



OPTIMAL

Automated Maskless Laser Lithography Platform for First Time Right Mixed Scale Patterning

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= Deliverable D6.5 =

Environmental impacts of photoresist material

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1. Executive Summary

This deliverable 6.5 “Environmental impacts of photoresist material” is the first out of three LCA reports in the OPTIMAL project. The objective is to assess environmental impacts of first- and second-generation positive and negative tone photoresist materials and related developer materials. This deliverable lays the basis for assessing the impacts of the OPTIMAL platform and expected environmental benefits of the “First-time-right” production concept in subsequent deliverables D6.6 and D6.7.

The link between the results reported in this document and the activities planned in OPTIMAL Task 6.5 are reported in section 2.

The assessment is based on the method of LCA (Life Cycle Assessment). The working steps are described in section 0. Section 3.1 describes the environmental impact categories assessed. This LCA includes the following relevant life cycle impact categories relevant in relation to the technical project targets: global warming potential, cumulated energy demand and abiotic resource depletion. The impacts are assessed in a cradle-to-gate LCA and calculated per kg resist respectively developer material.

Sections 3.2 to 3.4 describe the resist materials and typical synthesis paths in chemical industry, in order to increase the transparency and support the interpretation of the results.

Section 4 describes the data sources used. As data source for background processes, the LCA database ecoinvent (V3.10) is used. Due to confidentiality of the resist composition, foreground data are not included in this report, and impact results are presented in ranges.

In section 5 the LCA results are presented. The main results are summarized in Table 2:

Table 1: Summary of the main LCA results of resist and developer materials

	Positive resist PR	Developer PR	Negative resist NR	Developer NR	Unit
GWP total	5.5 – 6.0	0.79	6.6 – 7.4	5.9	kg CO ₂ e/kg
CED total	132 – 135	17.59	133 – 135	128	MJ/kg
CED fossil	115 – 116	15.26	115 – 116	113	MJ/kg
Fossil resources	3.4 – 3.6	0.129	3.1 – 3.2	3.5	kg/kg
Non-fossil resources	4.1 – 4.9	1.626	6.7 – 10.0	5.1	kg/kg
Metals/Minerals	5.7 E-05 – 6.6 E-05	5.55	7.3 E-05 – 8.5 E-05	7 E-05	kg Sb-e/kg

The results of this deliverable will be used in subsequent LCA work (Deliverable 6.6 and 6.7), assessing the OPTIMAL laser lithography platform for master production as well its transfer to metal shims for series production, and the expected benefits of material waste reduction during manufacturing due to the OPTIMAL “first time right” concept.

2. Introduction

This deliverable D6.5 is reporting an assessment of the environmental impacts of the photoresist materials developed by the company micro resist GmbH, as planned in Task 6.5 “Life Cycle Assessment and optimization of process parameters” of the OPTIMAL project description. This is the first of three deliverables related to the environmental impact assessment of the OPTIMAL “First-time-right” production concept and integrated platform. Effects of the “First-time-right” production concept, compared to the state of the art, are waste reduction (reduction of iterations, tailored resins, larger active area) and energy savings (increased writing speed, lower electric power per laser power). The focus of D6.5 is the assessment of the photoresist materials developed in the project. This deliverable lays the basis for assessing the impacts of the OPTIMAL platform in subsequent deliverables D6.6 and D6.7.

The impact assessment is based on the method of life cycle assessment (LCA) following the ISO 14040 standard (ISO 2006). LCA is a method to investigate the environmental impacts of a product or service due to the use of natural resources and the release of emissions during the various stages of its life cycle. The life cycle stages include extraction of raw materials, manufacturing, distribution, product use, recycling and final disposal from “cradle to grave”.

LCA is structured in four consecutive stages (Figure 1):

- (i) goal and scope definition (including a clear description of the function of the system and its boundaries);
- (ii) life cycle inventory (the compilation of all the inputs and outputs respectively from and back to the natural environment associated to all processes that form part of the system’s life cycle);
- (iii) life cycle impact assessment (in which the full inventory of inputs and outputs is translated into a number of aggregated metrics of environmental impact); and
- (iv) interpretation (in which results are discussed and compared to suitable benchmarks).

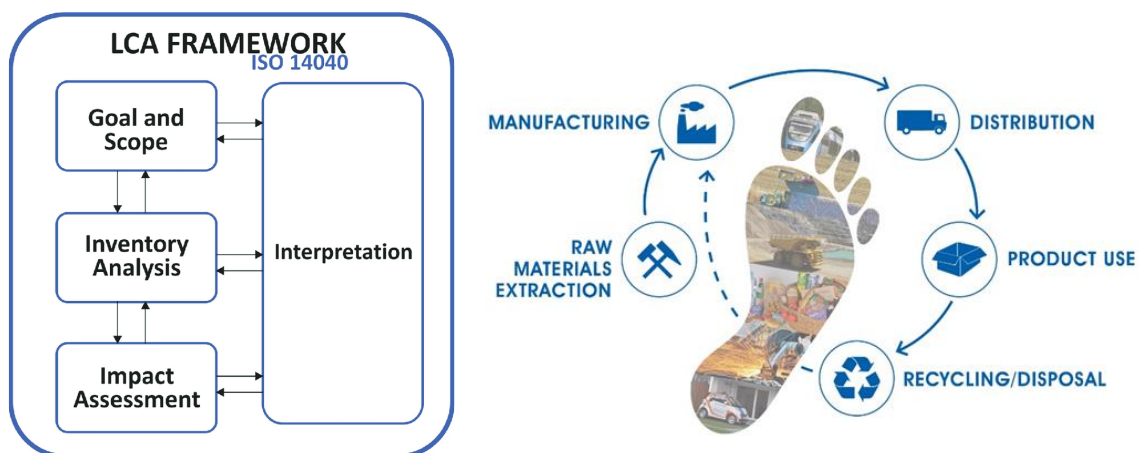


Figure 1: Method of Life Cycle Assessment according to the ISO standard 14040

Life cycle assessment is a horizontal project activity in the OPTIMAL project and therefore a responsibility of all project partners, led by JOR as Task-leader and with the partners providing input data to the life cycle inventories. The assessment of the photoresist materials has been performed in cooperation with partner MRT.

3. Goal and Scope of the OPTIMAL LCA

The goal of this first out of three LCA reports in the OPTIMAL project is to assess environmental impacts of first- and second-generation positive and negative tone photoresist materials and related developer materials (details see section 3.2) as applied in the four OPTIMAL use cases.

The scope of LCA studies is defined by the life cycle phases included. A full cradle-to-grave LCA includes all phases from resource extraction ('cradle') to the use phase and disposal phase ('grave'). Cradle-to-gate is an assessment of a partial product life cycle from resource extraction to the factory gate (i.e., before it is further processed or used).

