BHET monomer production based on PET packages

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Preface

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Karin Lindqvist, project manager, RISE AB

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1. Summary

The societal problem that a big part of post consumer PET packaging is used linearly, i.e. it is not recycled and is incinerated, has been addressed in this project. The purpose was to prepare the establishment of a plant for the production of the monomer and chemical bishydroxyethyl terephthalate (BHET), which uses PET plastic from sorted post-consumer packaging as raw material. Plastic from sorting facilities in Sweden, Norway and Denmark was mapped to be used circularly by recycling the plastic into a new product. The project's purpose was also to position the chemical BHET on the market and develop applications as binders for paint and varnish, in the plasticizer segment and as a monomer for specific grades of PET. The mapping of PET packages as a source for a production plant, preliminary placed in Stenungsund, showed that beside PET packages from Swedish Plastics Recycling in Motala, there is a need for packages also from Norway and Denmark.
The results from experiments for upscaling showed the tradeoff between using recycled ethylene glycol (EG), containing a few percent of water, and the resulting purity of the monomer obtained, as well as the tradeoff between removing color from the monomer and adding processing steps and energy costs. The process simulations for optimization and LCA calculations showed that for applications where a less pure monomer can be accepted the GHG emssions will be 2.0 kg CO_2 eq. per kg BHET, while purer monomer will generate GHG of 2,5 CO_2 eq. per kg BHET. LCA also showed that the chemical recycling of PET waste to BHET (scenario of the purest BHET) had a 20% lower climate impact than the scenario of BHET production from fossil source and todays' PET waste management.

150kg BHET was produced by one of the project partners, proving the possibility to prepare the chemical in pilot scale. The BHET monomer was synthesized to different binders for paint, and to plasticizer for flooring and automotive parts. It was also used in polymerization of PET for foaming and a special grade of PET for vacuum forming of packages. The conclusions from evaluations of the BHET based products can be summarized in the following points:

- For binder, further product development is needed among others the viscosity of the products. Very positive response to the fact that a product with properties very close to current products was obtained.
- For plasticizers, further product development is also needed, again related to the viscosity of the product but thermal stability was also an issue. Despite these needs for further development, the plasticizer performed well when blended in the flooring av plastic for components.
- Polymerized PET based on recycled BHET behaved as a normal PET but had a darker color when based on PC-PET. Thermofomed cups based on pressing of film with 30% rPET based on r BHET behaved almost identical to virgin PET in the process at the project partner, and the color difference was very little compared to the results with virgin PET.
- The foaming of PET with up to 75% of rPET based on rBHET showed no significant differences in the end result except the color that was darker. The color was no issue for the application of foams.

An important conclusion from the project is that LCA shows that the suggested process can have a 20% lower climate impact compared to a scenario where BHET is based on fossil sources assuming todays' waste handling of PET. Chemical recycling is in that sense clearly competitive with todays' alternatives. The results from application developments are very promising, though they show that further product developments are required.

Thorough work on developing a plan for industrialization of a complete production has shown that several points need to be dug into much deeper before a decision can be made about setting up a plant.

PET packages recycled through depolymerization turned into the monomer and chemical Bis Hydroxy Ethylene Terephtalate -BHET

2. Sammanfattning

Samhällsproblemet, att en stor del av post-konsument-PET-förpackningar används linjärt, det vill säga att de inte återvinns och förbränns har tagits upp i detta projekt. Syftet var att förbereda etableringen av en anläggning för tillverkning av monomeren och kemikalien bishydroxietyltereftalat (BHET) som använder PET-plast från sorterade post-konsumentförpackningar som råvara. Plast från sorteringsanläggningar i Sverige, Norge och Danmark kartlades för att användas cirkulärt genom att plasten återvinns till en ny produkt. Projektets syfte var också att positionera kemikalien BHET på marknaden och utveckla applikationer som bindemedel för färg och lack, inom mjukgöraresegmentet och som monomer för specifika kvaliteter av PET. Kartläggningen av PET-förpackningar som källa till en produktionsanläggning, preliminärt placerad i Stenungsund, visade att det förutom PET-förpackningar från Svensk Plaståtervinning i Motala finns ett behov av förpackningar även från Norge och Danmark.

Resultaten från experiment för uppskalning visade avvägningen mellan att använda återvunnen etylenglykol (EG), innehållande några få procent vatten, och den resulterande renheten hos den erhållna monomeren, såväl som avvägningen mellan att ta bort färg från monomeren och tillsätta bearbetning steg och energikostnader. Processimuleringarna för optimering och LCA-beräkningar visade att för applikationer där en mindre ren monomer kan accepteras kommer växthusgasutsläppen att vara 2,0 kg CO2-ekv. per kg BHET, medan renare monomer genererar växthusgaser på 2,5 CO2-ekv. per kg BHET. LCA visade också att den kemiska återvinningen av PET-avfall till BHET (scenariot för det renaste BHET) hade en 20 % lägre klimatpåverkan än scenariot med BHET-produktion från fossila källor och dagens PET-avfallshantering.

150 kg BHET producerades av en av projektpartnerna som bevisade möjligheten att bereda kemikalien i pilotskala. BHET-monomeren syntetiserades till olika bindemedel för färg och till mjukgörare för golv och bildelar. Det användes också vid polymerisation av PET för skumning och en speciell kvalitet av PET för vakuumformning av förpackningar. Slutsatserna från utvärderingar av de BHET-baserade produkterna kan sammanfattas i följande punkter:

- För bindemedel behövs ytterligare produktutveckling bland annat produkternas viskositet. Mycket positiv respons på att en produkt med egenskaper som ligger mycket nära nuvarande produkter erhölls.

- För mjukgörare behövs också ytterligare produktutveckling, återigen relaterat till produktens viskositet men termisk stabilitet var också ett problem. Trots dessa behov av vidareutveckling presterade mjukgöraren bra när den blandades i golvbeläggningen av plast för komponenter.

- Polymeriserad PET baserad på återvunnet BHET betedde sig som en vanlig PET men hade en mörkare färg när den var baserad på PC-PET. Termoformade koppar baserade på pressning av film med 30 % rPET baserad på r BHET betedde sig nästan identiskt med ny PET i processen vid projektpartner, och färgskillnaden var mycket liten jämfört med resultaten med ny PET.

- Skumningen av PET med upp till 75 % rPET baserat på rBHET visade inga signifikanta skillnader i slutresultatet förutom färgen som var mörkare. Färgen var inget problem för appliceringen av skum.

En viktig slutsats från projektet är att LCA visar att den föreslagna processen kan ha 20 % lägre klimatpåverkan jämfört med ett scenario där BHET baseras på fossila källor förutsatt att man idag antar avfallshantering av PET. Kemisk återvinning är i den meningen klart konkurrenskraftig med dagens alternativ. Resultaten från applikationsutvecklingen är mycket lovande, även om de visar att ytterligare produktutveckling krävs.
Ett grundligt arbete med att ta fram en plan för industrialisering av en komplett produktion har visat att ett antal punkter behöver grävas mycket djupare innan beslut kan fattas om etablering av en anläggning.

3. Introduction and background

3.1. Background

Packaging of PET from Swedish and Norwegian sorting facilities have, through chemical recycling on a lab scale, been used to produce the chemical and monomer bishydroxyethyl terephthalate (BHET). Repolymerization of BHET into new PET has resulted in a polymer with properties on par with new raw material. LCA calculations from a recently completed project showed a reduction in greenhouse gas emissions when linear use of PET was compared to circular use, based on the recycling method used at RISE. The proposed demonstration project aims to prepare the establishment of a process for the production of the monomer and the chemical bishydroxyethyl terephthalate (BHET) which can be produced from PET plastic from sorted post-consumer packaging as a raw material, and which thus substantially contributes to a more sustainable use of resources. The goal is to develop a basis for an economically profitable process with the lowest possible emissions of greenhouse gases (GHG) and to develop applications based on BHET together with end users. Plastic packaging is collected via recycling stations and sorted at Swedish Plastic Recycling's facility in Motala.

The plastic is sorted by type of polymer for further material recycling, but the largest proportion of PET is sent for incineration with energy recovery. Previous and ongoing projects carried out at RISE, have shown that depolymerization of PET packaging through glycolysis, which is based on the use of the solvent ethylene glycol (EG), is a robust process that has given high yield and high purity of the product BHET. The solvent has been recovered and reused in the process and the LCA carried out showed, as mentioned above, positive results. Perstorp AB has been one of the partners since the start of these projects, with an interest in producing and further developing applications based on BHET. At Perstorp's facility in Stenungsund, natural gas is used as a raw material to produce aldehydes, alcohols, carboxylic acids and esters, which are then used for special chemicals for the paint, varnish and plastic processing industry.

Results from the previously mentioned project showed the potential for the development of plasticizers based on recycled BHET and Perstorp has further ideas for how BHET can be used in paint and varnish binders, which means replacing fossil-based raw materials with recycled raw materials. This project proposal intends to develop these ideas on a scale that allows to demonstrate the possibilities in some different applications but also prepare for an industrialization intended for Stenungsund where Perstorp already has resources in the form of facilities. Potential rebuilding and reuse of existing resources therefore makes Stenungsund particularly interesting. For the production of BHET to be profitable, at least 10 kton of BHET must be able to be produced per year, which requires at least 14kTon of sorted PET packaging, because around 20% of the packaging consists of corks, labels, film, etc. and the direct yield is 75-80%. This means that the PET that is currently sorted out at Swedish Plastic Recycling is not enough without packaging from Norway and Denmark will be needed as raw material.

This opens the possibility of contributing to more sustainable resource use through real material recycling, reduced emissions of greenhouse gases through reduced combustion and brings us closer to a circular economy. The life cycle assessment carried out by the IVL Swedish Environmental Institute in a previous project showed that the climate impact could be reduced by 36% with a circular use of PET compared to a linear one that ends with incineration. In this project proposal, the process will be simulated for scaling up from batch to continuous production and LCA calculations will be carried out to minimize climate impact. There is great potential for further reduction of the process' climate impact. Roughly speaking, a facility as described above will emit 39% of the amount of GHG that is currently generated through combustion.

In this project, RISE has contributed with project management and resources in lab and pilot scale as well as software for process simulation. IVL, The Swedish Environmental Institute, has experience in mapping plastic waste and calculating LCA. Swedish Plastic Recycling contributed with expertise on sorting and qualities of PET. Perstorp AB, potential owner of a facility, has been the partner to the development of applications based on BHET. Recyctec (SME), has recycled glycol and has unique expertise in solvent purification. Synpo, a research company, has produced BHET for application development. Recipient of monomer, Selenis, contributed with polymerization of PET, and end user Klöckner Pentaplast has vacuum formed packaging from PET film. End user of adhesives, Sherwin Williams is the partner that has performed the application evaluation in paint and varnish. Tarkett has performed evaluations of plasticizers. National Sweden has evaluated BHET based plasticizers for rubber parts. Diabgroup has received high molecular weight PET and has tested PET for sandwich constructions. Stenungsund municipality has represented the public sector in the consortium.

3.2. State of knowledge

PET is the fourth most used plastic in the world, mainly because of the excellent mechanical properties, processability and low price which makes it suitable for many applications such as fibers, bottles and film. The global production of PET in 2016 was estimated at 77 million tons, of which approx. 60% was used for the manufacture of polyester fibers and 30% for various types of packaging. In Europe, 5.5 million tons of PET packaging is put on the market annually. Of all this plastic, only 24% is material recycled, mainly through deposit systems. A large proportion of PET is sent for incineration due to low quality caused by impurities such as paint, labels and other plastics (e.g. in laminates), which makes mechanical recycling problematic and unprofitable. There are alternatives to mechanical recycling because PET is one of the plastics that can be depolymerized in a chemical recycling process that breaks down the polymer molecules into monomers, i.e. the original building blocks of the plastic. Monomers can then be re-polymerized; the resulting plastic has the same properties and quality as new raw material based on monomer from oil. Depolymerization is a process that restores the quality of the plastic, which has also been shown in previous projects carried out at RISE.

There is a great awareness of the need to make PET and polyester products more circular. This is evident, among other things, through the start-up companies that have developed innovative recycling processes based on depolymerization, but also through the fact that even the largest global producers of PET present technologies for how future PET is planned to be based on both fossil-based and recycled monomer. Some processes are at the prototype stage, but plans for industrialization are presented to come within the next few years. The conclusion is that the PET industry has a strong commitment to the development of chemical recycling, to increase the circular use of PET. The results of previous projects at RISE demonstrate that simulation to optimize process flows and yields, reduce energy consumption and costs is the next step for the development of depolymerization of PET so that a competitive process for the production of the monomer BHET is obtained. Life cycle assessment (LCA) is used to map energy consumption and environmental impact and to be able to assess products and processes from a broader perspective. Process simulation needs to be included in a system analysis in order to perform LCA on a process that is similar to a process on an industrial scale. Process simulation provides data that can be used in the LCA. Studying the environmental impact of a product and process at an early stage means that changes in process design can be studied and its potential contribution to environmental improvements can be identified. Analysis of changes in process design can then be carried out using process simulation without having to build facilities.

To reduce the climate footprint and oil dependence, the use of alternative raw materials, bio-based or recycled, is very important. Recycled raw materials contribute to circular use of the molecular building blocks needed for chemical production. BHET is a monomer/chemical that is currently manufactured on a limited scale and is not used industrially as a raw material for products. BHET is generated on a large scale in situ from ethylene glycol and terephthalic acid as the first step in the manufacture of PET but is never isolated. Consequently, extensive application work is required to position the molecule's utility and performance in various potential markets. However, as mentioned above, there are many ongoing initiatives to start facilities for the production of BHET, but then mainly with the intention of producing PET. Perstorp, as a manufacturer of specialty chemicals, has, with its innovative ideas on the development of applications in the segments of plasticizers and binders for paint and varnish, a very good chance to create competitive products from recycled raw materials and thus demand, in more areas. This gives high potential for the project to contribute to an economically viable solution.

3.3. The Challenge

The problem that the project aims to solve is primarily that PET packaging is used linearly, i.e. it is incinerated and not recycled. . Associated problems are also about GHG emissions. The purpose and goals of the project to contribute to a solution are described below.

The purpose of the project is to prepare the establishment of a plant for the production of the monomer and the chemical bishydroxyethyl terephthalate (BHET), which uses PET plastic from sorted post-consumer packaging as raw material. Plastic from sorting facilities in Sweden, Norway and possibly Denmark will thus be used circularly by recycling the plastic into a new product. Through the project's scale-up experiments, process simulations and environmental impact calculations using LCA, the production process with the lowest possible energy consumption and greenhouse gas emissions will be proposed. This results in minimized operating costs, which is a prerequisite for an economically viable solution.

The project's purpose is also to position the chemical BHET on the market and develop applications in binders for paint and varnish, in the plasticizer segment and as a monomer for specific grades of PET. Furthermore, the production of BHET in volumes will demonstrate its competitiveness, and the cooperation in the supply chain will provide the conditions for the development required to create demand in the market, as well as give a markedly increased durability to several products, whose raw material will be recycled. This fulfills the purpose of achieving sustainable resource use and getting closer to a circular economy. Completed project should result in a plan for industrialization of the concept "PET to BHET" based on economically and resource-wise sustainable solutions.

3.3.1. Project goals

1. Develop the recovery/recirculation and purification of solvents in the process based on alternative methods for product separation. Process simulate and calculate LCA for batch process, with alternative developed solvent recovery. The results from the identified process must be below 2.3 kg CO_2/kg monomer, i.e. will be lower than the results from the previous project. The goal includes reducing the use of activated carbon for cleaning solvents
2. Calculate the climate footprint and propose the design of a continuous process for the production of 10kTon BHET/year. Energy consumption and emissions of greenhouse gases should give 30% better results than the batch process.
3. Produce 150 kg of BHET for polymerization of new PET and development of applications. Develop 3 applications for BHET and prove lower climate footprint for developed product compared to today's equivalent.
4. Design a timed plan for industrialization with handling of raw materials, process selection, techno-economic analysis and business model, REACH registration, permit and impact analysis and investment application

Figure 1 shows the monomers that can be obtained when PET is depolymerized. It is, as mentioned, the monomer BHET that is the desired product in this project.

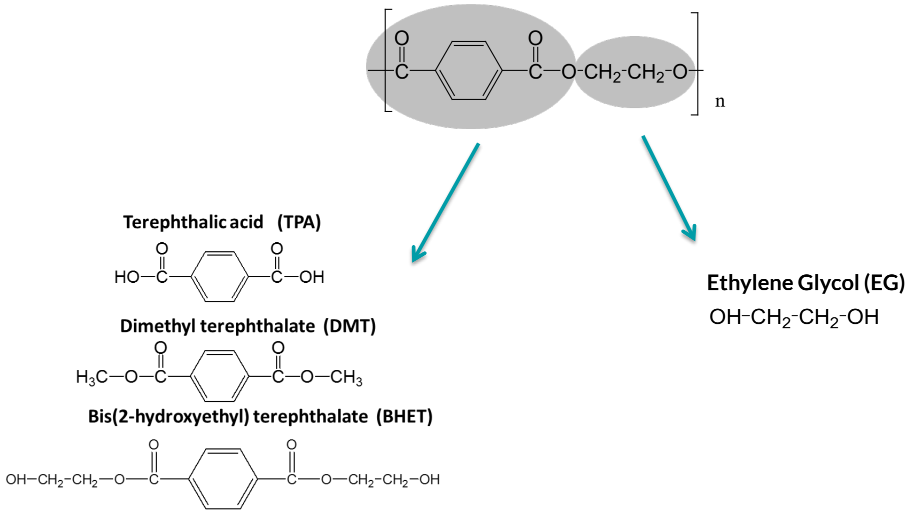

Figure 1 Depolymerization of PET can result in 3 different monomers and ethylene glycol. It is bishydroxy ethylene terephthalate (BHET) that is the product desired in the present project.

4. Implementation

The project was implemented mainly according to the description of work packages in the application as given below. Note that the grammar tense, describing the implementation is mainly written as future due to origin from the application. Chapter 5, describing the results, contains comments on deviations from the original plan where this was relevant for focusing on the project objectives.

4.1. Raw Material Supply

Based on an imagined location for a future plant for BHET production, the project will analyze different scenarios for raw material supply. It includes mapping volumes of PET waste generated and where they are generated, as well as the quality of the generated PET waste. The work includes making contacts with raw material suppliers and clarifying how far from the facility one needs to go to be able to collect the required amount of raw material. The goal is to design proposals for arrangements to supply the BHET facility with recycled raw materials. Partners involved were: i) IVL – performing interviews with relevant actors in the packaging recycling value chain; ii) Swedish Plastic Recycling- potential supplier of sorted PET packages

4.2. Experiments for Up-scaling

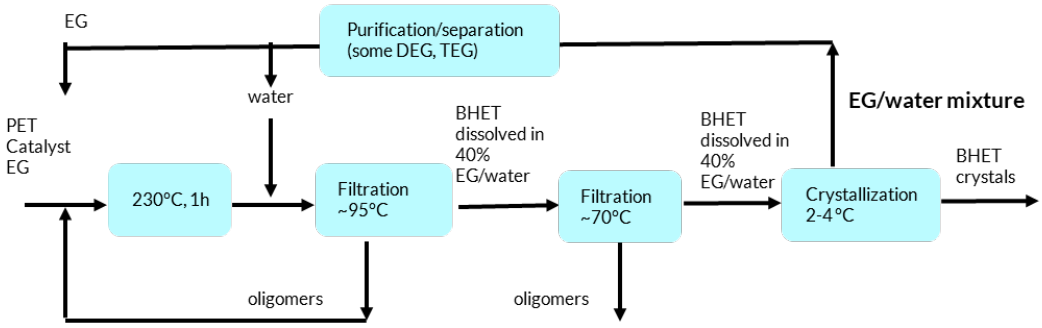

Figure 2 Schematic of the batch process for depolymerization through glycolysis of PET. PET/EG ratio 1:5. EG will be consumed (5,87%) and must be replaced in every new batch. Oligomers will be residue on filter paper around 5 wt%..Previous LCA has shown that oligomers must be recycled

The experiments for up-scaling contains several tasks:

Figure 2 shows a schematic drawing of the batch process for depolymerization through glycolysis of PET. Experiments for up-scaling aimed at creating results for a relevant simulation of the up-scaled process in WP3.

A. Recovery (recycling) of ethylene glycol (EG): purification and circulation of the solvent have a large impact on energy consumption. Streamlining recycling includes the following elements: Analysis of contaminations and identification of method for purification, i.e. identify which steps in Recyctec's process are necessary (amount of activated carbon, possibly membrane filtration, etc.). This is performed on existing depolymerization process with recovery of residual i.e. non-depolymerised material. Recovery of EG for alternative batch process with evaporation at high temperature, and subsequent purification will be tested. Investigation of possible continuous recycling process for EG in column.

B. Design of the reactor in a continuous process. Laboratory experiments to reduce the reaction temperature and avoid overpressure, as overpressure makes reactor design more difficult. Laboratory tests of the reaction in different reactor designs, e.g. extruder. Cooperation with task A for analysis of contaminations and necessary steps for purification.

   During the project a study was initiated to obtain a carbon mass balance as input to the simulation performed in WP 3 (described in section 4.4). The study included evaluation of the influence of reaction temperature (which influences the yield of BHET), the purity (i.e. water content) of the ethylene glycol as well as the need of decolorization of the monomer. The activities included in the study will influence the final carbon balance.

C. Filtering study. The oligomers can be difficult to filter as they are not crystalline. The filtration needs to be studied over time so that the filterability can be calculated with linearization of filtrate weight against time and the curve adjusted, so that parameters are obtained for calculating scale-up.

D. Crystallization study: Solubility study is carried out to produce basic data for a cold crystallization. Different ratios between ethylene glycol and water are tested. Next, the crystallization is studied in a batch reactor with oscillating baffles. This will show if the process is possible to run in a continuous cooling crystallization in baffled tube reactor with oscillating flow. Analysis of purity on BHET crystals is carried out with NMR, LC-MS and LC-UV, ICP, color measurement and possibly GC-MS.

Partners active in this work package were: RISE, performing experiments for up-scaling mainly focusing on reaction conditions and mass balance; Recyctec performing analyses and purification experiments on ethylene glycol and IVL recipient of data to be used in work package 3.

4.3. Simulation, Optimization and LCA

The process is currently not optimized regarding energy consumption. There are large temperature differences that can be heat exchanged, possibly with the help of heat pump technology. To get better energy efficiency, as well as volume efficiency at large volumes, the process will be transferred from batch to continuous. Simulations using the software Aspen Plus will be performed on both the existing batch process and a continuous process to investigate the development potential of the process.

A) Simulations of existing batch process and alternative process with evaporation of ethylene glycol near reaction temperature.

B) Simulation – of continuous process (40-50kTon/year) which is based on relevant knowledge from batch process and verifying experiments.

C) Simulation of the recovery of EG with input from 2A

D) LCA for batch process: update activated carbon production data used in previously performed LCA, update previous LCA with respect to yield and energy use when simulation using Aspen Plus has been performed i.e. input from 3A; Analysis recirculation of waste streams

E) LCA of decolorization: Collect monomer decolorization data, from previous projects, and add to the LCA model

F) LCA of continuous process; With input from simulation scenarios 3B and 3C, a continuous process for the production of BHET from PET waste is defined and IVL designs an LCA model to calculate the environmental impact. Input from AP-1 regarding transportation of PET packages is included in the model.

Partners in this work package: RISE that performs simulation of the process, Recyctec that contributes with data for purification of ethylene glycol, IVL that performs the life cycle assessment for several scenarios. Perstorp receives the results and data and uses the results for continued work in work package 6.

4.4. Market development-150kg BHET in pilot scale

The objective of this task is to produce 150kg of the monomer /chemical BHET. It is also a demonstration of the feasibility to depolymerize a larger quantity of BHET

A. Raw material - sorting and washing of PET packages. At Swedish Plastic Recycling's facility in Motala, PET packaging is sorted into different qualities. From these grades, raw material for BHET production will be taken. Which fraction is most suitable for depolymerization on a pilot scale will be decided during the project. For the process (the depolymerization of PET) to be as efficient as possible, the sorted PET packaging must be pre-treated in the form of washing. In the washing process, product residues and other contamination such as labels, glue etc. will be washed away. The washing will be carried out at the test facility of the washing process manufacturer. In the washing process, contaminations of PE and PP will also be separated by density baths or "wind shifters".

B. Depolymerization, separation and characterization of monomer: Depolymerization of washed PET will take place at Synpo using the parameters and catalysts developed in previous projects for the reaction. To produce 150 kg of BHET, around 200 kg of PET will be needed. This is done in batches of approx. 20kg per batch with delivery to AP 5A, 5B and 5C. Produced BHET is characterized by RISE according to previously established methods (NMR, LC-MS, LC-UV, ICP; potentiometric titration) and compared to known specifications

C. Decolorization: As the PET waste will be colored, the produced BHET will also be discolored. In previous projects we have developed methods to remove this discoloration. In the present project, we will investigate the possibilities of using the decolorization method and develop it to have as low energy consumption as possible.

Partners active in this task are the following: Swedish Plastics Recycling that sorts the PET fraction which is sent to a washing pilot plant owned by a washing process producing company, Synpo who depolymerizes the washed PET. Perstorp is involved in managing the distribution of BHET to different partners including themselves for further work performed in WP 5.

4.5. Market development – Applications

The cooperation between the partners in WP5 is performed iteratively, which is the reason for the activities being extended over time. The applications to be further developed are plasticizes and binders

A. Plasticizers: development of BHET esters which are building blocks for plasticizers for PVC. Synthesize 2-ethylhexanoic acid (2-EHA, octanol) esters of BHET, characterization of product, minimization of by-product and purification of the plasticizer (Perstorp). The evaluation in commercial formulations of the end users (Tarkett, National).

B. Binders for paint and varnish: BHET is being investigated as a substitute for phthalic anhydride in alkyd emulsions and as a building block in coil coatings as well as liquid polyester and powder paints. Study of the ethylene glycol contribution (difficult to remove) of BHET in the formulation work, as well as any influence of the presence of contaminations in BHET. Esterification and modification of BHET for evaluation in UV curing paints for wood (Sherwin Williams, France) as well as evaluation of experimental binders at the Wood R&D Center in Sweden.

C. PET: repolymerization of BHET by polycondensation reaction where ethylene glycol is boiled away. BHET is also copolymerized with a rigid aliphatic diol (Pentaspiroglycol PSG) to produce a modified PET with higher heat resistance. Repolymerized PET will be characterized by thermal properties, processing properties, rheological and color properties. The characterization will give results regarding the quality of PET and will have significance for how and where it can be used. Repolymerized PET will be evaluated in packaging applications by production of "plates" which are tested in a vacuum forming process (Klöckner Pentaplast). Repolymerized PET will also be evaluated PET for foaming and will undergo solid-state polymerization to raise IV. Evaluation by foaming trials (DiabGroup) and characterization of foamed structure will be performed.

Partners involved in the development of applications: Perstorp synthesizing plasticizers and binders, Tarkett and National Sweden evaluating the prepared plasticizers in their product formulations, Sherwin Williams preparing varnish and paint formulations that are evaluated, Selenis performing polymerization od different PET qualities, Klöckner Pentaplast testing the processability of polymerized PET in vacuum forming processes for packaging, Diab Group performing foaming experiments with PET polymerized from the prepared BHET.

4.6. Plan for implementation

The project results will give the technical data to estimate the cost and schedule for industrialization. The plan forward will contain the following parts:

A. Raw materials supply (i.e. sorted PET packages) based on input from L1, secure volumes of PET from sources whose quality is judged to be sufficiently uniform in terms of sorting and volume. The need for logistics solutions and storage should be identified. Proposal for the design of the washing facility - based on the collaboration with the washing facility supplier (input from task 4A), a design and a cost estimate are produced. Facility permits are planned, including a treatment plant for wash water.

B. Process selection: development of product specification(s) based on input from WP 4. Preliminary design of process (input from WP3): LCA for continuous process). The ATEX certification of the BHET factory for handling chemicals, dust and explosive solids.
C. Techno-economic analysis and business model: Deeper market analysis (input from WP 5 among others) and preliminary product specifications, this includes assessing the market potential and possible price. Plan for application tests with selected customers. Development of growth plan.
D. Permits and impact analysis: this includes concession permits, work with REACH registration and information collection for environmental assessment.
E. Investment application: Based on all parts of WP6 a cost analysis and an investment plan is formed.

This work package has mainly been performed by Perstorp but with input from RISE and IVL.

5. Results and discussion

5.1. Raw Material Supply

5.1.1. Summary of results

The aim of this study was to investigate potential suppliers of PET packaging waste within the Scandinavian area (Sweden, Norway and Denmark) and present estimations of potential volumes for a future depolymerization plant in Stenungsund. The study was conducted during the latter half of 2022 and the results presented below are based on what was known at that point. After the summary of results and recommendations of this study, there is also a short summary of some more recently available information, which has become publicly available since the study was conducted.

The data presented here has been collected through interviews and conversations with selected actors within the Scandinavian waste plastic sorting industry and a survey of relevant literature. Based on the information gathered from the interviews as well as data that was received from sorting and recycling plants in Scandinavia, estimations of the total generated PET packaging waste from households and the estimated volumes from specific suppliers that could be used for depolymerization were made.

The results show that there is an estimated generation of 85 000 tonnes of PET packaging waste from households within Scandinavia, excluding the PET bottles that are collected within the deposit scheme. Sweden is the biggest generator of household PET although the per capita amount is higher in Norway.

The estimated supply available, when the supplying sorting plants are at full operation (2025), for depolymerization is 18 500 – 20 500 tonnes for all countries, which is seen in Table 1. The two certain and largest volumes of sorted PET come from Swedish Plastic Recycling in Motala and Plastretur in Østlandet, with upwards of 15 000 tonnes of PET available for depolymerization when combined. Combining the PET supply volumes from Swedish Plastic Recycling and Plastretur the desired volumes (15 000 tonnes) can be reached within the distance of 522 km.

Table 1. Summary of the results from mapping of PET packaging waste.

TONNES	**Generation of PET packaging waste from households (excluding deposit scheme)**	**PET from suppliers**	**PET collected within the deposit scheme**
Sweden	39 000	9 000-11 000	24 000
Norway	29 000	5 500	23 000
Denmark	18 000	4 000	15 000
Total	85 000	18 500-20 500	62 000

The supply from Swedish Plastic Recycling and Plastretur can be complemented with PET from IVAR and ROAF with an additional 2 000 tonnes. It is important to note that these estimations include food waste and other materials stuck to the PET packaging after sorting, such as labels, bottlecaps and film.

As for the quality of PET available from the suppliers, 60% of the volumes available from suppliers consist of trays whereof transparent trays represent 52% and opaque/coloured trays 8%. Out of the bottle share (40%), 21% are transparent, 9% are colored (translucent) and 10% are opaque.

Regarding Denmark, it is likely that there will be some sort of central sorting plant for Danish plastic packaging, however, it is still uncertain how that will look like or where it will be located. A sorting plant in Denmark, sorting only Danish plastic packaging waste, we estimate should be able to deliver around 4 000 tonnes of mixed PET per year.

Quantafuel is building a plant in Esbjerg that will have a high capacity and can also be an important source of raw material. Although the exact quantity of PET that Quantafuel will be able to supply once it is completed has not been presented, the volumes are estimated to be significant. It is possible that the Quantafuel plant will be the sorting plant in Denmark that handles all the Danish packaging waste. Regarding polyester and its inclusion as a raw material for depolymerization, the total amount of possible fraction of mixed PET sorted for depolymerization could increase by 100% or more if polyester textiles are included, from some of the actors surveyed.

5.1.2. **Recommendations**

This study has focused on future flows of PET packaging waste, which inevitably leads to some uncertainty. The most certain sources of PET were, when conducting this survey, Swedish

Plastic Recycling in Motala and Plastretur in Østlandet. Those two plants will most likely be able to provide 10 000 – 15 000 tonnes of mixed PET per year. Swedish Plastic Recycling has, so far, the most ambitious plans for sorting, which means that their supply of PET to depolymerization compete less with mechanical recycling compared to smaller sorting plants with less ambitious plans. The plans for Plastretur are not fully decided yet, but it seems likely that their sorting plant will result in about the same level of sorting (of PET) as Swedish Plastic Recycling, which also means that the level of competition with mechanical recycling will be roughly the same. That will, on the other hand, lead to a more difficult fraction of PET to handle for the depolymerization plant, with a higher percentage of multilayer materials and coloring that needs to be rinsed out. If the amount of opaque and multilayer material gets too high, it should be possible to discuss higher quality criteria for the material but that will inevitably lead to a higher price (per ton) and a lower total amount from these two plants. We recommend that Swedish Plastic Recycling and Plastretur are the priority for deliveries of PET to a future depolymerization plant in Stenungsund.
The supply from Swedish Plastic Recycling and Plastretur can be supplemented with PET from IVAR and ROAF for an additional 2 000 tonnes.

There will be some sort of sorting plant for plastic packaging in Denmark, but it is still uncertain how that will look or where it will be located. A sorting plant in Denmark, sorting only Danish plastic packaging waste, should be able to deliver around 4 000 tonnes of mixed PET per year if it is built to have the same level of sorting as Swedish Plastic Recycling and what we expect from Plastretur. This also assumes that all source separated plastic packaging, as well as some MRF plastic, in Denmark goes to this future sorting plant. We recommend that the Danish market should be monitored since a lot can happen within a near future.

The Quantafuel plant in Esbjerg will have a high capacity and can also be an important source of raw material. Although the exact quantity of PET that Quantafuel will be able to supply once it is completed has not been presented, partly because the input material will have an impact on the volumes and qualities available from this plant. The volumes are estimated to be significant. It is possible that the Quantafuel plant will be the sorting plant in Denmark that handles all the Danish packaging waste. If that is the case, the 4 000 tonnes of mixed PET that we expect from Danish households will increase to 6 000 – 7 000 tonnes, since Quantafuel has so far only decided to build one sorting line for all PET plastic. If the IVAR and ROAF plants in Norway decide to keep the same setup as today and deliver their mixed plastic to Quantafuel, instead of sorting out some fraction of PET to depolymerization, we can expect an additional 1 000 – 1 500 tonnes of mixed PET from Quantafuel out of the IVAR and ROAF material. That amount is lower than the 2 000 tonnes of mixed PET from those two plants that we expect can go to depolymerization since they will in this scenario have sorted out the transparent bottles and trays before the mix is sent to Esbjerg. If Quantafuel starts sorting packaging waste from Finland, Germany, Netherlands, Great Britain or any other country outside of Scandinavia, the amount of PET from Esbjerg could increase even further. Quantafuel, as part of the Danish market, should be observed since a lot can happen within a near future. They could become a significant supplier of PET, but we expect that the quality of their material could change rapidly depending on where they source their material from.

For additional information about the Danish market, follow up discussions can be held with the three current sorting plants in Denmark that can sort out PET – Dansk Affald, Nordværk and Nomi4s, although the volumes of PET from these plants are today estimated to be lower than most of the previously mentioned plants.

5.1.3. **Short summary of some more recently available information**

In May 2024, Quantafuel opened their sorting plant in Esbjerg, called ReSource Denmark[1], which is now sorting most of the Danish plastic packaging waste. This means that the scenario with 6 000-7 000 tonnes of PET packaging from Danish households is more likely than the scenario with 4000 tonnes, due to fewer sorting steps of PET fractions at Quantafuel than assumed from the theorized plant. The size of the plant means that it will need to take in more plastic waste than we have here estimated from Danish households, to run at full capacity, which means that the amount of PET could increase even further but it will depend on the source of the material.

