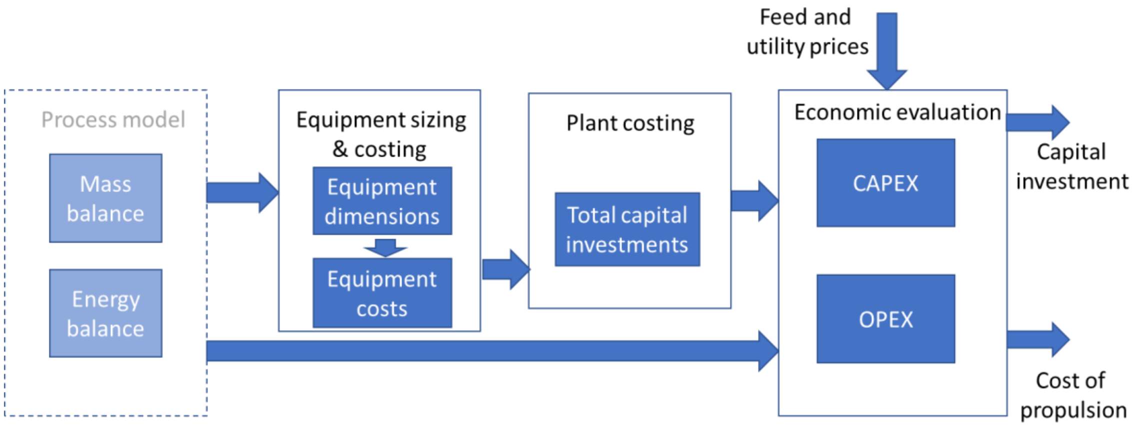


Figure 4.1: Methodology.

## 4.2.2 Fuel scenarios

The fuel scenarios are taken those as defined in Table 3.1 and Figure 3.2. Case 1 and 2 were fully evaluated using APEA modelling approach. Cases 3 and 4 were be evaluated using a shortcut method.

The process performance of the MeOH to DME system in cases 3 and 4 is equal to case 2. The investment costs for the scaled down process plant estimated using the Williams scaling rule:

$$C_b = C_b * \left(\frac{\emptyset_{m,b}}{\emptyset_{m,b}}\right)^n$$

With $C_a$ and $C_b$ the costs of two scenarios, $\Phi_{m,a}$ *and* $\Phi_{m,b}$, the mass flow throughput rates of the two scenarios and n the scaling factor (n=0.5-1, here taken 0.7).

Using the downscaled investments, the total costs of DME-crude are calculated. The total cost of fuel to engine are calculated using the energy weighted average of the DME-crude and secondary fuel methanol.

## 4.2.3 Scope and system limits

The economic evaluation assumes retrofit of an existing ship, as defined in the use case in chapter 3. The system limits are from the methanol tank up to the engine. The methanol tank is excluded (assuming that an existing diesel tank can be used as the methanol tank), the day tank needs to accommodate pressurized (crude) DME and is included.

The feed system limits are the following:
- Methanol connection from feed tank to feed line
- Heat utility in
- Cooling water utility in (sea water)
- Power utility in

The product system limits are:
- DME/DME-crude from the day tank to the engine
- Methanol to the engine, if required
- Waste water to surface water discharge
- Cooling water utility out (discharge to sea)
- Vent to atmosphere (stack included)

In the estimations, it was assumed a new day tank is required, capable of storing DME at pressure.

For the economic evaluation, the process models have been extended with some equipment that affects costs but not performance.
- Day tank
- Vent stack
- Start-up heater upstream the methanol reactor
- Cooling water mass flow calculation and cooling water pump

The total cooling water demand was calculated based on a 10 °C temperature difference.

### 4.2.4 Key performance indicators

For following key performance indicators were selected for the economic analysis:
- Breakdown of the distribution of total equipment costs and total investment costs.
- Total capital investments
- Costs per $GJ_{LHV}$ of total fuel delivered to the engine

As indicated above, the scope of the costs includes the conversion plant and day tank but exclude any engine modifications.

### 4.2.5 Uncertainties in the economic assessment

Estimating investments and costs for a process is inherently associated with uncertainties. Typical values for the accuracy of the methods for economic evaluation are listed in Table 4.1. The accuracy classification for economics is estimate at the high end of class 4, which makes that corresponding accuracy estimated at -20 to +50% for the investment. Additional uncertainties are caused by the small throughput, use of a packaged unit, and specific marine related costs factors. In addition to the uncertainty in capital cost estimates there is an uncertainty in the variable costs (predominantly costs of feedstock) and fixed costs that impact the key performance indicators.

Table 4.1: Accuracy classification[21].

| | Primary Characteristic | Secondary Characteristic | | |
|---|---|---|---|---|
| ESTIMATE CLASS | MATURITY LEVEL OF PROJECT DEFINITION DELIVERABLES<br>Expressed as % of complete definition | END USAGE<br>Typical purpose of estimate | METHODOLOGY<br>Typical estimating method | EXPECTED ACCURACY RANGE<br>Typical variation in low and high ranges [a] |
| Class 5 | 0% to 2% | Concept screening | Capacity factored, parametric models, judgment, or analogy | L: -20% to -50%<br>H: +30% to +100% |
| Class 4 | 1% to 15% | Study or feasibility | Equipment factored or parametric models | L: -15% to -30%<br>H: +20% to +50% |
| Class 3 | 10% to 40% | Budget authorization or control | Semi-detailed unit costs with assembly level line items | L: -10% to -20%<br>H: +10% to +30% |
| Class 2 | 30% to 75% | Control or bid/tender | Detailed unit cost with forced detailed take-off | L: -5% to -15%<br>H: +5% to +20% |
| Class 1 | 65% to 100% | Check estimate or bid/tender | Detailed unit cost with detailed take-off | L: -3% to -10%<br>H: +3% to +15% |

## 4.2.6 Starting points and costing data

Sizing and costing of the components are done using the stream property and equipment performance results from the process modelling.