The LCA presented here is classified a cradle-to-gate study, ending with the photoresist materials at the factory gate of MRT. In the subsequent LCA studies (D6.6, D6.7) it will be linked to further processing (see Figure 2) and will also include end-of-life treatment processes of the final products and production wastes, to form a complete cradle-to-gate evaluation.

3.1. Selected impact categories

The selection of environmental impact categories for this LCA is related to the expected technical effects of the OPTIMAL laser lithography platform for master production: 1) reduction of iterations required to produce an optimized structure due to the development of self-learning algorithms for the optimization of the virtual photomask, 2) reduction of the required time for quality analysis due to implementation of real time quality monitoring system, and 3) increase of writing speed due to the upgraded laser lithography modules. In comparison to state-of-the-art manufacturing technologies, these effects translate to material waste reduction during manufacturing (reduction of iterations, tailored resins, larger active area) and energy savings (increased writing speed, lower electric power per laser power) per kilogram of product manufactured.

This LCA therefore includes the following relevant life cycle impact categories:

- the Global Warming Potential (GWP) in [kg CO₂-equivalent or CO₂e], as a metric reflecting the project's contribution to the EU climate targets:

The GWP is a metric for the relative potential of different greenhouse gases to absorb radiation in the atmosphere over a given period of time, relative to carbon dioxide (CO₂). The GWP allows analysts to add up emissions and to compare emissions reduction measures across the different gases. CO₂ as reference gas has a GWP of 1 by definition, regardless of the time period used (commonly 100 or 20 years). Methane (CH₄) is estimated to have a GWP of 27-30 over 100 years. CH₄ decays within a decade on average, which is shorter than the decay time of CO₂ (with up to several thousand years in the atmosphere), but CH₄ also absorbs much more energy than CO₂. Nitrous Oxide (N₂O) has a GWP 273 times that of CO₂ for a 100-year timescale. N₂O emitted today remains in the atmosphere for more than 100 years, on average. Chlorofluorocarbons (CFCs), hydrofluorocarbons (HFCs), hydrochlorofluorocarbons (HCFCs), perfluorocarbons (PFCs), sulphur hexafluoride (SF₆) and Nitrogen Trifluoride (NF₃) are high-GWP gases because they trap substantially more heat than CO₂. The GWPs for these gases can be in the thousands or tens of thousands.

- the Cumulated Energy Demand (CED) in [MJ], as metric reflecting the energy efficiency of the OPTIMAL manufacturing concept and platform:

The CED is the sum of all primary energy inputs required for the production and utilisation of a product or service including all upstream processes. It is calculated as fossil primary energy (coal/oil/natural gas), renewable primary energy (wind/sun/hydro/biomass) and other primary energy sources (nuclear/waste/geothermal). According to the ISO standard, CED is not an environmental impact, but it is an important supplementary indicator for assessing energy efficiency.

- the Abiotic Resource Depletion in [kg], as metric reflecting the material efficiency of the OPTIMAL manufacturing concept and platform:

The primary resource requirement is based on the final energy and material requirements in the life cycle of the assessed resist materials. Primary resources are natural resources that are categorised into a) abiotic finite resources (mineral raw materials and fossil energy raw materials), b) abiotic renewable resources (groundwater, surface water and air), c) biotic finite resources (tropical timber and endangered animal and plant species), d) biotic regenerative resources (wild plants and animals), and e) natural space. For this study, the abiotic finite resources mineral raw materials are assessed. Biotic resources as well as water and natural areas have no specific relevance in the systems analysed and are therefore not included. The calculation of the abiotic resource depletion follows two methods. The method of the "Cumulative Raw Material Demand" (Giegrich 2012) is based on the absolute masses of natural

resources in the life cycle inventory. Primary fossil energy demand is converted to mass via the calorific value. The second method “Material Resources: metals/minerals” is part of the Environmental Footprint (EF v3.1¹) method by the European Commission’s Joint Research Centre (JRC). It also considers the scarcity of materials as concentrations and reserves of elements in the earth’s crust in the assessment using characterisation factors such as the ratio of extraction to reserve base, standardised to the element antimony (Guinée 2016) and expressed in the unit [kg sb-eq].

The environmental impacts are calculated per 1 kg of the resist or developer material as so-called functional unit.

This deliverable is a publicly available report. Since the LCA is based on partly confidential data on exact resist material composition as proprietary know-how within the project, some restrictions apply in the presentation of the impact assessment results (see also section 4).

3.2. Materials assessed

Figure 2 shows the OPTIMAL process chain with photoresist material production (assessed in this Deliverable 6.5), the OPTIMAL lithographic platform for master production (assessed in Deliverable 6.6) and the process for the transfer of the master pattern to the metal shim and series product manufacturing (assessed in Deliverable 6.7).