In November 2023, Swedish Plastic Recycling opened their updated and extended sorting plant in Motala, now called Site Zero[2]. This update was included in the estimation of possible PET packaging waste from this supplier. The estimation did however include some uncertainty since it was uncertain how (and if) Site Zero would be able to work at full capacity. In August 2023, Swedish Plastic Recycling announced[3] that they will recycle Finnish plastic packaging waste at Site Zero. This brings us closer to the estimate of 11 000 tonnes of PET packaging from this site.

The latest news about IVAR in Norway is that it will be rebuilt around the turn of the year 2026/2027[4].

5.2. Experiments for Upscaling

The purpose of experiments for up-scaling is to experimentally gather the necessary data for a simulation of a production process.

A) Recycling of ethylene glycol

Recyctec analysed the ethylene glycol (EG) that was used for depolymerization to understand the impurities generated in the process. No diethylene- or triethylene glycols were found. A certain amount of BHET (the desired monomer) and MHET (a non-desired monomer i.e. a by-product) will remain in the EG but these substances are harmless when entering a new depolymerization reaction. “Harmless” refers to not being accumulated. Color will accumulate unless removed from the EG. Active Carbon (AC) from Jacobi, was added to the EG/water mixture which is the filtrate from the first filtration during the process of isolating the monomer (process scheme in figure 2). Color purification trials with AC loadings between 0.5 to 1.5 g/100 mL EG was done, where 1.5g/100 mL EG represents the amount Recyctec usually uses in their process. It is important to minimize the amount of AC added since the consumption of AC will have a large impact on the GHG emissions. An addition of 0,5 g AC/ 100 ml of solvent blend resulted in a Hazen color number of 70,

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[1] https://www.quantafuel.com/media#/pressreleases/resource-denmark-officially-opens-a-leap-forward-in-sustainability-3326249

[2] https://www.svenskplastatervinning.se/fordubbling-av-plastatervinningen-med-site-zero-2/

[3] https://www.svenskplastatervinning.se/finska-plastforpackningar-ska-atervinnas-cirkulart-i-motala/

[4] https://www.aftenbladet.no/lokalt/i/69Lgoz/skal-staa-ferdig-om-tre-aar-bruker-ekstra-penger-paa-brannsikkerhet

corresponding to a discoloration of the EG that is barely detectable by the eye. Figure 3 shows the change in Hazen color scale vs amount of AC. The untreated EG had a Hazen color number of 360. L*a*b* Color space measurements would be an alternative analysis to Hazen color number.

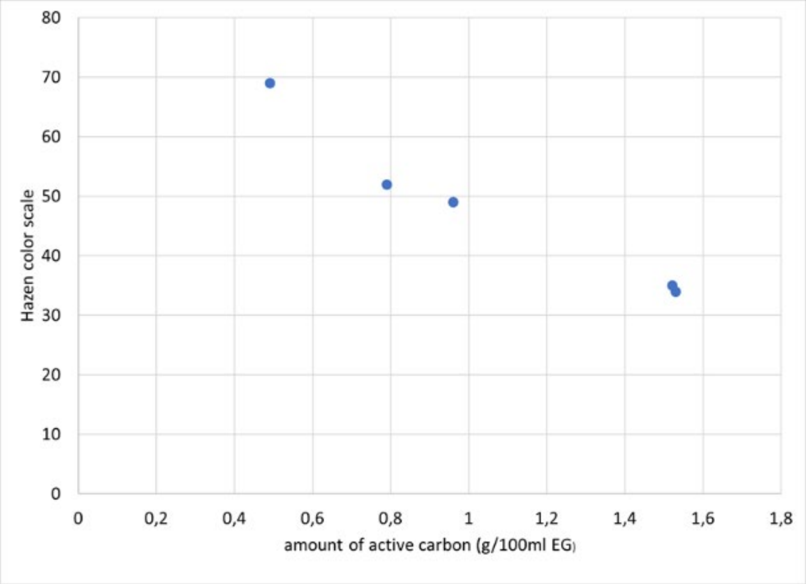


Figure 3 Hazen number vs amount of active carnon added to 100ml solvent blend (40%EG in water) for color removal. Starting value of Hazen color number was 360. A value of 60 means a by human eye barel detectable tint of yellow.

Recyctecs purification process is based on batch-wise active carbon treatment with a following step of filter pressing to separate the ethylene glycol for further treatment. The active carbon is then deposited as solid waste. An alternative treatment would be a continuous treatment with active carbon granulates packed in columns that would allow for a regeneration of the active carbon to remove adsorbed colors. The continuous process was discussed with Jacobi, the active carbon supplier. A continuous process requires several columns in parallel as the adsorption processes usually are slow and may requires the same liquid to pass several times. It is not obvious that a continuous process will save energy, since the regeneration of the active carbon require temperatures of > 700°C. No experiments were performed as the process was disregarded.

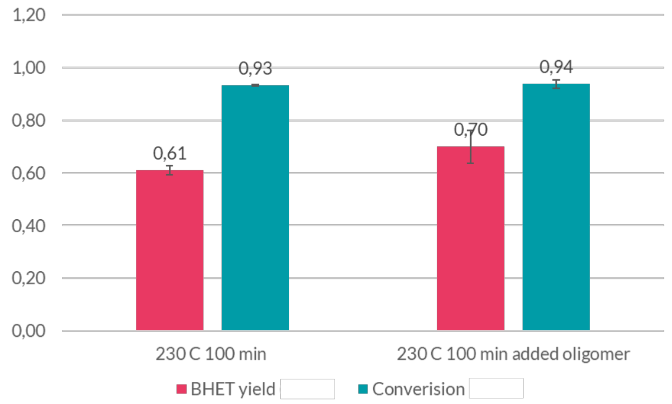


Figure 4. Results from recirculating oligomers in the glycolysis process. The results given in fraction of mol for BHET and in fraction of weight for the conversion.

During workup, non-depolymerized oligomers are recovered on the filtration step. Previous LCA has spotted recirculation of those as one of the prerequisites to get a favorable carbon footprint from the process. Recirculation of oligomers was tested by adding 1g of oligomers, previously collected from a filter cake to the PET charged for a new glycolysis batch reaction. The results are shown in Figure 4. The yield as expressed in mole fraction increased as well as the conversion expressed in weight fraction. Recycling the oligomers several times means that a certain amount of catalyst will be circulated. This means that the amount of catalysed charged for a new batch can be decreased.

Recovery of EG for alternative batch process with evaporation at high temperature as planned and described in section 4.2 was performed. The typical workup of BHET involves adding water to the reaction solution to reach a EG/water ratio of 0.4. By careful selection of temperature of the EG/water solution, oligomers and dimers of PET can be separated from BHET by filtration. The added water must be evaporated to recirculate the EG. Trials were made to reduce the amount of water in the EG stream.

An attempt to evaporate EG prior to addition of water was made. The temperature of the reaction solution was first decreased from 230°C to 180°C and EG was evaporated. The experimental set-up is shown in Figure 5. About 75% ethylene glycol was evaporated with a slight vacuum while keeping the reaction solution at 180°C. The remaining reaction solution had a very high viscosity as shown in Figure 6. To separate BHET from oligomers and dimers water was added so that the ratio of EG/water would be about 0,4. The viscosity was very high and impossible to filter.

Further experiments showed that double amount of water was needed to be able to filter the dissolved BHET and separate it from oligomers and the yield was decreased by 18 mol %. Since BHET dissolves in hot water (> 70°C), it means that the energy saved by evaporating EG while still at high temperature will be lost when heating large volumes of water. Thus, the alternative process would not save energy compared to the “normal” procedure for isolating the monomer. However, the evaporated EG was very pure and would not require purification by active carbon. On the other hand, larger volumes of a solvent blend of EG/water, with lower EG concentration (around 7 % EG in water) would require distillation of the water to recover the smaller volume of EG. The alternative batch process was deemed unsuitable for up-scaling.

Figure 5. Experimental set-up for evaporation of ethylene glycol from reaction solution at 180°C.

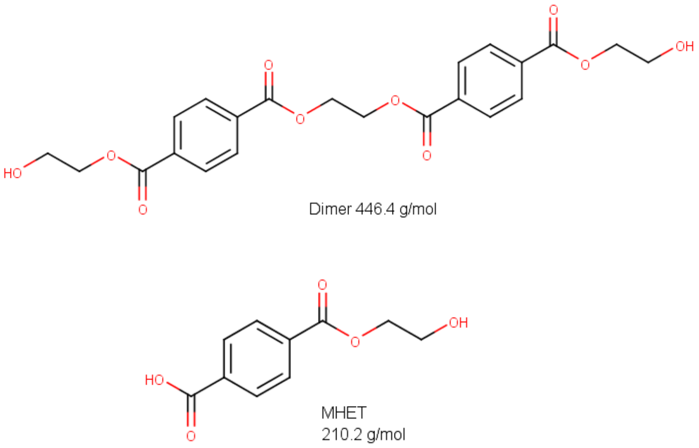
Figure 6. Reaction solution after evaporation of about 70% of the EG.

B) Design of the reactor in a continuous process:

A continuous process was considered and planned by collecting expertise on the glycolysis process performed in laboratory scale and expertise on up-scaling. The original plan to run the reaction at lower temperature to avoid overpressure would require very large tank-reactors and reaction times of 5-6 hours. A substantial problem with this concept would be a semi-continuous emptying of the reactor. A continuous process based on an extruder/tube reactor working at a slight over pressure would allow for a better overall technical solution.

It was decided to perform a study on the required reaction time at different temperatures as the results would help in understanding how to design a reactor for a continuous process as well as establishing the carbon balance needed for simulation in WP3.

The study was performed in glass vials of 20 ml that were microwave heated, thus allowing to reach the desired reaction temperature quickly while minimizing the heat losses. A carbon mass balance for the reaction was performed in parallel with results from a 2 liter batch reactor. The mass balance would help to identify and measure the yield, and losses of BHET to filtrates, the amount of oligomers, as well as by-product small molecules.


Dimer 446.4 g/mol

MHET
210.2 g/mol

Figure 7. Molecular structure of the dimer of BHET and of the non-desired monomer with only one side group substituted

*Table 2. Results from glycolysis run in microwave reactor in 20 ml glass vials with approximately 2 min heating up/cooling down time. The yields are based on LC-MS analysis with error ca ± 1 % point. BHET and the dimer available as reference material. The loading of catalyst corresponds to 0,14*m^2*cat/gPET. Experiments were performed with recyled EG (3,5%water content).*

Exp No	Temp (° C)	Time (min)	P (barg)	EG:PET (vol:wt)	Cat** (wt%)	BHET LCMS Yield (%)	Dimer LCMS Yield (%)	MHET LCMS Yield (%)*
22E2969	230	60	4	5:1	0.50	68	2.6	7
22E2993	230	60	4	5:1	**No**	7.0	1.1	1
22E3184	**250**	**5**	**6**	**5:1**	**0.50**	**87**	**4.0**	**7**
22E3099	250	10	6	5:1	0.50	86	4.0	7
22E3206	250	10	6	5:1	**0.25**	78	4.6	6
22E3098	250	20	6	5:1	0.50	84	3.4	7
22E3144	**250**	**30**	**6**	**5:1**	**0.50**	**91**	**4.0**	**7**
23E0134	270	3	9	5:1	0.50	74	5.4	6
22E3149	**270**	**5**	**9**	**5:1**	**0.50**	**86**	**4.0**	**6**
22E3148	270	10	9	5:1	0.50	87	4.0	6

The results from a number of experiments performed in microwave reactors are shown in table 2. For experiment No 22E3184 performed at 250°C for 5 min, show a yield of 87% BHET after 5 min but the the longer reaction time of 30 min (Exp No 22E3144) show that a higher yield can be obtained. Data at 270°C indicate that the equilibrium has a low temperature dependency (within the LC error margin) as the yield for Exp No 22E3149 run at 270°C for 5 min is about the same as for 22E3184 run at 250°C for 5min. However, this is true only for temperatures above 250°C. The molecular structures of dimer and byproduct molecules are shown in Figure 7. The yield of these substances does not vary very much and seem to be independent of the reaction temperature.

To investigate the formation of MHET, glycolysis experiments in anhydrous EG or EG/water 90/10 addition of 10 wt% water were performed. Table 3 shows that the yield of MHET is low when pure (>99%) EG was used as solvent while considerably more MHET was formed when 10wt% of water was added to the EG. The results are compared to earlier results with recycled EG (water content <3%), shown in light grey). It was concluded that the formation of MHET is strongly dependent on the water content in the EG and is recovered together with BHET

Table 3. Results from glycolysis with varying content of water in the ethylene glycol.

Sample	Form	Weight-%		
		BHET	Dimer	MHET
EG>99%	Reaction solution	21	1.7	0.5
EG>99%	Filter cake (2nd cryst)	99	3.3	0.7
EG/H_2O 90/10	Reaction solution	18	1.4	5.3
EG/H_2O 90/10	Filter cake (2nd cryst)	76	2.2	26
EG/H_2O 97.5/2.5	Reaction solution	14	1	1
EG/H_2O 97.5/2.5	Filter cake (2nd cryst)	95	3	4

Figure 8. BHET decolorized by active carbon. The amount of carbon is given as as percentage of the weight of BHET treated.

Decolorization of BHET was performed by dissolving BHET in boiling water and adding active carbon (ColorSorb XFP 21 from Jacobi) at 0,1-0,4wt% based on the amount of monomer. The solution was held at 80°C for 30 min during magnetic stirring, using 10g of monomer in 100 ml water.

Color measurement was performed on the final product, i.e. the crystals, in a spectrophotometer (Konica Minolta CM-3600A) as presented in Table 4. The light source used was Standard illuminant D65 which uses average daylight with ultraviolet wavelength region included. By illuminating the sample and measure the reflectance, numerical values are calculated and presented as three values: *L*, *a* and *b*. Value *L* indicates lightness in a range of 0 to 100, where 100 is the lightest. Value *a* indicates color direction ranging from green (negative direction) to red (positive direction) and value *b* indicates color direction ranging from blue (negative direction) to yellow (positive direction). Both *a* and *b* ranges from -60 to 60. As a reference, depolymerized PET from transparent plastic packaging was used. A gradually lighter shade of BHET is achieved with increased AC charging (Figure 8). Unfortunately, not only color, but also BHET is adsorbed onto AC, resulting in a yield loss.

*Table 4. L*a*b* color space measurements on decolorized BHET after active carbon treatment.*

	L*(D65)	a*(D65)	b*(D65)	Weight loss %
Reference BHET	89	-1,8	5,3	
0,1% AC	77	6,8	14	12,1
0,2%AC	79	6,2	14	16,3
0,4% AC	85	3,4	10	9

Coming back to the discussion about design of a reactor for a continuous process the following conclusions were made based on the results from the experiments:

- The original handling of ethylene glycol, as schematically shown in Figure 2 was the best process i.e. no evaporation of EG at high temperature.
- It is mainly color that needs to be removed from EG during the purification and 0,5 g of AC to 100 ml solvent blend resulted in a good purification.
- The most efficient reaction temperature is 250-270°C with a reaction time of 5-30 minutes.
- The formation of MHET depends on the water content of the ethylene glycol.
- Decolorization of the BHET monomer required 0,4w% active carbon on the weight of BHET when dissolved as 10% in hot water (80°C) i.e.10g BHET in 100 ml of water.

Figure 9 shows a schematic drawing of a suggested continuous process. The PET will be fed into the compounder and melted at 275°C. The EG will be mixed with catalyst and pre-heated to the reaction temperature 250-270°C. PET, EG and catalyst will be fed into the continuous tube reactor and the reaction can be completed in 5 minutes. The process will work at 6-9 bars.

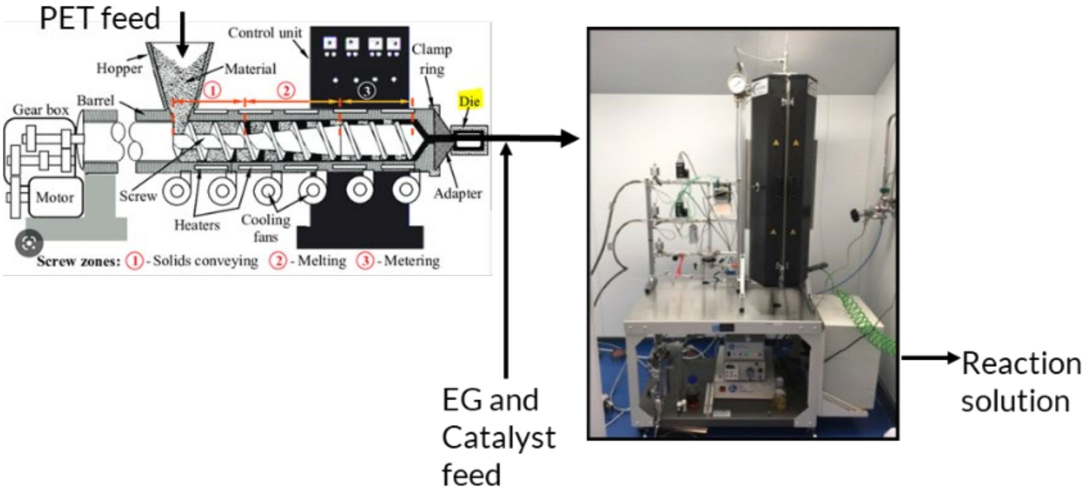
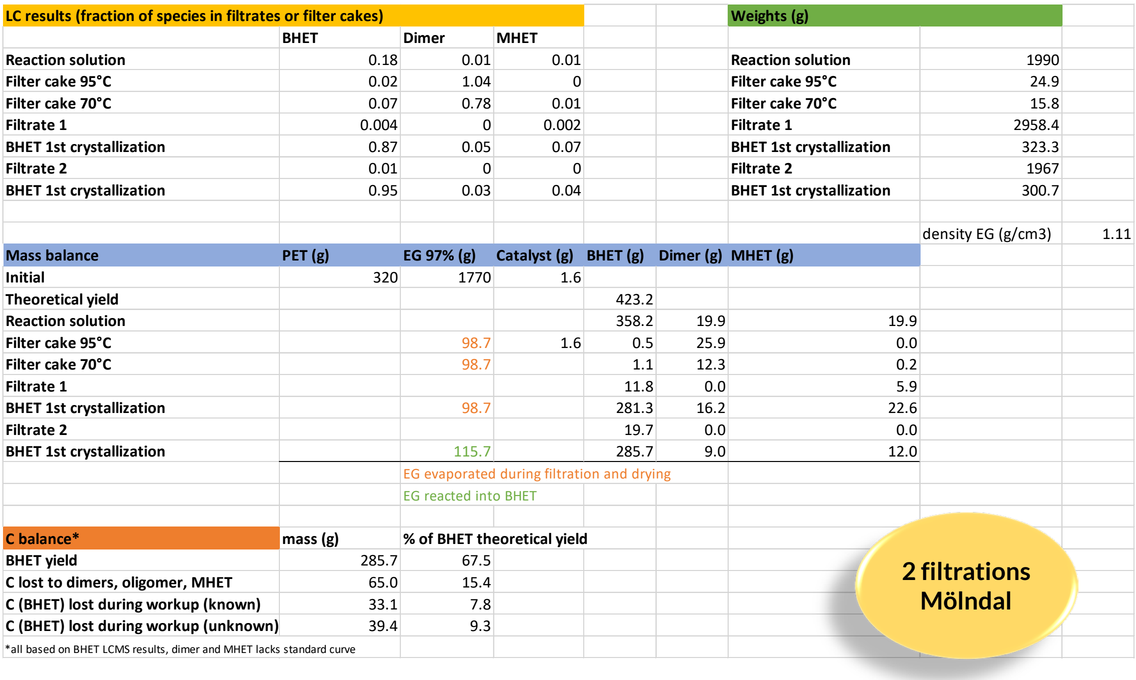


Figure 9. Schematic suggestion a continuous glycolysis process starting with PET being fed through a compounder so that a melted PET is fed together with EG and catalyst into a tubular reactor. A reaction time of 5 minutes means there will be a continuous flow of reaction solution from the tube reactor.

A *mass balance* was completed by performing a depolymerization in a 2-liter reactor, weighing all input and output materials. The results complemented the experiments and were performed in microwave heated reactors. The amount of BHET, dimers and MHET in each reaction step was taken from the LC-analysis of MW-reactor experiments (Table 2) and was combined with measures on yields and losses from a complete work up in the 2 liter reactor. Loss of BHET happened in several process steps: residue of reaction solution in the reactor, BHET crystallizing in the filtration funnel or flask, BHET in the solid residue recovered in filtration, BHET dissolved in EG-water blend removed as filtrate after the first crystallization and BHET dissolved in water removed as filtrate after the second crystallization. A further contribution to weight loss will be the decolorization of BHET by use of active carbon as described above.

Table 5. Results as input to mass balance.



LC results (fraction of species in filtrates or filter cakes)	BHET	Dimer	MHET		Weights (g)	
Reaction solution	0.18	0.01	0.01		Reaction solution	1990
Filter cake 95°C	0.02	1.04	0		Filter cake 95°C	24.9
Filter cake 70°C	0.07	0.78	0.01		Filter cake 70°C	15.8
Filtrate 1	0.004	0	0.002		Filtrate 1	2958.4
BHET 1st crystallization	0.87	0.05	0.07		BHET 1st crystallization	323.3
Filtrate 2	0.01	0	0		Filtrate 2	1967
BHET 1st crystallization	0.95	0.03	0.04		BHET 1st crystallization	300.7

density EG (g/cm3) 1.11

Mass balance	PET (g)	EG 97% (g)	Catalyst (g)	BHET (g)	Dimer (g)	MHET (g)
Initial	320	1770	1.6			
Theoretical yield				423.2		
Reaction solution				358.2	19.9	19.9
Filter cake 95°C		98.7	1.6	0.5	25.9	0.0
Filter cake 70°C		98.7		1.1	12.3	0.2
Filtrate 1				11.8	0.0	5.9
BHET 1st crystallization		98.7		281.3	16.2	22.6
Filtrate 2				19.7	0.0	0.0
BHET 1st crystallization		115.7		285.7	9.0	12.0

EG evaporated during filtration and drying

EG reacted into BHET

C balance*	mass (g)	% of BHET theoretical yield
BHET yield	285.7	67.5
C lost to dimers, oligomer, MHET	65.0	15.4
C (BHET) lost during workup (known)	33.1	7.8
C (BHET) lost during workup (unknown)	39.4	9.3

*all based on BHET LCMS results, dimer and MHET lacks standard curve

2 filtrations Mölndal

Table 6. Mass balance from the depolymerization. The results are based on BHET results from LC-MS. Dimer and MHET lacked standard curves.

	Mass (g)	**Molar yield (%)**
BHET yield	285.7	67.5
C lost to dimers, oligomers, MHET (easy to recover)	65.0	15.4
C (BHET) lost during workup (dissolved - difficult to recover)	72.5	17.1

The mass balance is based on the assumption that the BHET molar yield in reaction is 85% and 95% purity of the monomer. The results from several calculations on the mass balance are shown in Table 5. A final carbon balance seen from the formation of BHET is presented in table 6.

C) Filtering study

The original batch process for glycolysis was based on two steps of filtration as shown in Figure 1. This set-up was based on filtration with heated reaction solution but equipment at room temperature aiming at getting a filtrate free from oligomers, containing pure BHET ready for subsequent crystallization. Hot filtration i.e. having a heated filtering equipment that also can be pressurized (Nutsch filter) would be an alternative making it possible to only perform one filtration at 70°C. The results from filtration experiments showed that one filtration with controlled temperature can replace two filtrations.

D) Crystallization study:

A separate crystallization study was not performed. BHET crystallizes readily and continuous crystallization is a well-known process which will be included in the production line for BHET.

5.3. Simulation, Optimization and LCA

5.3.1. **Simulation**

The process that was used in the setting up of the Aspen simulation is depicted in Figure 1. Results from batch experiments were used to set up the mass balance in Excel. For the simulation in Aspen a continuous process was set up using data from the batch experimental results. Figure 9 is a proposal on how a continuous PET depolymerization reactor could be set up. The proposed reaction time is 5 minutes at reaction temperature 270°C.

The mass balance data, combined with operational details (for example temperature, flows, etc.) were used to set up the first draft version of the Aspen simulation. This first draft version contained the main unit operations. The flowsheet of the first draft version of the Aspen simulation is given in Figure 10.

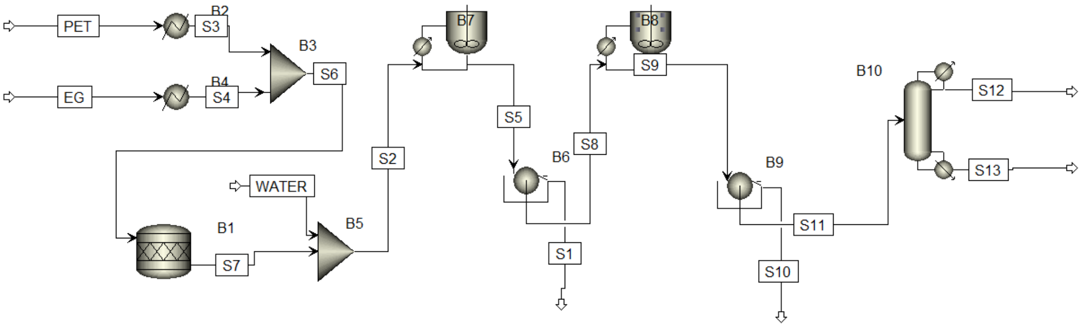


Figure 10. First draft version of the Aspen Simulation depicting the main unit operations

In Figure 10, the “original” process can be described as follows:

1. Streams PET and EG, at room temperature, is fed to heaters B2 and B4. The streams are heated up to the reaction temperature of 270 C (stream S3 heated PET and S4 heated EG).
2. The streams are mixed in mixer B3, the combined mixed and heated stream being S6.
3. Stream S6 is fed to the reactor B1, where the reaction PET to BHET takes place, resulting in stream S7.
4. Water is added to stream S7 in mixer B5, resulting in dimers and unreacted PET to precipitate, forming stream S2.
5. Stream S2 is further cooled down in crystallizer B7, to precipitate all dimer, forming stream S5.
6. The precipitated dimer/unreacted PET in stream S5 is filtered off in filter B6. The mother liquor containing the BHET product remains in stream S8, the filtered dimer stream S1.
7. The dissolved BHET product in stream S8 is cooled in crystallizer B8. BHET product is filtered off in filter B9. This isolated BHET product remains in stream S10, with the EG/water mixture , stream S11, being transferred to distillation column B10 where the water is distilled off from the EG. The water overhead stream being S12, with the EG exiting the bottom of the distillation column as stream S13.

5.3.2. Optimization

After completion of the first draft Aspen simulation a more detailed Aspen simulation was set up to even include a second crystallization step, and inclusion of heat exchangers to optimize energy usage. See Figure 11 for a flowsheet of the “detailed” Aspen simulation.

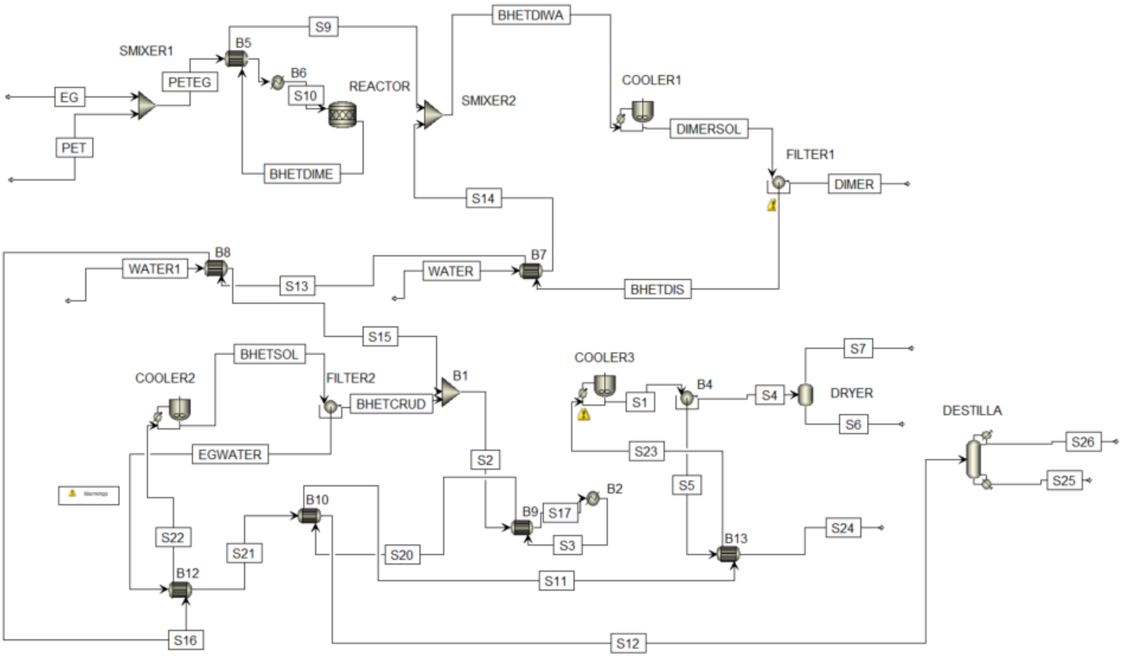


Figure 11. “Detailed” Aspen Simulation, including heat exchange/energy optimization

In Figure 11, the process even containing heat exchange/energy optimization can be described as follows:

1. Streams PET and EG, at room temperature, is mixed in mixer SMIXER1, the mixed stream being PETEG.
2. Stream PETEG enters heat exchanger B5, where heat from the reaction mixer exiting the reactor REACTOR (stream BHETDIME) is heat exchanged with stream PETEG. The heated stream PETEG is then further heated to the reaction temperature in heater B6, before entering reactor REACTOR where PET is reacted to BHET. The reaction mixture exiting REACTOR is named BHETDIME (a mixture of BHET and dimer). Stream BHETDIME after heat exchange in heat exchanger B5 is called S9.
3. Water (stream WATER) is heated in heat exchanger B7 (heat exchange with stream BHETDIS), the heated water stream S14. Heated water (stream S14) is mixed with stream S9 in mixer SMIXER2, resulting in dimers and unreacted PET to precipitate, forming stream BHETDIWA (BHET, dimers and water).
4. Stream BHETDIWA is further cooled down in crystallizer COOLER1, to precipitate all dimer, forming stream DIMERSOL.
5. The precipitated dimer/unreacted PET in stream DIMERSOL is filtered off in filter FILTER1. The mother liquor containing the BHET product is called stream BHETDIS, the filtered dimer stream being DIMER.
6. The stream BHETDIS is heat exchanged in heat exchanger B7 (exit stream S13), B8 (exit stream S16) and B12 (exit stream S22) before entering the second crystallizer (COOLER2), where the product BHET is crystallized. The mixture exiting the crystallizer is stream BHETSOL.
7. Crude BHET product in stream BHETSOL is filtered off in filter FILTER2. This isolated BHET product remains in stream BHETCRUD, with the EG/water mixture, stream EGWATER, is heat exchanged in heater B12 (exit stream S21) and B10 (exit stream S12). Stream S12 (EG water mixture) is transferred to distillation column DISTALLA where the water is distilled off from the EG. The water overhead stream being S26, with the EG exiting the bottom of the distillation column as stream S25.
8. The crude BHET (stream BHETCRUD) is recrystallized in water to form a pure BHET product. This is performed by first heating up water stream WATER1 through heat exchanger B8, the heated water stream being S15, before mixing this water stream S15 with BHETCRUD in mixer B1 to form stream S2. Stream S2 is heat exchanged in heat exchanger B9, B10 and B13 and then finally cooled in crystallizer COOLER3 to crystallize out the pure BHET. The pure BHET in stream S1 is filtered off in filter B4 resulting in pure BHET (stream S4) that is dried in dryer DRYER. The product dry BHET is stream S6, with the water dried off in stream S7. The mother liquor, mainly water with dissolved BHET (stream S5), is heat exchanged in heat exchanger B13, with the wastewater outlet after heat exchange being stream S24.

The Aspen simulation, combined with the mass balance created in Excel were used to investigate how 3 different parameters impacted production of BHET. The results from this investigation were used to perform LCA's on the different scenarios.

The following 3 parameters were investigated:

- EG water content (1 % or 2,5 %): High water content in the EG used has a negative effect on the quality and yield of the BHET formed, as water reacts with PET to form MHET. On the other hand recycling of EG is easier (less costly, less energy use, reduction on LCA footprint) if more water remains in the recycled EG.
- Activated carbon treatment to remove color or no activated carbon treatment: Removal of color with activated carbon increases quality of the product, but reduces yield as some of the product is filtered off during this operation.
- 1 or 2 crystallization steps to purify the product: One crystallization step is required to isolate the product. A second crystallization step mainly removes EG (purer product), but also reduces yield as some product remains in the mother liquor.

The following scenarios were investigated:

1. EG 2,5 % water, activated carbon treatment for color removal, 2 crystallizations.
2. EG 2,5 % water, activated carbon treatment for color removal, 1 crystallization.
3. EG 2,5 % water, no activated carbon treatment for color removal, 2 crystallizations.
4. EG 2,5 % water, no activated carbon treatment for color removal, 1 crystallization.
5. EG 1 % water, activated carbon treatment for color removal, 2 crystallizations.
6. EG 1 % water, activated carbon treatment for color removal, 1 crystallization.
7. EG 1 % water, no activated carbon treatment for color removal, 2 crystallizations.
8. EG 1 % water, no activated carbon treatment for color removal, 1 crystallization.

The "detailed" Aspen simulation was transferred to Perstorp, where further modifications were introduced to optimize energy usage, and to perform the techno-economic evaluation.

5.3.3. **LCA**

This report shows the results of the life cycle assessment (LCA) of chemical recycling of polyethylene terephthalate (PET) waste to bishydroxyethyl terephthalate (BHET). It was carried out by IVL Swedish Environmental Research Institute in the research project "Kemisk återvunnen PET/polyester som råvara för additiv och ny polymer" funded by the Swedish Energy Agency.

Lab scale testing and process simulation data carried out at RISE for the chemical recycling of PET waste BHET were used as input to the LCA model. Three different process parameters were tested to generate 8 different process configurations. The parameters tested were -

- Water content in recycled ethylene glycol.
- Decolouring of BHET.
- Number of crystallisations steps.

The base case was defined as the scenario in which there is 1% water content in recycled Ethylene Glycol, the addition of a decolouring step and the addition of a crystallization step.

The results show that the climate change impact of recycling PET waste to BHET ranges from 2.0-2.5 kg CO_2 eq. per kg BHET across the 8 different scenarios studied. It was observed that the most desired scenario i.e.m1 % water in the EG, decolorized BHET crystallized twice, had the highest impact. Major hotspots within the process were identified to be use of Ethylene glycol, and particularly the energy use during its recycling step.

Sensitivity analysis was also conducted on the electricity grid mix used as well as the source of energy in the process. It was found that PET washing is sensitive to the Electricity grid mix used and using an EU average grid mix increases the climate change impact by about 20%. Using biomass as a source of energy was found to potentially reduce the climate change impact by 60%.

The results were also compared to current market conditions of PET waste management and BHET production. Chemical recycling of PET waste to BHET has 20% lesser climate impact when comparing to current market conditions.

The LCA results on the chemical recycling of PET waste to BHET indicates that the climate change impact is between **2.0-2.5 kg CO_2 eq. per kg BHET** for the different scenarios studied. Scenario 5, the scenario with the highest climate change impact and highest purity, has process settings with 1% water content of the recycled EG, decolourisation of BHET and two crystallisation steps.