The main assumptions for the costing are as follows:
- Costs are in EUR for year 2023, first year of operation is 2023.
- Investments are subject to deprecation of the equipment over 15 years, with zero salvage value.
- Cost of capital are included at 5%.
- Taxes are excluded.

The yearly fuel consumption is calculated from ship data as reported by Jager[22]. The calculation is listed in Table 4.2 and results in a yearly demand of 1525 ton of diesel per year during 5580 design load equivalent operating hours.

[21] Christensen, P. & Dysert, L. Cost estimate classification system. AACE International recommended practice No. 17R-97. *Association for the Advancement of Cost Engineering, Morgantown, WV* (2011).
[22] Jager, A. d. Analyse vaargegevens 3000GT ARKLOW VENTURE. (Marin, 2022).

Table 4.2: Calculation of engine fuel demand

| Parameter | Value | Unit |
|---|---|---|
| Timespan | 2 | Years |
| # Trips | 186 | # |
| Average trip duration | 60 | Hrs |
| Average trip propulsion demand | 1400 | kW |
| Average trips/year | 93 | #/year |
| Hrs/year of operation | 5,580 | hrs/yr |
| Propulsion demand/year | 2.81E+13 | J/yr |
| Propulsion demand/year | 7.81E+06 | kWh/yr |
| Specific energy use | 195.2 | gr/kWh |
| Diesel use/yr | 1.52E+06 | kg/yr |
| Diesel use/yr | 1,525 | ton/yr |
| LHV diesel | 42.8 | MJ/kg |
| Diesel use/yr | 6.53E+07 | MJ/yr |
| Propulsion demand/year | 2.81.E+07 | MJ/yr |
| Check: engine efficiency | 43% | J_fuel/J_propulsion |

Methanol prices are subject to large varieties due to variation in natural gas feedstock prices and market demand as well as other factors, such as the pricing of $CO_2$ emitted during production. Table 4.3 lists the price ranges over recent years for the spot and contract market for grey methanol (from natural gas feedstock). Based on this a base scenario value of 450 EUR/t (22.4 EUR/$GJ_{LHV}$) was selected with a range of 200-600 EUR/t for the sensitivity studies. Renewable methanol from biogenic sources or from hydrogen and captured $CO_2$ is expected to have a higher price level.

Table 4.3: Methanol market price ranges 2021-2023[23].

| Year | Spot [EUR/t] | Contract [EUR/t] |
|---|---|---|
| 2023 | 200-350 | 475-500 |
| 2022 | 300-450 | 500-550 |
| 2021 | 300-475 | 400-500 |

The price of heat was based on combustion of methanol at an efficiency of 90%, arriving at 24.9 EUR/GJ. A scenario study will be performed for the scenario where the heat can be obtained from a waste heat boiler installed downstream the main engine, or the auxiliary

[23] ICIS. Chemical profile reports. *ICIS chemical business magazine* (2023).

engine on the ship, for which the heat will be assumed available at zero costs (neglecting the investment for the waste heat boiler as a simplification).
The price of power was calculated assuming that this will be generated from methanol, assuming the price of methanal of 450 EUR/t and a conversion efficiency of 40%.

Catalyst costs were chosen 33 EUR/kg, based on using an alumina catalyst for the reaction and catalyst costs data from[24].

It was assumed that the plant can be run by the existing ships crew without the need for additional crew members. Operating and maintenance costs were taken 2% for labor and 2% for materials costs.

For the reference scenario the price of fuel was based on the price of VLSFO (very low sulphur fuel oil, see Figure 4.2. Based on an average of 625 USD/ton and using an exchange rate of 1.1 USD/EUR and heating value of 42.8 MJ/kg, the price used was 568 EUR/ton or 13.3 EUR/GJ.

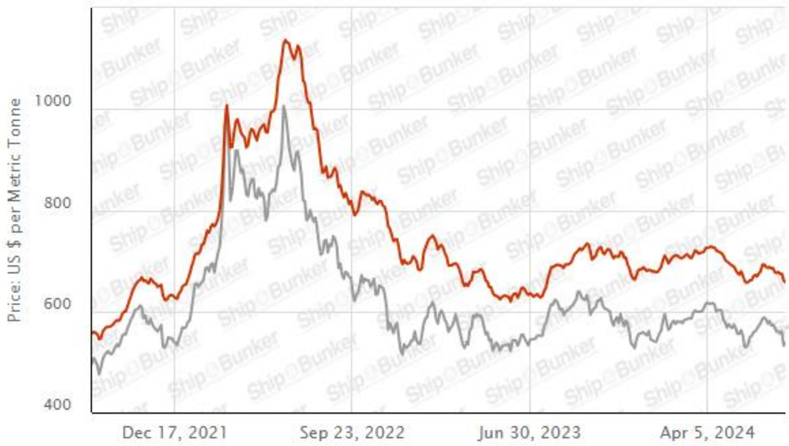


Figure 4.2: Bunker fuel prices 2021-2024, VLSFO Rotterdam (red) and global average bunker price (grey)[25].