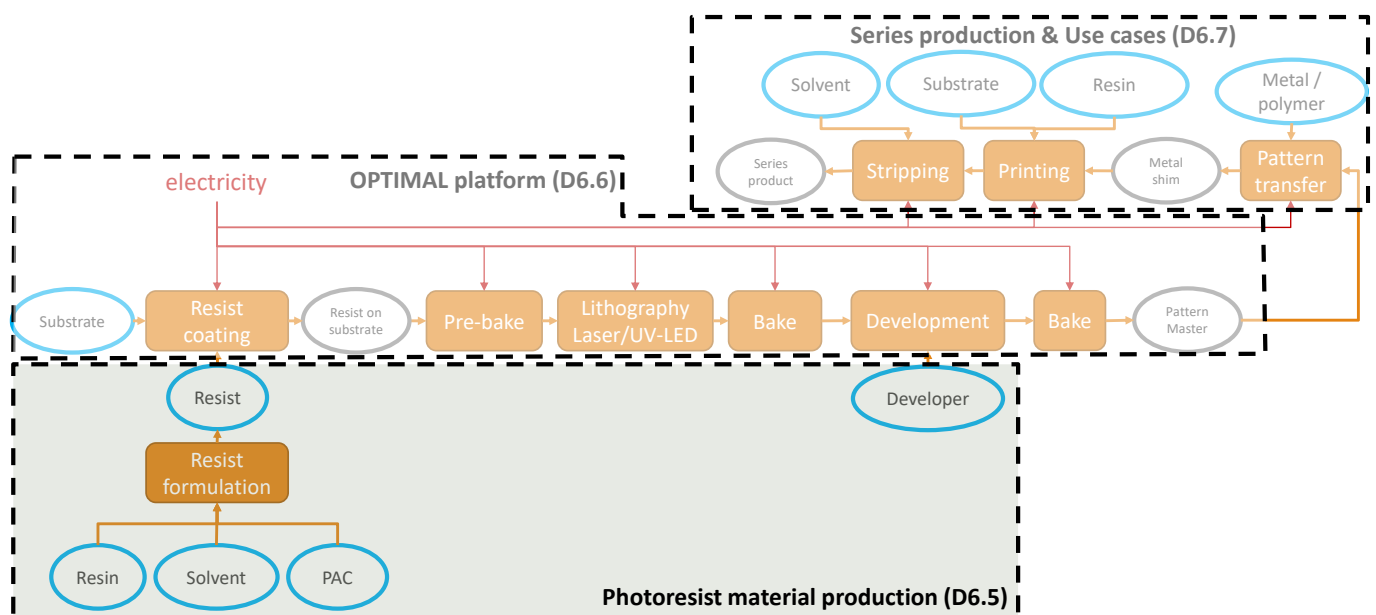


Figure 2: System diagram of the OPTIMAL process chain

Photoresists are light-sensitive materials, composed of a polymeric binder, a photoactive compound (PAC) dissolved in a solvent. Each component has a particular function. The polymer is the matrix for the PAC and responsible for the generation of a certain thickness, and controls, together with the PAC, the photochemical reaction of the negative resist type. The solvent is responsible to dissolve all resists components and allows the photoresist to be spun and to form homogeneous films on the substrate surface. The PAC is activated/ decomposed when exposed and starts the photochemical reaction resulting in a solubility change.

Photoresists can be classified as positive or negative. In a negative resist, the decomposed PAC starts a crosslinking of the polymer, and therefore the exposed areas of a negative resist remain on the surface of the substrate, whereas the developer solution removes the unexposed areas. In a DNQ/ novolak positive resist the solubility in the developer solution becomes higher in the exposed areas and hence, the exposed areas are removed during development.

The following photoresist materials are assessed in this LCA:

- Positive resist formulations
 - first generation (=state of the art materials): ma-P 1200G resist series with 4 different viscosity types
 - second generation (=material developed in the project): mr-P 22G_XP with optimized properties for the patterning of very thick resist films
- Negative resist formulations
 - first generation (=state of the art materials): mr-DWL resist series with 3 viscosity types

¹ <https://eplca.jrc.ec.europa.eu/LCDN/developerEF.html>

- second generation (=materials developed in the project): mr-DWL_100_HT_XP with lower sensitivity

The main chemical components of the positive and negative resists are listed below.

Components such as the DNQ/-novolak system have been used in resist production for more than 50 years. First and second generation positive resists are regarded as a product family, since they have both a DNQ-based PAC and a novolak resin as polymeric binder. Also first and second generation negative resists are regarded as a product family. Generally, the polymeric binder and the solvent dominate total resist mass. The exact formulation and recipes of these resist materials are classified confidential, and are therefore not documented in this report.

- Positive resists: ma-P 1200G series and mr-P 22G_XP series
 - Polymeric binder: Novolak resin
 - Solvent: 2-Methoxy-1-methylethyl-acetate (PGMEA)
 - PAC: Diazonaphthoquinone (DNQ)
- Negative resists: mr-DWL-series and mr-DWL_120_XP series
 - Polymeric binder: Epoxy resin
 - Solvent: Gamma Butyrolactone (GBL), Propylene carbonate
 - PAC: A photoinitiator system based on a photo acid generator (PAG) and a sensitizer

The developers have the following components:

- Developer for positive resists: ma-D_5xxseries
 - Tetramethylammoniumhydroxide TMAH
 - Solvent: Ultrapure water
- Developer for negative resists: mr-Dev_600
 - Solvent: 2-Methoxy-1-methylethyl-acetate (PGMEA)

These components are produced in conventional chemical industrial synthesis processes, the final formulation step of mixing the above listed components is done by project partner MRT.

3.3. Synthesis processes of positive resists

This section describes the synthesis processes of the assessed resist materials and their chemical components, including environmentally relevant processes and intermediate chemical products from the extraction of raw materials from natural environments to the manufactured photoresist materials and developers.

Several literature sources have been used for identifying common industrial synthesis processes of organic chemical materials (Weissermel 2003, Mc-Graw-Hill 2019, Falcke 2017, Langhorst 2023). In addition, the synthesis chains have been matched with the documentation of process chains in the LCA database ecoinvent (see section 4).

- Novolak resin (positive resist materials / Polymeric binder):

Novolak is a phenolic resin, which is commonly produced by poly-condensation of phenol and formaldehyde. Phenol is produced in the Hock process by partial oxidation of cumene, which in turn is a product of alkylation of benzene and propylene. Formaldehyde is the product of methanol oxidation. A typical overall synthesis path is presented in Figure 3.

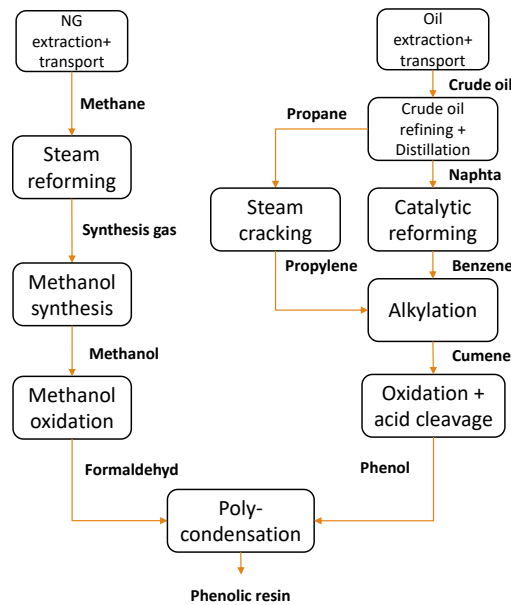


Figure 3: Typical synthesis path of Novolak resin

- PGMEA (positive resist materials / solvent):

Methoxypropanol acetate (PGMEA) is produced in an esterification reaction of methoxypropanol (PGME) and acetic acid. PGME in turn is the product of a reaction and distillation process of propylene oxide and methanol. Acetic acid is produced by butane oxidation. A typical overall synthesis path is presented in Figure 4.