The main climate change impact, for all scenarios, comes from the depolymerization step. In the depolymerization step it is mainly the use of ethylene glycol (both fresh and recycled) contributing to the impact. The impact of ethylene glycol ranges from 0.3 (recycled) to 0.8 kg CO_2 eq. per kg. Fresh EG has been modelled using virgin EG dataset that is fossil based. However, this need not be the case in the future, as there could be other sources of ethylene glycol with a lower climate impact, for instance biobased EG or EG from other recycled sources. The other main conclusion to point out is that the recycling of EG currently uses fossil energy sources, which affects the environmental performance. The hotspot analysis further justifies on why it is important to consider the source of ethylene glycol used in the system. Since large quantities of ethylene glycol are used in the depolymerization step, efforts should be put on exploring the possibilities of reducing the amount of ethylene glycol use and investigate if it is possible to reuse the ethylene glycol within the same process before being sent for recycling. Further studies must also explore ways to optimize energy use in the recycling of EG at Recyctec, which could potentially lower the climate impact as well.

In the sensitivity analysis the effect of using EU electricity mix instead of the Swedish electricity mix was tested. The EU electricity mix has a higher share of fossil energy compared to the Swedish electricity mix, resulting in higher climate change impact. For all scenarios, the climate change impact increased approximately by 20% when the system was modelled with EU electricity mix. This shows the importance of using cleaner electricity sources. The increase of the climate change impact is mainly because of the electricity use in the washing of PET waste. The data use for the washing of PET are based on washing tests at the company Herbold Mecksheim GmbH. The PET waste was treated in several steps, and in future work it is recommended to study the washing further, trying to understand which washing steps are necessary.

A sensitivity analysis was also done to study changing the source of energy from natural gas to biomass and the results indicate that approximately 60% reduction can be observed in the climate change impact bringing it down to less than 1 kg CO_2 eq. per kg BHET.

The efforts, in this project, of trying to optimise the process have influenced the outcome of the LCA. In the project, *Material circularity through recycling of PET/polyester in preparation for BHET monomer production in Sweden*, in year 2021, the LCA identified the use of ethylene glycol, incineration of oligomers, and energy usage as hotspots (Lindqvist, 2021). The use of ethylene glycol is still a main hotspot of the system, but incineration of oligomers and electricity usage are not. In this project it was identified that the oligomers could be recycled back into the depolymerization reactor, which means that no incineration of the flow is necessary. Also, in this project heat optimisation was studied, and it was concluded that the energy used in the foreground process has minor impact. However, the use of fossil-based energy in the recycling of EG, is a hotspot identified and optimization of the overall energy consumption as well as choice of energy source should be studied further.

The purity and colour of the final product is a known factor in the industry for product quality. The LCA study results indicate that de-colouring has low climate change impact.

Figure 12 shows how the LCA results for the studied system compares with a comparative scenario today. Scenario 5, i.e., Base case (BC), was used in the comparison. In the incineration of PET waste, 41.3% of the impacts are allocated to the waste handling of PET waste and the remaining 58.7% to energy production (Avfall Sverige, 2014). The climate change impact has been expressed as kg CO_2 eq./kg BHET produced and 1.1 kg PET waste handled. This is to reflect the dual functionality of both waste management and production of 1kg BHET.

The yield for producing BHET from PET waste is 90% and so we need 1.1 kg of PET to produce 1kg of BHET which is reflected in the functional unit for the comparative scenario (CS). The results show that the chemical recycling of PET waste to BHET (BC scenario) has a 20% lower climate impact than the scenario of BHET production based on DMT from fossil source and todays' PET waste management. It is also important to note that the impacts from other pre-processing steps with regards to waste management of PET are excluded as they are assumed to be similar for both the scenarios (base case and comparative). The complete LCA report is found in Appendix A.

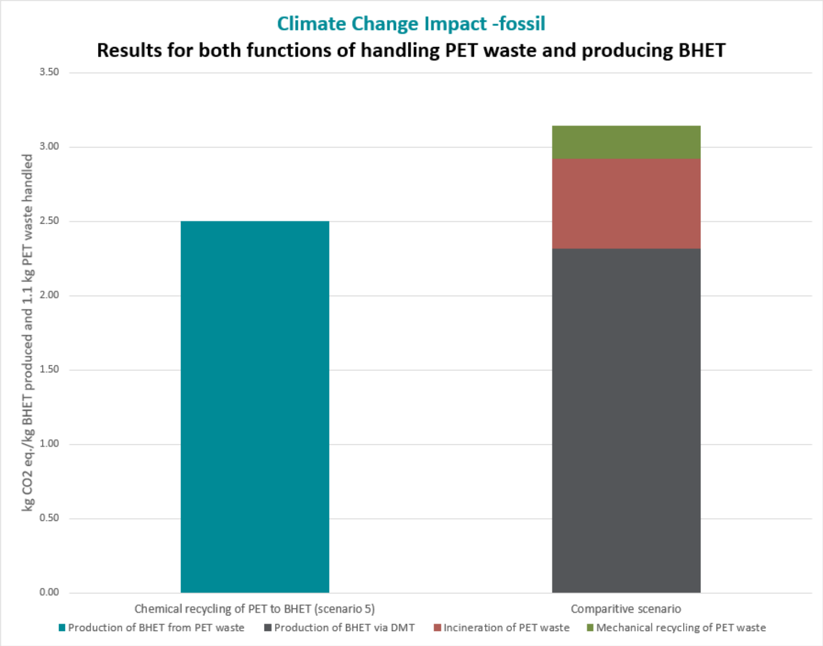


Figure 12. Climate Change impact for Chemical recycling of PET to BHET compared to Comparative scenario. Note: This figure represents two functions of a system and so the results must be interpreted accordingly.

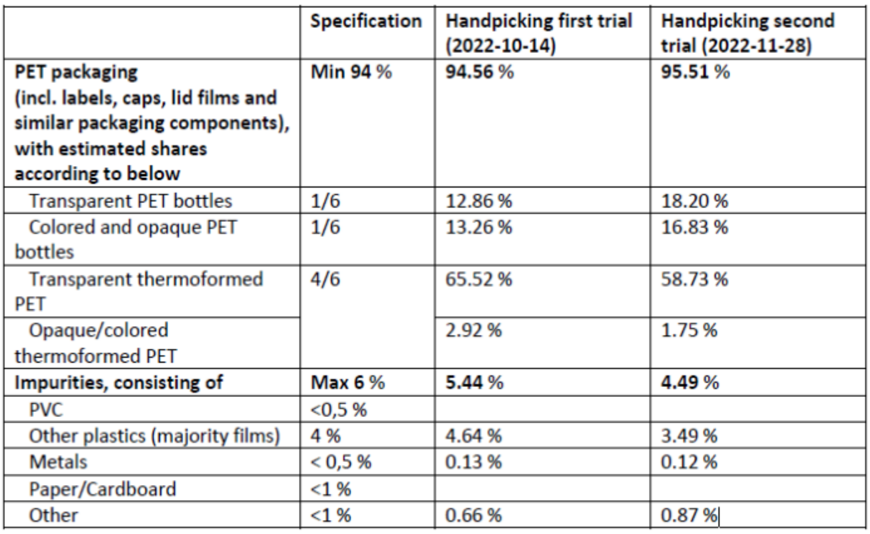
5.4. Market development-150kg BHET in pilot scale

5.4.1. Raw material - sorting and washing of PET packages

Swedish Plastics Recycling sorted PET to send a bale for washing and further separation. A PET share of > 94% was targeted to make it possible to transport the mix easily under the the waste shipment regulation (Annex VII of the EU Waste Shipment Regulation). Figure 13 show the sorted PET packages ready to be sent for washing. Table 7 shows the estimated composition of the PET waste and Figure 14 some examples of packages from handpicking trials.

Figure 13. The PET packages sorted at Swedish Plastics Recycling that was sent for washing at Herbold Meckesheim GmbH.

Table 7. Estimated composition of sorted PET waste



	Specification	**Handpicking first trial (2022-10-14)**	**Handpicking second trial (2022-11-28)**
PET packaging (incl. labels, caps, lid films and similar packaging components), with estimated shares according to below	**Min 94** %	**94.56** %	**95.51** %
Transparent PET bottles	1/6	12.86 %	18.20 %
Colored and opaque PET bottles	1/6	13.26 %	16.83 %
Transparent thermoformed PET	4/6	65.52 %	58.73 %
Opaque/colored thermoformed PET		2.92 %	1.75 %
Impurities, consisting of	**Max 6** %	**5.44** %	**4.49** %
PVC	<0,5 %		
Other plastics (majority films)	4 %	4.64 %	3.49 %
Metals	< 0,5 %	0.13 %	0.12 %
Paper/Cardboard	<1 %		
Other	<1 %	0.66 %	0.87 %

Figure 14. Example of PET packages from handpicking trial performed at Swedish Plastics Recycling.

Washing of PET packages was performed at Herbold Meckesheim GmbH in Germany, in their pilot scale washing unit with the different steps included as shown in Figures 15 and 16.

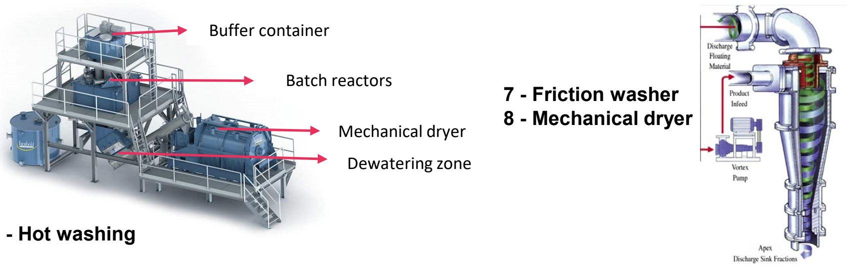
1 - Shredder

2 - Prewashtank

3 - Wet grinder with
4 - Friction washer

5 - Mechanical dryer
(OR step dryer)

Figure 15. Washing PC-PET at Herbold Meckesheim GmbH: shredder, prewash, wet grinder with friction wash and mechanical drying.



6 - Hot washing

7 - Friction washer
8 - Mechanical dryer

9 – Separation
-Hydrocyclone

10 - Friction washer
11 - Mechanical dryer

Figure 16. Washing PC-PET at Herbold Meckesheim GmbH: hot washing, friction washing, mechanical drying, separation hydrocyclone and final friction washer and dryer.

Table 8. Results from washing and separation of sorted PET packages at Herbold Meckesheim.

Material/position in process	Mass (kg)	Res.moisture (%)	Dry mass (kg)	Percent of total input (%)
input			344	100
Output good materials	166	1,21	164	47,6 clean PET
Sieving at hydrocyclone	115	43,97	64	18,6
Heavy mat cyclone	6	14,03	5	1,5
Water treatment, sieving machines	120	71,1	35	10,2
Sink of pre-washer	164	53,72	76	22,1

Table 8 shows the results from washing and separation as the fraction of various streams. It is a surprisingly low amount that is output as good (i.e. washed) material. A fact confirmed by other sources, is that PC packages contain a considerable amount of product residues which contribute to the weight of the sorted packages. Another unfortunate fact is that the total amount of packages sent to Herbold was too small for the size of the pilot plant. Too much of the original weight was “lost” in the plant and could never be collected as washed PET. The volume going in should have been at least the double (two bales instead of one). The results in Table 8 can therefore not be used as a base for “mass balance” for a washing operation.

Results from FTIR analysis performed on different fraction from the separation steps in the washing process, are shown in Table 9. The results indicate the various contaminations and confirm the effectiveness of the separation steps.

Conclusions from the washing are that the washed PET is clean and does not seem to contain any large amounts of polyolefins. The amount sent to Herbold was too small and there were big losses of packages in their machinery. The information for LCA is insufficient when it comes to data on their machinery and a much better mass balance is needed.

Table 9. Results from FTIR analysis of different fractions from the washing of PC-PET

Sample	#samples	#PET	#others	identity others
Heavy cyclone good material	10	10	0	
Heavy cyclone good material after glycolysis	10	9	1	NBR rubber
Heavy cyclone bad material	10	8	2	metal spring, unidentified plastic
Light cyclone	10	0	10	PP and PE films
Sieve	10	10	0	

5.4.2. Depolymerization, separation and characterization of monomer

The washed PC-PET from Herbold was sent to Synpo for depolymerization. A certain volume of virgin PET (75 kg) was also supplied by RISE since the volume of washed PC-PET was smaller than expected. The raw materials at Synpo are shown in Figure 18. The desired and possible reactions that take place during depolymerization are shown in Figure 17.

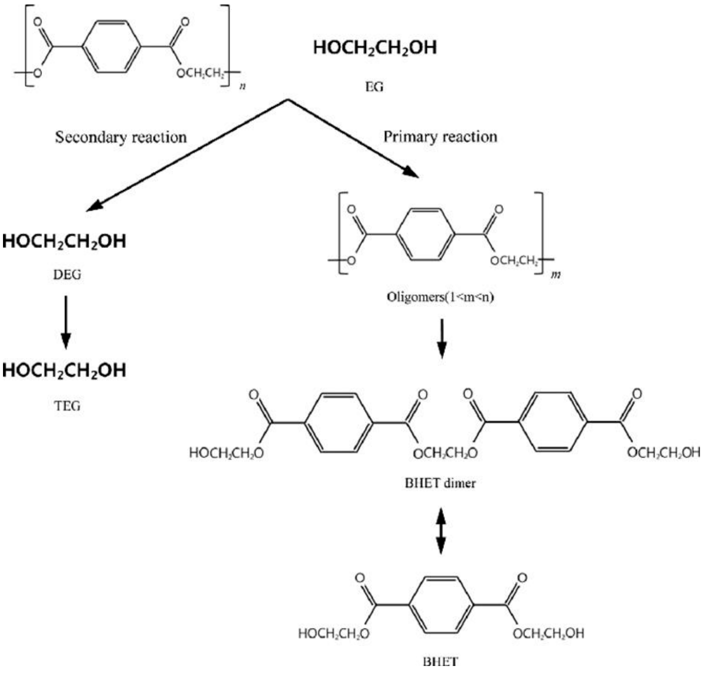


Figure 17. Reaction sceme for the glycolysis process. The ethylene glycol may form some di-ethylene glycol a/o tri-ethylene glycol, as biproducts. The oligomers formed during depolymerization further react to form dimers and finally monomers.

Figure 18. Materials depolymerized at Synpo: Virgin PET to the left and washed PC-PET to the right

Depolymerization experiments were first performed in lab scale and then in a 350 liter reactor at 200°C. The yield was 84% on molar basis when depolymerizing virgin PET while the yield was lower, 72% on molar basis for the PC-PET. One explanation for the lower yield is a certain amount of polyolefins remaining in the PC-PET. The polyolefins were found as residues in the reactor, adhering to the reactor walls or the stirrer. The residues were removed by mechanical cleaning with some solvent.

5.4.3. Decolorization of BHET

The crude BHET obtained from lab scale experiments with PC-PET at Synpo are shown in Figure 19.

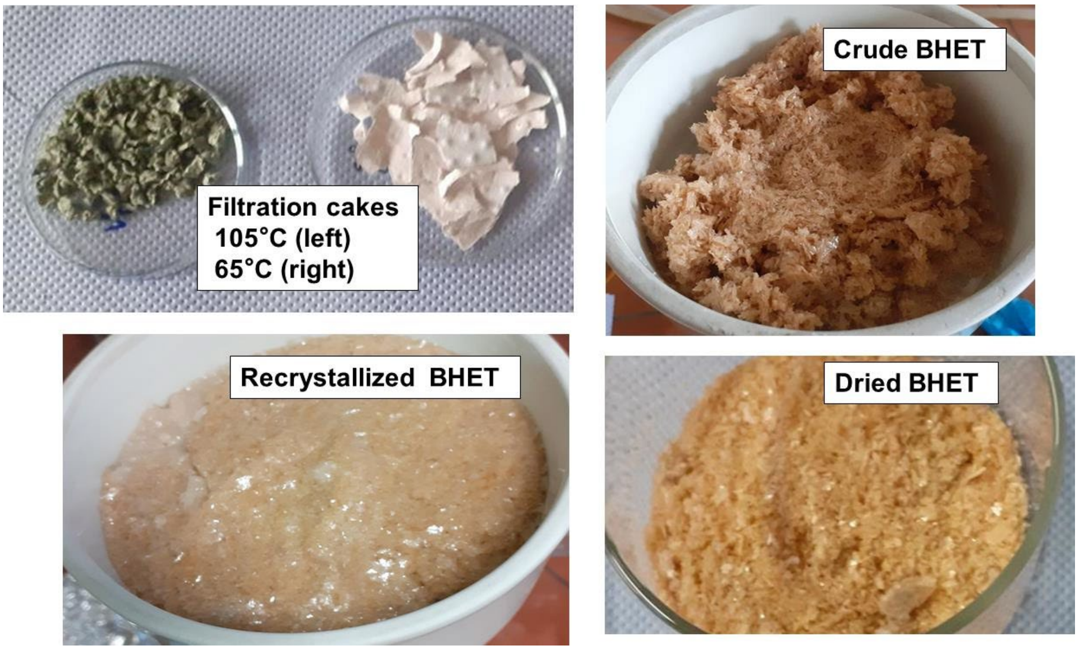


Figure 19. Results from the process of isolating the BHET. Filter cakes to the upper left are made up of residues and oligomers and to some extent BHET that mya crystallize on the filter paper due to cooling. The recrystallized BHET is brighter than crude BHET, partly since crude BHET contain a residue of EG.

The decolorized BHET as shown in Figure 20 was treated with 0,2 and 0,4 w% AC based on the amount of BHET. There has been a loss in yield of BHET of about 10% after active carbon treatment. There may be a certain amount of BHET adsorbed on the active carbon or, it may be due to loss during filtration. Further studies with hot filtering should be performed.

Figure 20. BHET decolorized with 0,4w% active carbon BHET to the left and 0,2w% active carbon to the right.

5.5. Market development – Applications

BHET from Synpo was sent to project partners for application development. Perstorp received BHET for synthesis of plasticizer to be evaluated by Tarkett and National Sweden. Perstorp also synthesized binders for paint to be evaluated by Sherwin Williams and Celenis received BHET for polymerization of PET to be further evaluated by KP Film, pressing trays or cups, and by Diab that performed experiment by foaming the PET.

5.5.1. Syntheses performed by Perstorp

Binders for coatings:

Perstorp synthesized BHET based polyester that can be used for coatings but also be further synthesized to form BHET based polyester acrylate which also is a type of binder. Schematic reactions to form these binders are shown in Figures 21. TMP is added in the reaction to form a network. Also, BHET based urethane acrylates were synthesized.

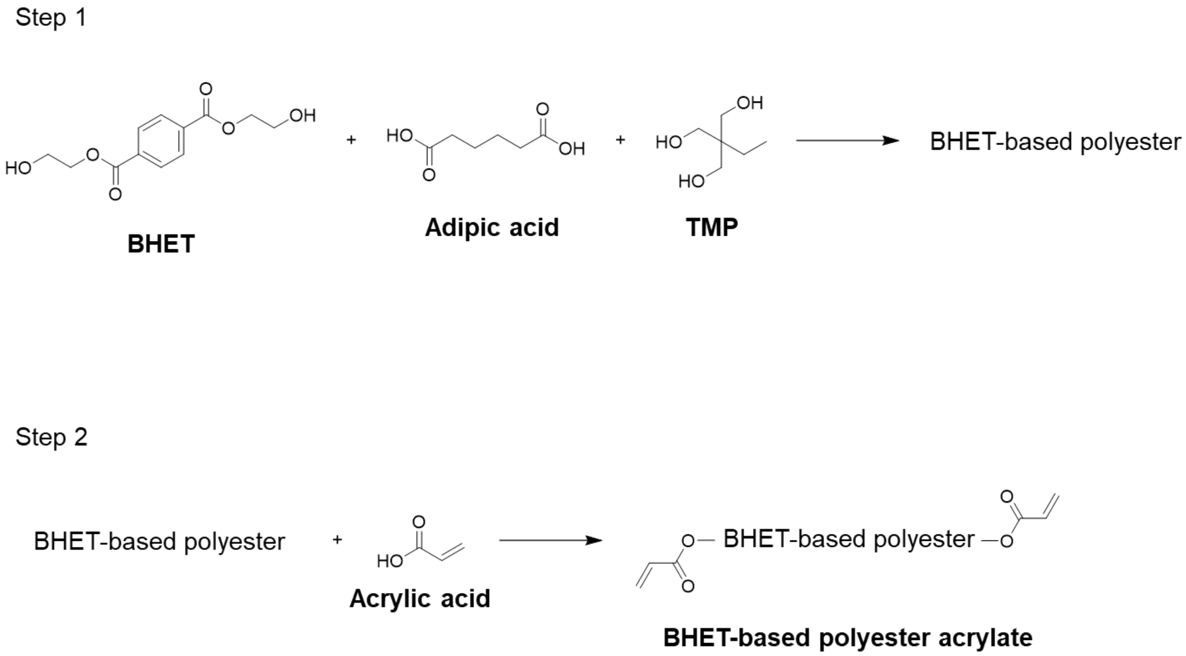


Figure 21. Synthesis of **BHET**-based polyester acrylate.

Four BHET-based polyester batches and 4 BHET-based polyester acrylate batches were successfully produced. The results from analyses of the reaction products are shown in Table 10. Analyses concerned acid number, hydroxyl number, molecular weight, amount of TMP, mono ethylene glycol (MEG) and colour. Importantly, the amount of TMP found in the product was below the accepted limit since trimethylol propane TMP is classed as toxic chemical. The polyesters were also analyzed by LC-MS, which showed typical distribution for polyesters production as seen in Figure 23. Figure 22 show the prepared polyesters to be used as binders.

Table 10. Analytical results of the BHET based polyesters

BHET grade	**AN, mg KOH/g**	**OH number, mg KOH/g**	**MW main peak, Mn/Mw/Pd**	**TMP, %m/m**	**MEG, %m/m**	**Colour, visual**
23Mar10, Decolorized BHET	3.3	95	2800/4400/1.6	0.07	0.9	White/yellow
23Mar11, Colored BHET	1.4	104	2700/4100/1.5	0.06	0.8	Brown
23Mar17b, **rBHET**	2.3	111	2000/4400/2.2	0.06	0.8	Brown
23Mar19, **rBHET**	4.6	124	2200/4400/2.2	0.06	0.8	Brown

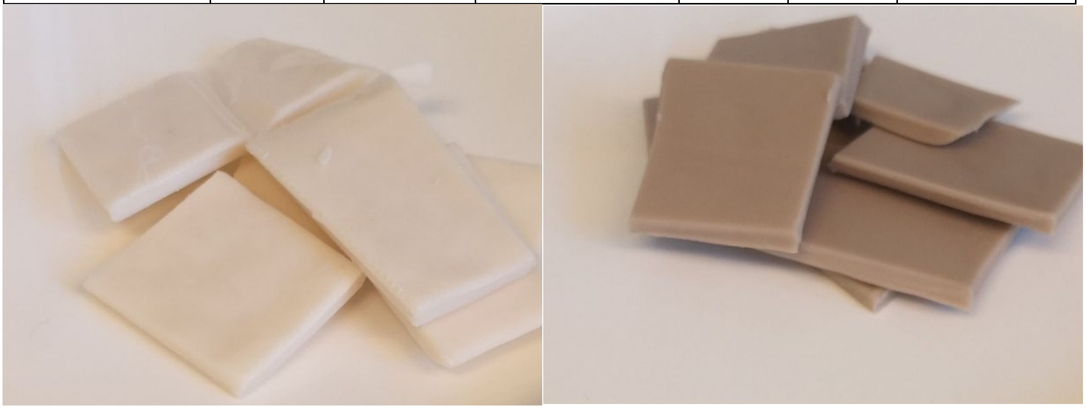


Figure 22 To the left polyester as binder made with decolorized BHET and to the right made with colored BHET

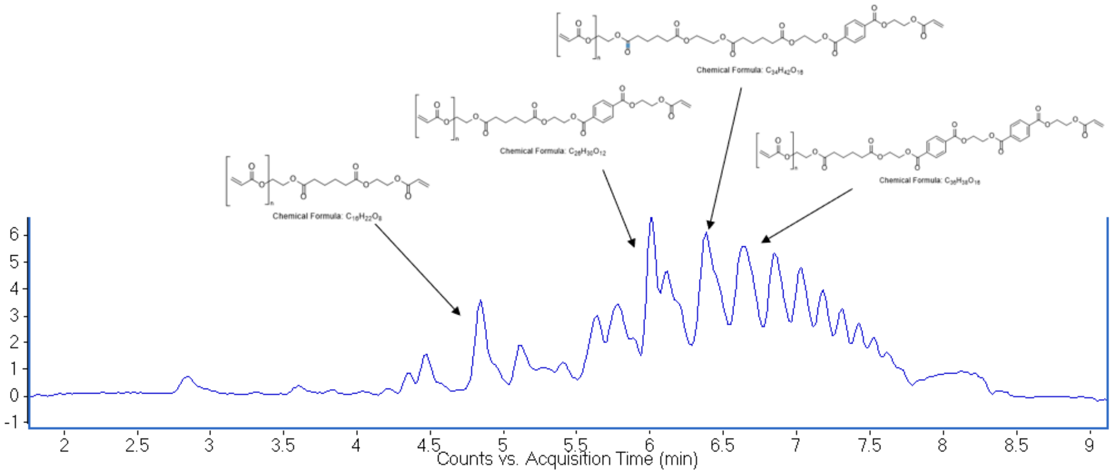


Figure 23. LC-MS chromatogram of the polyester acrylates.

The urethane acrylates were produced in two steps according to Figure 24. In the first step an adduct is produced from the reaction of 2-EHA and IPDI. In the second step, BHET is added to the acrylate-containing adduct to form the targeted compound. Finally, removal of the reaction solvent afforded the BHET-based urethane acrylate.

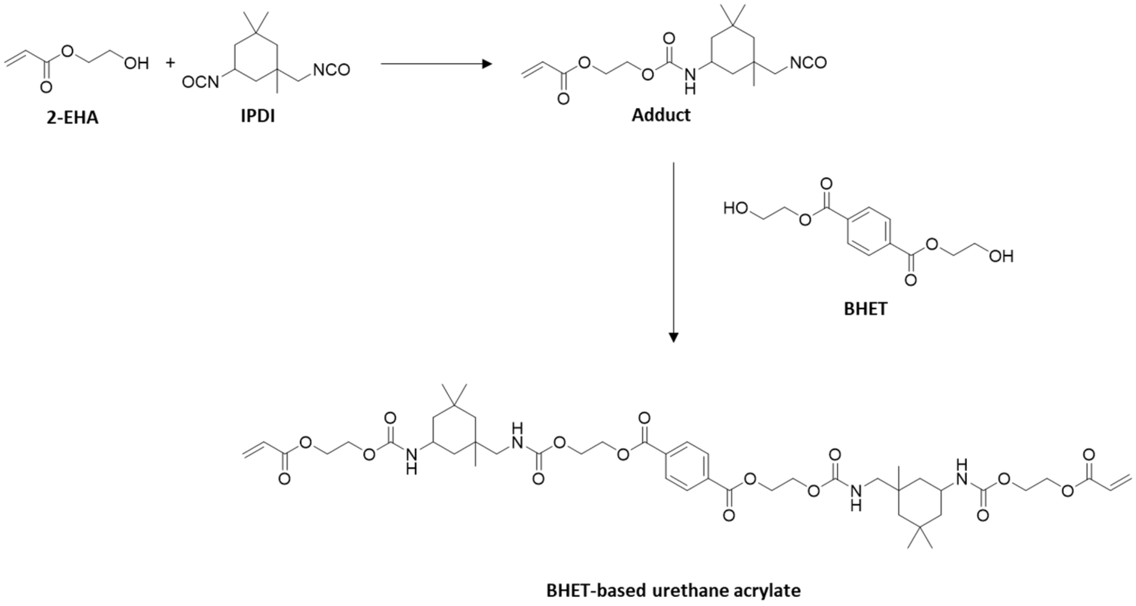


Figure 24. Synthesis of BHET based urethane acrylate.

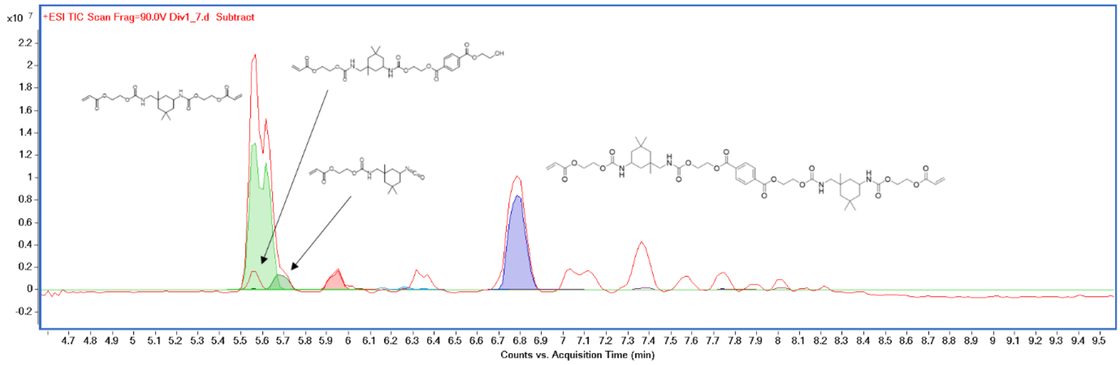


Figure 25. LC-MS chromatogram of th BHET based urethane acrylate reaction mixture.

Figure 25 shows the identification of reaction products formed during synthesis of BHET based urethane acrylate.

There were no significant differences between products produced form BHET form Sigma Aldrich and rBHET except for the color which is shown in Figure 26.

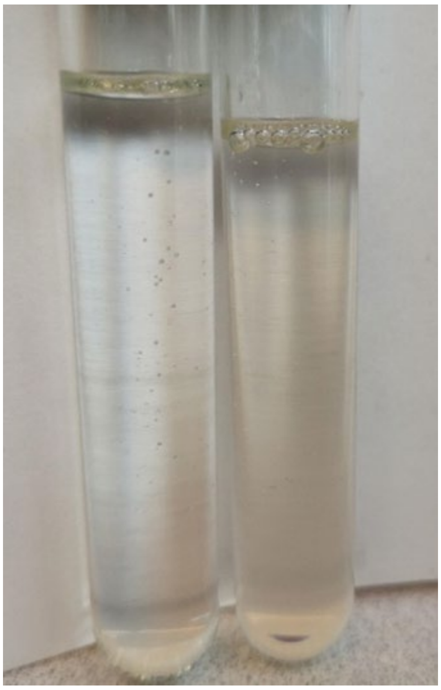


Figure 26. BHET based urethane acrylates produced from BHET (Sigma Aldrich (left) and rBHET (right).

Plasticizer

Perstorp also synthesized plasticizers based on BHET to be blended in compound for flooring or rubber. Figure 27 shows the schematic reaction and Figure 28 show the experimental set up used during synthesis of plasticizer. The effects of temperature and reaction time were studied as a start.

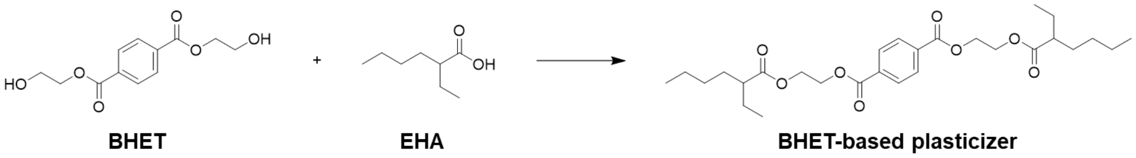


Figure 27. Synthesis of BHET based plasticizer.

Figure 28. Experimental set-up for synthesis of plasticizer

The effect of the reaction temperature was small in terms of the final composition of the product. Increasing reaction temperature yields higher amounts carboxylic acid-containing products, which difficult the work up as it acts as surfactant during the extraction. Interestingly, oligomerization of BHET was favored by decreasing temperatures. The targeted compound was found at about 20 Area%, and even though the yield was low, the total amount of EHA-containing BHET and BHET oligomers amounted to ca 90 Area%. This was considered, together with National and Tarkett, good enough and preparation of this product was pursued at higher scale. Finally, ca 2 kg BHET-based plasticizer was obtained. The reaction was performed using sodium hypophosphite at 180 ºC and the final acid value of the product was 9.45 mg KOH/g.

5.5.2. PET synthesis by Selenis

Table 11. Results from polymerizations at Selenis

Sample						MSP - Poly				MSP - Colors			MSP-I.V.	SSP-I.V.	CEG	DEG	T_g
N°	BHET type	BHET quantity used (kg)	Theoretical polymer produced (kg)	Total amount of polymer cut (kg)	Final State process	Time	Final Poly Temp. °C	% Final Torque	RPM Final speed	L*	a*	b*	dL/g	dL/g	meq/kg	%	°C
1	**Virgin**	32.0	24.2	12.8	SSP	60	283.0	35.0	500	57.1	-1.1	6.8	0.673	0.730	29	0.9	80.1
2	**Virgin**	30.0	35.5	30.0	MSP	64	282.7	80.0	290	57.5	2.4	16.4	0.631	N.A.	33	0.7	105.4
3	**Virgin +rBHET**	60.0	45.4	28.4	SSP	55	282.4	35.0	500	69.1	-1.0	13.6	0.648	0.800	48	0.8	81.1

Polymerization into PET and Akestra 110 using BHET and rBHET was successfully achieved as observed by their final intrinsic viscosities IV, see results in Table 11 (MSP-I.V.). Increase of the IV of PET to bottle grade (0.8 IV) was also successfully attained using solid state polymerization SSP. Interestingly, generation of diethylene glycol DEG was minimized compared with conventional production of PET due to fact that the first step for the production of polyesters is omitted by the use of BHET, which is where most of the DEG is generated. The presence of DEG-containing repeating units within polymer causes a dramatic drop in the glass transition temperature T_g. The most significant difference between the two PET grades (sample 1 and 3 in Table 11) is, again, the color, as observed in Figure 29. The PET produced for the project, otherwise, exhibited typical thermal and rheological properties.

MSP		
L*	a*	b*
57.1	-1.1	6.8
I.V. 0.673		
Tg=80.1°C		

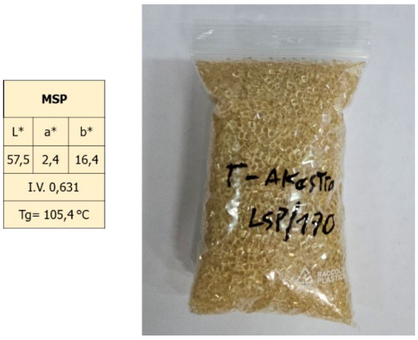
SSP		
L*	a*	b*
72.3	-1.4	3.1
I.V. 0.730		
Tg=81.6 °C		

MSP		
L*	a*	b*
69.1	-1.0	13.6
I.V. 0.648		
Tg= 81.1°C		

SSP		
L*	a*	b*
55.5	1.5	6.2
I.V. 0.800		
Tg= 83°C		

Figure 29. PET produced from BHET (a), and a mixture of BHET and rBHET (b). The Picture also contains information about the color properties, IV, and T_g, before and after SSP.

Akestra 110 was also successfully prepared despite being a less conventional procedure as compared to PET production. Figure 30 shows pellets of Akestra 110 as well as color indexes, IV and T_g. Except for the color, IV and T_g fell within the expected values. It is worth mentioning that polyesters produced in the pilot plant at Selenis tend to color. On top of that, addition of toners was avoided, which help to mask colored material. Big scale production would most probably have resulted in much clearer products.



MSP		
L*	a*	b*
57,5	2,4	16,4
I.V. 0,631		
Tg= 105,4 °C		

Figure 30. Pellets of Akestra 110

GPC measurements showed molecular weight and molecular weight distribution within the required specifications, which resulted in 25000 and 67000 g/mol for M_n and M_w, respectively, and polydispersity index PDI of 2.7. DSC of Akestra 110 showed no thermic event at temperatures above T_g confirming that the polyester was amorphous. Otherwise, as it was the case of PET, the Akestra 110 produced from BHET showed typical thermal and rheological behavior.