# 4.3 Equipment sizing and costing

## 4.3.1 Sizing results

For the sizing and costing the area definition selected in APEA was "OPEN", indicating that all the equipment is connected to a steel structure. All items were specified to be hung in the structure. The standard size of the structure was adapted to the dimensions of two stacked standard ISO 45 foot high cube container. 12.0x2.33x2.65 m with a max net load 28500 kg. For the day tank a separate "OPEN" area was created (3x3x3 meters).

[24] Baddour, F. & Snowden-Swan, L. in *U.S. Department of Energy (DOE)Bioenergy Technologies Office (BETO) 2019 Project Peer Review* (2019).
[25] Ship&Bunker. *Global average bunker price*, <https://shipandbunker.com/prices/av/global/av-glb-global-average-bunker-price> (2024).

Starting points for the sizing and costing are listed in Table 4.4 and Table 4.5. Most equipment is constructed from stainless steel, in alignment with literature[26]. The selected grade for most equipment was AISI 304. Though expensive, this steel grade protects against generalized corrosion, pitting corrosion, stress corrosion cracking, hydrogen induced cracking, as well as product contamination[27].

Table 4.4: Starting points for equipment sizing and costing, Case 1 (pure DME).

| Equipment | Specification | Material | Comment |
|---|---|---|---|
| Feed pump | Centrifugal pump | SS304 | |
| Heat exchanger | Standard heat exchanger | SS304 | HX1, 5.7 m2 |
| Heater | Downterm heater, duty 305 kWth<br>Dowtherm heat exchanger 5.7 $m^2$ | SS304<br>SS304 | <br>HX2 Heat exchanger area chosen equal to heat exchanger HX1 |
| Catalytic reactor | Vertical vessel<br>WHSV =2.4 $hr^{-1}$<br>Catalyst density 1.47 $kg/dm^3$<br>Bed porosity 0.4 -<br>L/D=5 | SS304 | [28]<br>Catalyst density unit adjusted to kg/dm3.<br><br>Resulting volume 0.50 m3 |
| Column | Single diameter packed distillation column<br>Structured packing M107YB<br>Kettle type reboiler<br>TEMA HX type Condenser | SS304<br><br>SS304<br>Titanium | Height 3 meter (see text)<br>Diameter 0.4 meter (calculated) |
| Cooler | Standard heat exchanger Titanium (Sea water) | Titanium | See text |
| Product DME pump | Centrifugal pump | SS304 | |
| Recycle pump | Centrifugal pump | SS304 | |
| Cooling water pump | Centrifugal pump | 316L | [29] |
| Day tank | 7 m3 7 m3 (1.44D,4.31H) | SS304 | |

The reactor volume was based on a weight hourly space velocity WHSV (g methanol feed / h / g catalyst). In literature the space velocity varies significantly. High values (WHSV=are seen in academic studies using powder catalyst: WHSV=15-30[30] and WHSV = 35[31]. An engineering

[26] Ellis, J. *et al.* Spireth–End of project report. Activities and outcomes of the Spireth Project. (2014).
[27] Methanol Institute. Methanol safe handling manual. (2020).
[28] Bercic, G. & Levec, J. Catalytic dehydration of methanol to dimethyl ether. Kinetic investigation and reactor simulation. *Industrial & Engineering Chemistry Research* **32**, 2478-2484 (1993). https://doi.org:10.1021/ie00023a006
[29] Morrow, S. J. MATERIALS SELECTION FOR SEAWATER PUMPS. *Turbomachinery Laboratory, Texas A&M University* (2011).
[30] Ghavipour, M. & Behbahani, R. M. Fixed-bed reactor modeling for methanol to dimethyl ether (DME) reaction over γ-Alumina using a new practical reaction rate model. *Journal of Industrial and Engineering Chemistry* **20**, 1942-1951 (2014). https://doi.org:10.1016/j.jiec.2013.09.015
[31] Hosseini, S. Y. g. & Nikou, M. R. K. Investigation the effect of temperature and weight hourly space velocity in dimethyl ether synthesis from methanol over the nano-sized acidic gamma-alumina catalyst. *Journal of American Science* **8** (2012).

study by NREL[32] provided conflicting information so was not used. The original data for this study used industrial specifications for a catalyst, listing WHSV= 6 $hr^{-1}$ [33]. The most extensive study addressed kinetics, mass transfer and reactor profiles[28]. It was found that intraparticle diffusion resistance is the dominating mechanism. The WHSV of this study is the most conservative found with WHSV=2.4 $hr^{-1}$.

Given the restrictions in available space on board, it was initially considered to select compact heat exchangers. These are common in marine service, offer a low temperature approach[34,35]. It was however found that the process temperature exceeds the maximum temperature allowed. Therefore, common shell and tube heat exchangers were selected. The cooler is being constructed of titanium to mitigate corrosion issues[36]. The cooling water pump selected was constructed from 316L stainless steel[29].