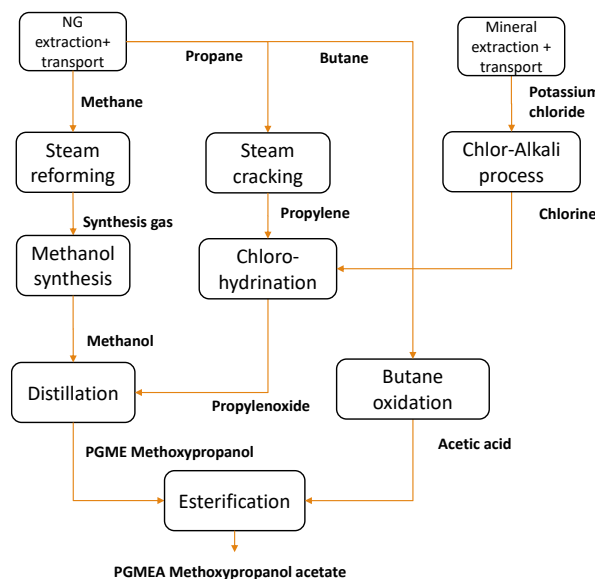


Figure 4: Typical synthesis path of PGMEA

- DNQ (positive resist materials / photoactive compound):

The production of the PAC Diazonaphtoquinone (DNQ) requires a complex process chain. DNQ is produced by a reaction of Naphthalene-2-sulfonyl chloride (NAC) with phenol. NAC is produced by reaction of Naphthalene-2-sulfonic acid with Thionylchlorid. Naphthalene-2-sulfonic acid in turn is produced by sulphonation of naphthalene with sulphuric acid, and Thionylchlorid by reacting sulphur dioxide, chlorine and sulphur dichloride. Naphthalene is produced from coal tar by fractional distillation. The overall synthesis path is presented in Figure 5.

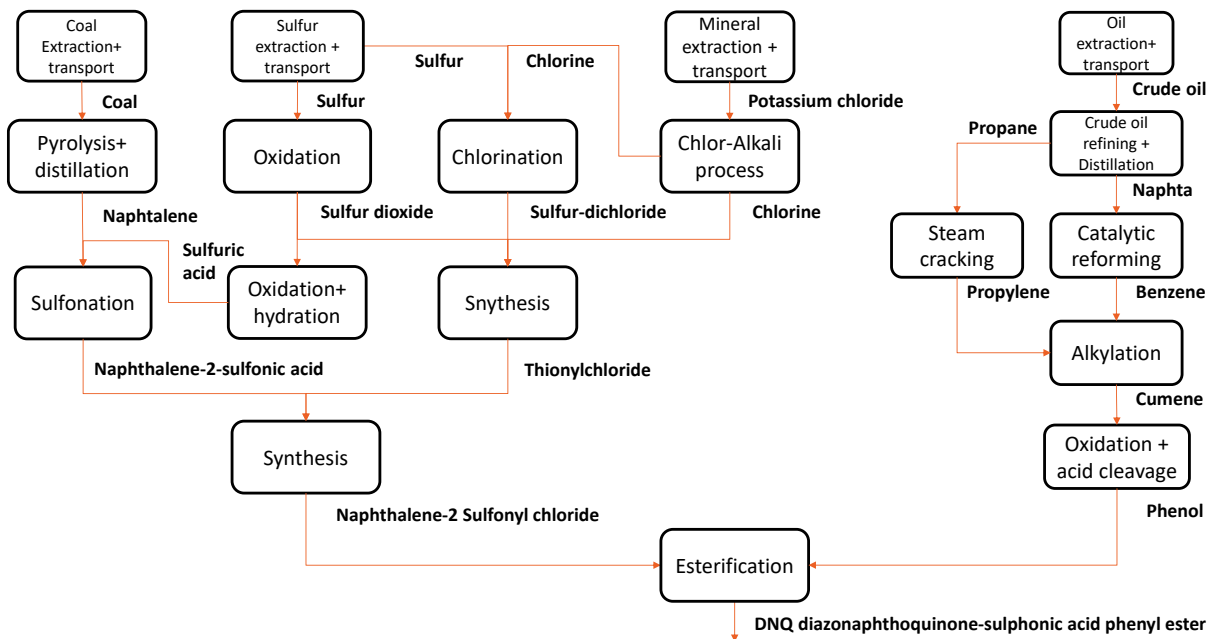


Figure 5: Typical synthesis path of DNQ

3.4. Synthesis processes of negative resists

- Epoxy resin (negative resist materials / Polymeric binder):

Epoxy resins are commonly produced by reacting bisphenol A with epichlorohydrin. Bisphenol A is produced by condensation of phenol with acetone. Acetone in turn is the product of dehydrogenation of isopropyl alcohol. Epichlorohydrin is produced in a reaction of allyl chloride, chlorine and quicklime. Allyl chloride in turn is produced from a reaction of chlorine with propene. A typical overall synthesis path is presented in Figure 6.

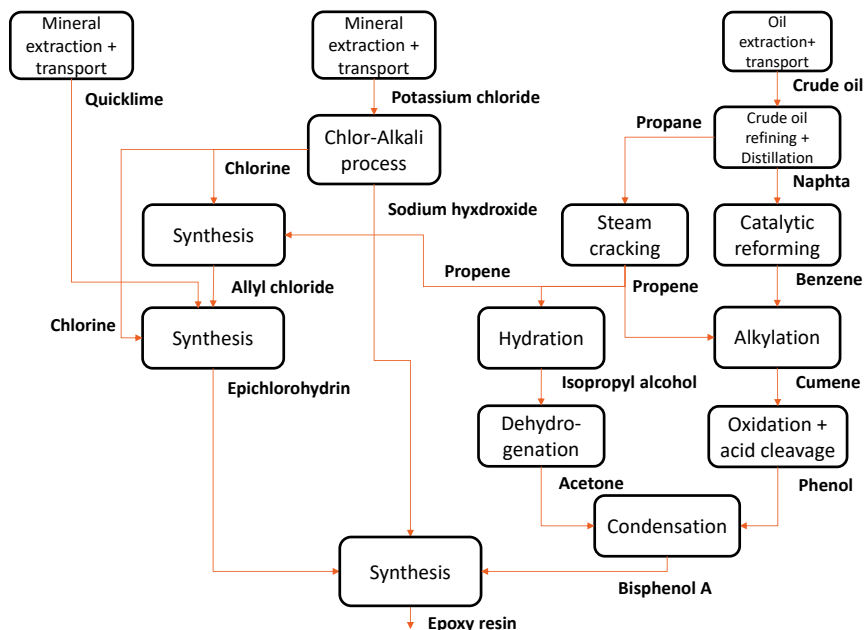


Figure 6: Typical synthesis path of epoxy resin

- GBL, propylene carbonate (negative resist materials / solvent):

GBL Gamma-Butyrolactone is produced by dehydrogenation of Butane-1,4-diol. Butane-1,4-diol is produced by a reaction of formaldehyde and acetylene. Propylene carbonate is produced from propylene glycol and CO₂. Propylene glycol in turn is derived from propylene oxide and water. Typical overall synthesis paths are presented in Figure 7.