Conclusions - Syntheses

In this project, BHET obtained from post-consumer PET rBHET was employed to successfully produce polyester acrylates, urethane acrylates, and EHA-containing plasticizer. More importantly, rBHET, together with BHET obtained from depolymerization of virgin PET, was repolymerized into PET and Akestra 110, which, except for the color, all measured properties (M_n, M_w, PDI, T_g, IV, TGA, and rheological data) fell within the desired specification values. As diol building block, BHET had a tendency to oligomerization during the conditions used for the formation of the polyester acrylate and plasticizer, whereas it was reduced for the production of the urethane acrylate due to lower reaction temperatures. Consequently, all the BHET derivatives produced presented wide molecular distribution, which did not hinder their further evaluation at the end user's facilities. In the case of the synthesis of a BHET-based diacrylate, however, the wide molecular distribution obtained during its production entailed a significant deviation from the expected outcome, and its pursue was abandoned. In summary, BHET generated from glycolysis of PC-PET can be employed to produce suitable albeit colored polyesters (PET and Akestra 110), as well as to be further modified for the production of polyester acrylates, urethane acrylates and plasticizers.

Plasticizers - evaluation

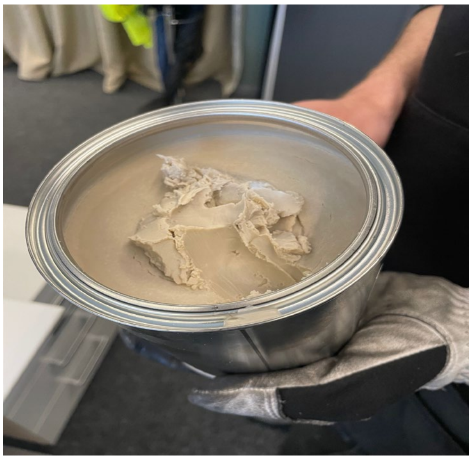


Figure 31. The plasticizer delivered to National Sweden and Tarket had viscosity as a paste.

The plasticizer from Perstorp was evaluated by National Sweden and Tarkett. The plasticizer had a viscosity much like a paste which is shown in Figure 31. Figure 32 shows the set-up of rheological measurements of the plasticizer.

Figure 32. Evaluation of the rheology at National Sweden

The following conclusion conclusions were made:

1. Slight increase in density. (1.26 to 1.29 g/cm³)
2. Increase in hardness, + 10 Sh A, requires a higher load of plasticizer.
3. Mechanical properties similar to existing compound. (within reach)
4. Viscosity differs from existing plasticizer. (Paste contra liquid)
5. Rheometric properties, requires change in curing-system and load.
6. Volume change in IRM 901/903 std oils, acceptable. (Swelling in naphtenic 903)
7. Further testing required with different adhesive-systems and ageing. (product)

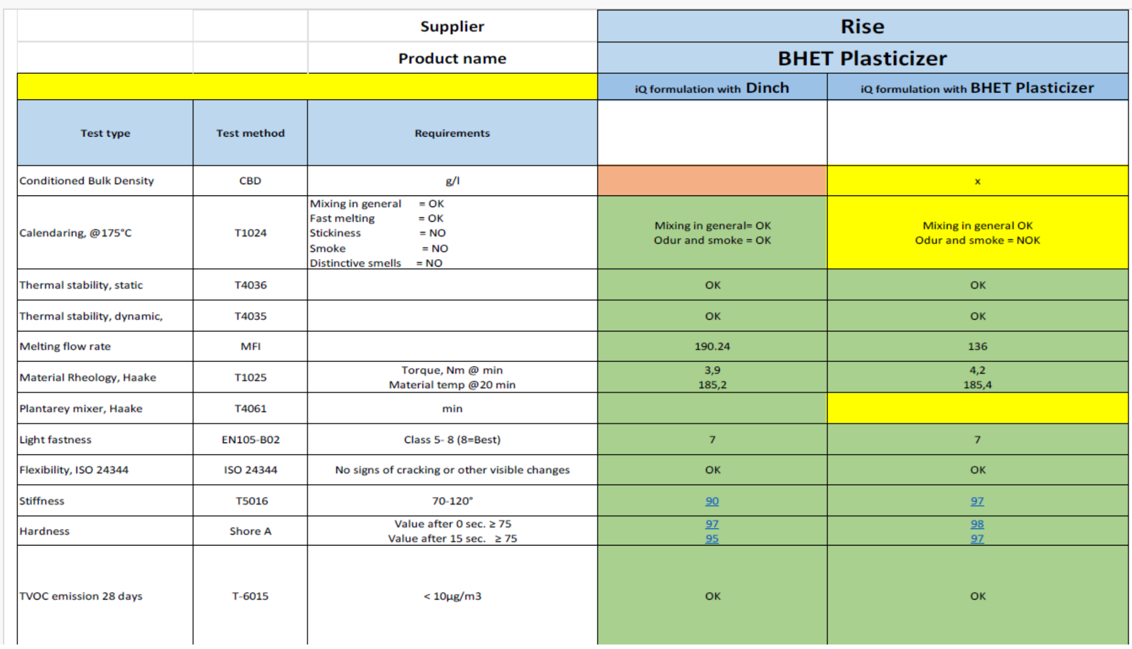
Tarkett received the same plasticizer as National Sweden and the experimental plan for evaluation is shown in table 12.

Table 12. Experimental plan for evaluation of plasticizer based on BHET at Tarkett.

	Reference	1	2	3	4	5
Poly Vinyl Chloride	Same %					
Current plasticizer, Dinch	15	0	0	0	0	0
Epoxidised soya bean oil	4	0	0	4	4	4
BHET plasticizer	0	20	25	15	22	15
Stabilizer	0.54	0.54	0.54	0.54	0.54	0.7
Mineral fillers	Same %					

The normal dry blending of the substances in the plasticized flooring was not possible due to the high viscosity of the BHET based plasticizer, so wet blending was necessary. Table 13 show a summary of the evaluation of the BHET based plasticizer in a PVC formulation for flooring, as compared to the reference sample. Overall, it could be concluded that many properties were acceptable in the BHET based plasticizer but thermal stability, processability and viscosity need to be improved. Another aspect is that more plasticizer i.e. large amount was needed in order to get the desired properties of the final product. It is shown in Table 10 as 22 w% of BHET based plasticizer was needed instead of 15 w% as shown in the recipe for the reference.

Table 13. Summary of the evaluation of the BHET based plasticizer in a PVC formulation for flooring, as compared to the reference sample.



		Supplier	Rise	
		Product name	BHET Plasticizer	
			iQ formulation with **Dinch**	iQ formulation with **BHET Plasticizer**
Test type	**Test method**	**Requirements**		
Conditioned Bulk Density	CBD	g/l		x
Calendaring, @175°C	T1024	Mixing in general = OK Fast melting = OK Stickiness = NO Smoke = NO Distinctive smells = NO	Mixing in general= OK Odur and smoke = OK	Mixing in general OK Odur and smoke = NOK
Thermal stability, static	T4036		OK	OK
Thermal stability, dynamic,	T4035		OK	OK
Melting flow rate	MFI		190.24	136
Material Rheology, Haake	T1025	Torque, Nm @ min Material temp @20 min	3,9 185,2	4,2 185,4
Plantarey mixer, Haake	T4061	min		
Light fastness	EN105-B02	Class 5- 8 (8=Best)	7	7
Flexibility, ISO 24344	ISO 24344	No signs of cracking or other visible changes	OK	OK
Stiffness	T5016	70-120°	90	97
Hardness	Shore A	Value after 0 sec. ≥ 75 Value after 15 sec. ≥ 75	97 95	98 97
TVOC emission 28 days	T-6015	< 10µg/m3	OK	OK

5.5.3. Binders for paint and varnish – evaluation by Sherwin Williams

The first part of the test experiment performed at Sherwin Williams was to test the binder compared to four references and check the performance and similarity in terms of viscosity, hardness, chemical resistances, yellowing, gloss and reactivity. Where each sample was mixed with a standard photoinitiator and monomer. While the second part of the experiment consisted of testing the BHET sample in formulations and perform standard tests on film performance in comparison to reference products.

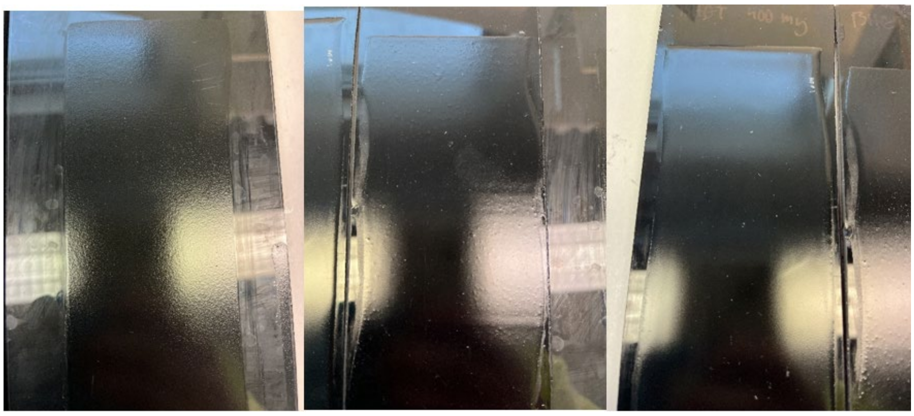


Figure 33. BHET samples applied with 60 µm, 150 µm and 400 µm, from left to right respectively

It was found that the BHET samples contained particles of a size of at least 100 µm. An application amount of 400 µm was good enough to get a smooth surface for testing, as shown in Figure 33. All samples, references and BHET, were therefore applied with a thickness of 400 µm. The following tests could thereafter be performed: viscosity, hardness, reactivity (UV hardening), gloss, chemical resistance and yellowing

Conclusions were made after evaluation of the BHET based polyester binder: The current BHET raw material contained a large number of crystallized particles, posing problems for it to be used in paint formulations in its current state. Preheating of the raw material was necessary to dissolve the particles before mixing it into a formulation, where 1h in 70°C was found to be enough to obtain smooth surfaces. Initially, the preheating caused a significant drop in reactivity and hardness when investigating only the raw material, but these issues were resolved when mixed into a formulation. The final performance in terms of viscosity, hardness, chemical resistances, yellowing, gloss and reactivity of a 1:1 substitution of binder to BHET turned out to be equal to the reference sample. On a lab-level, it is not an issue to preheat the sample to 70°C; however, such a preparation would be inconvenient in scaling up for usage in a production plant. For future work, BHET would be of great interest if the raw material itself could be stabilized by the manufacturer. There is also some more aspect to be aware of. Regarding molecular weight and its distribution in this BHET polyester, there can be restrictions both regarding REACH and other regulatory limitations on residues and low molecular weight monomers in the mixture.

5.5.4.Re polymerization of BHET – evaluation by Klöckner Pentaplast KP Films

Figure 34. Pilot plant used for polymerization of BHET performed at Selenis.

Klöckner Pentaplast-KP Films evaluated the PET type called Akestra based on polymerization with BHET (performed by Selenis) as shown in Figure 34. KP Film mixed 30% BHET Akestra with 70% virgin to be tested and compared to 100 virgin Akestra in their production of cups. FTIR and DSC analyses showed very small differences between BHET containing and virgin Akestra. A slightly higher moisture was found in BHET containing material compared to 100% virgin but BHET sample was still below threshold.

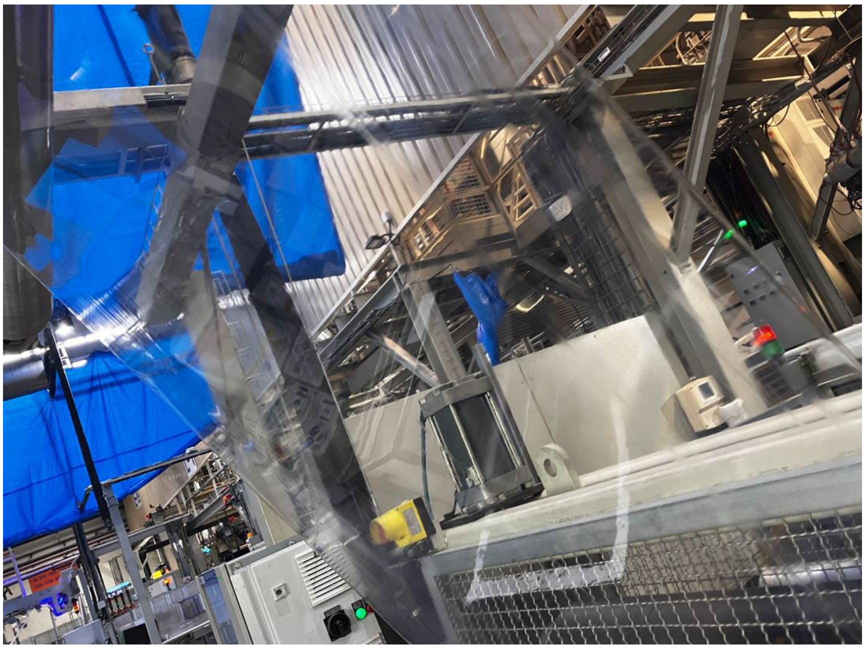


Figure 35. Film extrusion of BHET based Akestra mixed as 30/70 with virgin Akestra at KP Films.

Figure 35 shows the film extrusion of the Akestra containing 30% BHET based polymers. The evaluation and comparison with 100% virgin Akestra showed almost identical properties with just some small differences as shown below.

Figure 36 shows slightly lower tensile impact strength observed with the material produced with the mix 30%BHET Akestra 110 + 70% Virgin Akestra 110, nevertheless the results are acceptable for the final application purpose.

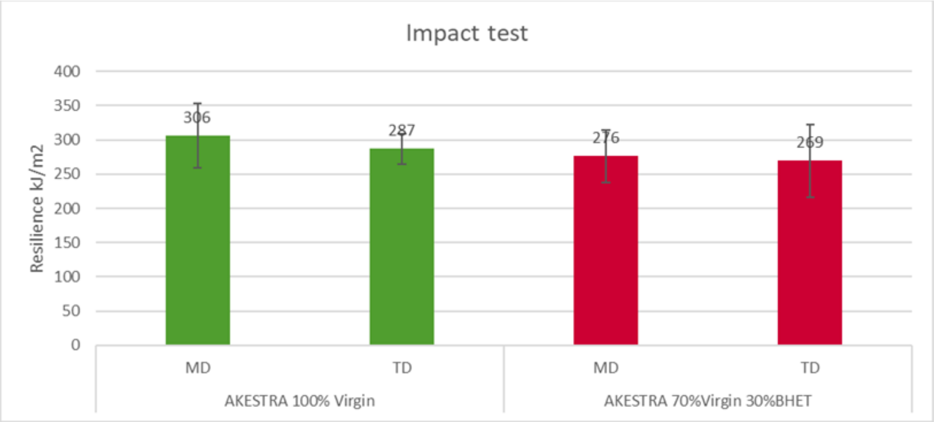


Figure 36. Results from pendulum impact measurement.

Table 14. Color measurement with CIE Lab Color Space on films prepared at KP Films.

Reference	L	a	b
Akestra 110 100% virgin 2mm	82,01	0,55	3,51
Akestra 110 70% virgin 30% BHET 2mm	81,72	0,42	4,51

Table 14 shows Color Delta is observed to be 1 (mainly difference in b* i.e.blue-yellow range), what is a very low variation, we observe a little tendency to yellowness (higher b) with the material produced with the mix 30/70 (when measured in a 2mm thick overlapped samples). Figure 37 show cups formed from the previously extruded film. Standard settings for the product were used for both materials (no change in thermoforming conditions).

Figure 37. Thermoformed cups prepared at KP Films

Figure 38 show the thermoformed cups after evaluation. The cups were hot filled with olive oil at different controlled temperatures. The following results were obtained: cups of both materials are behaving in the same manner, slight deformation when reaching the 90ºC. We conclude that both materials have the same heat resistance stability.

The following summary was made for the results obtained at KP Films:

The BHET obtained Akestra 110 shows same signals under IR analysis as standard virgin and thermal properties are almost identical. The BHET containing sample exhibits a characteristic yellowness which differs from virgin neutral color. The BHET Akestra 110 can be easily processed in extrusion line as standard virgin product. The material produced with the mix 30%BHET AKESTRA + 70%vAKESTRA shows same mechanical properties as the one produced with virgin material. Only slightly lower impact resistance is observed, but this is not considered relevant. Optical properties of both materials are very similar, slightly higher yellowness for BHET containing film which is not visible with naked eye. The film produced is easy to thermoform and there is no need to change thermoforming parameters when processing the product with the BHET Akestra 110. The cups produced with both materials have the same thermal properties when tested under application conditions.

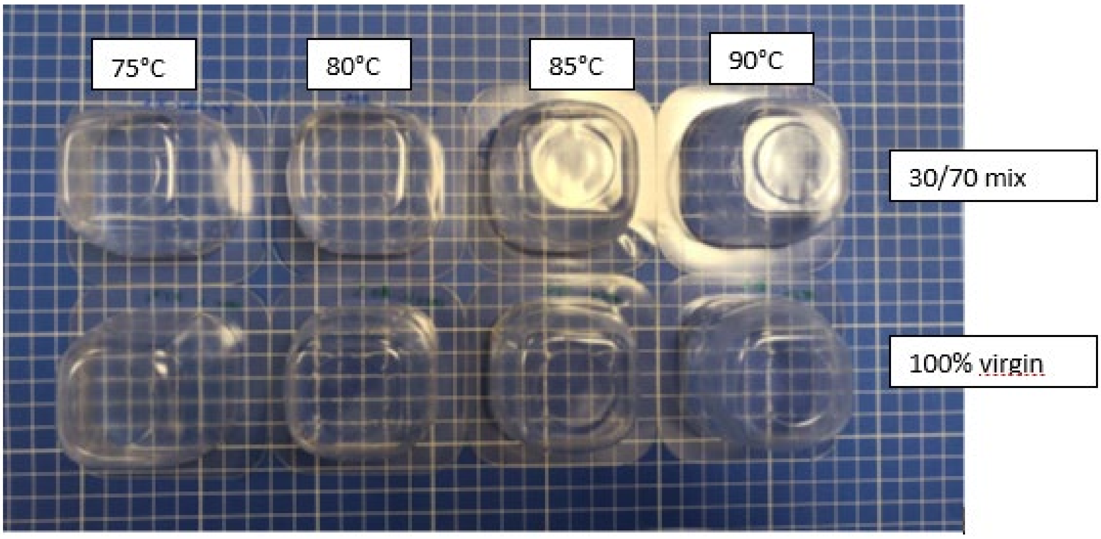


Figure 38 Thermofomed cups tested for filling with hot olive oil. Very similar results for the different samples.

DIAB received PET based on rBHET (colored) from Selenis as shown in Figure 39 where also a standard PET is shown.

Figure 39 . rBHET based PET to the left and vPET to the right.

Thermal analysis showed no important differences between the BHET based PET and the reference. The foaming tests performed at DIAB included the following blends:

Production of a 110 kg/m3 foam:

- After 1h of stable production, replacement of 25% vPET with BHET rPET (5 kg/h) [5kg / 33kg]

☐ After 1h of stable production, replacement of 50% vPET with BHET rPET (10 kg/h) [10+5kg / 33kg]
☐ After 1h of stable production, replacement of 75% vPET with BHET rPET (15 kg/h) [15+10+5kg / 33kg]

The output was extrusion signals as torque and meltpressure (values and stability). The foamability was another output including characterization of the foam measuring cellularity i.e. cell size and closed cells, as well as the mechanical testing including compression and shear. The foams produced at DIAB are shown in Figure 40.

Figure 40 Foaming test performed at DIAB. Samples from top contain 75%, 50%, 25% and 0% rBHET PET.

The following conclusions were made by DIAB:
☐ PET produced with virgin + post-consumer BHET shows IV and Acidity in line with common virgin PET;
☐ Melting and crystallization temperature are slightly higher than reference;
☐ The extrusion foaming gave acceptable quality w/out any changes to settings or equipment at different percentages;
☐ Melt pressures and extruder torque increased, proper settings expected to give more stability;
☐ New pilot trials required to:

- ☐ confirm the possibility of scaling up to industrial process;
- ☐ provide information regarding batch to batch repeatability;
- ☐ allow a study to determine the behavior at recipe changes (reagents content, line settings, blowing agent content to change foam density).

5.6. Plan for implementation

The present report summarizes the work collected in Work package 6 done around transferring the results from the laboratory trials performed by RISE and Synpo and use these to develop block and process flow diagrams and then implement these in the process simulator Aspen Plus® where various operating and design scenarios are simulated and studied. The mass and energy balances resulting from the process simulations are used as basis for a techno-economic analysis in which the direct variable cost (DVC), a useful measure of the operating expenditure (OPEX), and the capital cost (CAPEX) are evaluated. These concepts and how they are estimated will be described here and further in Appendix B.

In the techno-economic analysis of the depolymerization unit, four operating cases with different levels of stream integration and purity of recycled MEG were evaluated as presented in Table 15.

Table 15. Operating cases evaluated in technoeconomic analysis.

Operating case	Specifications
Case 1	99 wt% MEG from column, no recirculation of process water
Case 2	97 wt% MEG from column, no recirculation of process water
Case 3	99 wt% MEG from column, process water recirculated
Case 4	97 wt% MEG from column, process water recirculated

5.6.1. CAPEX

The flowsheet developed was ran through the application Aspen Process Economic Analyzer^{TM} to provide a first estimate of the CAPEX cost for the depolymerization unit. Aspen Process Economic Analyzer^{TM} was used to map, size, and price the equipment.

Equipment costs were evaluated for carbon steel and multiplied by 2 to convert to stainless steel. For process equipment cost differences between stainless steel and carbon steel vary widely depending on equipment type and the fraction of the equipment that requires stainless steel. A shell and tube heat exchanger may for example have a carbon steel shell and stainless steel tubes. The material conversion factor is then 1.67[5] while if the entire exchanger is made of stainless steel the factor would be 2.86. Similar reasoning can be applied to other equipment as well. A pump for example has a factor of 1.7 while 2” Raschig rings have a factor of about 3. For simplicity and consistency, a value of 2 was selected for the present evaluation.

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[5] H. P. Loh, U.S. Department of Energy/National Energy Technology Laboratory and Jennifer Lyons and Charles W. White, III, EG&G Technical Services, Inc; *Process Equipment Cost Estimation Final Report*, **2002, DOE-NETL/1169**

For a complete plant cost, an experience-based factor-approach is used in which the sum of the equipment cost is multiplied by a factor (16) to arrive at the final investment cost. The factor includes costs such as project management, installation, instrumentation, electricity, foundations, etc. Depending on the project such a factor can vary widely, typical values may range from 2 to 12. For larger projects with good project management factors are typically in the 6-8 range. In the present project a factor of 6 is assumed, see Table 16.

In work package 6, tanks, office buildings, shipping, raw material handling including washing and sorting of the PET waste are not included. The economic concept presented here will thus only include the depolymerization unit. The complete cost for a processing unit including the above features and facilities may be twice that presented here but has to be investigated in more detail. The total plant cost is hence evaluated according to [Eq. 1].

$$CAPEX = MF \times LF \times \sum C_{Equipment} \qquad \text{[Eq. 1]}$$

Where C is cost.

Table 16. Plant cost from factor-based approach.

Parameter	**Source/Value**
Carbon steel equipment cost	Aspen Process Economic Analyzer™ (SEK)
Material factor (*MF*)	2
Lang factor (*LF*)	6

CAPEX – 10 ktonnes BHET per year

The difference in between the four operating cases was minimal with regards to the equipment cost and the final cost for building the depolymerization unit as described above was roughly 315 MSEK. There was no effect on CAPEX when recirculating the water streams while the plant cost decreased by about 8% when the operated using a lower MEG purity specification (97 wt% instead of 99 wt%). The cost reduction was close to entirely allocated to the distillation column.

Taking the entire plant into consideration, the distillation column represents approximately 23% of the total CAPEX for operating cases 1 and 2. In operating case 3 and 4 when the MEG purity is lowered to 97 wt%, the distillation column cost reduces by 30-35% compared to case 1 and 2 which in turn reduces the fraction of the cost constituted by the distillation column to approximately 18% (Figure). It should be noted that the bars in Figure 41 are related to the total cost for each scenario and that the total CAPEX for operating case 1 and 2 is approximately 8%

higher than that of operating case 3 and 4. As mentioned in the text, the only unit operation that has a changed cost is the distillation column and the lower cost of the column alters the fraction of the cost represented by the other unit operations.

In terms of the individual equipment costs, the crystallisers stand out making up close to half of the total CAPEX and optimising crystalliser operation and design should be investigated further. The filters also represent a large portion of the cost and must be investigated further with equipment trials to determine the most suitable and cost efficient solid-liquid separation technology. The heat exchangers are not highly significant given that there are many (10) and in total constitute only 8-10% of the CAPEX and that they, as will be seen in later, are important for the operating costs. Finally, the distillation column making up 18-23% of the CAPEX is impactful, and its exact cost will be determined in detail during the basic engineering phase of a plant project (exact diameter, type of internals, type of phase contacting equipment (plates or packing and which type of each)). The distillation column represents the only actual equipment where the operating cases with reduced MEG purity can reduce the CAPEX. Hence determining the most suitable MEG purity has the potential to save roughly 8% on the CAPEX.

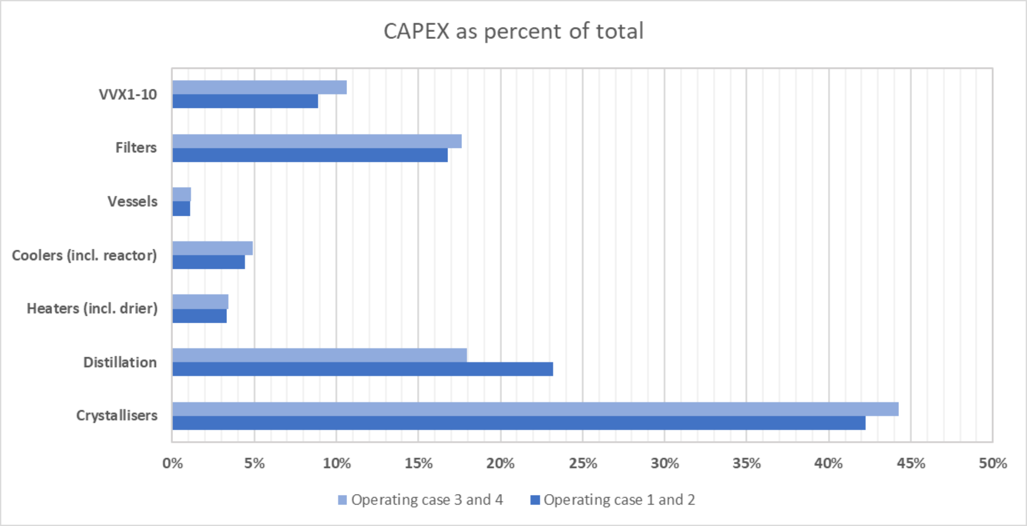

Figure 41 Equipment cost represented as fractions of total CAPEX.

The 10 000 tonnes per year plant concept was scaled up to a BHET production of 100 000 tonnes per year and the corresponding development of the CAPEX studied (Figure 42). A plant producing very small volumes can see a tremendous decrease in the capital cost per tonne produced product when the size of the plant is increased. As the size of the plant increases the decrease in capital cost per tonne product reduced. That means that when prospecting a new plant, an evaluation of this sort can assist in determining a suitable production volume for the plant. There are several ways this can be accomplished. A well-established and straight-forward method is to apply the Rule of Six-tenths, [Eq. 2], which normally is accurate to within 20% and highly useful in the initial phases of a project.

$$\frac{CAPEX_2}{CAPEX_1} = \left(\frac{Production_2}{Production_1}\right)^{0.6} \qquad \text{[Eq. 2]}$$

Where *CAPEX* in [Eq. 2] refers to the capital cost of the plant and *Production* to the production volume of BHET. The subscripts *1* and *2* refer to the present/available and estimated plant sizes respectively. When estimating the cost for higher and lower production volumes, the chosen plant size of 10 000 tonnes annual production volume is in the start of the flattening of the CAPEX per volume curve.

Preferably, a 3-5 times higher production volume (i.e., 30-50 ktonnes per annum) should be targeted as it can close to half the CAPEX cost per tonne produced BHET. Going to production volumes in excess of 50 ktonnes does not significantly reduce CAPEX per volume cost and unless the demand for product and the quantity of available raw material can justify it, there is no direct need to size the plant capacities as large as 80-100 ktonnes per annum.

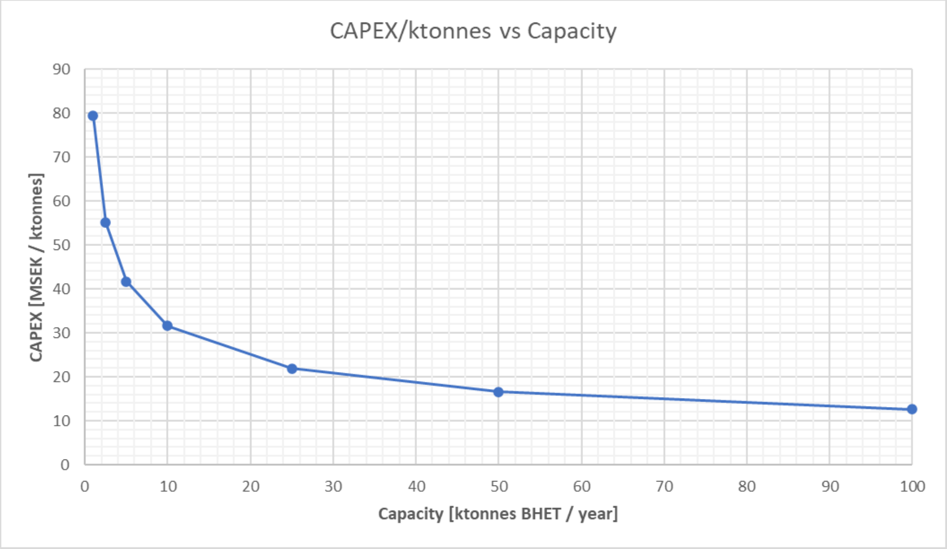

Figure 42 Variation of CAPEX with BHET production volume.

Summary CAPEX

- recirculation of the process water does not have a negative impact on CAPEX
- the crystallisers constitute the largest fraction of the CAPEX and optimization of the crystallisation process and crystalliser design will be important in the industrial implementation
- reduced MEG purity from the distillation reduces the cost of the distillation column by 30-35% and the total plant cost by approximately 8% and its operability should be investigated
- plant size should preferably be larger by 3-5 times, i.e., 30 000 – 50 000 tonnes BHET production per year, to reach a point where capital cost per produced BHET does not significantly reduce with increased BHET production volume

5.6.2. OPEX

When evaluating the operational costs Perstorp use a term we call Direct Variable Cost (DVC). The DVC is calculated by taking the costs of all raw material and utilities (steam, electricity, process water, cooling water, etc.) that is added to the production and divide that by the production rate. This results in a DVC with units of SEK per kg BHET. This value must then be compared with the sales price and the difference is the margin or when divided by the sales price, the profit margin. The details from this part of WP 6 are found in Appendix 2.

5.6.3. Conclusions and further work

A concept for a post-consumer PET depolymerization plant to produce BHET through glycolysis was developed and modelled in Aspen Plus®. The functionality of the technology using an actual industrial feedstock was demonstrated in the earlier work packages of the project. The use of the depolymerised PET in downstream applications was demonstrated in work package 5 and a holistic view of the depolymerization unit in terms of production and equipment costs as well as energy usage was presented in the present report concerning work package 6.

The main outcome from work package 6 is a depolymerization concept that can be used as a basis for a plant project. To ensure successful implementation of a large-scale plant, there are additional topics that needs to be considered and potentially addressed in further studies. These can be loosely grouped as either pertaining to the equipment/process, the economic/logistical side of the design and operation of a depolymerization unit, or to the legal side. Below are the topics identified in the implementation phase (in no particular order of importance):

Equipment-Process considerations

- *Experimentally measure solubilities of BHET in MEG, water, and MEG/water solutions at various temperatures*

Rationale: The costliest unit operation by far are the crystallisation steps and the most important aspect of crystallisation in terms of fluid properties is the substrate's solubility and the temperature dependence of said solubility.

- *Investigate BHET fouling tendency in process equipment (pipes, valves, heat exchangers)*

Rationale: As a process operating with substrate solubilities, particle precipitation and the possible associated fouling is important to understand to design process equipment for long uptime and reduced maintenance.

- *Develop alternative(s) to active carbon for decolourisation*

Rationale: The active carbon treatment results in approximately 10% BHET losses. If the produced BHET whiteness requirement is low, the activated carbon treatment can be reduced or bypassed altogether. When this is acceptable, it should be used to reduce DVC and the environmental footprint. It may then be sufficient to wash the crystals from the first crystalliser and bypass also the second crystalliser, thus further reducing operating costs and energy usage.

- *Detailed design of process equipment*

Rationale: To further sharpen the CAPEX estimation and to provide viable designs for the crystallisers, the reactor, and many of the heat exchanger positions, more detailed designs and equipment selection is necessary. When executing larger projects this is a step in either a feasibility study or basic engineering. In the present project, given the complexity of the feedstock and the somewhat uncertain nature of some of the process streams, a more detailed study of these topics as well as the MEG regeneration is preferably performed at the development stage.

- *Investigation around reactor types suitable for the process*

Rationale: The exact type and configuration of the reactor is at present not determined and should be investigated further.

- *Investigation around solid-liquid separators for oligomer and monomer separation*

Rationale: Successful separation of solids in the oligomer separation stage and after each of the crystallisers is required. The characteristics of the crystals, especially the particle size distribution does govern the equipment design. A second aspect is the amount of washing necessary and how it will be accomplished. Typically, it is done in the separator and the design must then allow and account for that.

Economic-Logistic considerations

- *Larger plant size recommended*

Rationale: The presently investigated plant size of 10 ktonnes per year falls on the part of the capacity vs cost curve where there still is a significant rate of decrease in cost per unit capacity and it is recommended to target a plant size that is 3-5 times the size of the currently considered capacity. This has a significant impact on pay-back time.

- *Increased PC PET collection radius*

Rationale: As a consequence of the larger plant size suggested in the above item, the collection radius for the PC PET most be increased. This means longer transportation, which may negatively impact the carbon footprint.

- *Study process robustness*

Rationale: Due to the larger plant size and consequently wider PC PET collection radius, a more wide-ranging feedstock quality will likely result. It is therefore important to study the effect of large feedstock variations on the process stability and product quality.

- *BHET sales price*

Rationale: The DVC for producing BHET from PC PET is higher than for virgin PET, which in turn means that any products made from the BHET will be more expensive than if virgin raw materials were used. Hence a price premium is needed to make the process financially viable. The exact magnitude of the price premium must be decided based on the end-product in question.

- *External costs*

Rationale: Raw material costs (MEG and PC PET), logistic, etc., must be optimized to increase competitiveness against fossil PET and allow for the realization products based on BHET from depolymerized PET sources.

Legal aspects

- *Freedom to operate (FTO)*

Rationale: an FTO is always conducted in relation to the realization of novel ideas that are to be transferred from idea stage to actual development projects with the aim of construction new production capacity. An FTO is an extensive search in the patent literature to ensure that there are no obstacles or other legal hinderance in constructing and operating a plant using the suggested technology.