To limit the height of a the DME distillation column, a stainless-steel structured packing was used, with an estimated height equivalent theoretical packing of 0.1 m. This value needs to be further verified with modelling and/or experiments.

Table 4.5: Starting points for equipment sizing and costing, Case 2 (DME-crude).

| Equipment | Specification | Material | Comment |
|---|---|---|---|
| Feed pump | Centrifugal pump | SS304 | |
| Heat exchanger | Standard heat exchanger | SS304 | HX1, 2.5 $m^2$ |
| Heater | Dowtherm heater, duty 117 $kW_{th}$<br>Dowtherm heat exchanger<br>2.5 $m^2$ | SS304<br><br>SS304 | <br><br>HX2 Heat exchanger area chosen equal to heat exchanger HX1 |
| Catalytic reactor | Vertical vessel<br>WHSV =2.4 $hr^{-1}$<br>Catalyst density 1.47 kg/$dm^3$<br>Bed porosity 0.4 -<br>L/D=5 | SS304 | [28]<br>Catalyst density unit adjusted to kg/$dm^3$.<br><br>Resulting volume 0.35 $m^3$ |
| Cooler | Standard heat exchanger<br>Titanium (Sea water) | Titanium | See text |
| Product DME pump | Centrifugal pump | SS304 | |
| Cooling water pump | Centrifugal pump | 316L | [29] |
| Day tank | 7 $m^3$ (1.44D,4.31H) | SS304 | |

[32] Tan, E. C. *et al.* Process design and economics for the conversion of lignocellulosic biomass to hydrocarbons via indirect liquefaction. Thermochemical research pathway to high-octane gasoline blendstock through methanol/dimethyl ether intermediates. (National Renewable Energy Lab (NREL), Golden, CO (United States), 2015).

[33] Phillips, S. D., Tarud, J. K., Biddy, M. J. & Dutta, A. Gasoline from Woody Biomass via Thermochemical Gasification, Methanol Synthesis, and Methanol-to-Gasoline Technologies: A Technoeconomic Analysis. *Industrial & Engineering Chemistry Research* **50**, 11734-11745 (2011). https://doi.org/10.1021/ie2010675

[34] Araner. *Seawater Heat Exchanger: Different Models*, <https://www.araner.com/blog/comparison-heat-exchange-technologies-seawater-applications> (2024).

[35] Hofmann. *Marine Heat Exchanger - Plate Heat Exchanger For Marine Applications*, <https://www.hofmann-heatexchanger.com/solutions/plate-heat-exchanger-for-marine> (2024).

[36] Andersson, H. Shift to Compact Heat Exchangers For optimized heat recovery, efficient cooling and reduced chiller load. *Chemical Industry Digest* (2010).

The results do not give an exact estimation of the total volume of the system, but based on the number of unit operations and the volume of the largest equipment a first indication on the relative volume of main equipment of all unit operations (excluding the day tank) the two options can be obtained. The total volume has been estimated based on the equipment sizing results and assumed specific volume for pumps and a specific surface area for the heat exchangers (pumps 0.1 $m^3$, heat exchangers 50 $m^2/m^3$). Here is found that Case 1 (pure DME) is significantly larger with a facto 1.3 more unit operations and a factor 2.25 more total equipment volume than Case 2 (crude DME). In addition, Case 2 requires significant height for the distillation column that is estimated to be 3 meter high.

## 4.3.2 Costing results

A breakdown of the purchased equipment costs for the Case 1 (pure DME) depicted in Figure 4.3. The total bare equipment costs amount to 596 kEUR. The costs are distributed over several elements, with the column, the DME reactor and the pumps being the three largest contributors. The choice for stainless steel as a construction material contributes to the significant investments.

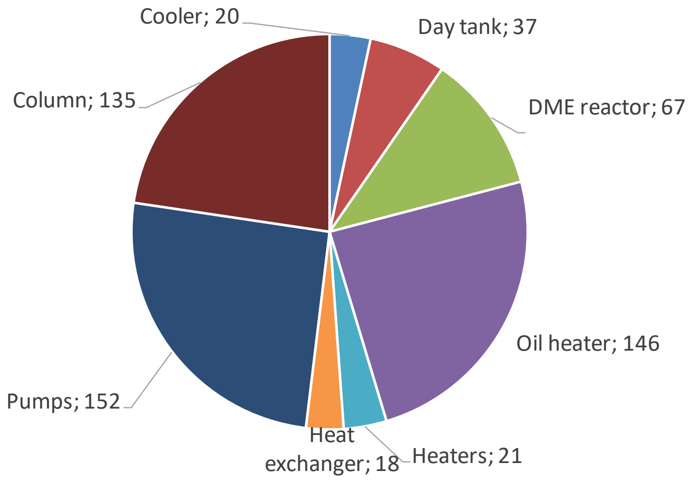


Figure 4.3: Breakdown of bare equipment costs (kEUR) for Case 1, pure DME. Total bare equipment costs 596 kEUR.

A breakdown of the purchased equipment costs for the Case 2 (DME-crude) as depicted in Figure 4.4. It is again seen that the different elements all contribute with relatively equal contributions, with none of the items dominating the costs. The total equipment costs amount to 370 kEUR, which is almost half that of Case 1 Pure DME. This as a result of the fewer pieces of equipment, and to a lesser extent to the smaller equipment size as a result of the absence of a recycle.