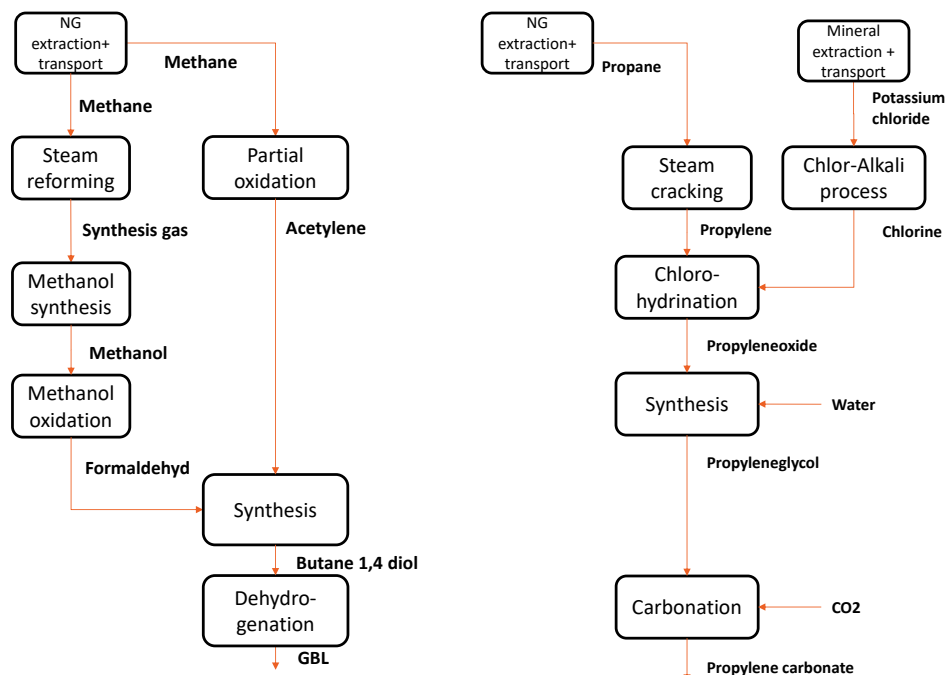


Figure 7: Typical synthesis of GBL and Propylene carbonate

- Photo initiator system based on photo active generator (PAG) and a sensitizer:

Since the chemical specification of this component is classified as sensitive information, the overall synthesis path is not presented herein.

4. Data collection

Data required for LCA calculations are collected in the so-called Life Cycle Inventory (LCI). A LCI includes all inputs and outputs passing the system boundaries, which are energy and material flowing into the system as well as emissions and wastes leaving the system.

The compilation and quantification of the LCI includes foreground and background data. Foreground data are process- and site-specific data, e.g. from process monitoring or simulation. In this LCA, such data include for example the specification of the (confidential) material composition or the energy demand of the resist formulation at MRT. Foreground data are linked to background data, which cover and quantify input and output flows of up- and downstream process chains, for example, the average extraction, processing and transports of primary energy sources or primary resources, or the upstream production of certain intermediate chemicals in refineries. Background data are supplied by so-called LCA-databases, which are provided by third parties, such as the Swiss company ecoinvent.

Relevant LCA databases with chemical datasets (ecoinvent, carbonmind.chemicals, sphera) have been screened for use in this project, based on criteria such as coverage of relevant chemicals, details of documentation, transparency and disaggregation of datasets, data quality, and the option to adjust datasets. In this LCA, ecoinvent (V3.10) has been chosen as background database, together with the LCA software openLCA (V2.1), due to the coverage of chemical products required for this LCA, the high transparency of dataset documentation and the option to adjust datasets in case more specific process data become available.

When compiling chemical process background data, significant challenges may exist, due to the diversity of chemical products, complex production processes and supply chains, the confidentiality of process information and inconsistent modelling principles (Righi 2020). While chemical reaction equations and their heat balance resulting in endo- or exothermic reactions are well defined, the overall energy balance of chemical production processes in an industrial environment, also including subsequent material purification and separation steps, depend on the individual setup of a chemical refinery. For inputs of electricity and heat to refinery processes, all LCA databases partly use proxy data, which are derived by course approximations from single or few specific chemical sites with aggregated production data publicly reported. Obviously, data from a chemical proxy approach have a limited representativeness for the entire chemical sector. Oberschelp 2023 conclude that the proxies used in the ecoinvent database tend to overestimate the electricity demand whereas the heat demand may be underestimated, in more than 20% of the chemical datasets in the database. Therefore, LCA results, especially in the context of complex chemical production,

need to be interpreted as approximation. As a general outlook for improving such data in LCA databases, additional production data from different refineries will become publicly available in future due to the increasing legal environmental reporting requirements in the EU.

As a general rule within the process chains of industrial organic chemistry, the (commonly fossil) energy and related GHG intensity generally decreases starting from the separation of natural sources crude oil, coal or natural gas, to raw materials, base materials, intermediates and fine products (Figure 8). Separation processes for splitting long hydrocarbon chains of natural sources require high process temperatures in boilers or kilns, whereas the synthesis of fine products at the end of the value chains often requires only low reaction temperatures or electricity e.g. for mixing components.

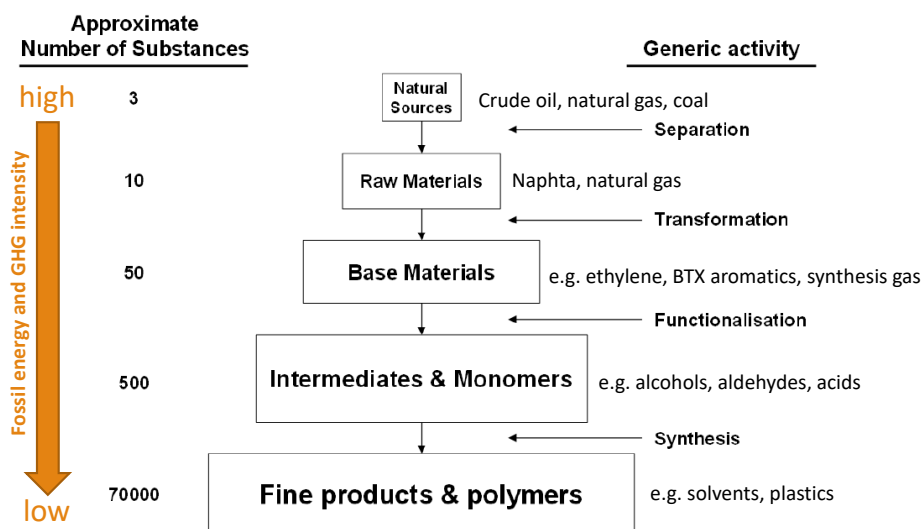


Figure 8: Structure of industrial organic chemical production (Falcke 2017)

Typical processes and energy carriers involved in today's industrial organic chemistry are presented in Figure 9. In organic industrial chemistry, heat dominates over electricity as energy carrier in the overall process chain.