- *Reach registration*

Rationale: a chemical that is not currently being sold by Perstorp is always investigated for how to in the correct way register the chemical with the right authorities. It is a process that may take up to a year and does incur certain costs that are non-negligible.

- *Environmental permit*

Rationale: an environmental permit must be in place before construction of a plant can commence and getting a permit for a new plant may take around 3 years.

6. Conclusions, values and next step

The project highlights the potential of chemical recycling for PET, particularly its ability to convert post-consumer PET, unsuitable for mechanical recycling, back into useful BHET with a lower carbon footprint compared to virgin PET. The positive feedback from end users reinforces its viability for certain applications. However, significant challenges remain, including economic competitiveness, scalability requirements, the need for improved decolorization processes, and expanded PET collection efforts. Addressing these bottlenecks through continued research and development is crucial for enhancing process robustness and achieving a more sustainable circular economy, ultimately benefiting both society and commercial sectors.

Positive outcomes:

- It has been demonstrated that PET that is unsuitable for mechanical recycling can be recycled back into PET, copolyesters and other applications through chemical recycling.

- Chemical recycling of PC-PET into BHET showed 20% lower carbon footprint than having produced the BHET on fossile based resource and having handles the PET waste according to the procedures used today (mechanical recycling and incineration).
- Colored BHET or colored re-polymerised PET is not always an issue but depends of the application.
- End user's feedback was mainly positive though more application development is needed.

Negative outcomes:

- Economically, it is not competitive compared to conventional production of PET.
- The production must be scaled up from 3 to 5 times of what it was investigated in the project for the CAPEX to be sensible.
- There is a need to improve the decolorization process in order to secure process performance and stability with varying raw feedstock, sources and varying quality.
- Increase the collection radius of PET in order to ensure sufficient feed-stock for larger depolymerization process plants.

The project has had a very strong focus on technical process development to build knowledge and understand bottle necks. This means that the results have laid a foundation for further development rather than directly having a societal impact today. The results will be used for another iteration of a development of the process, for further investigation of the process, and for further investigation of feedstock sources.

There is need for further intensify the research development of the technology in order to address bottle necks such as further reduction of carbon footprint, and robustness of the process technology. The results, although not complete, supports the transition to circular economy.

7. Project Communication

The project was presented at "Klimatledande Processindustri" 9 September 2022 at their member meeting. The organizer is hosted by Västsvenska Kemi- och Materialklustret with about 50 organized members and with more than 100 organiztions within the chemical and plastics industry and beyond. About 40 persons attended the meeting.

The project was presented by David James, Pertorp AB in November 2022, for a group of students from Chalmers University of Technology when they visited Stenungsund and their cluster of Chemical Industries.

The project has been presented at the meeting for the Network connected to the testbed for Plastics Recycling, hosted by RISE, during 2022 and 2023. The network contains more than 100 individuals from 40-50 organizations, mainly companies.

The project produced a "story" published on RISE home page: https://www.ri.se/en/our-stories/chemical-pet-recycling-creates-new-products

The project was presented by a poster at the inauguration of “Site Zero” 15 Nover 2023 at Swedish Plastics Recycling plant in Motala where more than 500 people had been invited. The invited persons came from many parts of business life such as packaging and waste management industry but also innovation companies using recycled plastics in their products.

Christian Andersson from Perstorp AB held a presentation in the webinar with the title” Chemical recycling of plastics: How does additives and polymer blends influence the recycling?” arranged 19 June 2024 by Klimatledande ProcessIndustri. The organizer is hosted by Västsvenska Kemi- och Materialklustret with about 50 organized members and with more than 100 organiztions within the chemical and plastics industry and beyond. More than 70 persons participated in the webinar. The presentation concerned the implementation, i.e. how to upscale a chemical process based on recycled raw material.

8. Appendices

Appendix A. LCA

Appendix B. Implementation, a plan for industrialization

Life cycle assessment

Chemical recycling of PET waste to BHET

Josefin Neuwirth, Manuel Parayil, Tomas Rydberg, Henric Lassesson and Elisabeth Hallberg

IVL Swedish Environmental Research Institute

Working draft 2024-08-21

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Summary

This report shows the results of the life cycle assessment (LCA) of chemical recycling of polyethylene terephthalate (PET) waste to bishydroxyethyl terephthalate (BHET) carried out by IVL Swedish Environmental Research Institute in the research project "Kemisk återvunnen PET/polyester som råvara för additiv och ny polymer" funded by the Swedish Energy Agency.

Lab scale testing and process simulation data carried out at RISE for the chemical recycling of PET waste BHET were used as input to the LCA model. Three different process parameters were tested to generate 8 different process configurations. The parameters tested were -

- Water content in recycled ethylene glycol.
- Decolouring of BHET.
- Number of crystallisations steps.

The base case was defined as the scenario in which there is 1% water content in recycled Ethylene Glycol, the addition of a decolouring step and the addition of a crystallization step.

The results show that the climate change impact of recycling PET waste to BHET ranges from 2.0-2.5 kg CO_2 eq. per kg BHET across the 8 different scenarios studied. It was observed that the most desired scenario had the highest impact. Major hotspots within the process were identified to be use of Ethylene glycol and in particular the energy use during its recycling step.

Sensitivity analysis was also conducted on the electricity grid mix used as well as the source of energy in the process. It was found that PET washing is sensitive to the Electricity grid mix used and using an EU average grid mix increases the climate change impact by about 20%. Using biomass as a source of energy was found to potentially reduce the climate change impact by 60%.

The results were also compared to current market conditions of PET waste management and BHET production. Chemical recycling of PET waste to BHET has 20% lesser climate impact when comparing to current market conditions.

1. Introduction

This report shows the results of the life cycle assessment (LCA) of chemical recycling of polyethylene terephthalate (PET) waste to bishydroxyethyl terephthalate (BHET) carried out by IVL Swedish Environmental Research Institute in the research project "Kemisk återvunnen PET/polyester som råvara för additiv och ny polymer" funded by the Swedish Energy Agency.

Experimental data for upscaling the chemical recycling and process simulations data were made available in the project. These results were used as input to the LCA and herein the results from the LCA are presented and described.

The most important information and results are found in the main chapters of the report. Additional details concerning the LCA method applied, and modelling information can be found in the Appendices.

1.1 Goal of the study

The main goal of this LCA is to evaluate the environmental performance of the various chemical recycling scenarios based on the different process configurations identified in the experimental and simulation work carried out by RISE for the chemical recycling of PET waste to BHET. An additional goal of the study is to identify which process in the chemical recycling of PET waste to BHET contribute the most to climate change impact. This is often referred to as hotspot analysis. The intended audience of this report are all project partners who have participated in various research activities and the main stakeholder being the Swedish Energy Agency.

2. Studied system

The studied system, referred to as the base case scenario, is illustrated in Figure 1. First, the PET waste is transported 370 km by truck from different sorting plants in Scandinavia to the intended chemical recycling plant at Stenungsund, Sweden. This distance was calculated based on the PET waste mapping work carried out in WP1 in the project (Lassesson, H and Ghasemi, A, 2023). At the plant, the PET waste is washed and dried before entering the depolymerisation reactor. In the depolymerisation step, the PET waste is mixed with ethylene glycol (both fresh and recycled) and a catalyst. The mixture is heated to 270 °C before entering the depolymerization reactor. The output from the depolymerisation step are monomers of BHET and oligomers in ethylene glycol. After depolymerisation, the mixture is cooled to 70 °C and filtered to remove the oligomers from the mixture. The oligomers are then recycled back into the reactor.

The BHET mixture, from the cooling and filtration step, is transferred to the decolouring step to remove colour from the mixture using activated carbon. The colour comes originally from the PET waste mixture used as raw material input. Some of the BHET becomes attached to the activated carbon, and this together with the used activated carbon are sent to disposal (incineration).

Thereafter, the decoloured BHET mixture is sent to the first crystallization step. In the first crystallization step, the BHET mixture is purified by removing ethylene glycol and water (referred to as mother liquor). The mother liquor consists of approximately 40% ethylene glycol. The ethylene glycol is purified in a recycling step by removing colour using activated carbon and dried to remove moisture content before being sent into the depolymerisation reactor.

The wet BHET crystals from the first crystallisation step is further purified in a second crystallisation step. In the second crystallisation step, water is added, and the mixture heated, causing water to leave the system. The water is sent to wastewater treatment (WWT). After crystallization, BHET crystals are dried to get the final desired product. The water dried is further sent to wastewater treatment (WWT).

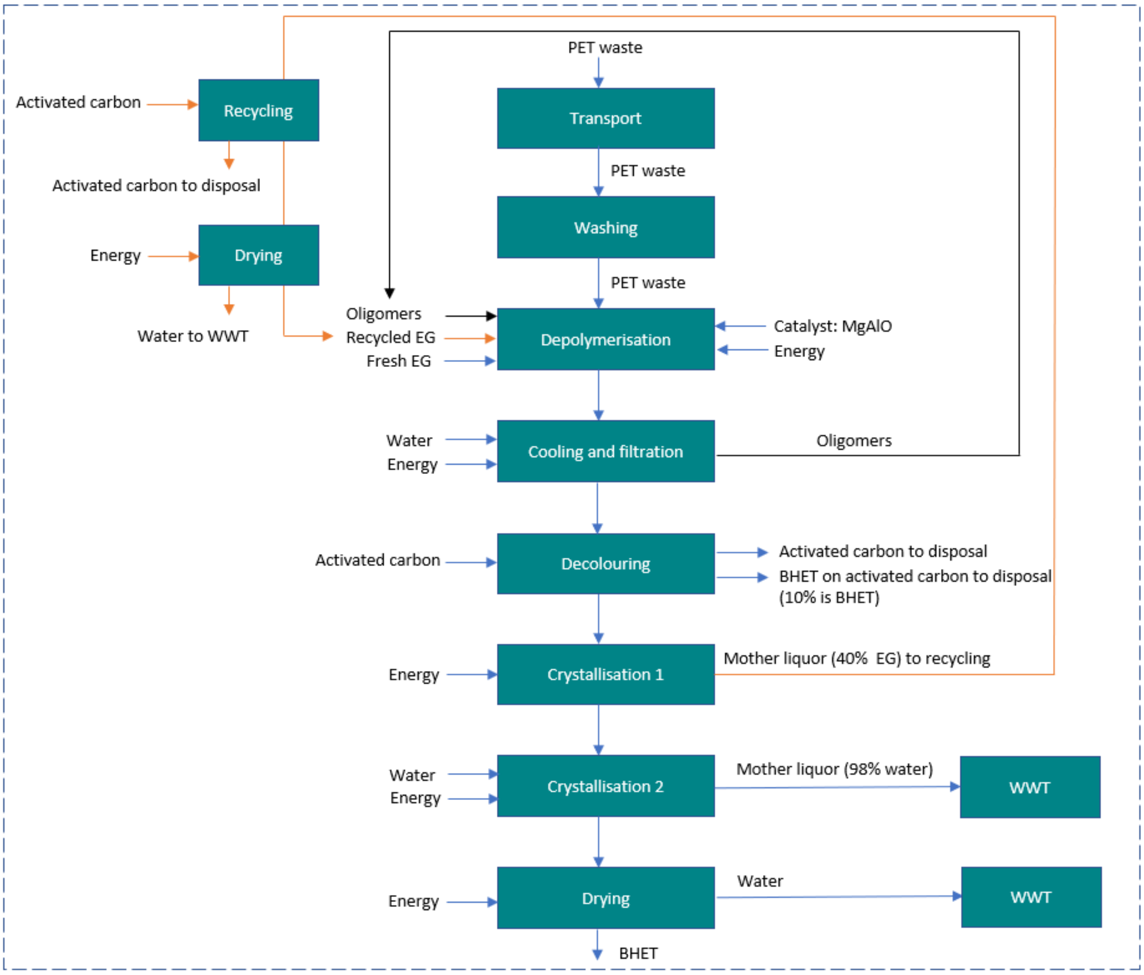

Figure 1: Overview of studied system (base case scenario).

2.1 Chemical recycling scenarios

In the scenario analysis different process settings have been assessed. The process settings that have been modified are:

- Water content in recycled ethylene glycol.
- Decolouring of BHET.
- Number of crystallisations steps.

The EG and water mixture (mother liquor) from the first crystallisation step consist of approximately 60% water. After this mixture is sent to recycling, we get EG with a water content of 2.5%. Water in the depolymerisation reactor has been identified to create unwanted by-products, lowering the BHET yield. Because of this, removal of water to reach 1% water content in EG after recycling, is studied in the scenarios 5-8, as specified in Table 1. In scenarios 1-4 the recycled EG consist of 2.5% water. The base case (scenario 5) is modelled with 1% water content in the recycled EG.

The decolouring of BHET is included in the scenarios 1, 2, 5 and 6. Decolouring of BHET is necessary for the use of BHET in some applications, but decolouring also lowers the yield. The base case is modelled with decolouring.

The addition of one extra crystallisation step, results in a product with higher purity. For the use of BHET in some applications, a higher purity is necessary. In scenarios 1, 3, 5, and 7, two crystallisation steps are studied. If only one crystallisation step is included (as in scenario 2, 4, 6, and 8) the wet BHET crystals go directly to drying. This is, however, not illustrated in the overview of the studied system (Figure 1).

Table 1: Scenarios studied. EG=Ethylene glycol. BHET= Bishydroxyethyl terephthalate

Scenario	Water content recycled EG	Decolouring of BHET	Number of crystallisations
1	2.5%	Yes	Two
2	2.5%	Yes	One
3	2.5%	No	Two
4	2.5%	No	One
5 (base case)	1%	Yes	Two
6	1%	Yes	One
7	1%	No	Two
8	1%	No	One

2.2 Sensitivity analysis

To expand the scope of the LCA and to test the robustness of some key assumptions/parameters in the study, a sensitivity analysis was included. The recycling of PET to BHET is assumed to take place in Stenungsund, Sweden and thus the electricity is modelled with the Swedish electricity consumption mix. The Swedish electricity consumption mix consist mainly of renewable energy sources and hence has a low climate change impact. In the sensitivity analysis the system is modelled with the average EU electricity mix that has a higher climate change impact compared to the Swedish mix. The EU electricity mix is generated from 42.28% fossil fuels, 25.32% nuclear fuels and 32.4% renewables. The reason for including this sensitivity analysis is to investigate the contribution of electricity use when less renewable electricity sources are used. Additionally, using biomass instead of natural gas was also tested.

2.3 Comparative Scenario

In order to analyse the results in context with the situation of PET waste handling today, a comparative scenario was also modelled. The system under study which recycles PET waste to BHET fulfils two functions –

1. The production of a certain amount of BHET
2. The waste management of a certain amount of PET waste

These functionalities need to be assessed and compared to a system that provides the same functions as per current market conditions. This comparative scenario (CS) was modelled with a system that produces BHET via dimethyl terephthalate (DMT) and ethylene glycol (equivalent to function 1 above) and an incineration process plus mechanical recycling that takes care of PET waste (equivalent to function 2). It was assumed that 42% of PET waste goes to mechanical recycling and 58% of the PET waste to incineration.

In reality, the reaction between DMT and ethylene glycol produces virgin PET with BHET as an intermediate. We assume in this study that the reaction does not proceed to completion and produces BHET instead. Commercial production of BHET is very limited and there is a lack of publicly available data and hence the assumption was made.

7.4 Review procedure

This study and report have been internally reviewed and approved in accordance with IVL's audited and approved management system. No third-party review has been performed.

7. Results and discussion

A functional unit is used to relate the results to a fixed factor, that reflects the function of the system studied. If the function of the product is not assessed within the study the term declared unit is used. A declared unit is a quantity of a product.

In this study, a declared unit is used. The declared unit is **one kg BHET product mixture.**

The impact category studied in the LCA is the climate change impact. Details concerning the impact category are found in Table 2.

Table 2: Impact category studied in the life cycle impact assessment.

Impact category	Category indicator	Unit	Method
Climate change (fossil)	Radiative forcing as global warming potential	kg CO_2 eq.	IPCC baseline, 100 years, 2013

In the sections below results are presented and discussed. First, the result for the base case (scenario 5) is presented, followed by the results for the different scenarios. Lastly, the results for the sensitivity analysis and comparative scenario are described.

3.1 Climate change impact of the base case scenario

The climate change impact of BHET produced from PET waste in the base case (scenario 5) is **2.5 kg CO_2 eq. per kg BHET product**. The main impact arises from the depolymerisation step, whereas the other steps have insignificant contributions to the climate change impact (Figure 2).

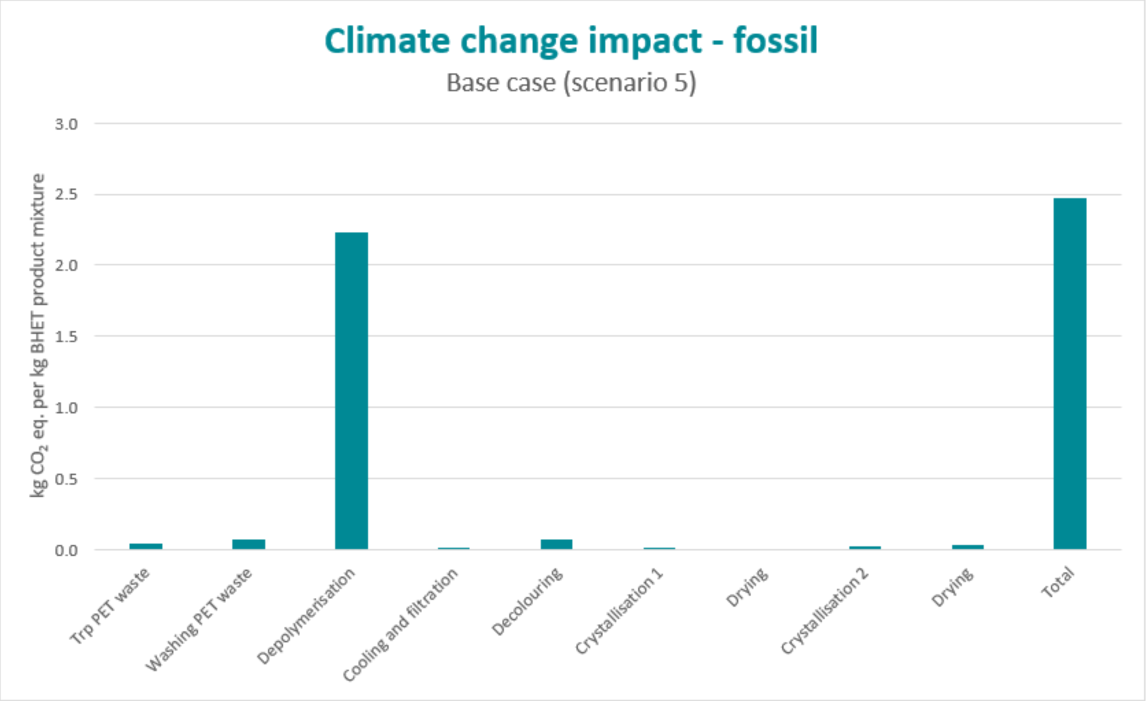

Figure 2: Climate change impact (fossil) of recycling PET waste to BHET in the base case (scenario 5). The result is presented for one kg BHET product mixture.

A closer look into the results for the depolymerisation step indicates that it is the use of EG that contributes to the climate change impact. It is interesting to note that recycled EG use has a higher contribution to the climate change impact of the depolymerisation step than the use of fresh EG (Figure 3). There are two reasons for this; one, the depolymerisation step uses more recycled EG than fresh EG. Two, the source of energy used in the recycling process is fossil based. The climate change impact per kg of fresh EG is 0.8 kg CO_2 eq. and for recycled EG it is 0.3 kg CO_2 eq.

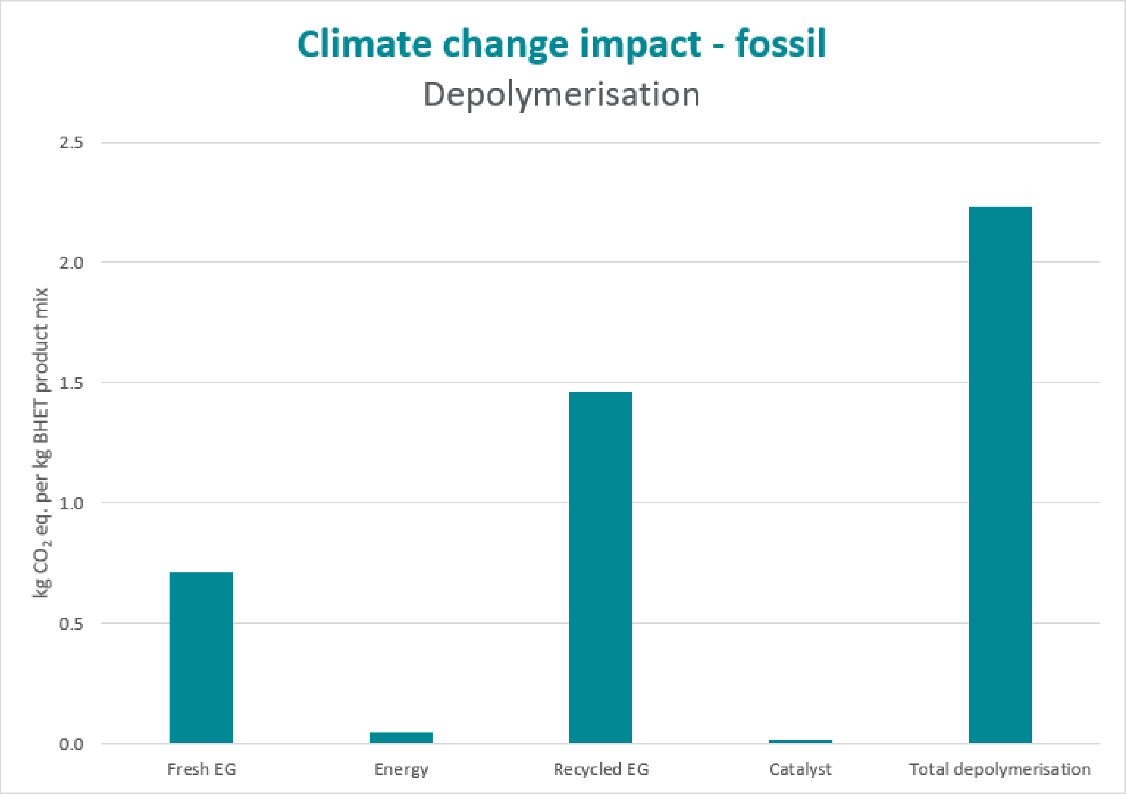

Figure 3: Climate change impact (fossil) of the depolymerisation step. The result is presented for one kg BHET product mixture.

3.2 Climate change impact of different recycling scenarios

The results for the climate change impact (fossil) across all studied scenarios are presented in Figure 4 along with the purity of BHET crystals obtained. The base case (scenario 5) has the highest climate change impact compared to all scenarios, while scenario 4 has the lowest. The difference in the climate change impact between them is 25%. It is interesting to note that scenarios 5 and 4 have the highest and lowest purities respectively among the scenarios, indicating the possible trade-off between purity and the climate change impact. Scenario 7 also has a high purity of BHET crystals (97%) and lower climate impact compared to scenario 5. The lower impact of scenario 7 is due to exclusion of BHET decolouring. However, this scenario might not always be applicable as in some applications it is important to have a decolourised product.

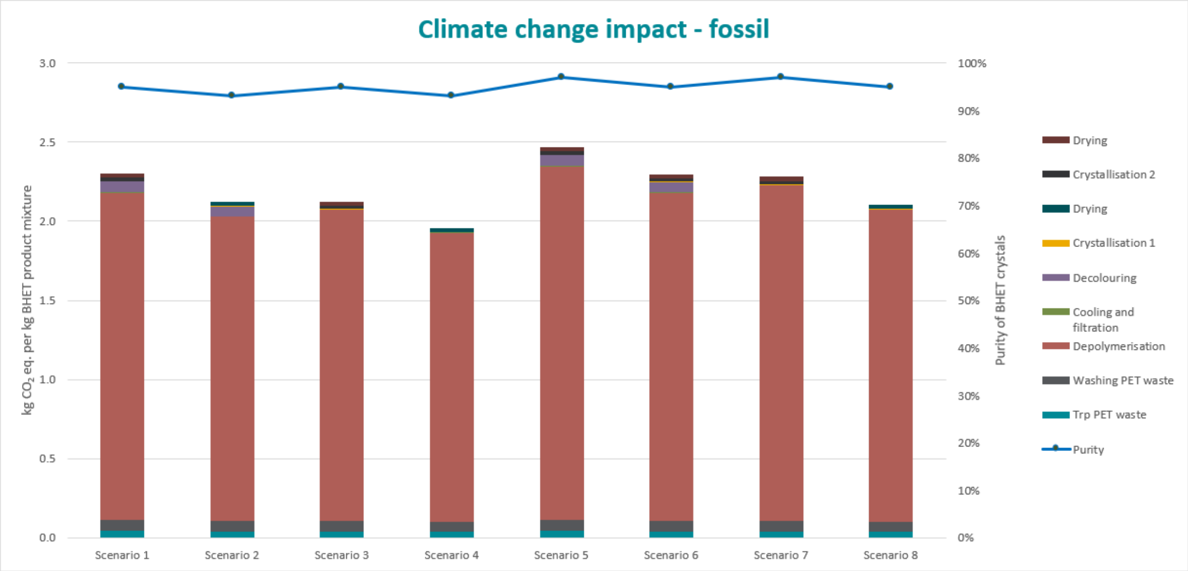

Figure 4: Climate change impact (fossil) for all scenarios studied. Blue line indicates purity of BHET crystals under the studied scenarios.

3.3 Sensitivity analysis

3.3.1 Electricity mix – EU grid mix

The results from the sensitivity analysis in using average EU electricity mix instead of the Swedish mix is shown below in Figure 5. The use of an EU electricity mix increases the climate change impact of BHET approximately by 20%. The increase is because of the electricity mainly used in the washing of PET waste. The data for washing is based on a test run conducted at Herbold Meckesheim GmbH. More details regarding how the washing of PET has been modelled is described in Appendix A.

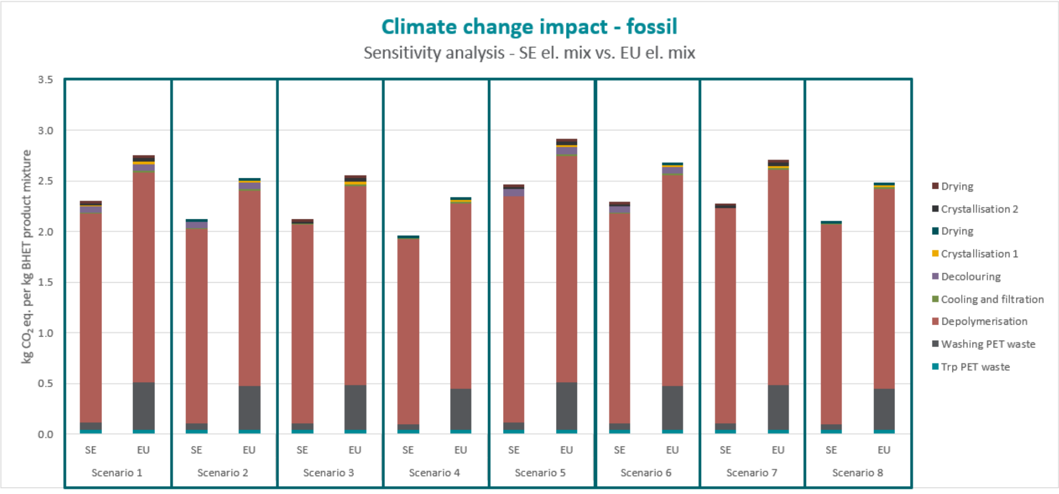

Figure 5: Climate change impact (fossil) for the different scenarios when using SE and EU electricity mix .

3.3.2 Energy – Biomass

Changing the energy source from natural gas to biomass reduces the climate change impact by almost 60%. The results are shown in Figure 6.

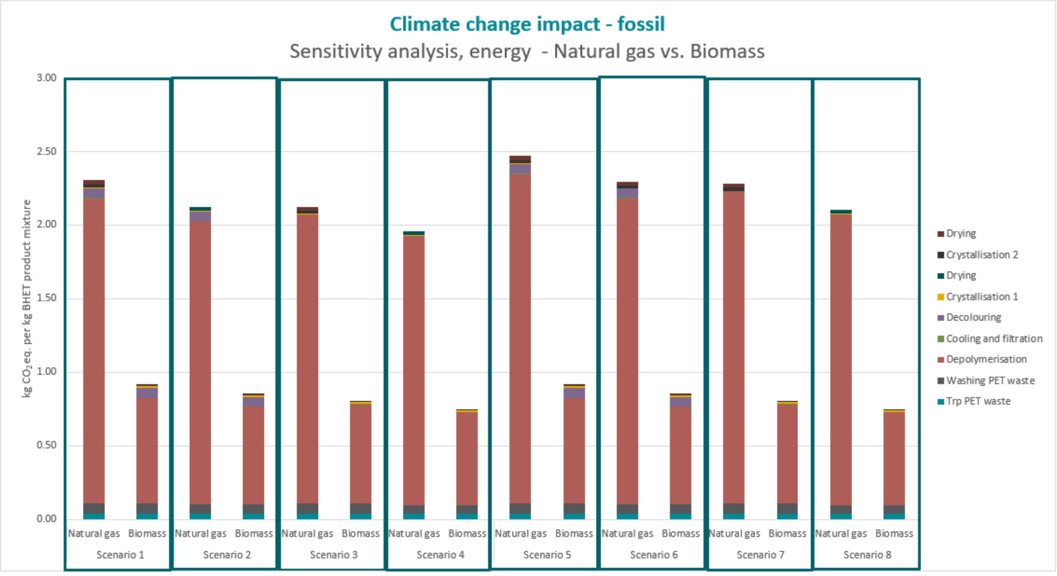

Figure 6: Climate change impact (fossil) for the different scenarios when using energy from natural gas and biomass.

3.4. Comparative scenario

Figure 7 shows how the LCA results for the studied system compares with a comparative scenario today. Scenario 5, i.e., Base case (BC), was used in the comparison. In the incineration of PET waste, 41.3% of the impacts are allocated to the waste handling of PET waste and the remaining 58.7% to energy production (Avfall Sverige, 2014). The climate change impact has been expressed as **kg CO_2 eq./kg BHET produced and 1.1 kg PET waste handled**. This is to reflect the dual functionality of both waste management and production of 1kg BHET.

The yield for producing BHET from PET waste is 90% and so we need 1.1 kg of PET to produce 1kg of BHET which is reflected in the functional unit for the comparative scenario (CS). The results show that the chemical recycling of PET waste to BHET has a lower climate change impact (20%) than the base case (BC) scenario of BHET production and PET waste management. It is also important to note that the impacts from other pre-processing steps with regards to waste management of PET are excluded as they are assumed to be similar for both the scenarios (base case and comparative).

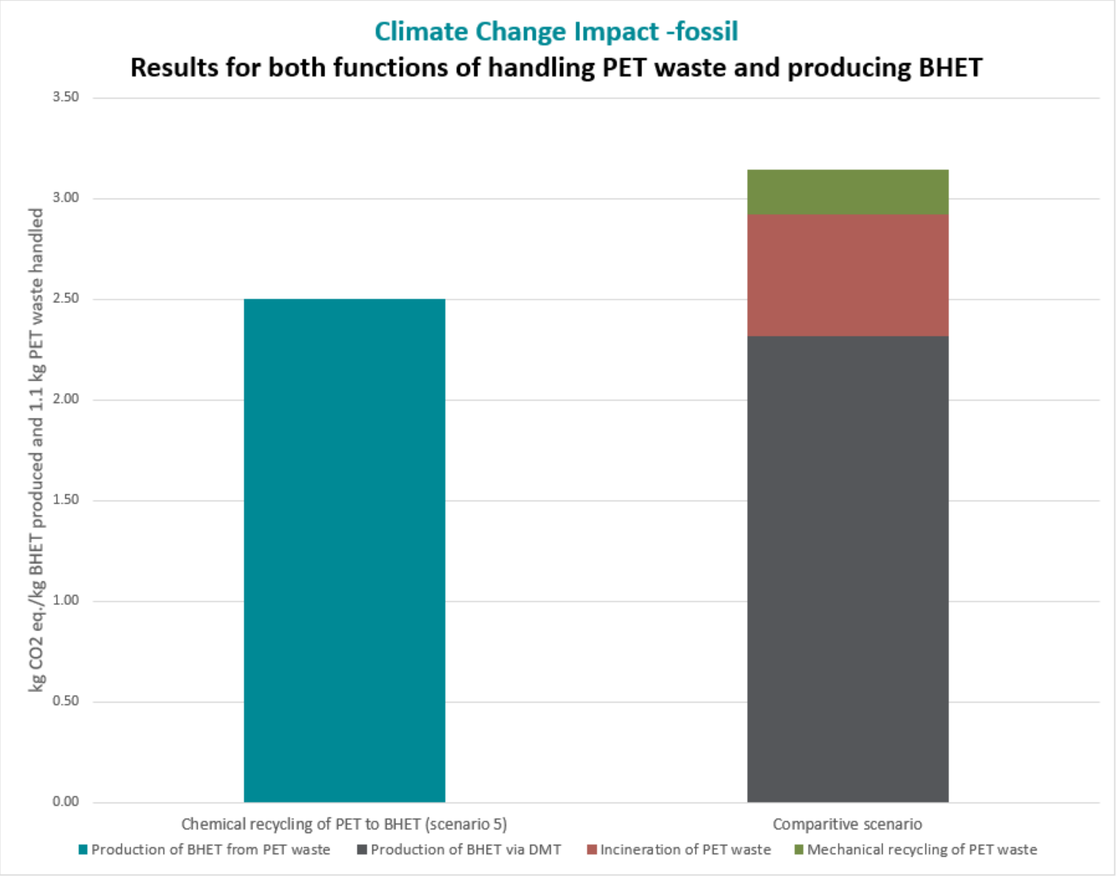

Figure 7: Climate Change impact for Chemical recycling of PET to BHET compared to Comparative scenario. Note: This figure represents two functions of a system and so the results must be interpreted accordingly.

4. Conclusions and recommendations

The LCA results on the chemical recycling of PET waste to BHET indicates that the climate change impact is between **2.0-2.5 kg CO_2 eq. per kg BHET** for the different scenarios studied. Scenario 5, the scenario with the highest climate change impact and highest purity, has process settings with 1% water content of the recycled EG, decolourisation of BHET and two crystallisation steps.

The main climate change impact, for all scenarios, comes from the depolymerisation step. In the depolymerisation step it is mainly the use of ethylene glycol (both fresh and recycled) contributing to the impact. The impact of ethylene glycol ranges from 0.3 (recycled) to 0.8 kg CO_2 eq. per kg. Fresh EG has been modelled using virgin EG dataset that is fossil based. However, this need not be the case in the future, as there could be other sources of ethylene glycol with a lower climate impact, for instance biobased EG or EG from other recycled sources. The other main conclusion to point out is that the recycling of EG currently uses fossil energy sources, which affects the environmental performance. The hotspot analysis further justifies on why it is important to consider the source of ethylene glycol used in the system. Since large quantities of ethylene glycol are used in the depolymerisation step, efforts should be put on exploring the possibilities of reducing the amount of ethylene glycol use and also investigate if it is possible to reuse the ethylene glycol within the same process before being sent for recycling. Further studies must also explore ways to optimize energy use in the recycling of EG at Recyctec, which could potentially lower the climate impact as well.