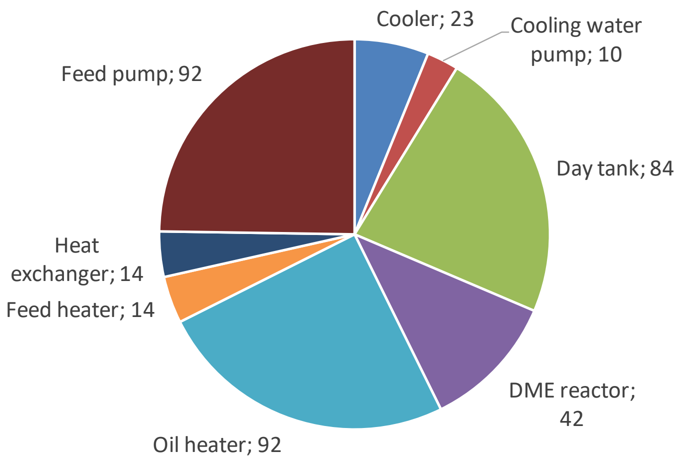


Figure 4.4: Breakdown of bare equipment costs (kEUR) for Case 2 DME-crude. Total bare equipment costs 370 kEUR.

The breakdown of Total Capital Investments for Case 1 pure DME (2.0 MEUR) and Case 2 DME-crude (1.2 MEUR) are depicted in respectively Figure 4.5 and Figure 4.6. These results from the surcharges as recommended by the AACE, but adapted for the purpose of this study, see section 4.2.6. A significant part of the costs are for process and project contingencies, as recommended for early-stage development technologies. The total investment costs amount to 1.2 MEUR for the Case 1 pure DME and 2.0 MEUR, for case 2 crude DME.

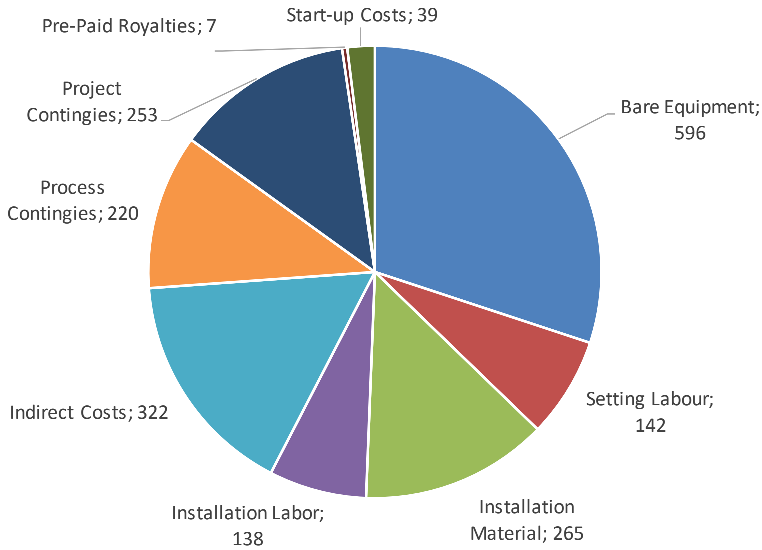


Figure 4.5: Breakdown of Total Capital Investments for Case 1 pure DME, 2.0 MEUR total investment costs.

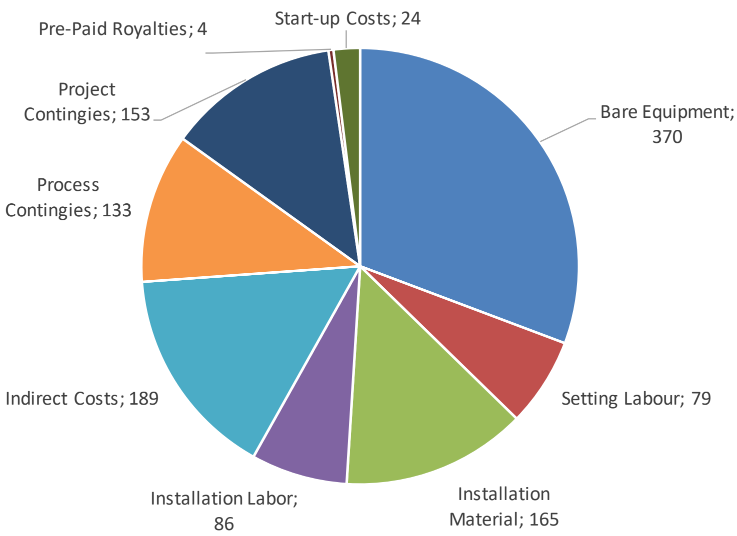


Figure 4.6: Breakdown of Total Capital Investments for Case 2 DME-crude, 1.2 MEUR total investment costs.

## 4.4 Economic evaluation results

Total cost of fuel to engine and a breakdown thereof is listed in Table 4.6. The main contribution by far is from the methanol feed for both scenarios. Capital related costs are however also significant, especially for Case 1 pure DME. The heat needs assumed to be generated from combustion of methanol are again higher for Case 1, but much smaller for Case 2 as a result of the lower heat demand. The contribution of catalyst costs is in both cases negligible.