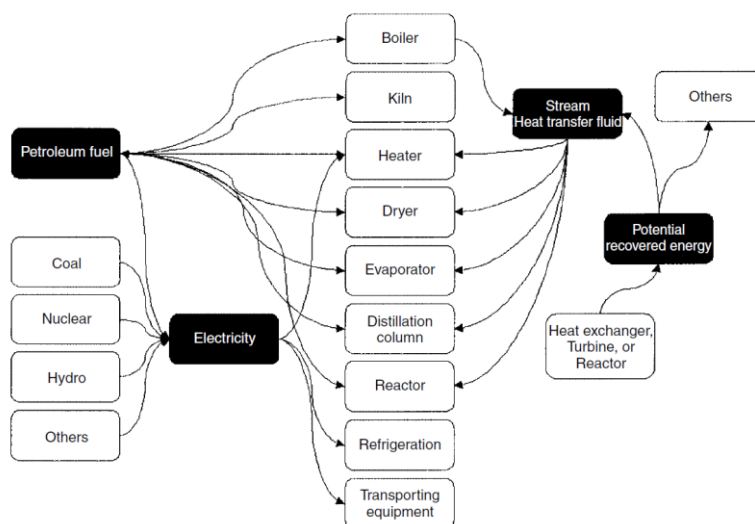


Figure 9: Processes and energy carriers in industrial organic chemical production (Kim 2003)

In addition to energy consumption and carriers, other factors such as process yields of products and co-products, the use of reactants or solvents in large excess, catalysts and also the end-of-life treatment of production wastes can have an influence on the use of resources and environmental impacts. These factors are considered in the background datasets of the ecoinvent database (Wernet 2012, Althaus 2007), with the same limitations concerning the use of proxy data as discussed above for the energy demand.

Finally, this LCA builds on state-of-the-art industrial chemical processes, which still largely use fossil energy resources. The development and use of "green materials or chemicals" was out of scope of this project and therefore not considered here.

Appendix 1 lists the background datasets from the ecoinvent database used for the calculation of the LCI. Reactions not covered by the ecoinvent database were added by the authors based on a literature search (sources see section 3.3) and the use of the general proxy data used in ecoinvent for electricity and heat demand.

5. Impact assessment

For Life Cycle Impact Assessment (LCIA), different methods are available for calculating certain environmental impacts. The methods differ in relation to the characterisation models, which translate emissions to impacts on environment. As most relevant method framework for this LCA, the EU Environmental Footprint (EF v3.1) method has been chosen. In addition, the Cumulated Energy Demand (CED) method, developed by ecoinvent, has been used to present the primary energy demand with the shares of fossil, biogenic and other primary energy, and the method for Cumulative Raw Material Demand (Giegrich 2012) to present the abiotic resource depletion (see section 3.1).

Total environmental impacts as results of LCIA are presented as ranges between two values (“V1”, “V2”), reflecting the range of mass shares of the chemical components: polymeric binder, solvent and PAC within the analysed family of resist materials. For an exemplary resist composition, a Sankey flow diagram shows the relative contributions to the GWP of the main processes and intermediate materials within the resist synthesis process chain.

5.1. Positive resists

5.1.1. Global warming potential

The GWP of the positive resist family is between 5.5 and 6.0 kg CO₂e per kg positive resist material (Figure 10). The range is due to different mass shares of the main components such as polymeric binder, solvent and PAC, which is confidential information, and therefore it is not displayed here. The specific GWP of these components are also presented in Figure 10, with 5.9 kg CO₂e per kg solvent PGMEA, 4.6 kg CO₂e per kg Novolak resin and 3.5 kg CO₂e per kg PAC. In addition, the GWP related to the electricity demand for resist formulation is 0.3 kg CO₂e per kg resist.

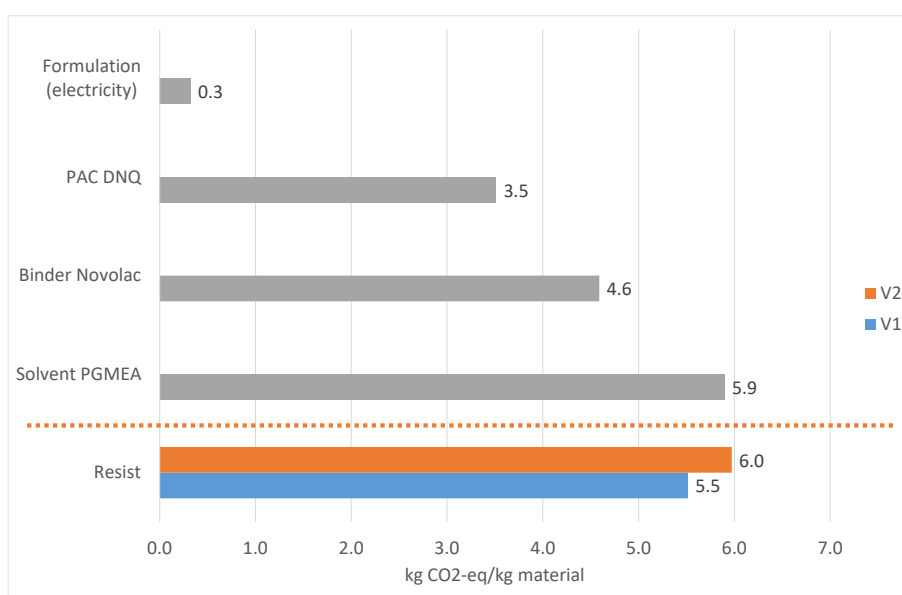


Figure 10: Global Warming Potential of positive resist material family and components

For the resist synthesis process chain of an exemplary resist composition, Figure 11 shows the relative individual and Figure 12 the cumulated contributions of the main processes and intermediate materials to the total GWP. As discussed in Figure 8, the energy intensive production processes of base materials and intermediates (e.g. Benzene, Propylene, Methanol, Phenol) contribute around 80% of the GWP.