In the sensitivity analysis the effect of using EU electricity mix instead of the Swedish electricity mix was tested. The EU electricity mix has a higher share of fossil energy compared to the Swedish electricity mix, resulting in higher climate change impact. For all scenarios, the climate change impact increased approximately by 20% when the system was modelled with EU electricity mix. This shows the importance of using cleaner electricity sources. The increase of the climate change impact is mainly because of the electricity use in the washing of PET waste. The data use for the washing of PET are based on washing tests at the company Herbold Mecksheim GmbH. The PET waste was treated in several steps, and in future work it is recommended to study the washing further, trying to understand which washing steps are necessary.

A sensitivity analysis was also done to study changing the source of energy from natural gas to biomass and the results indicate that approximately 60% reduction can be observed in the climate change impact bringing it down to less than 1 kg CO_2 eq. per kg BHET.

The efforts, in this project, trying to optimise the process have influenced the outcome of the LCA. In the project, *Material circularity through recycling of PET/polyester in preparation for BHET monomer production in Sweden*, in year 2021, the LCA identified the use of ethylene glycol, incineration of oligomers, and energy usage as hotspots (Lindqvist, 2021). The use of ethylene glycol is still a main hotspot of the system, but incineration of oligomers and electricity usage are not. In this project it was identified that the oligomers could be recycled back into the depolymerisation reactor, which means that no incineration of the flow is necessary. Also, in this project heat optimisation was studied, and it was concluded that the energy used in the foreground process has minor impact. However, the use of fossil-based energy in the recycling of EG, is a hotspot identified and optimization of the overall energy consumption as well as choice of energy source should be studied further.

The purity and colour of the final product is a known factor in the industry for product quality. The LCA study results indicate that de-colouring has low climate change impact.

The comparison of chemical recycling of PET waste to BHET to the current situation today was also studied. The results indicate that it is potentially better to chemically recycle PET waste to BHET rather than the business-as-usual state of waste management along with a separate production of BHET from virgin sources. It must be noted that there are some major assumptions in this comparative model and the consequences of this have not been studied in this project as it was beyond the current scope. Further research into this should be conducted.

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Appendix A: LCA method

In this appendix, the LCA, is as much as possible, reported according to the format specified in the ISO 14044 standard. The 4 steps of the LCA report are goal and scope definition, inventory analysis, impact assessment and interpretation. In the appendix the goal and scope and inventory analysis are presented, while the impact assessment and interpretation of the result are found in the chapter result and discussion above.

A1 Goal and scope

In this section, the goal and scope of this LCA are defined and explained. It is in this part of the report where the primary objectives of the study are listed and where the scope of the project is described. The goal and scope should act as guidelines to perform the assessment as well as helping the reader of the report to understand key assumptions, system boundaries, limitations and other aspects influencing the results. Another important element of the goal and scope is the definition of the functional unit, which is the reference unit by which the inputs and outputs of the LCA is scaled.

Goal

The main goal of this LCA is to evaluate the environmental performance of the various process scenarios according to the different process configurations identified in the experimental and simulation work carried out by RISE for the chemical recycling of PET waste to BHET. A second goal with the study is to identify which activities in the chemical recycling of PET waste to BHET, contribute the most to climate change impact. This is often referred to as a dominance or hotspot analysis.

The outcome of this study is intended to inform various stakeholders within the project, of the potential climate change impact that could arise from the proposed recycling process.

Scope

The studied system, referred to as the base case scenario, is illustrated in Figure 8. First, the PET waste is transported 370 km by truck from different sorting plants in Scandinavia to the intended chemical recycling plant in Stenungsund, Sweden. At the plant, the PET waste is washed and dried before entering the depolymerisation reactor. In the depolymerisation the PET waste is mixed with ethylene glycol (both virgin and recycled) and catalyst. The mixture is heated to 270°C before entering the depolymerization reactor. The output from the depolymerisation is monomers of BHET and oligomers in ethylene glycol. After the depolymerisation, the mixture is cooled to 70 °C and filtered to remove the oligomers from the mixture. The oligomers are recycled back into the reactor.

The BHET mixture, from the cooling and filtration step, is transferred to the decolouring step to remove colour from the mixture using activated carbon. The colour comes originally from the PET waste mixture used as raw material input. Some of the BHET gets attached to the activated carbon, and this together with the used activated carbon are sent for incineration.

Thereafter, the decoloured BHET mixture is sent to the first crystallization step. In the first crystallization the BHET mixture is purified by removing ethylene glycol and water (referred to as mother liquor). The mother liquor consists of approximate 40% ethylene glycol. The ethylene glycol is purified in a recycling step by removing colour using activated carbon and dried to remove the water before being sent into the depolymerisation reactor.

The wet BHET crystals from the first crystallisation step is further purified in a second crystallisation. In the second crystallisation water is added and the mixture is heated, making the water to leave the system. The water is sent to wastewater treatment (WWT). After the crystallization the BHET crystals is dried, and the removed water is sent to WWT. After the drying step the final product containing BHET is obtained.

In this study, the process has been analysed in different process scenarios. The scenarios are described in the next section.

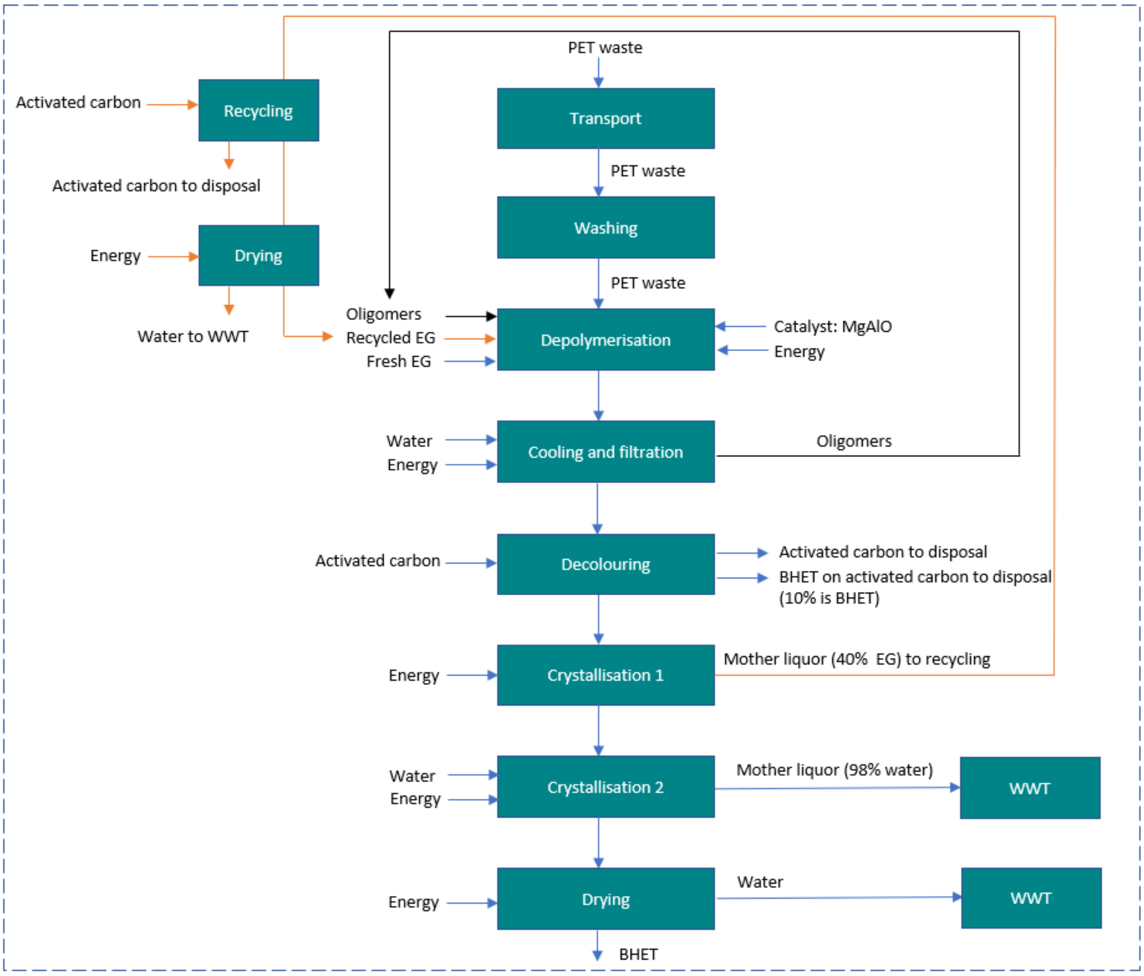

Figure 8: Overview of studied system (base case scenario).

Scenario analysis

In the scenario analysis different process settings have been assessed. The process settings that have been modified are:

- Water content in recycled ethylene glycol.
- Decolouring of BHET.
- Number of crystallisations steps.

The EG and water mixture (mother liquor) from the first crystallisation step consist of approximate 60% water. In the recycling step, a water content of 2.5% is obtained. Water in the depolymerisation reactor have been identified to create unwanted by-products, lowering the BHET yield. Because of this, removal of more water to reach 1% water content in recycled EG is added in scenarios 5-8, as specified in Table 3. In scenarios 1-4 the recycled EG consist of 2.5% water. The base case (scenario 5) is modelled with 1% water content in the recycled EG.

The decolouring of BHET is included in the scenarios 1, 2, 5 and 6. Decolouring of BHET can become necessary for the use of BHET in some applications, but the decolouring also lowers the yield. The base case is modelled with decolouring.

The addition of one extra crystallisation step, result in a product with higher purity. For the use of BHET in some applications a high purity is necessary. In scenarios 1, 3, 5, and 7, two crystallisation steps are studied. If only one crystallisation step is included (as in scenario 2, 4, 6, and 8) the wet BHET crystals goes directly to drying. This is, however, not illustrated in the overview of the studied system (Figure 8).

Table 3:Scenarios studied. EG=Ethylene glycol. BHET= Bishydroxyethyl terephthalate

Scenario	Water content recycled EG	Decolouring of BHET	Amount of crystallisations
1	2.5%	Yes	Two
2	2.5%	Yes	One
3	2.5%	No	Two
4	2.5%	No	One
5 (base case)	1%	Yes	Two
6	1%	Yes	One
7	1%	No	Two
8	1%	No	One

Sensitivity analysis

To expand the scope of the LCA and to test the robustness for some key assumptions/parameters in the study, sensitivity analysis is introduced and included in the study. The recycling of PET to BHET is assumed to take place in Stenungsund in Sweden and thus the electricity is modelled with the Swedish electricity consumption mix. The Swedish electricity consumption mix consist mainly of renewable energy and has, because of that, a low climate change impact. In the sensitivity analysis the system is modelled with the EU electricity mix since it has a higher climate change impact compared to the Swedish mix. The EU electricity mix is generated from 42.28% fossil fuels, 25.32% nuclear and 32.4% renewables. The reason for including this sensitivity analysis is to investigate if electricity becomes a hotspot when electricity with high climate change impact is used. In addition to this, a sensitivity analysis was studied to analyse the climate change impact when changing energy sources from natural gas to biomass.

A.1.3 Comparative Scenario

In order to analyse the results in context with the situation of PET waste handling today, a comparative scenario was also modelled. The system under study which recycles PET waste to BHET fulfils two functions –

1. The production of a certain amount of BHET
2. The waste management of a certain amount of PET waste

In order to compare these two functionalities in today's scenario, the comparative scenario was modelled with a system that produces BHET via dimethyl terephthalate (DMT) and ethylene glycol (equivalent to function 1 above) and an incineration process plus mechanical recycling that takes care of PET waste (equivalent to function 2). It was assumed that 42% of PET waste goes to mechanical recycling and 58% of the PET waste to incineration.

In reality, the reaction between DMT and ethylene glycol produces virgin PET with BHET as an intermediate. We assume in this study that the reaction does not proceed to completion and produces BHET instead. Commercial production of BHET is very limited and there is a lack of publicly available data and hence the assumption was made.

Type of LCA

For this study an attributional LCA was performed, meaning that the assessment estimates the environmental impact that belongs to the studied system.

Functional unit or declared unit

A functional unit is used to relate the result to a fixed factor, to enable comparison of different cases based on the prerequisites of a certain function. This is important both when comparing results, but also important to understand in what cases the LCA results are valid as the results showing the environmental impacts are given in relation to this function. If the function of the product is not assessed within the study the term declared unit is used instead. A declared unit is a quantity of a product.

The declared unit of this study is: **one kg of BHET product mixture.**

System boundaries

In this section the applied system boundaries of the LCA are specified. Aspects such as boundaries towards nature and geographical boundaries, as well as methodological aspects concerning system expansion and allocation are defined and explained.

Boundaries towards nature

This study covers the value chain from waste PET to the production of BHET. The waste PET is considered to be "free of burden" from the upstream environmental impact, but the impact for producing all the other inputs, to the processes described above, are included. This study is a cradle to gate assessment. The production of raw material, generation of fuels and electricity are followed from the cradle where natural resources (e.g. crude oil) are extracted from the ground. The life cycle also covers all relevant transportation as well as the waste management of the production waste produced i.e. the "grave" in terms of the soil (after human activity has ceased), the air (e.g. emissions from combustion of fuels) or water (e.g. water emissions from wastewater treatment).

Geographical boundaries

The waste PET recycling is assumed to take place in Sweden, at Perstorp, in Stenungsund. The electricity is modelled with Swedish electricity grid mix and the heat is modelled with thermal energy from natural gas.

Allocation

Often allocations are required in LCA studies. This is, for instance, relevant for multioutput processes generating several products and co-products, where it is necessary to distribute (allocate) the environmental impact between these. For this LCA, allocation is not applied (not needed) since the processes studied are not multioutput processes.

Important methodology choices

The most important methodology choices are summarised below:

- The LCA performed is attributional.
- The system boundary is cradle to gate.
- No system expansion is applied.
- No allocation of environmental impact is conducted.
- The declared unit is kg BHET product mixture.
- The waste PET is considered to be "free of burden" from upstream environmental impact.
- Sorting of PET waste is not included.

A2 Life cycle inventory analysis

This section gives an overview of the data collection process, data, modelling and information collected and used in the analysis. The modelling of the systems has been conducted using the LCA-software LCA for Experts by Sphera.

Through the project, experiment in the laboratory for upscaling the chemical recycling and simulations in Aspen have been made. The result from that work is used as input to the LCA. The data collected from the simulation are found in the data collection file provided as electronic appendix.

Transport of waste

The transport of waste PET was based on the work conducted in WP1 of the project, in which a mapping was conducted to identify possible sources and quantities of post-consumer PET waste within Scandinavia. The transportation of PET waste to Stenungsund was modelled with a truck and an average distance of 374 km.

Washing of PET waste

For the washing of PET waste, a test sample consisting of post-consumer PET waste was sent to Herbold Meckesheim GmbH from Svensk Plaståtervinning, where washing was carried out. Herbold provided data concerning material flows and energy requirement for each step in the washing (Klein, 2022). The data can be found in the data collection file for washing provided as electronic appendix and report from Herbold Mecksheim GmbH. From the washing, cleaned PET fines and PET trays are obtained.

The washing steps conduced on the PET waste sample are:

- Shredding
- Prewash tank
- Wet grinder
- Friction washer 1
- Mechanical dryer 1
- Hot washing
- Friction washer 2
- Mechanical dryer 2
- Separation
- Friction washer 3
- Mechanical dryer 3
- Drying

In the separation step, polyolefins and dirt are removed. Treatment of these flows are not accounted for in this LCA.

Depolymerisation

Important details are summarised below:

- Data for the depolymerisation step was provided by RISE from the simulations in Aspen.
- The virgin EG was modelled with a generic dataset from the LCA for Experts database.
- The recycled EG is based on data and information from Recyctec. The data are found in the data collection file provided as electronic appendix.
- The information and data for the production of the activated carbon are found in the report *Screening Life Cycle of recycled glycol, 2018, by Elisabeth Olsson, Swerea IVF*.
- The production of catalyst was modelled based on data from RISE, provided as an electronic appendix. RISE produced the catalyst at a lab scale using magnesium and aluminum hydroxide and then this data was used to estimate industrial level values for reactants and utilities used (Piccinno et al., 2016).
- The energy requirement is heating, and it was modelled as thermal energy from natural gas.

Cooling and filtration

Important details are summarised below:

- Data for the cooling and filtration step was provided by RISE from the simulations in Aspen.
- The energy requirement is cooling, and it was modelled with electricity (Swedish grid mix).

Decolouring

Important details are summarised below:

- Data for the decolouring step was provided by RISE from the simulations in Aspen.
- The production of the activated carbon is based on data from the report by Olsson, 2018.

- The spent activated carbon and BHET absorbed on activated carbon are sent to disposal (hazardous waste incineration).

Crystallisation 1

Important details are summarised below:

- The energy requirement is cooling, and it was modelled with electricity (Swedish grid mix).
- The mother liquor (EG and water) is recycled using Recyctec technology.

Drying

Important details are summarised below:

- The energy requirement is heating, and it was modelled as thermal energy from natural gas.
- The removed water is sent to WWT.

Crystallisation 2

Important details are summarised below:

- The energy requirement is heating and cooling. Heating was modelled as thermal energy from natural gas, while cooling was modelled with electricity (Swedish grid mix).
- The mother liquor containing mainly water is sent to WWT.

Drying

Important details are summarised below:

- The energy requirement is heating, and it was modelled as thermal energy from natural gas.
- The removed water is sent to WWT.

Dataset used in modelling

Table 4: Datasets used in modelling the various process steps in the studied system.

Process step	Material/process	Dataset	Reference
Transport of PET waste	Mode of transport : Truck	Truck, Euro 6 A-C, 28 - 32t gross weight / 22t payload capacity (Global)	Sphera
Washing	Detergent	Sodium hydroxide (100%) (Europe)	Sphera
Depolymerisation	Virgin Ethylene glycol	Ethylene glycol (Europe)	Sphera

	Catalyst	Magnesium oxide production (Europe) Aluminium hydroxide production (China)	Ecoinvent
	Energy heating	Thermal energy from natural gas (Europe)	Sphera
Cooling and filtration	Process Water	Tap water from ground water (Sweden)	Sphera
	Energy cooling	Electricity grid mix 1kV-60kV (Sweden)	Sphera
Decolouring	Activated carbon	Electricity grid mix 1kV-60kV (Sweden) Heavy fuel oil at refinery (1.0wt.% S) (Europe)	Sphera
Crystallization 1	Energy cooling	Electricity grid mix 1kV-60kV (Sweden)	Sphera
Drying 1	Energy heating	Thermal energy from natural gas (Europe)	Sphera
Crystallization 2	Process Water	Tap water from ground water (Sweden)	Sphera
	Energy cooling	Electricity grid mix 1kV-60kV (Sweden)	Sphera
	Energy heating	Thermal energy from natural gas (Europe)	Sphera
Drying 1	Energy heating	Thermal energy from natural gas (Europe)	Sphera
Wastewater treatment plant (WWTP)		Municipal waste water treatment (Europe)	Sphera

Activated Carbon disposal	Hazardous waste incineration	Hazardous waste in waste incineration plant (Sweden)	Sphera

Table 5: Details on datasets and distances used for the different transport activities in the studied system.

Transport of Material	Mode of Transport	Distance (km)
Catalyst	Truck - Euro 6 A-C, 28 - 32t gross weight / 22t payload capacity (Global)	1000
Activated Carbon	Ship Bulk commodity carrier, (Global)	14000

A.3 Life cycle impact assessment

Selected impact categories

The impact category studied in the LCA is the climate change impact. Details concerning the impact category are found in Table 6.

Table 6: Impact category studied in the life cycle impact assessment.

Impact category	Category indicator	Unit	Method
Climate change (fossil)	Radiative forcing as global warming potential	kg CO_2 eq.	IPCC baseline, 100 years, 2013

Appendix B – LCA model in LCA for experts

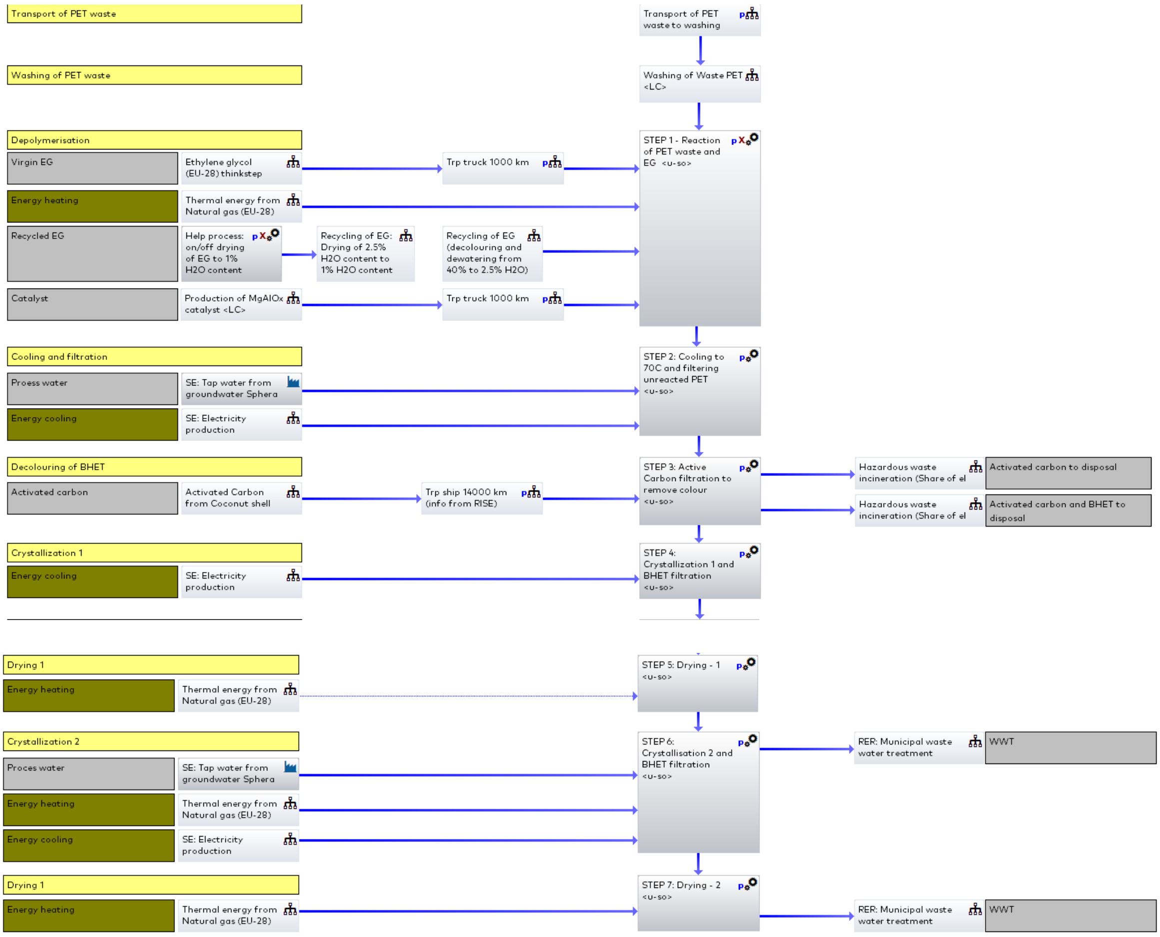

Figure 9: LCA Model for the chemical recycling of PET to BHET

Work package 6 - Implementation, a plan for industrialisation

Project ID: 766

Christian Andersson, 2024-09-24

EXECUTIVE SUMMARY

A concept for a post-consumer PET depolymerisation plant to produce BHET through glycolysis was developed and modelled in Aspen Plus®. The functionality of the technology using an actual industrial feedstock was demonstrated in the earlier work packages of the project. The use of the depolymerised PET in downstream applications was demonstrated in work package 5 and a holistic view of the depolymerisation unit in terms of production and equipment costs as well as energy usage was presented in the present report concerning work package 6.

The main outcome from work package 6 is a depolymerisation concept that can be used as a basis for a plant project. To ensure successful implementation of a large-scale plant, there are additional topics that needs to be considered and potentially addressed in further studies. These can be loosely grouped as either pertaining to the equipment/process, the economical/logistical side of the design and operation of a depolymerisation unit, or to the legal side. These are:

Equipment-Process considerations

- *Experimentally measure solubilities of BHET in MEG, water, and MEG/water solutions at various temperatures*
- *Investigate BHET fouling tendency in process equipment (pipes, valves, heat exchangers)*
- *Develop alternative(s) to active carbon for decolourisation*
- *Detailed design of process equipment*
- *Investigation around reactor types suitable for the process*
- *Investigation around solid-liquid separators for oligomer and monomer separation*

Economic-Logistic considerations

- *Larger plant size recommended*
- *Increased PC PET collection radius*
- *Study process robustness*
- *BHET sales price*
- *External costs (MEG, PC PET, logistics, etc.)*

Legal aspects

- *Freedom to operate (FTO)*
- *Reach registration*
- *Environmental permit*

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BACKGROUND

The present report summarises the work collected in Work package 6 done around transferring the results from the laboratory trials performed by RISE and Synpo and use these to develop block and process flow diagrams and then implement these in the process simulator Aspen Plus® where various operating and design scenarios are simulated and studied. The mass and energy balances resulting from the process simulations are used as basis for a techno-economic analysis in which the direct variable cost (DVC), a useful measure of the operating expenditure (OPEX), and the capital cost (CAPEX) are evaluated. These concepts and how they are estimated will be described in the Techno-Economic analysis.

The report does not go into detail regarding the work performed in the other work packages in the project. The results and conclusions relevant to the implementation phase are used in the present report. For the interested reader, please refer to the other project material and reports associated with the implementation phase according to the below bullet list with the executing organisation in parenthesis:

- Raw material supply
    - Work package 1. Supply of raw material – volumes, quality, and distance (IVL, SPÅ)
- Laboratory experiments, life cycle assessment (LCA), and basic flowsheet development
    - Work package 2. Experiments for upscaling (RISE)
    - Work package 3. Simulation, optimisation, and LCA (RISE, IVL)
- Details regarding mono ethylene glycol (MEG) regeneration outside of distillation
    - Work package 2. Experiments for upscaling (Recyctec)
- Evaluation of depolymerisation process in pilot scale
    - Work package 4. BHET in pilot scale (Synpo)
- Downstream use of depolymerised polyethylene terephthalate (PET)
    - Work package 5. Applications (Perstorp, end-users)

PROCESS

In this section the process and the function of each of the unit operations is discussed together with representations of the process by block flow (Figure 1) and process flow diagrams (Figure 2). The flowsheet has been developed from the block flow diagram by including process stream recycles and heat recovery position. The process flow diagram is taken directly from the process simulation and includes only the main equipment and streams and not the control loop often shown in a process flow diagram.

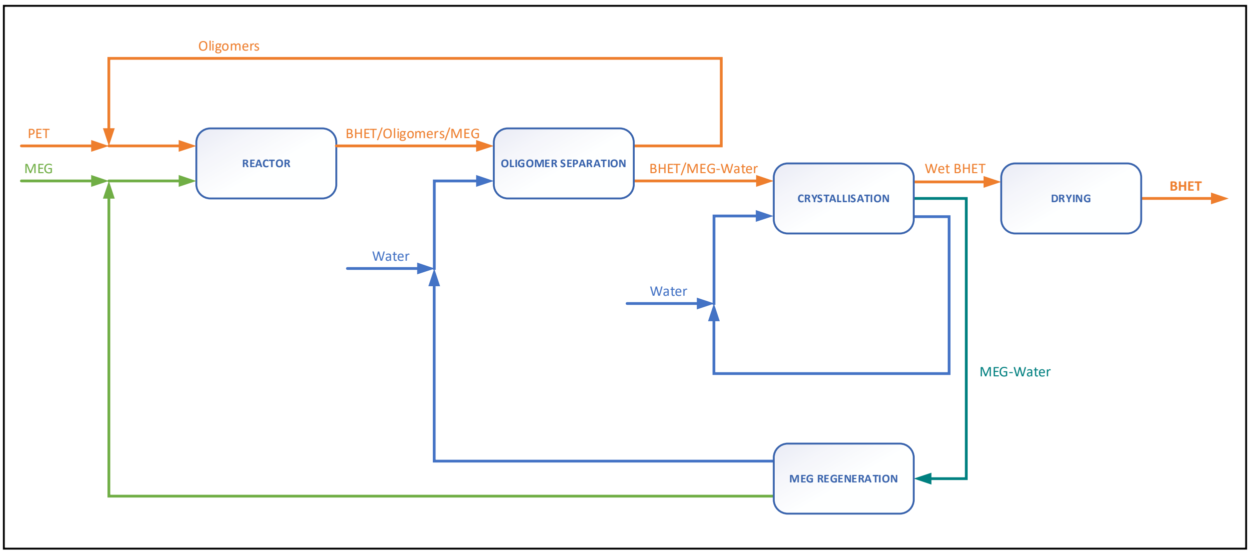

Figure 1. Block flow diagram of glycolysis depolymerisation unit. Orange streams represent streams containing PET/BHET, green represents MEG, blue represents water, and dark blue-green a MEG-water mixture.

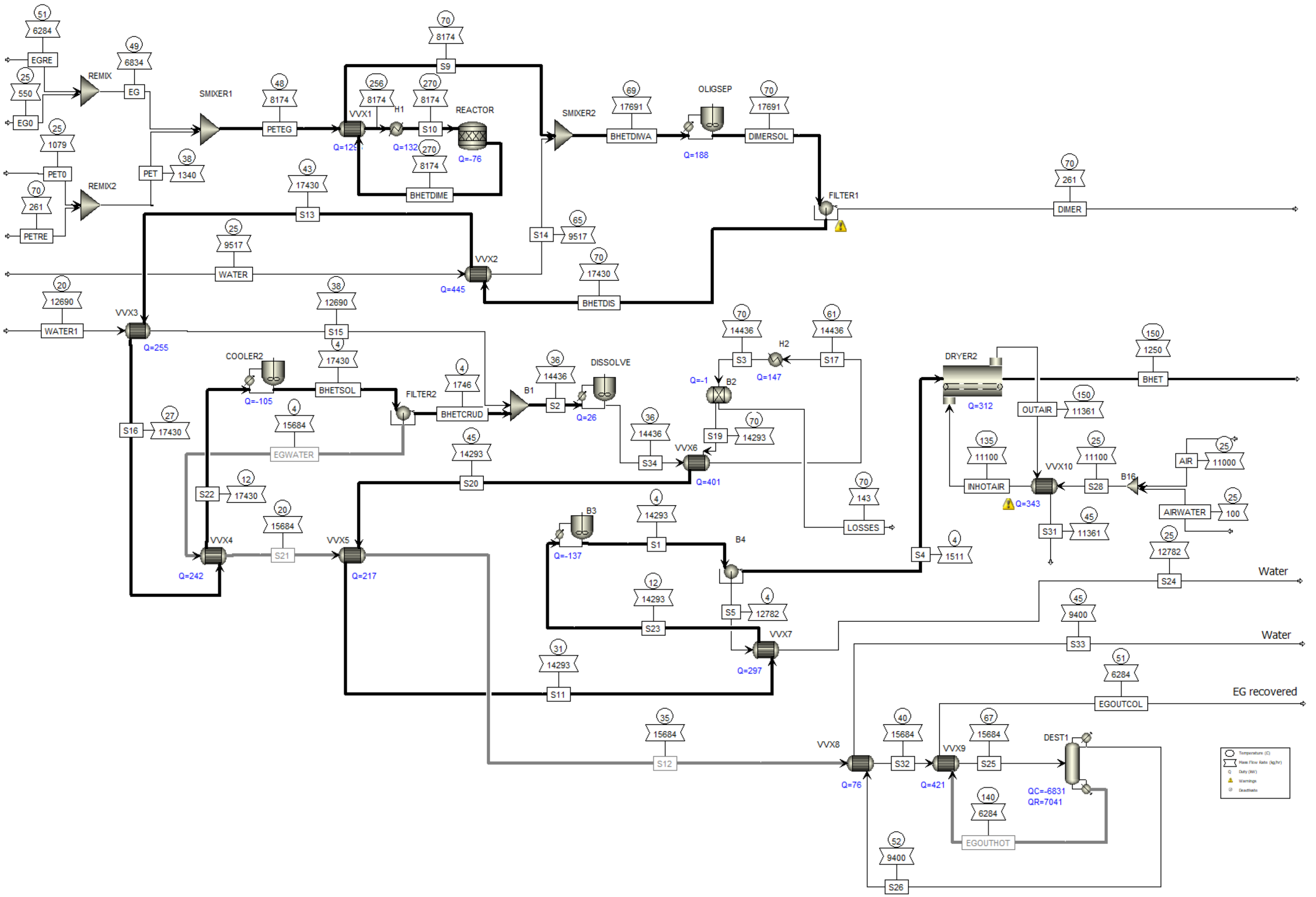

Figure 2. Process flow diagram of glycolysis depolymerisation unit. The bold line shows the path of the PET/BHET.

1. Process description

Depolymerisation of post-consumer (PC) PET to bis(2-hydroxyethyl) terephthalate (BHET) by glycolysis as described in the present report entails a rection section, an oligomer separation section, a crystallisation section, a product drying section, and a MEG regeneration section. In this part of the report, the different process sections will be discussed in terms of their process configuration, function, and equipment considerations.

1. Reaction section

In the reaction section, finely divided PET waste is mixed with MEG and fed to the reactor. The mixture is preheated in two steps, first by a feed-effluent exchanger taking the hot reactor effluent, approximately 270 °C and heat exchanging it with the cold feed at approximately 50 °C (Figure 3). This step is essentially a heat recovery step helping to minimise the plant energy consumption. It brings the feed temperature up to approximately 250 °C. The exact temperature will depend on the heat exchanger design and the proclivity of the process fluid to foul the heat exchanger.

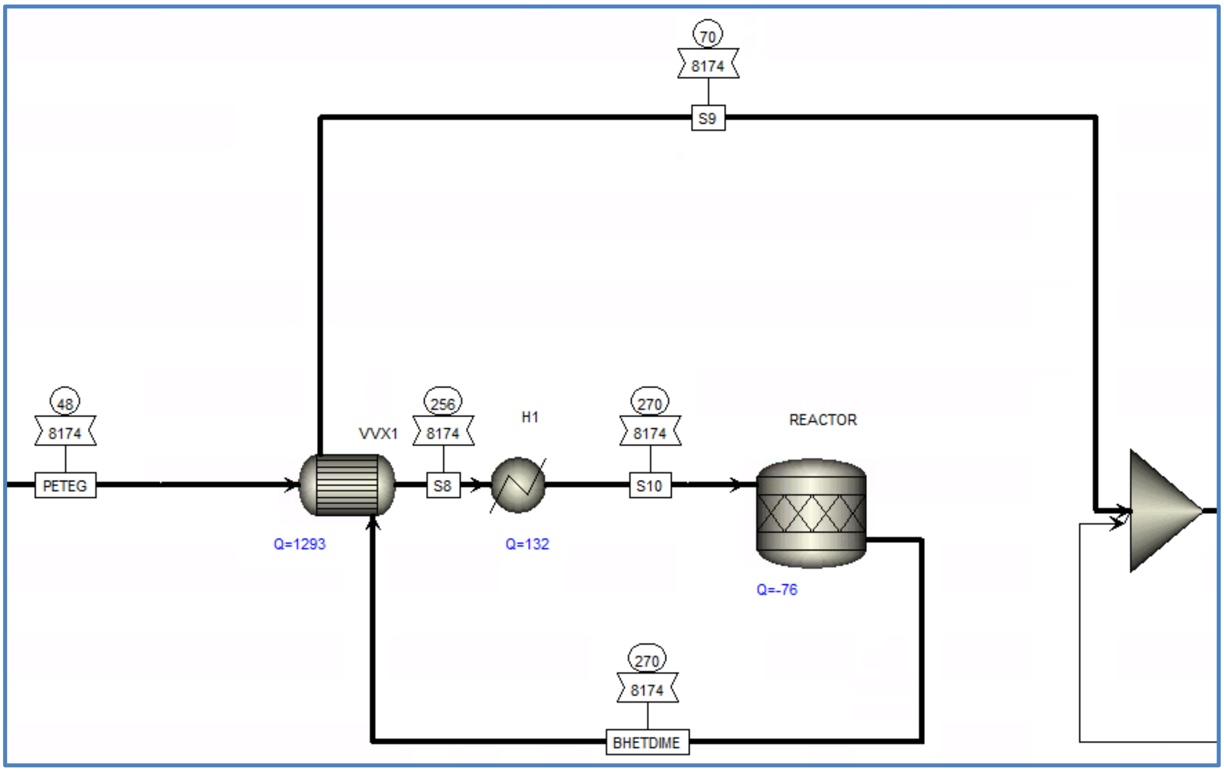

Figure 3. Cut-out showing the reactor and preheating section.