Table 4.6: Breakdown of costs of fuel to engine (EUR/$GJ_{LHV}$).

| | **Case 1**<br>**Pure DME**<br>**[EUR/GJ_Fuel LHV to engine]** | **Case 2**<br>**DME-crude**<br>**[EUR/GJ_Fuel LHV to engine]** |
|---|---|---|
| Feedstock | 21.7 | 21.8 |
| Heat & power | 2.1 | 0.8 |
| Catalyst | 0.0 | 0.03 |
| Maintenance | 1.2 | 0.7 |
| Depreciation | 2.0 | 1.2 |
| Cost of capital | 1.5 | 0.9 |
| **Total costs of fuel to engine** | **28.5** | **25.5** |

## 4.5 Sensitivity and scenario studies

Figure 4.7 depict the result of a sensitivity study towards the impact of selected parameters. The range of variations for the investments was taken from the typical uncertainty for the classification (not taking into account additional specific aspects for the current project) and variations seen for methanol price in recent years. Zero cost for heat production correspond with obtaining waste heat within the ship by installing a waste heat boiler while neglecting the investments for that.

Putting the cost for heat at zero will reduce the cost to a limited amount, and most significant for the case 2 DME-crude. Case 2 has the highest contribution of capital related costs and is also most sensitive for the variations in investment. The largest impact is seen from the variation of methanol price. In total variations are seen between 16.5 and 35.8 EUR/GJ for Case 1 and 13.4 and 32.8 EUR/GJ for Case 2 when varying a single parameter, both indicating a significant uncertainty for the results obtained.

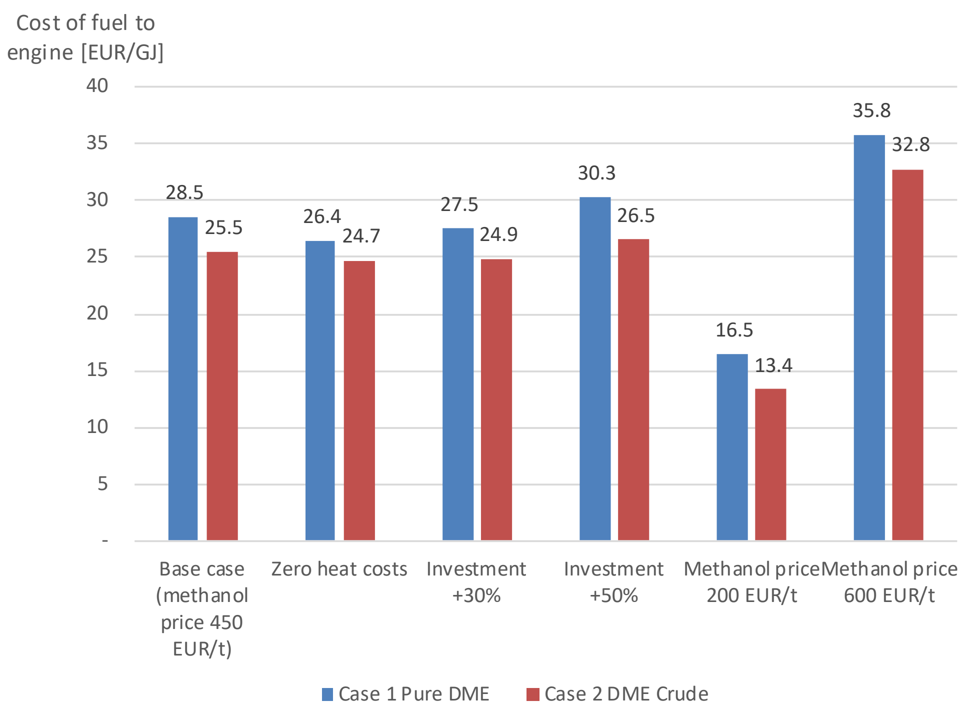


Figure 4.7: Sensitivity study, impact of selected parameters on cost for fuel to engine. For reference: Methanol prices for base scenario, high and low scenario respectively 450/200/600 EUR/t, corresponding with respectively 10.0/22.4/28.9 EUR/GJ.

The results for the fuel scenario studies are depicted in Table 4.7. Based on the detailed investments estimations for the DME-crude, a shortcut method was used to estimate the total capital investment costs for scenarios 3 and 4. This is then combined with the total cost of additional methanol to arrive at the total cost of fuel to engine.

The results show that the investment is significantly reduced. The uncertainty of the investments is expected to be higher for the smaller size. Also, equipment availability for smaller is advised to be further assessed. The costs for fuel to engine are lower for the use

Cases 3 and especially for Case 4, both approaching further to the costs for methanol (22.4 EUR/GJ).

Table 4.7: Results fuel scenario studies. Specific DME-crude costs for downscaled system and resulting total costs of fuel to engine ($GJ_{LHV}$).

| Fuel case # | Fuel case | Share of DME (crude) | Total capital investments | Crude DME costs | Cost of fuel to engine |
|---|---|---|---|---|---|
| | | GJ/GJ | MEUR | EUR/GJ | EUR/GJ |
| 0 | Diesel reference | - | - | | 13.3 |
| 1 | Pure DME | 100% | 2.0 | | 28.5 |
| 2 | DME-crude | 100% | 1.2 | 25.5 | 25.5 |
| 3 | Dual fuel (DI of DME-crude, rest MeOH) | 30% | 0.52 | 28.2 | 24.1 |
| 4 | Fumi / GANE (PFI of DME-crude, rest MeOH) | 10% | 0.24 | 34.4 | 23.6 |

An overview of the final results for the scenario studies are summarized in Figure 4.8. It lists the total capital investments for the fuel conversion plant (MEUR, excluding costs for engine modification) and the total costs of fuel to engine ($GJ_{LHV}$). This is done for all scenarios as listed defined in Table 3.1 and includes the price of diesel (VLSFO) as a reference scenario, and the costs of methanol as a theoretical minimum value for reference too. It is seen that the highest costs are for Case 1 Pure DME, which is found only to be viable if for technical reasons pure DME is required. The system is more complex, has a higher investment and higher operating costs as result of having a higher heat demand.