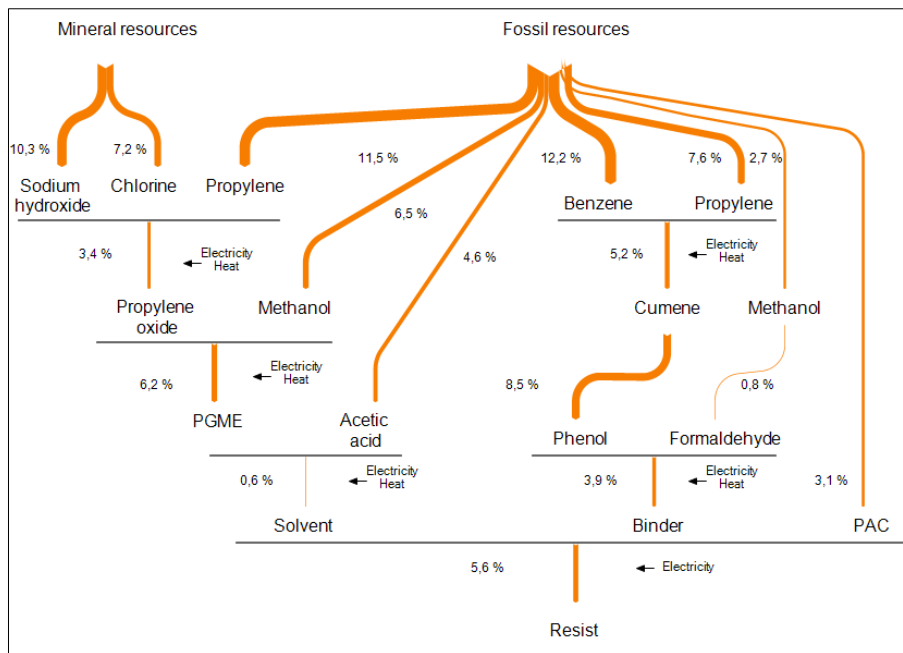


Figure 11: Relative individual contributions of processes and intermediates to the GWP of an exemplary positive resist composition

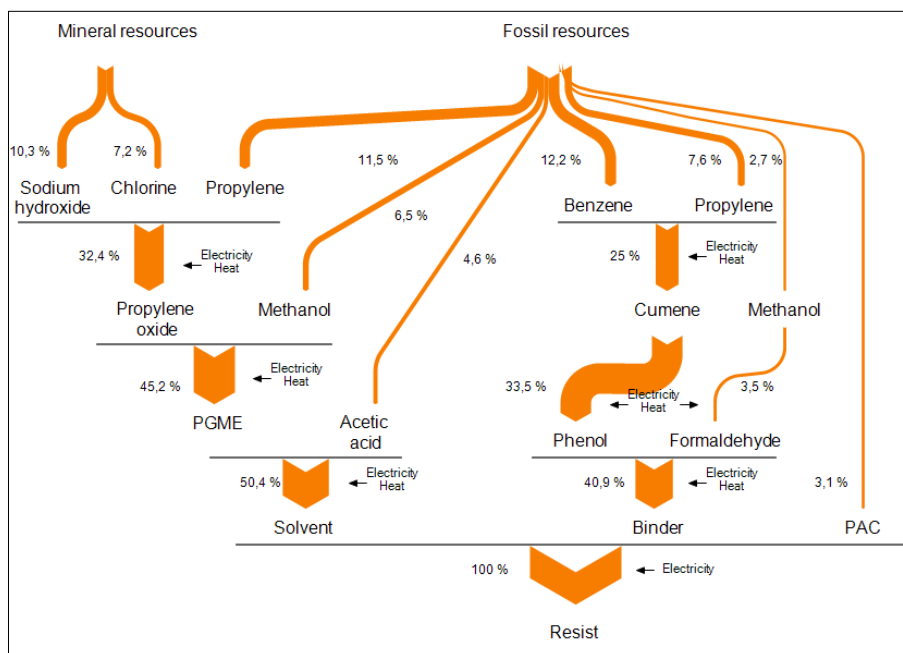


Figure 12: Relative cumulated contributions of processes and intermediates to the GWP of an exemplary positive resist composition

5.1.2. Cumulated energy demand

The cumulated energy demand (CED) of the positive resist family is between 132 and 135 MJ per kg positive resist material (Figure 13). The cumulated energy demand includes all primary energy inputs required for the production of the resist including all upstream processes. It is presented as fossil CED (coal/oil/natural gas), renewable CED (wind/sun/hydro/biomass) and nuclear CED. The fossil CED has the largest share of about 87% or 115 MJ per kg positive resist, where the renewable CED is about 5% and the nuclear CED about 8%. The large share of fossil CED is obviously the main contribution to the GWP of the resist material.

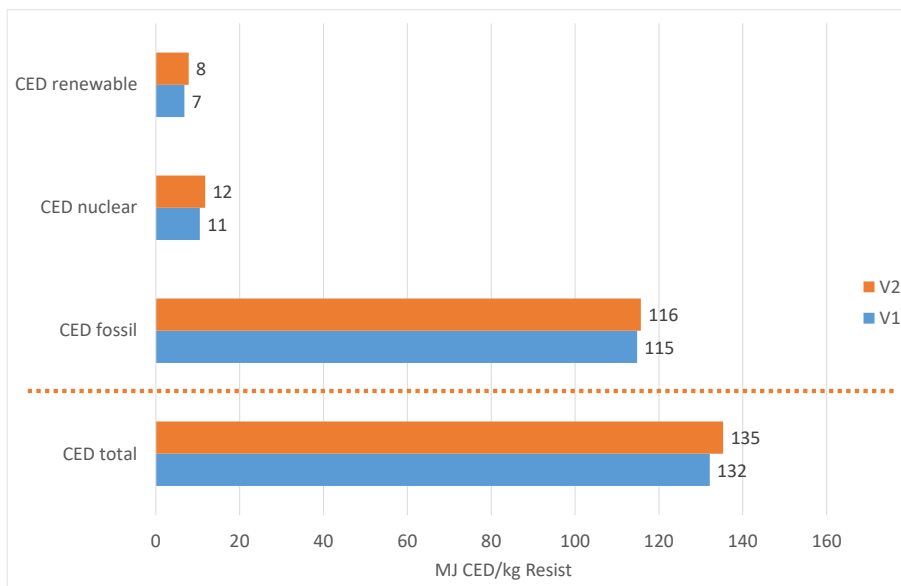


Figure 13: Cumulated Energy Demand of positive resist material family

5.1.3. Abiotic resource depletion

The life cycle abiotic resource depletion of the positive resist family is between 7.5 and 8.4 kg resources per kg positive resist material (Figure 14). It includes non-fossil-energy material resources with 4.1 to 4.9 kg per kg resist and the fossil energy resources (converted to mass unit) with 3.4 to 3.6 kg per kg resist. Fossil energy resources in turn include coal (about 50%), crude oil (25%) and natural gas (25%).