At this point a 10 K hot end approach was used in the simulation (Figure 4). This specification was likely too tight given the uncertain nature of the fluid, especially in terms of its viscosity, thermal conductivity, and fouling tendency, and the long temperature program. The temperature program results in a heat exchanger effectiveness of a little more than 90%, which is very high. The heat exchanger effectiveness can, assuming constant specific heat capacities be calculated from [Eq. 1].

For a detailed design, a value between 70-80% is likely more realistic, i.e., a process fluid outlet temperature in the range of 210-230 °C instead of 250 °C. Anything above 80% is termed a high effectiveness heat exchanger and although excellent in terms of heat transfer, may be difficult to attain in a process heat exchanger working with complex fluids.

$$\epsilon = \frac{Q_{actual}}{Q_{max}} = \frac{T_{cold,out} - T_{cold,in}}{T_{hot,in} - T_{cold,in}} \quad \text{[Eq. 1]}$$

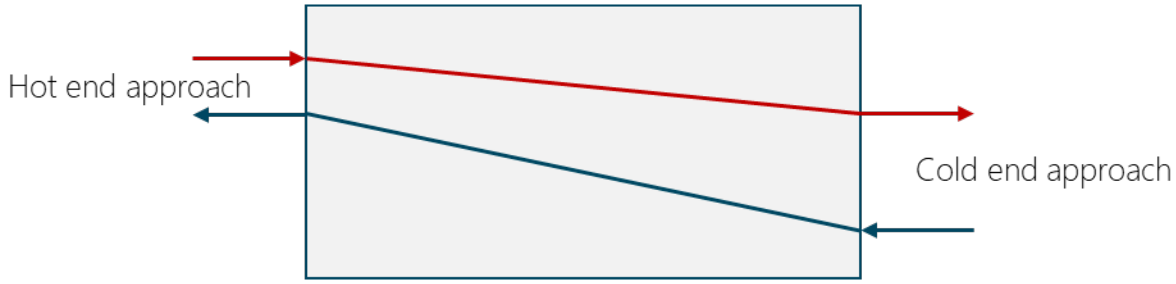

Figure 4. Schematic showing the hot and cold approach temperatures and temperature profiles through a heat exchanger without phase change and with constant specific heat.

For the current investigation the difference in effectiveness has minor impact on the results. In the present evaluation the main impact of a reduced effectiveness is a percentage reduction in heat recovery roughly the same as the reduction in effectiveness. On the other hand, a very high effectiveness, which is possible to design for, will lead to slightly higher energy recovery, but when the actual process is designed, such a high effectiveness would result in a very expensive and likely sensitive heat exchanger design. In the concept of sensitive, one must understand the impact of fouling and pressure drop on the thermal performance. A high effectiveness will, considering typical heat exchanger types (e.g., shell-and-tubes, hairpins, plate-and-frame), result in a large heat transfer area, which necessitates a high pressure drop to provide enough fluid velocity to generate turbulence and sufficient fluid-to-wall shear stress to maintain a low fouling tendency. Likely, the large heat transfer area required will result in low wall shear stress as sufficient pressure to drive the flow through a heat exchanger with long thermal length (multipass tubes/shells in series or long plates) at high enough velocity typically is not available and as a result the heat exchanger fouls. If the heat exchanger experiences fouling, the thermal performance will decrease and now the plant must operate with reduced performance while having invested significantly in heat transfer area that cannot be utilised fully.

The reactor feed-effluent exchanger is the most important heat exchanger in the process in terms of heat recovery and ensuring a correct and optimally functioning design will be important for the overall operation of the plant. Such a design may be based no redundancy (1x100%), half redundancy (2x50%), or full redundancy 2x100% or 4x50% design, or some other variant. The main benefit of using multiple smaller exchangers (50% alternatives) instead of one large (100% alternatives), is that it often is easier to maintain good wall shear stress also at reduced loads and that one exchanger can be taken out of service for maintenance (e.g., inspection, cleaning, repair) while the plant can still be in operation. In the present report only one heat exchanger is considered.

The second preheating step is included to raise the temperature from the feed-effluent exchanger exit temperature to the reactor operating temperature of 270 °C. This step can be done in any type of heater suitable for the operation, e.g., fired heater, electrical heater, or a heater powered by a thermal oil or a hot process fluid that may be available on the site. Due to the temperatures required, steam is unsuitable as heating medium as it would require steam at around 300 °C corresponding to a saturation pressure of approximately 85 bar. Such a high operating pressure would drive up the design pressure and thus equipment cost unnecessarily high.

The final heater should be designed with significant margin so that it can ensure full plant capacity even if the reactor feed-effluent exchanger is under-performing or in need of maintenance. This will bring the capital cost for the heater up in relation to what is presented in the current report. The degree of over-design necessary will depend on the design philosophy for the reactor feed-effluent exchanger. For example, if the feed-effluent exchanger is design as 2x50%, then it may be useful to design the heater to be able to handle the current capacity plus 50% of the capacity of the feed-effluent exchanger.

The reactor is at this point just simulated as a continuously stirred tank reactor (CSTR). The project has discussed possible reactor designs, and this remains an open point for further evaluation and trials.

2. Oligomer separation

Water is added to precipitate the oligomers not yet fully depolymerised into BHET monomers. This is done by adding water to stream S9 (Figure 3). The water is prior to addition heat exchanged with the stream combining the reactor outlet and added water post the oligomer separation stage (Figure 5). The oligomers can then be separated by a suitable solid-liquid separation operation, e.g., a vacuum belt filter or some type of centrifuge. The type and design of the solid-liquid separator depends on the characteristics of the particles, in particular the particle size distribution. The design of the solid-liquid separation equipment will have to be further investigated. To further cool the reactor effluent before the crystallisation section, another heat exchanger transferring heat from the process stream to the water to be used in the BHET redissolving step is installed.

Both heat exchangers are simulated using a 5 K hot end approach. Although, this is a tight approach, the streams in these exchangers are better defined than in the reactor feed-effluent exchanger. The thermal conductivities are higher, and the streams consist of water, MEG, and dissolved BHET. Since the solubility of BHET in 40 wt% MEG (aq) is higher than the concentration of BHET in the streams, it is expected that the process stream is either non- or minimally fouling. The resulting effectiveness for the first and second water heat exchangers are about 90% and 80%, which is realistic, especially considering that the temperatures are low enough to allow for the use of gasketed plate heat exchangers in which such effectiveness values are attainable without sacrificing hydraulic performance (turbulence and wall-shear).

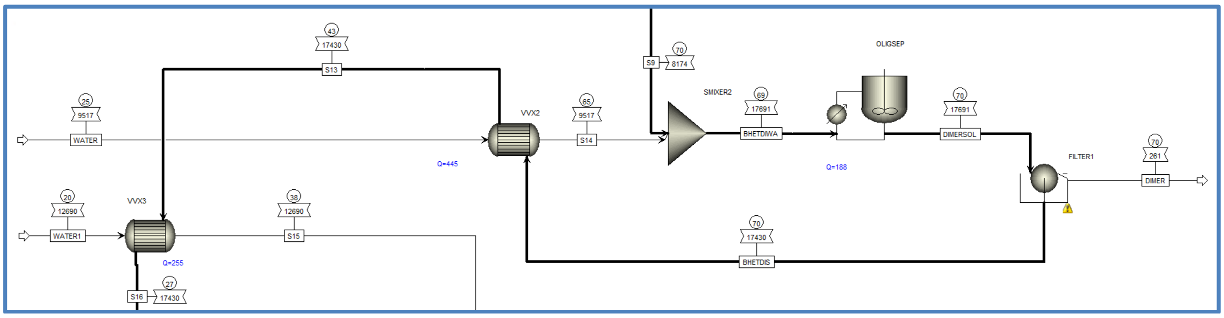

Figure 5. Water addition, oligomer separation, and heat exchange with MEG/Water/BHET stream from reaction section. The water added to the reactor effluent is charged through VVX2. The water charged through VVX3 is added to the BHET redissolving step.

3. Crystallisation section

The crystallisation section is built up around two crystallisers with an intermittent active coal treatment for colour removal from the BHET product. The crystallisation is accomplished by cooling crystallisation decreasing the fluid temperature to precipitate dissolved BHET (Figure 6).

In the crystallisation section, the BHET is first precipitated from the MEG-water stream and separated by solid-liquid separation. As with the oligomer separation equipment, also the separators in the crystallisation section will have to be investigated separately. In fact, each separation stage will require a separate investigation as the properties of the particles will differ, especially comparing the oligomer and monomer crystallisation steps.

After separation the BHET crystals are redissolved in water and treated with activated carbon to achieve the colour reduction required to result in on-spec end-products. It is thereafter again precipitated in a second crystalliser before being transferred to the drying section (Figure 7). The MEG-water from the first crystalliser is after passing through a series of heat exchangers sent to the MEG regeneration section.

The fluid from the second water heat exchanger in the oligomer separation section is further cooled by heat exchanging it with the cold crystalliser exit stream. The first crystalliser decreases the temperature to 4 °C. Given that the media is made up of a 40 wt% MEG solution it should be possible to further decrease the temperature and improve the BHET yield in the process by increasing the amount of BHET precipitation. It should be remembered that the BHET that is not precipitated in the first crystalliser does not enter the second crystalliser. Some of it may be recovered from the MEG regeneration column and returned to the reaction section, however, it would be preferable to crystalise more by further reducing the temperature.

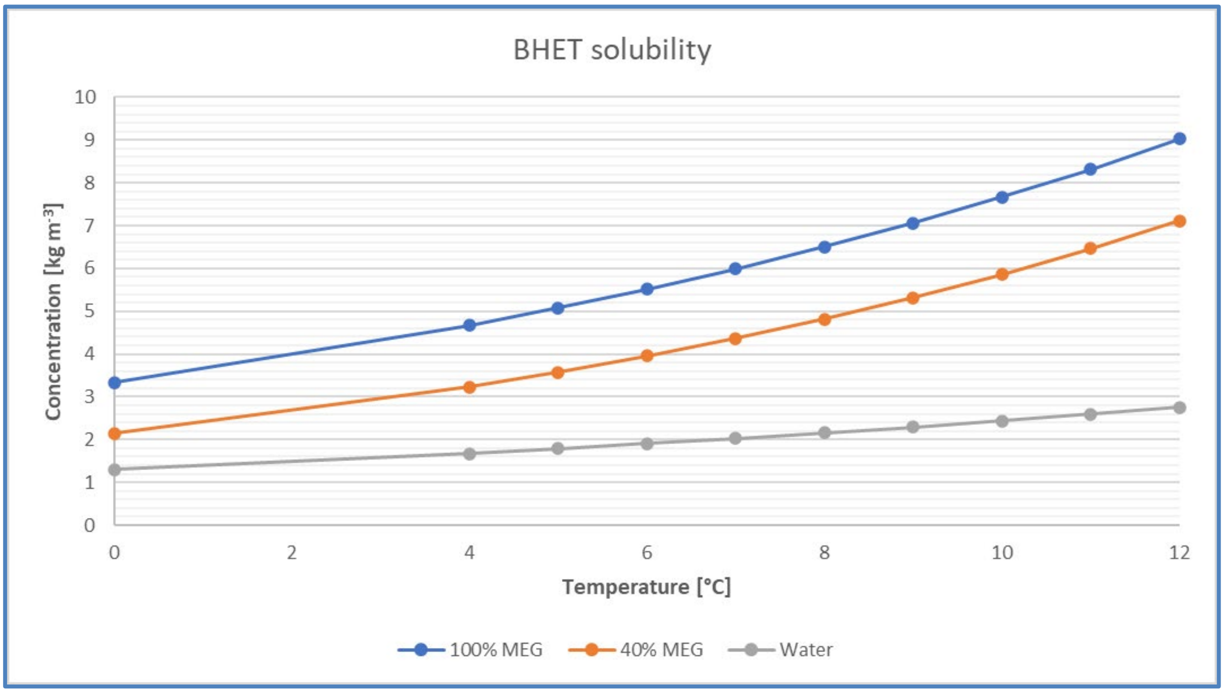

Figure 6. Solubility curves for BHET in water and 40 wt% and 100 wt% MEG.[1]

After the first crystalliser, the BHET is separated and dissolved in the water from the second water heat exchanger and treated with activated carbon. This treatment has been shown to result in overall BHET losses of approximately 10%. This is significant and improvements regarding decolourisation of the BHET with reference to reducing BHET losses should be investigated. The losses will depend on the extent of the colour reduction required by the requirements of the downstream users of the BHET. If low or no colour removal is required, the activated carbon step may be omitted. This also means that there is no need for the redissolving and second crystallisation steps and the BHET can go directly to the drying section.

Prior to the second crystalliser the stream is cooled to 12 °C by the cold exit stream from the crystalliser. When dissolved in water, the BHET solubility is much lower than in a MEG solution and BHET precipitation will likely start already in the heat exchanger, especially as the resulting wall temperature will be somewhere in the 6-10 °C range (lower than 12 °C, higher than 4 °C) and if the wall shear is low enough to allow for crystals to build up at the wall in the heat exchanger. The heat exchanger, if it should be kept, must therefore be designed to handle the formed crystals without choking. This includes high wall shear and possible a sufficiently large channel to allow for some crystal formation.

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[1] Haoyu Yao, Dongxia Yan, Xingmei Lu, Qing Zhou, Yinan Bao, Junli Xu, *Solubility determination and thermodynamic modelling of bis-2-hydroxyethyl terephthalate (BHET) in different solvents*, **Chinese Journal of Chemical Engineering, 45 (2022), 294-300**

In the second (water as solvent) crystalliser, the temperature of 4 °C should be maintained. In the design of the crystalliser, it will be important to ensure that the wall temperature in the cooler is above the water freezing point to prevent water from freezing in the cooler. To achieve temperatures below 25 °C chilled water is needed and to achieve temperatures below approximately 5 °C a special refrigeration system is needed. Such a system is assumed to be present. A simulation of a simple ammonia system was performed to provide OPEX estimates for the depolymerisation. The system was not included in the CAPEX estimates for the unit.

The heat exchangers in the crystallisation section are designed rather than with a specified approach temperature, with a certain process exit temperature. For the precooler to the first and second crystallisers, the process exit should be cooled to 12 °C, and as mentioned, for the second precooler a higher value may be necessary when more experimental solubility data is available. This means that the heat exchanger may need a control function, likely in the shape of a bypass on the cold side. This is easily done with a 3-way valve and a temperature controller. This should be safe as the cold side fluid mostly is non-fouling liquid. Effectiveness values for the heat exchangers range from 60% to almost 80%. These designs if done correctly accounting for possible BHET precipitation are realistic.

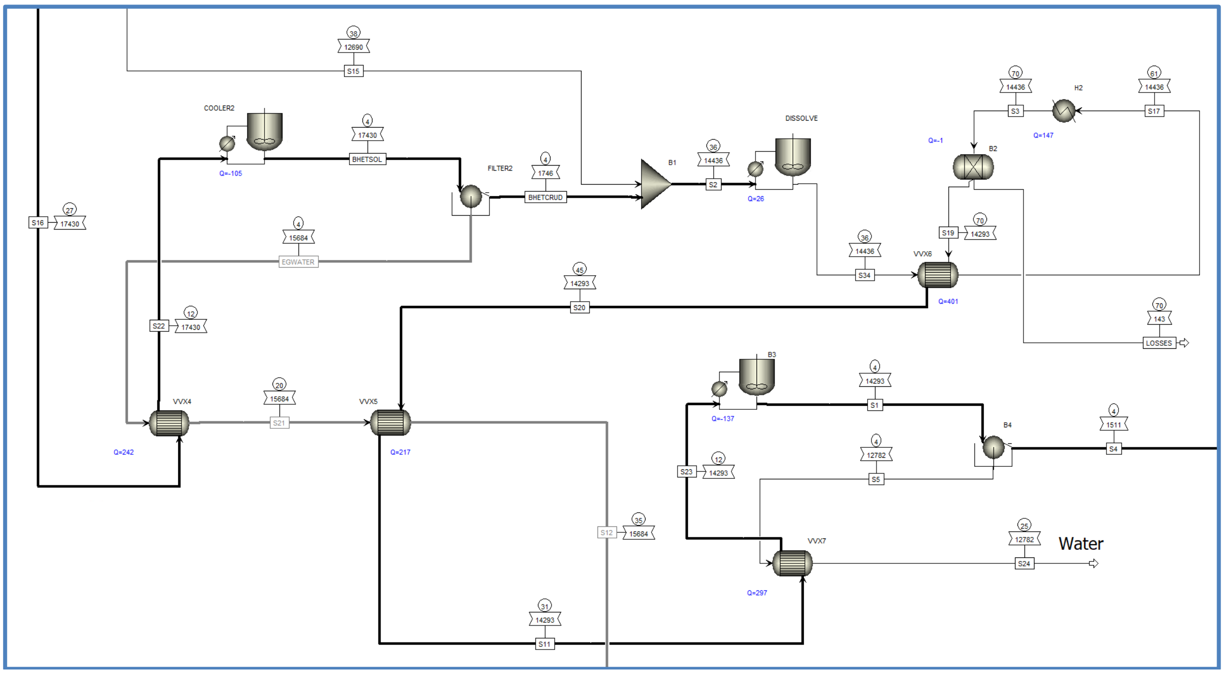

Figure 7. Cut-out showing the crystallisation section.

4. Drying section

The drying section (Figure 8) consist of a feed-effluent exchanger preheating the incoming air with the hot air exiting the drier. The drier is at this point just considered to be a continuous direct contact type drier.

The air-air exchanger being a heat exchanger with gas close to atmospheric pressure on both sides must be designed with minimal pressure drop. Since it is low pressure gases, the volumetric flow will be large and in addition, the thermal conductivity poor, hence the exchanger must be designed with a large heat transfer and cross-sectional area to allow for the heat transfer to be completed without using too much pressure drop.

The heat exchanger must also account for possible condensation of water evaporated from the BHET stream. The heat exchanger design is not difficult, but these aspects must be considered in the design.

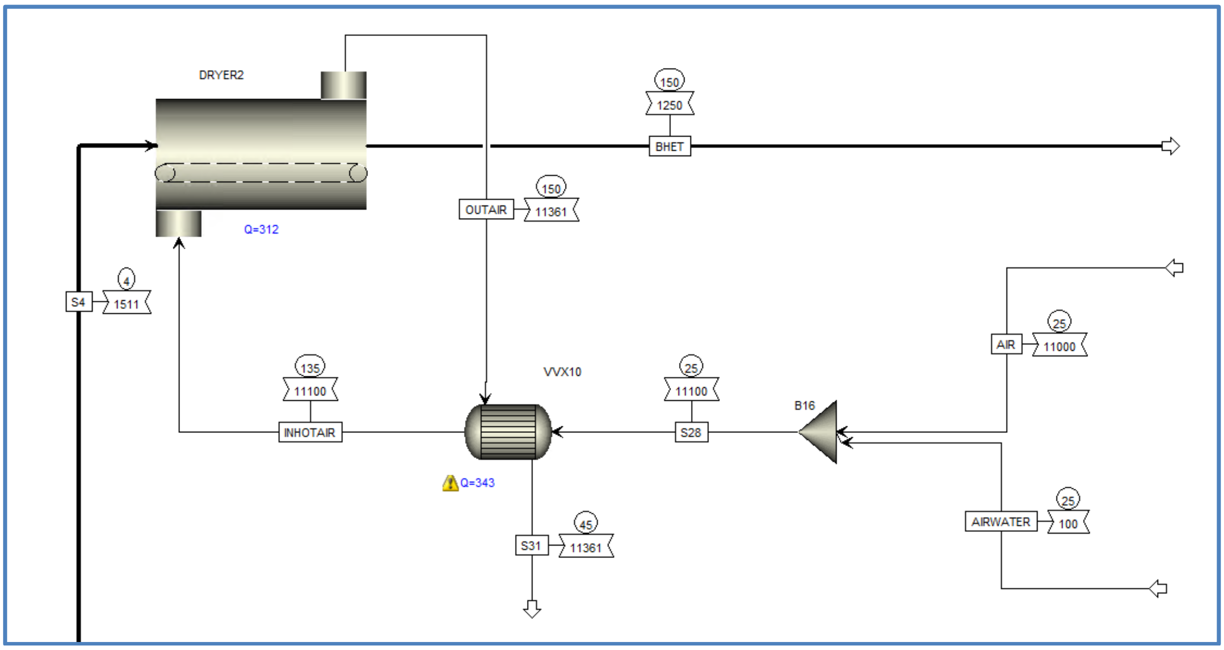

Figure 8. Drying section.

5. MEG regeneration section

The glycolysis process handles in relation to the product approximately 5 times the amount of MEG and 20 times the amount of water. These streams must be separated from the BHET product, each other, purified, and recycled for the process to be economically viable and environmentally relevant. The MEG-water stream separated from crystallised BHET in the first crystalliser must be purified to enable recirculation of the water and MEG streams to their respective feed points without negatively affecting process performance. This is mainly accomplished by distillation. The process is well-known and used extensively in e.g., natural gas processing. The MEG-water stream feeding the distillation unit may need pretreatment to remove salts or other chemicals that may interfere with the distillation or otherwise accumulate in the process. In the present investigation only the distillation column is included. Other necessary separation operations are reported in other work packages and included here simply as a unit block termed "Separations" (Figure 9).

To design the distillation unit, there are four main considerations needed. The first is to try to maintain a bottoms temperature below 165 °C. This is to avoid thermal degradation of MEG. As MEG has an atmospheric boiling point of 197 °C, the column must operate at sub-atmospheric pressure to facilitate the separation at a temperature below 165 °C. The second aspect is to ensure sufficient temperature difference between the boiling fluid and the heating medium to allow for boiling in a competitively sized reboiler. Perstorp primarily employ steam as heating medium in distillation columns. There are several pressure-ranges available and for the purpose of the present project Perstorp's medium pressure steam at 7 bar (saturation temperature 165 °C) is most suitable.

Depending on the type of reboiler and the process fluids, a temperature difference somewhere in the range of 10 K to 50 K generally results in a robust and competitive design. When designing a reboiler, it is necessary to ensure some degree of superheating at the wall to provide enough energy to form bubbles from the otherwise saturated liquid. That is, the temperature at the wall must be a couple of degrees higher than the saturation temperature to produce the phase change. To this, the boiling point increase due to static head (height difference between liquid level in column or draw of tray to the reboiler inlet) must be considered. This is especially important in vacuum columns as the effect of a pressure increase on the boiling point is significantly more pronounced at lower compared to higher operating pressures. So, when design a reboiler that both must operate under vacuum and with a limited temperature heating medium care must be taken to not provide excessive static head as it may limit the possibility to initiate boiling. This is an aspect of the detailed piping design and is at the present stage of the project not considered in detail, however, it is highlighted for future reference.

In addition, to the minimum necessary temperature difference including boiling point elevation due to static head, a temperature difference in excess of the bare minimum is generally preferable from a design perspective both to ensure operating robustness in the face of process variation (pressure, liquid level, etc.) and as it results in a smaller reboiler. The latter is beneficial from not only the equipment procurement cost but also from an installation cost as a small reboiler may be supported directly on the column and reduce the structural steel and foundation costs.

The fourth consideration pertains to the overhead condenser. The lowest column pressure that can be used depends on the temperature of the cooling medium. In the present project, regular cooling water should be used. In Sweden, a cooling water supply temperature of 25 °C can be used as the highest average temperature and hence a suitable design basis. A normal temperature increase for cooling water from supply to return is in the range of 10-15 K. That is, a cooling water outlet temperature of 40 °C can be used.

The temperature difference in a condenser can generally be slightly lower than in a reboiler since there is no equivalent to the static head component and vapour bubble formation energy present in the reboiler in the overhead condenser. Nevertheless, a temperature difference between the condensing overhead vapours and the cooling medium of at least 5 K is generally needed for a decent condenser design and 10 K or more is recommended if possible. To be evaluated in during basic engineering.

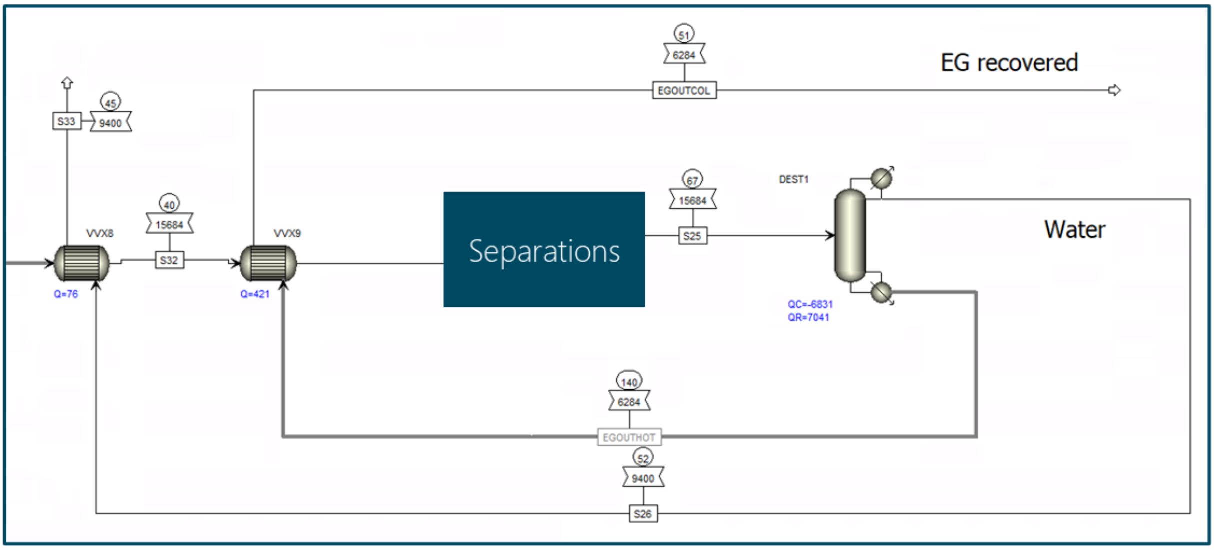

Figure 9. MEG regeneration section.

In the present project a column pressure of 0.15 bar was used. This is a standard vacuum rating and results in a bottom temperature of 140 °C and overhead temperature of approximately 50 °C. That is, the reboiler has a 20-25 K temperature difference between the steam and process fluid and the condenser operates with approximately a 10 K temperature difference.

With regards to the pressure there is also a minor trade-off in that the lower the pressure the higher the volumetric vapour flowrate and hence vapour velocity. The vapour velocity is the limiting factor for determining the column diameter and column diameter is very important for the cost of the column. One can consider that adding a plate or even a handful of plates only increases the height of the column by roughly 0.6 x number of extra plates. If you require for example 5 additional plates in 30 m column, you have increased the height and consequently the steel needed by 10%. Contrast that by increasing the diameter by e.g., 10% for the same 30 m column, now the entire column and every plate, collector, distributor, packed section increases in diameter by 10%, which results in a 20% increase in the amount of steel required, just from an area point. That said, the first priority should be to optimise or at least find an operable operating pressure for the separation at hand and second priority is to minimise the diameter.

In addition to the above, the distillation section contains two feed-effluent exchangers preheating the feed to the column by cooling the overhead and bottoms streams. The heat exchanger using the column bottoms stream is classified as a feed-bottoms exchanger. In terms of heat recovery in the process, the exchanger heat exchanging the feed against the overhead stream may be omitted as the heat recovery it represents is low. The bottom stream on the other hand provides significant thermal energy on par with the water exchangers in the oligomer separation section.

The heat recovery exchanger using the overhead stream is designed with a 5 K hot end approach. It has an effectiveness of about 45% and any type of heat exchanger could be used. One way to heat integrate a process unit is to use the condenser to preheat the feed by using the feed as cooling medium in the condenser. Doing this saves one heat exchanger from the capital expenditure but reduces the operability somewhat and it may be necessary to have a second water-cooled condenser to ensure full condensation.

In the present project, applying the above reasoning is not feasible as the temperature difference is small and although one could recover approximately double the heat that is recovered in the current design of the overhead feed-effluent exchanger, it is not a large energy saving and the concept suffers from a major flaw. The condenser requires a heat transfer rate close to 7 000 kW while the overhead feed-effluent exchanger recovers only about 80 kW or 160 kW if doubled (cold side exit temperature increased to 45 °C), so a little more than 1% of the total condenser duty. Additionally, any extra exchanger in the overhead system uses the available pressure drop and as this is a vacuum application, the available pressure drop is limited, thus the heat exchanger must be made very large to minimise the pressure drop. The consequence of this is that both the preheating condenser and the main cooling water cooled condenser must be made significantly larger than in the original concept, thereby increasing the plant CAPEX. The conclusion is to use the setup as envision in Figure 9 with or without including the overhead feed-effluent exchanger.

For the feed-bottoms exchanger the heat exchanger is design to bring the cold side (column feed) up to its boiling point. This results in an effectiveness of close to 90% which is attainable considering the low fouling tendency of the two streams. However, it may require additional booster pumps on both the hot and cold side to ensure that sufficient pressure drop is available to converge on a well-operating heat exchanger design.

2. Simulation report

The simulation model used in the present report was developed in Aspen Plus® v. 14. It is a continuation on a model developed by RISE for earlier work packages in the project. The original flowsheet was based on data from the laboratory trials in work package 2. In the flowsheet used for work package 6, the original model was modified to include the recycling of material streams (MEG, water, oligomers) post separation and recovery, scaled up to a production rate of 10 000 tonnes BHET per year using an annual operating time of 8 000 hours. This results in an hourly production rate of 1 250 kg BHET.

1. Scaling up and building a dynamic flowsheet

A design-spec block was used and set to vary the total amount of PET fed to the depolymerisation unit to reach the target capacity of 1 250 kg BHET h^{-1} (10 000 tonnes BHET $year^{-1}$). A calculator block was used to enforce the proportions between PET, MEG and water when varying the feedrate PET [Eq. 2], [Eq. 3], and [Eq. 4].

$$F_{MEG} = 5.35 \times F_{PET} \quad [Eq.\ 2]$$

$$F_{water} = 7 \times F_{PET} \quad [Eq.\ 3]$$

$$F_{water1} = 10 \times F_{PET} \quad [Eq.\ 4]$$

Where F is the flowrate in kg h^{-1}. The subscripts *MEG* and *PET* refers to the feedrate of the chemicals. The subscripts *water* and *water1* refers to the water added to the oligomer separation and redissolving steps respectively.

The recirculation loops in the flowsheet for unreacted PET and MEG from the distillation section were simulated using and open-loop approach where the outgoing streams of recovered PET and MEG were transferred to new inlet recirculation streams using CALCULATOR-blocks and mixed with the fresh feed (Figure 10). The processes often required several iterations to ensure mass balance convergence (Figure 11).

In principle, the simulation is run, and the flow of PET scaled to meet the desired BHET production capacity. The flows are then balanced according to [Eq. 2], [Eq. 3], and [Eq. 4], and the exiting PET and MEG streams calculated and transferred to the inlet recirculation streams where the PET feed and MEG make-up streams are recalculated. The simulation is run repeatedly until there is no change in the feed stream flowrate.

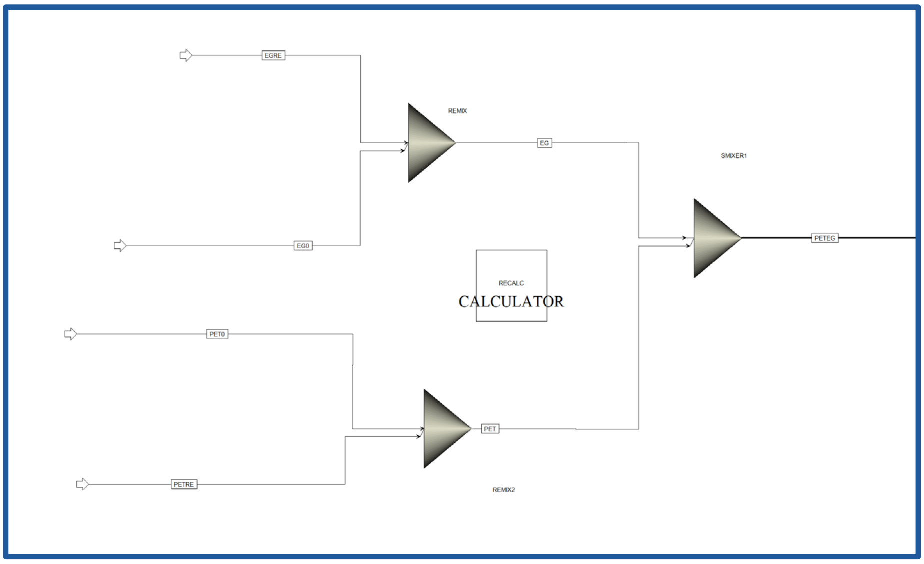

Figure 10. Simulation of PET and MEG recirculation with reactor feed.

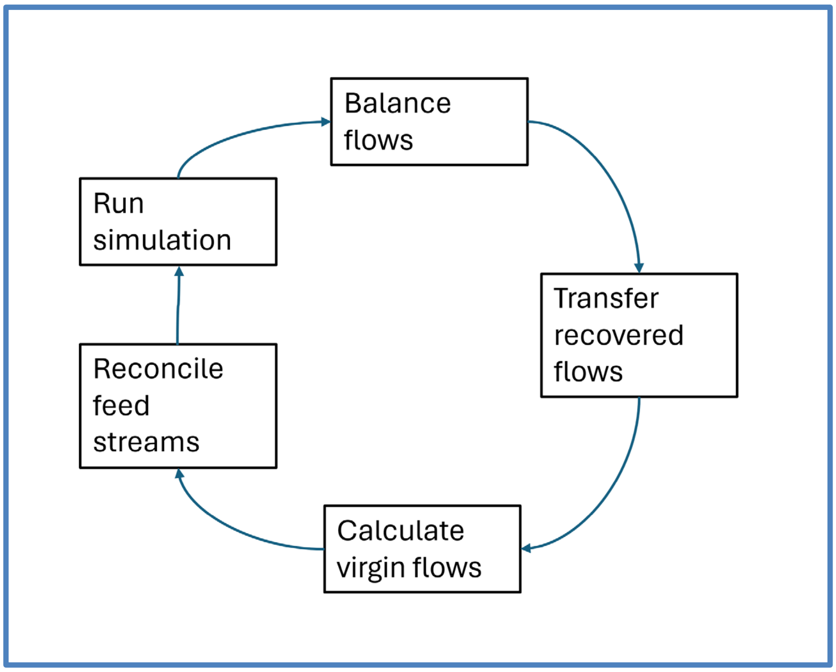

Figure 11. Work algorithm for material stream recirculation.

1. Artificial BHET losses

The activated carbon treatment between the first (MEG-water as solvent) and second (water as solvent) crystallisers induces a loss equivalent to 10% of the BHET contained in the stream. To include this in the simulation an activated carbon bed was simulated by using a separation unit from Aspen Plus® in which 10% of the BHET was removed as a loss (Figure 12). The remainder of the stream was heat exchanged against the circuit inlet. A heater was also included to increase the inlet temperature to an operating temperature of 70 °C, suitable for the activated carbon treatment.