Case 2 pure DME is more attractive than Case 1. It has lower investments as well as lower operating costs and thereby a lower cost of fuel to engine. The system requires that a mixture of DME, methanol and water can be used as an engine feed.

Case 3 Dual fuel using MeOH as pilot fuel (PFI) and DME as main fuel (DI) in a dual-fuel system benefits from downscaling of the DME system to 30% of its size resulting lower investments to less than half value of case 2. A modest reduction in cost to engine are achieved.

Case 4. The other dual fuel approach with port fuel injection of DME-crude and methanol as the main fuel (DI) allows for further downscaling of the system to 10% of its original capacity reducing the investments with again 50% compared to case 3. The resulting cost for fuel to engine are the lowest for all scenarios obtained, and the uncertainty in equipment costs for this system is high, and availability of equipment of this size needs to be assessed in more detail. A larger plant with reduced operating hours could be selected as an alternative approach.

For reference, the price of diesel (VLSFO) and that of methanol are depicted. Using methanol is seen to be the main contributor to increased cost for fuel to engine, especially for the cases 3 and 4 where for the latter the total costs approach the costs for methanol within 20%.

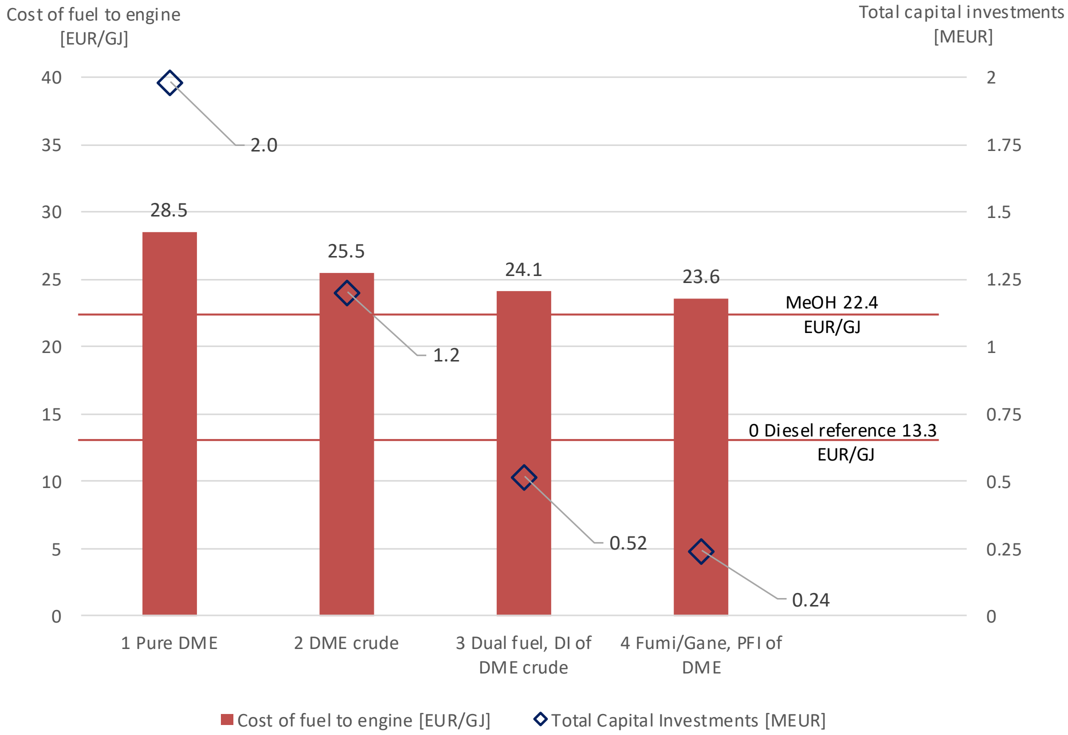


Figure 4.8: Final results for the key performance indicator for all fuel scenarios. Total cost of fuel to engine ($EUR/GJ_{LHV}$) and total investments (MEUR), for the scenarios defined. Excluding costs for engine modifications. For scenario definitions see Table 3.1, the price of methanol feed added as theoretical minimum price level.

# 5 Summarizing discussion and conclusions

In order to transition away completely from using marine diesel in a compression ignition engine, DME can be used as fuel or DME in combination with MeOH. As DME is not readily available and is a gas under standard conditions, DME can be obtained through the on-board conversion / dehydration of MeOH. Only MeOH has to be bunkered then on the ship. As a reference ship, the Arklow Venture was selected which currently contains a 1740 kW CI diesel engine. In this work it is assumed that only MeOH is bunkered, which is then (partially) converted to DME to supply the fuel to the engine at equal energy consumption as currently with diesel. Four DME-MeOH fuel cases were considered for the techno-economic analysis of the corresponding MeOH to DME conversion plant to be installed on board:

Case 1: DI of pure DME
Case 2: DI of DME-crude (DME/MeOH/$H_2O$ mixture)
Case 3: DI of DME-crude (30%) with PFI of MeOH
Case 4: DI of MeOH and PFI of DME-crude (10%)

In case 1, the bunkered MeOH needs to be converted completely to pure DME for which an additional distillation step is required downstream the catalytic converter. Cases 2-4 also convert the bunkered MeOH through catalytic dehydration, but these utilize the DME-crude product from the MeOH dehydration. This simplifies the conversion plant significantly and, considering operational difficulty, cases 2-4 are more realistic on board of a ship. Furthermore, as MeOH is co-fed in cases 3 and 4 in dual fuel mode, less MeOH has to be converted resulting in smaller conversion plants.

From the process models that were set up, the mass and energy balances were obtained as described in Chapter 3. It was found that the net conversion efficiency including the heating / cooling duty, of cases 2-4 were somewhat higher at 94.3% than the 90.9% of case 1, mainly due to the additional duty required for the distillation column in case 1 where pure DME needs to be produced.

In a consecutive sizing and economic assessment (Chapter 4), the total capital investment of these plants were determined at respectively 2.0, 1.2, 0.52 and 0.24 MEUR, also seen in the summarizing plot of Figure 4.8. When the average fuel consumption was considered, a specific price of fuel-to-engine could be determined at 28.5, 25.5, 24.1 and 23.6 EUR/GJ. Clearly cases 3 and 4 are priced lowest, due the absence of a distillation unit and the lower MeOH flow to be converted.

Considering the CI engine and accompanied retrofit costs (Chapter 2), only valid costing references were found for a diesel engine conversion to a MeOH-diesel dual fuel propulsion (STENA Germanica). For this reason, the retrofit costs were not considered because of the lack of costing information and accompanied high uncertainty for cases 1,2, and 4. Nonetheless, for case 3, being most similar, it was calculated that for the 1740 kW engine, an additional 783 kEUR capital investment should be assumed at an additional fuel to engine cost of 1.4 EUR/GJ. Retrofits for cases 1, 2 and 4 are not expected to cost much less, because these all require higher fuel flow rates for DI of the lower energy density fuel for which the injection system needs to be customized. Also, as these would be more pioneering, this would result in additional engineering costs for novel approaches.

The authors argue that case 3 is the best option considering the conversion plant efficiency and size, plant operation, overall fuel-to-engine costs and engine retrofit maturity. Although not necessarily the cheapest at 24.1 EUR/GJ, considering these factors, it provides a viable option to completely replace fossil diesel while using a CI engine.

When comparing this 24.1 EUR/GJ for case 3 to the price of MeOH (22.4 EUR/GJ) and diesel (13.3 EUR/GJ), this is of course a substantial premium. Without strict regulations on the (complete) substitution of fossil diesel, this will be too expensive and in the interim period MeOH-diesel dual fuel combinations will suffice. Moreover, only MeOH is bunkered in the scenarios of this work, meaning the dependency on the MeOH price fluctuations will increase, especially true for renewable MeOH. However, if towards 2050 mandates will indeed require a complete substitution of fossil fuels, the switch from diesel (or diesel-MeOH) to MeOH-DME can become crucial.

In this report, the authors have focused on engine scenarios that can be retrofitted on existing vessels. Since the goal is to transition away from fossil fuel use, future engines can be designed differently, to enable 100% MeOH operation via spark ignition or double high-pressure DI high using methanol as main fuel and DME as ignition fuel. The former is appealing as a conversion plant is no longer needed, yet thermal efficiency of SI engines is lower than that of CI engines.  The latter option is interesting given the high thermal efficiency and the increased methanol blend fractions compared to conventional dual fuel operation. It is advised to consider these options in future work.

**Main conclusions:**

- The net efficiency of the conversion plants 2-4 is somewhat higher 94.3% than the 90.9% of case 1, mainly due to the additional duty required for the distillation column.
- The total capital investments for cases 1-4 were respectively 2.0, 1.2, 0.52 and 0.24 MEUR.
- Case 1 producing pure DME is the most expensive, mostly due to the presence of a distillation unit. Case 2 requires fewer processing units and is therefore priced almost 2x lower. Cases 3 and 4 require less DME-crude, because MeOH is co-fed to the engine, therefore these are again priced lower based on the processing capacity needed.
- The costs of the fuel to engine were respectively 28.5, 25.5, 24.1 and 23.6 EUR/GJ. As expected from the TCIs, cases 2-4 are substantially cheaper.
- Retrofitting costs were not included as no costs were found similar to cases 1, 2 and 4, therefore the uncertainty would become too great. However, for a diesel-MeOH dual fuel engine a price of 450 EUR/kW was found. This would be a price to be expected most similar to case 3, adding 783 kEUR to the TCI of case 3 adding 1.4 EUR/GJ to the cost of fuel to engine.
- For cases 1,2 and 4, at least similar retrofit costs are to be expected as for case 3.
- The authors argue that case 3 is the most viable option, considering the conversion plant efficiency and size, plant operation, overall fuel-to-engine costs and engine retrofit maturity.

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