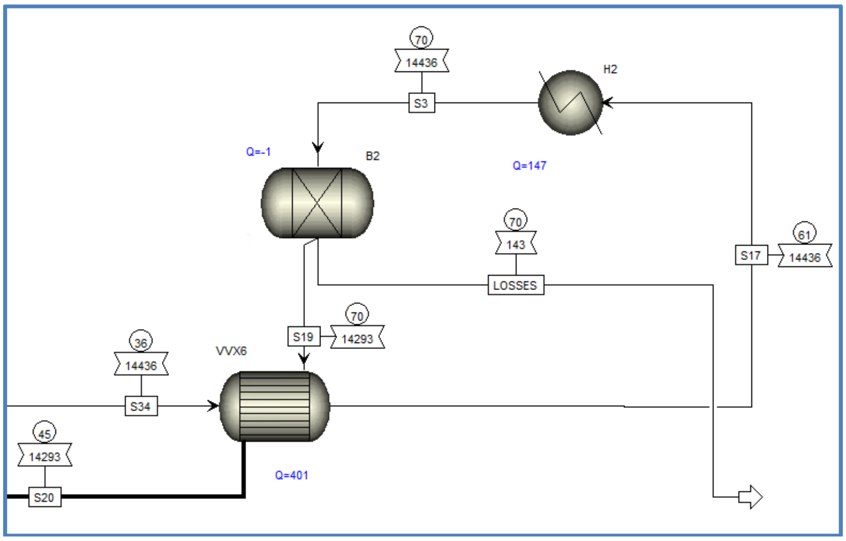

Figure 12. Activated carbon unit.

2. Ammonia refrigeration unit

To estimate the energy expenditure and operating cost of cooling to below 5 °C, an ammonia refrigeration system was simulated. The system consists of a compressor, condenser, JT-valve, separator, circulation pump, and a vaporiser (Figure 13). The power consumed by the compressor and circulation pump is used to estimate the electricity cost for operating the equipment while the cost for operating the condenser is estimated from its cooling water usage. The vaporiser is connected to the process equipment and assumed to directly cool the crystallisers.

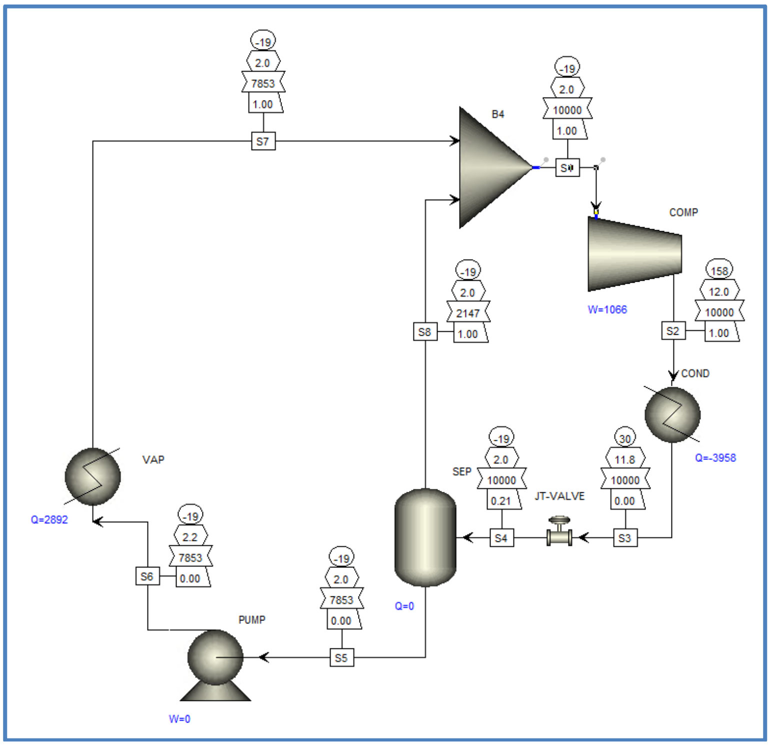

Figure 13. Ammonia refrigeration system.

TECHNO-ECONOMIC ANALYSIS

3. Cases

In the techno-economic analysis of the depolymerisation unit, four operating cases with different levels of stream integration and purity of recycled MEG were evaluated (Table 1).

Table 1. Operating cases evaluated in technoeconomic analysis.

Operating case	Specifications
Case 1	99 wt% MEG from column, no recirculation of process water
Case 2	97 wt% MEG from column, no recirculation of process water
Case 3	99 wt% MEG from column, process water recirculated
Case 4	97 wt% MEG from column, process water recirculated

4. CAPEX

The flowsheet developed was ran through the application Aspen Process Economic Analyzer^{TM} to provide a first estimate of the CAPEX cost for the depolymerisation unit. Aspen Process Economic Analyzer^{TM} was used to map, size, and price the equipment.

Equipment costs were evaluated for carbon steel and multiplied by 2 to convert to stainless steel. For process equipment cost differences between stainless steel and carbon steel vary widely depending on equipment type and the fraction of the equipment that requires stainless steel. A shell and tube heat exchanger may for example have a carbon steel shell and stainless steel tubes. The material conversion factor is then 1.67[2] while if the entire exchanger is made of stainless steel the factor would be 2.86. Similar reasoning can be applied to other equipment as well. A pump for example has a factor of 1.7 while 2" Raschig rings have a factor of about 3. For simplicity and consistency, a value of 2 was selected for the present evaluation.

For a complete plant cost, an experience-based factor-approach is used in which the sum of the equipment cost is multiplied by a factor (Table 2) to arrive at the final investment cost. The factor includes costs such as project management, installation, instrumentation, electricity, foundations, etc. Depending on the project such a factor can vary widely, typical values may range from 2 to 12. For larger projects with good project management factors are typically in the 6-8 range. In the present project a factor of 6 is assumed.

In work package 6, tanks, office buildings, shipping, raw material handling including washing and sorting of the PET waste are not included. The economic concept presented here will thus only include the depolymerisation unit. The complete cost for a processing unit including the above features and facilities may be twice that presented here but has to be investigated in more detail. The total plant cost is hence evaluated according to [Eq. 5].

$$CAPEX = MF \times LF \times \sum C_{Equipment} \qquad \text{[Eq. 5]}$$

Where C is cost.

Table 2. Plant cost from factor-based approach.

Parameter	Source/Value
Carbon steel equipment cost	Aspen Process Economic Analyzer^{TM} (SEK)
Material factor (*MF*)	2
Lang factor (*LF*)	6

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[2] H. P. Loh, U.S. Department of Energy/National Energy Technology Laboratory and Jennifer Lyons and Charles W. White, III, EG&G Technical Services, Inc; *Process Equipment Cost Estimation Final Report*, **2002, DOE-NETL/1169**

1. CAPEX – 10 000 tonnes BHET per year

The difference in between the four operating cases was minimal with regards to the equipment cost and the final cost for building the depolymerisation unit as described above was roughly 315 MSEK. There was no effect on CAPEX when recirculating the water streams while the plant cost decreased by about 8% when the operated using a lower MEG purity specification (97 wt% instead of 99 wt%). The cost reduction was close to entirely allocated to the distillation column.

Taking the entire plant into consideration, the distillation column represents approximately 23% of the total CAPEX for operating cases 1 and 2. In operating case 3 and 4 when the MEG purity is lowered to 97 wt%, the distillation column cost reduces by 30-35% compared to case 1 and 2 which in turn reduces the fraction of the cost constituted by the distillation column to approximately 18% (Figure 14). It should be noted that the bars in Figure 14 are related to the total cost for each scenario and that the total CAPEX for operating case 1 and 2 is approximately 8% higher than that of operating case 3 and 4. As mentioned in the text, the only unit operation that has a changed cost is the distillation column and the lower cost of the column alters the fraction of the cost represented by the other unit operations.

In terms of the individual equipment costs, the crystallisers stand out making up close to half of the total CAPEX and optimising crystalliser operation and design should be investigated further. The filters also represent a large portion of the cost and must be investigated further with equipment trials to determine the most suitable and cost efficient solid-liquid separation technology. The heat exchangers are not highly significant given that there are many (10) and in total constitute only 8-10% of the CAPEX and that they, as will be seen in later, are important for the operating costs. Finally, the distillation column making up 18-23% of the CAPEX is impactful, and its exact cost will be determined in detail during the basic engineering phase of a plant project (exact diameter, type of internals, type of phase contacting equipment (plates or packing and which type of each)). The distillation column represents the only actual equipment where the operating cases with reduced MEG purity can reduce the CAPEX. Hence determining the most suitable MEG purity has the potential to save roughly 8% on the CAPEX.

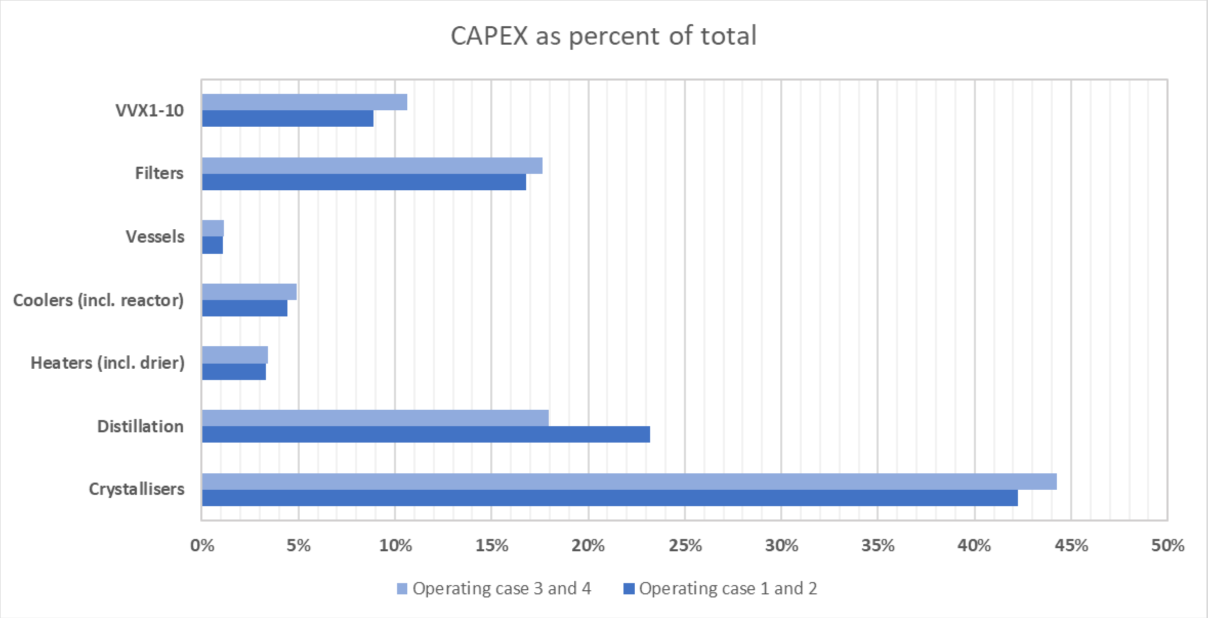

Figure 14. Equipment cost represented as fractions of total CAPEX.

2. Scale-up of concept plant

The 10 000 tonnes per year plant concept was scaled up to a BHET production of 100 000 tonnes per year and the corresponding development of the CAPEX studied (Figure 15). A plant producing very small volumes can see a tremendous decrease in the capital cost per tonne produced product when the size of the plant is increased. As the size of the plant increases the decrease in capital cost per tonne product reduced. That means that when prospecting a new plant, an evaluation of this sort can assist in determining a suitable production volume for the plant. There are several ways this can be accomplished. A well-established and straight-forward method is to apply the Rule of Six-tenths, [Eq. 6], which normally is accurate to within 20% and highly useful in the initial phases of a project.

$$\frac{CAPEX_2}{CAPEX_1} = \left(\frac{Production_2}{Production_1}\right)^{0.6} \qquad \text{[Eq. 6]}$$

Where *CAPEX* in [Eq. 6] refers to the capital cost of the plant and *Production* to the production volume of BHET. The subscripts *1* and *2* refer to the present/available and estimated plant sizes respectively. When estimating the cost for higher and lower production volumes, the chosen plant size of 10 000 tonnes annual production volume is in the start of the flattening of the CAPEX per volume curve.

Preferably, a 3-5 times higher production volume (i.e., 30-50 ktonnes per annum) should be targeted as it can close to half the CAPEX cost per tonne produced BHET. Going to production volumes in excess of 50 ktonnes does not significantly reduce CAPEX per volume cost and unless the demand for product and the quantity of available raw material can justify it, there is no direct need to size the plant capacities as large as 80-100 ktonnes per annum.

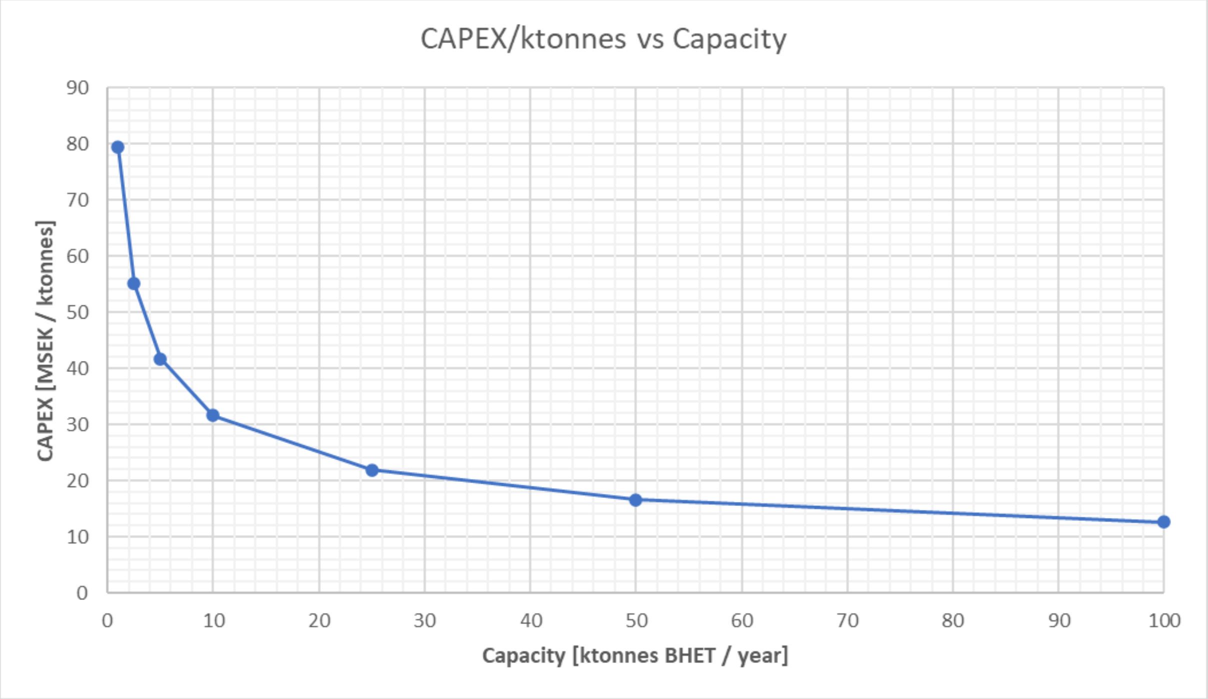

Figure 15. Variation of CAPEX with BHET production volume.

3. CAPEX study conclusions

- recirculation of the process water does not have a negative impact on CAPEX
- the crystallisers constitute the largest fraction of the CAPEX and optimisation of the crystallisation process and crystalliser design will be important in the industrial implementation
- reduced MEG purity from the distillation reduces the cost of the distillation column by 30-35% and the total plant cost by approximately 8% and its operability should be investigated
- plant size should preferably be larger by 3-5 times, i.e., 30 000 – 50 000 tonnes BHET production per year, to reach a point where capital cost per produced BHET does not significantly reduce with increased BHET production volume

5. OPEX

When evaluating the operational costs Perstorp use a term we call Direct Variable Cost (DVC). The DVC is calculated by taking the costs of all raw material and utilities (steam, electricity, process water, cooling water, etc.) that is added to the production and divide that by the production rate. This results in a DVC with units of SEK per kg BHET. This value must then be compared with the sales price and the difference is the margin or when divided by the sales price, the profit margin.

1. Calculation of DVC

The raw material costs are calculated as the stream flowrate times the unit price of the chemical in question and results in a stream cost per hour. The stream cost per hour is then multiplied by the yearly operating hours to obtain the yearly cost of the raw material. In the depolymerisation unit considered in work package 6, the unit is considered to have 8 000 operating hours per year.

$$C_{stream}[SEK\ year^{-1}] = \sum F_{component} C_{component} t_{year} \qquad \text{[Eq. 7]}$$

Where *F* is the flowrate of the component in kg h^{-1}, *C* the cost in SEK kg^{-1} for the component, and *t* the operating hours in a year. The stream cost in [Eq. 7] for each of the individual raw materials; MEG, PET, process water, and cooling water is summarised into the cost of all chemicals added to the process. Cooling water is considered a utility and is not consumed in the process, but its cost is calculated in the same manner as the raw materials and thus included in the stream cost.

The cost for the production power usage was evaluated as the sum of the power requirement for each respective unit operation times the cost of the energy type utilised, [Eq. 8]. In the investigation the cost of electricity, steam, and natural gas according to Perstorp data was used.

$$C_{power}[SEK\ year^{-1}] = \left(C_{elec}\sum Q_{elec} + C_{natural\ gas}\sum Q_{natural\ gas} + C_{steam}\sum Q_{steam}\right)t_{year} \qquad \text{[Eq. 8]}$$

Where *Q* is the power requirement in kW and *C* is the cost for the utility in SEK kWh^{-1}.

For coolers and condensers using cooling water the cost is in the cooling water. The simulations have been performed using the heater/cooler unit operation in which the process exit temperature is set and the duty required to reach it calculated. The cooling water inlet temperature used in the project is 25 °C and a cooling water temperature increase of 15 K is used. From the temperature increase and the heat transfer rate, the cooling water mass flowrate is calculated, [Eq. 9]. The cooling water cost is then calculated by [Eq. 7].

$$F_{CW}[kg\ h^{-1}] = \frac{Q_{CW}}{C_{p,CW}\left(T_{CW,out} - T_{CW,in}\right)} \times 3600 \qquad \text{[Eq. 9]}$$

Where *F* is the flowrate in kg h^{-1}, *Q* the heat transfer rate in kW, C_p the specific heat in kJ $kg^{-1}K^{-1}$ and *T* the temperature in K.

The DVC is then calculated according to [Eq. 10], where the cooling water cost is included in C_{stream}.

$$DVC[SEK\ kg\ BHET^{-1}] = \frac{C_{stream} + C_{power}}{Production} \qquad \text{[Eq. 10]}$$

Where *Production* represents the annual BHET output from the plant in kg $year^{-1}$.

2. Analysis of DVC and associated parameters

The DVC is a crucial parameter when it comes to the viability of a process or product. From a purely economic perspective, if the CAPEX is omitted from the reasoning, the DVC is the parameter that sets the profit of a production unit. The concept can be expanded to include labour and maintenance, but in its most simple for, as it is used here, then the DVC is a direct measurement of the effectiveness of the chemistry and unit operations in the manufacturing process.

The DVC can be broken down into three parts as described above:

- raw material – MEG, PET, process water
- energy – electricity, natural gas, steam
- utilities – cooling water

When discretising the DVC in this way, operating case 1 is used as the baseline cost, i.e., a plant without water recirculation and with a high MEG purity. This is a high-end plant in terms of the purity of the chemicals (water and MEG) used. The DVC cost for this plant setup is the highest and is set to 100%. The other operating cases are normalised against operating case 1.

In operating case 2 where the process water is recirculated and the MEG purity is maintained high at 99 wt%, the DVC decreases by 5% to 95% (Figure 16). Operating case 3 and 4 use 97 wt% MEG and both cases decrease the DVC by approximately 12-13%. As was seen when evaluating the CAPEX, the lower MEG purity cases resulted in lower CAPEX and the lower MEG purity also results in lower operating costs.

Again, as with the CAPEX, the DVC is not greatly affected by the water recirculation. In the analysis an arbitrary cost of process water has been used, however, when considering the rather large quantities of water in relation to the produced BHET, it would be necessary to analyse the wastewater treatment unit in detail to ensure that the water quantity can be treated effectively and cost efficiently. In an actual installation, it is recommended to recirculate the process water, as it does reduce the DVC and by its nature is beneficial for the environmental profile of the depolymerisation unit.

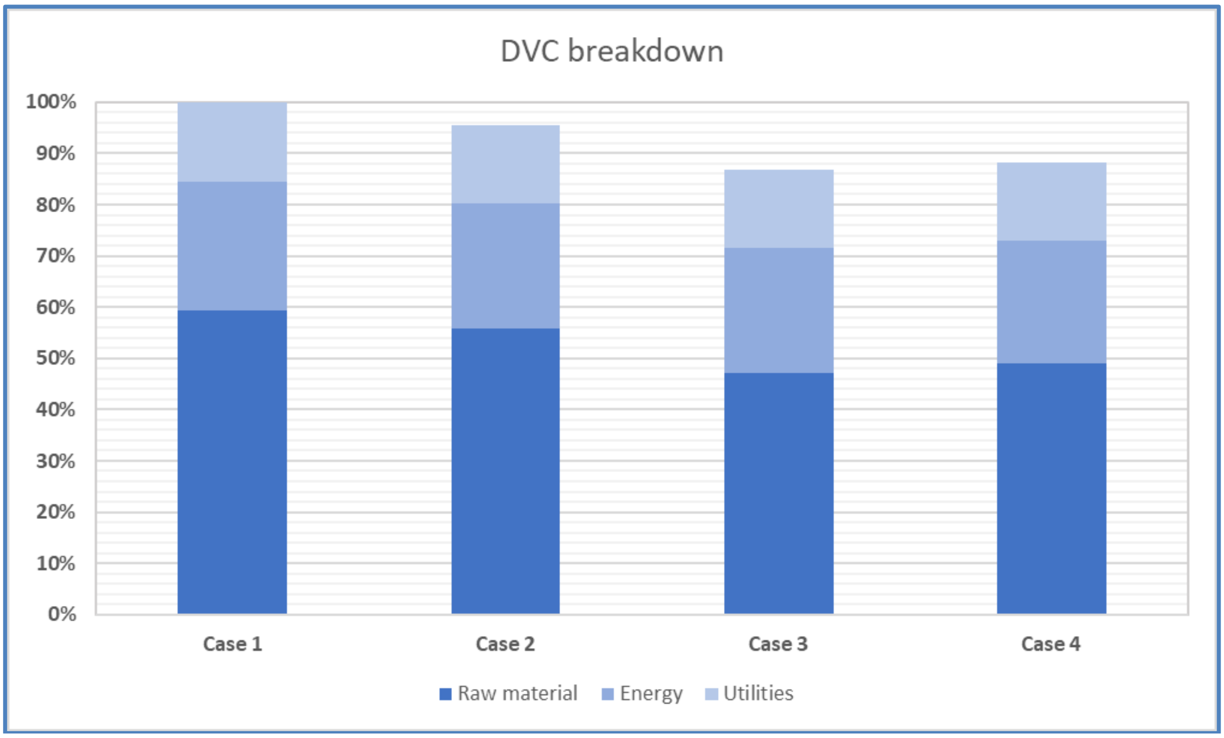

Figure 16. Breakdown of DVC in its constituents: raw material, energy, and utilities.

In the cost of the produced BHET roughly 60% originates from the raw materials. Out of that it is almost equal parts due to the MEG and PET with the MEG cost, even if it is just make-up volumes, being somewhat higher. The water cost is as has been alluded to, not having a significant impact on the DVC.

The energy usage represents 25% and the utilities 15%. For many products produced from virgin material, the part of the DVC that comes from the raw materials is typically well over 70%, closer to or above 90%. The ratio between the three categories is identical between the four operating cases.

In the process concept for the depolymerisation, there are many heat exchangers included to recover energy from the hotter process streams. If all the heat exchangers that were used in the flowsheet are included, about 21% of the heat in the shape of heating and cooling, can be recovered (Figure 17). As was mentioned under the Crystallisation section, two of the heat exchangers there were at risk of BHET precipitation and fouling. These were VVX4 and VVX7, both being cooled by cold effluent fluid from the crystallisers. If these are excluded, the percentage of the heat recovered decreases to 18%. This is not an extreme decrease, but it is noticeable. It can also be observed that the fraction of the energy used for heating and for cooling are approximately equal.

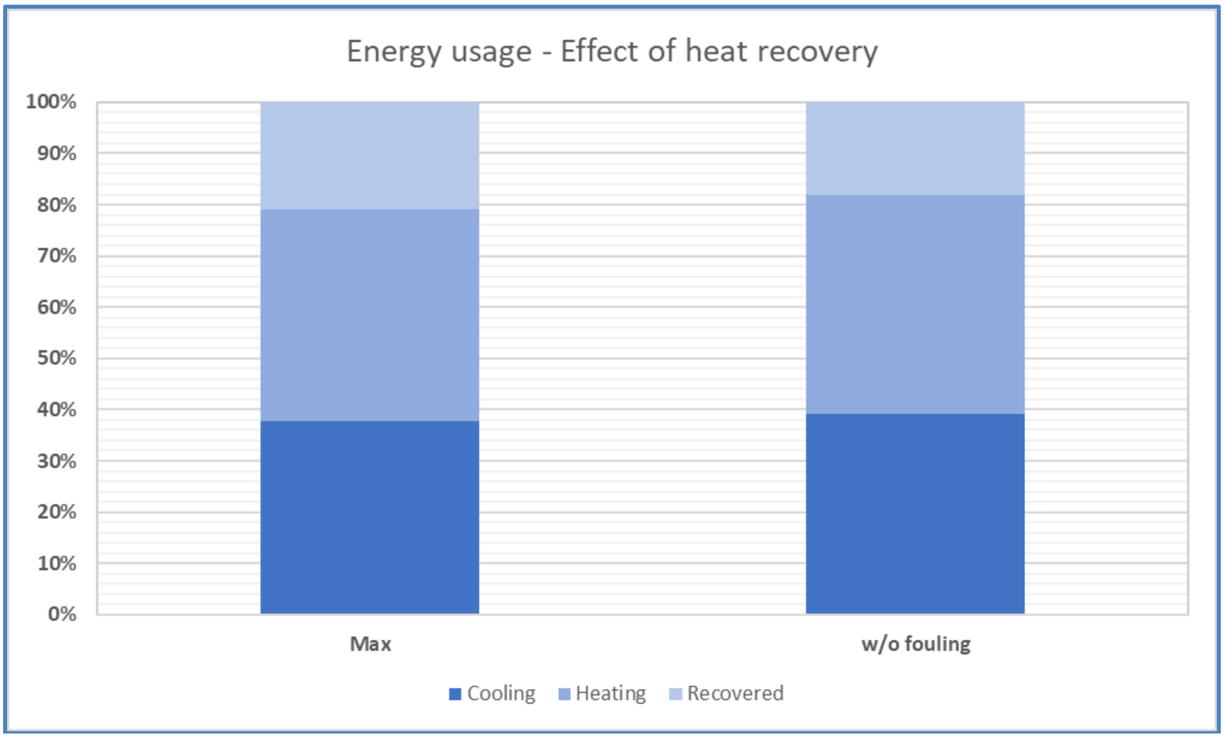

Figure 17. Distribution of energy utilisation and recovery

The process is not particularly energy intense except for the operation of the MEG-water distillation column. Excluding the heat exchangers that do not consume energy (feed/effluent of feed/bottoms exchangers), more than 90% of the total plant energy consumption is allocated to the distillation column reboiler and condenser (Figure 18). As the reboiler is powered by steam, it is a higher cost energy source than cooling water and contributes more to the overall DVC.

Considering the dominant contribution from the distillation unit, one should investigate ways to reduce the energy cost. For instance, by using vapour recompression technology to be able to use the overhead vapour (steam) as heating medium in the reboiler or utilise an air-cooled condenser to minimise cooling water usage.

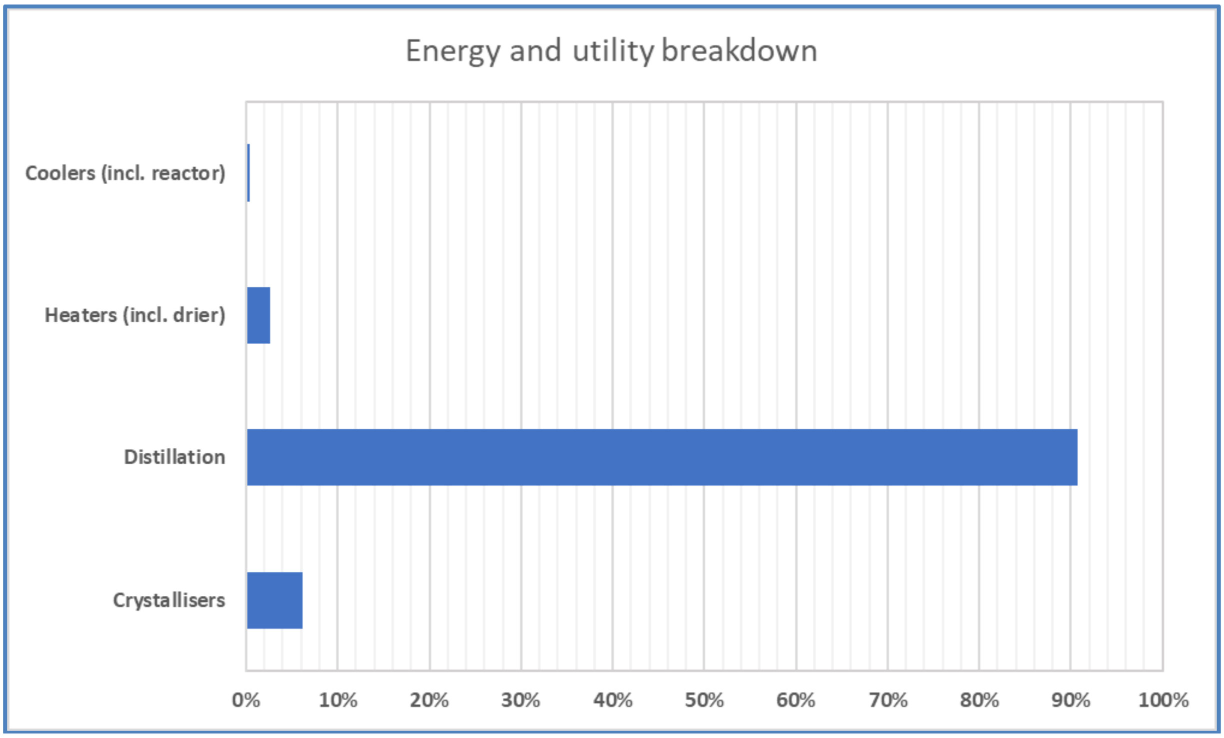

Figure 18. Energy usage per operation type.

CONCLUSIONS AND FURTHER WORK

A concept for a post-consumer PET depolymerisation plant to produce BHET through glycolysis was developed and modelled in Aspen Plus®. The functionality of the technology using an actual industrial feedstock was demonstrated in the earlier work packages of the project. The use of the depolymerised PET in downstream applications was demonstrated in work package 5 and a holistic view of the depolymerisation unit in terms of production and equipment costs as well as energy usage was presented in the present report concerning work package 6.

The main outcome from work package 6 is a depolymerisation concept that can be used as a basis for a plant project. To ensure successful implementation of a large-scale plant, there are additional topics that needs to be considered and potentially addressed in further studies. These can be loosely grouped as either pertaining to the equipment/process, the economical/logistical side of the design and operation of a depolymerisation unit, or to the legal side. Below are the topics identified in the implementation phase (in no particular order of importance):

Equipment-Process considerations

- *Experimentally measure solubilities of BHET in MEG, water, and MEG/water solutions at various temperatures*
  Rationale: The costliest unit operation by far are the crystallisation steps and the most important aspect of crystallisation in terms of fluid properties is the substrate's solubility and the temperature dependence of said solubility.
- *Investigate BHET fouling tendency in process equipment (pipes, valves, heat exchangers)*
  Rationale: As a process operating with substrate solubilities, particle precipitation and the possible associated fouling is important to understand to design process equipment for long uptime and reduced maintenance.
- *Develop alternative(s) to active carbon for decolourisation*
  Rationale: The active carbon treatment results in approximately 10% BHET losses. If the produced BHET whiteness requirement is low, the activated carbon treatment can be reduced or bypassed altogether. When this is acceptable, it should be used to reduce DVC and the environmental footprint. It may then be sufficient to wash the crystals from the first crystalliser and bypass also the second crystalliser, thus further reducing operating costs and energy usage.
- *Detailed design of process equipment*
  Rationale: To further sharpen the CAPEX estimation and to provide viable designs for the crystallisers, the reactor, and many of the heat exchanger positions, more detailed designs and equipment selection is necessary. When executing larger projects this is a step in either a feasibility study or basic engineering. In the present project, given the complexity of the feedstock and the somewhat uncertain nature of some of the process streams, a more detailed study of these topics as well as the MEG regeneration is preferably performed at the development stage.
- *Investigation around reactor types suitable for the process*
  Rationale: As alluded to in the Reaction section, the exact type and configuration of the reactor is at present not determined and should be investigated further.
- *Investigation around solid-liquid separators for oligomer and monomer separation*
  Rationale: Successful separation of solids in the oligomer separation stage and after each of the crystallisers is required. The characteristics of the crystals, especially the particle size distribution does govern the equipment design. A second aspect is the amount of washing necessary and how it will be accomplished. Typically, it is done in the separator and the design must then allow and account for that.

Economic-Logistic considerations

- *Larger plant size recommended*
  Rationale: The presently investigated plant size of 10 ktonnes per year falls on the part of the capacity vs cost curve where there still is a significant rate of decrease in cost per unit capacity and it is recommended to target a plant size that is 3-5 times the size of the currently considered capacity. This has a significant impact on pay-back time.

- *Increased PC PET collection radius*
  Rationale: As a consequence of the larger plant size suggested in the above item, the collection radius for the PC PET most be increased. This means longer transportation, which may negatively impact the carbon footprint.
- *Study process robustness*
  Rationale: Due to the larger plant size and consequently wider PC PET collection radius, a more wide-ranging feedstock quality will likely result. It is therefore important to study the effect of large feedstock variations on the process stability and product quality.
- *BHET sales price*
  Rationale: The DVC for producing BHET from PC PET is higher than for virgin PET, which in turn means that any products made from the BHET will be more expensive than if virgin raw materials were used. Hence a price premium is needed to make the process financially viable. The exact magnitude of the price premium must be decided based on the end-product in question.
- *External costs*
  Rationale: Raw material costs (MEG and PC PET), logistic, etc., must be optimised to increase competitiveness against fossil PET and allow for the realisation products based on BHET from depolymerised PET sources.

Legal aspects

- *Freedom to operate (FTO)*
  Rationale: an FTO is always conducted in relation to the realisation of novel ideas that are to be transferred from idea stage to actual development projects with the aim of construction new production capacity. An FTO is an extensive search in the patent literature to ensure that there are no obstacles or other legal hinderance in constructing and operating a plant using the suggested technology.
- *Reach registration*
  Rationale: a chemical that is not currently being sold by Perstorp is always investigated for how to in the correct way register the chemical with the right authorities. It is a process that may take up to a year and does incur certain costs that are non-negligible.
- *Environmental permit*
  Rationale: an environmental permit must be in place before construction of a plant can commence and getting a permit for a new plant may take around 3 years.

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