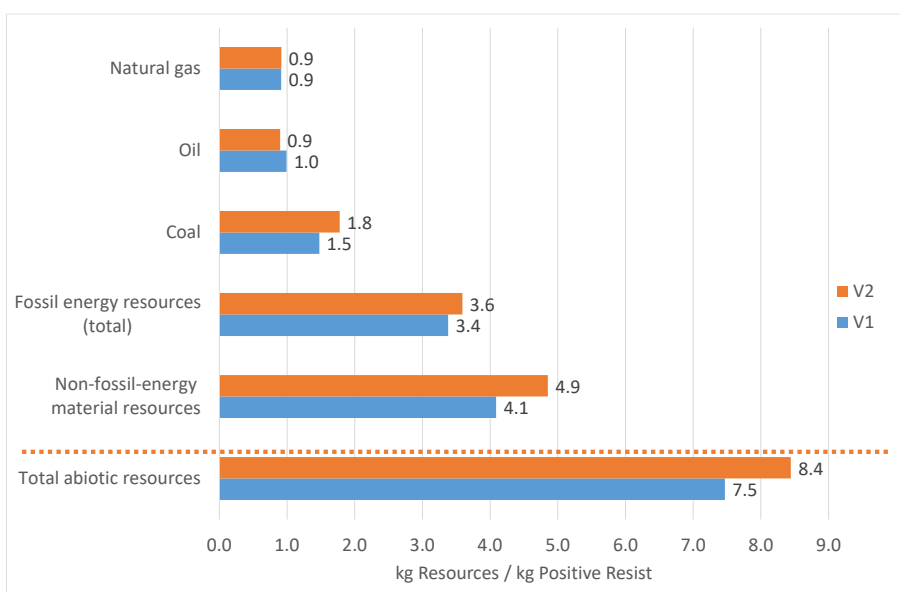


Figure 14: Abiotic resource depletion [in kg Resources] of positive resist material family

In Figure 15 the non-fossil-energy material resources are displayed as kg Sb-equivalent per kg of resist material. In comparison to other exemplary materials, such as the mineral resource concrete and the metal copper, as well as to the polymer polyethylene, the result of 6.0 E-05 kg Sb-e/kg resist indicates, that this impact assessment method is less meaningful for organic chemical products.

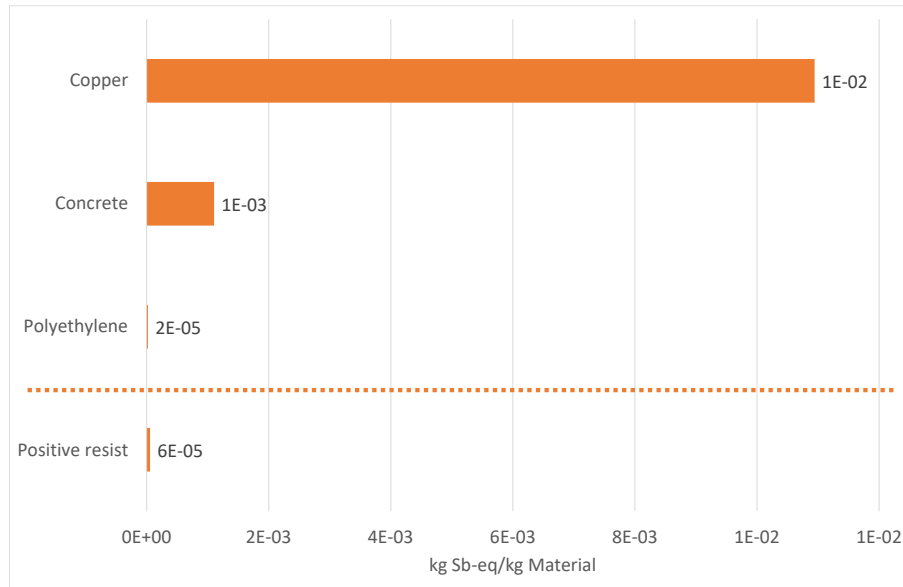


Figure 15: Abiotic resource depletion [in kg Sb-equivalent] of positive resist material family

5.2. Negative resists

5.2.1. Global warming potential

The GWP of the negative resist family is between 6.6 and 7.4 kg CO₂e per kg negative resist material (Figure 16). The range is due to different mass shares of the main components such as binder, solvent and PAC, which is confidential information, and therefore it is not displayed here. The specific GWP of these components is also presented in Figure 16, with 4.6 kg CO₂e per kg solvent, 6.0 kg CO₂e per kg resin and 11.0 kg CO₂e per kg PAC. In addition, the GWP related to the electricity demand for resist formulation is 0.3 kg CO₂e per kg resist.

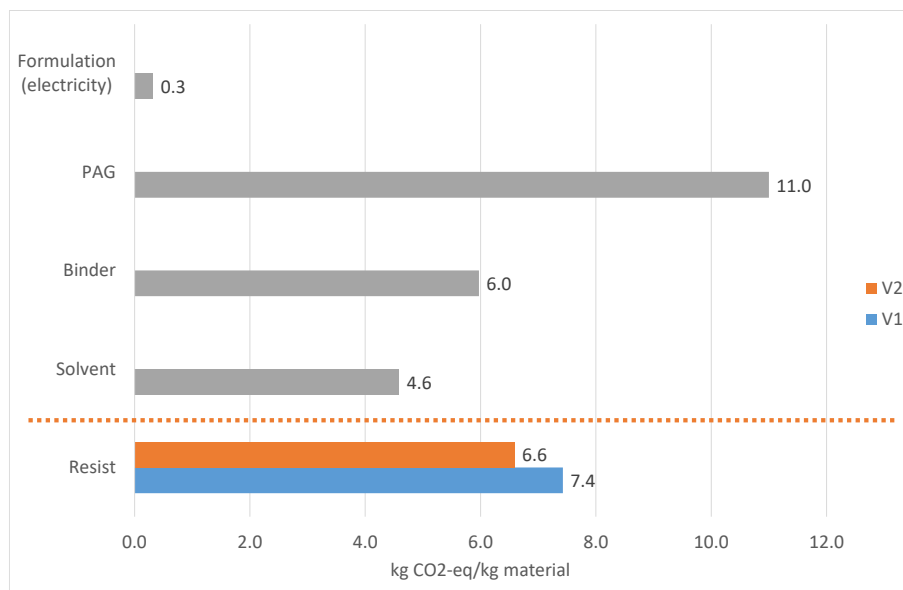


Figure 16: Global Warming Potential of negative resist material family

For the resist synthesis process chain of an exemplary resist composition, Figure 17 shows the relative individual and Figure 18 the cumulated contributions of the main processes and intermediate materials to the total GWP. As discussed in Figure 8, the energy intensive production processes of base materials and intermediates (e.g. Methanol, Acetylene, Cumene, Butane-1,4-diol) at the beginning of the chemical synthesis chain contribute about 60% of the GWP. The production of Butane-1,4-diol including upstream production of Methanol and Acetylene contributes about 50% of total GWP, due to the high process (fossil) heat demand of the so-called Reppe-process in the ecoinvent dataset. Currently, the heat demand (around 28 MJ/kg Butane-1,4-diol) could not be verified in other literature sources. The production of the PAC contributes about 22% of the GWP. Due to confidentiality, details of the synthesis processes are not discussed here.

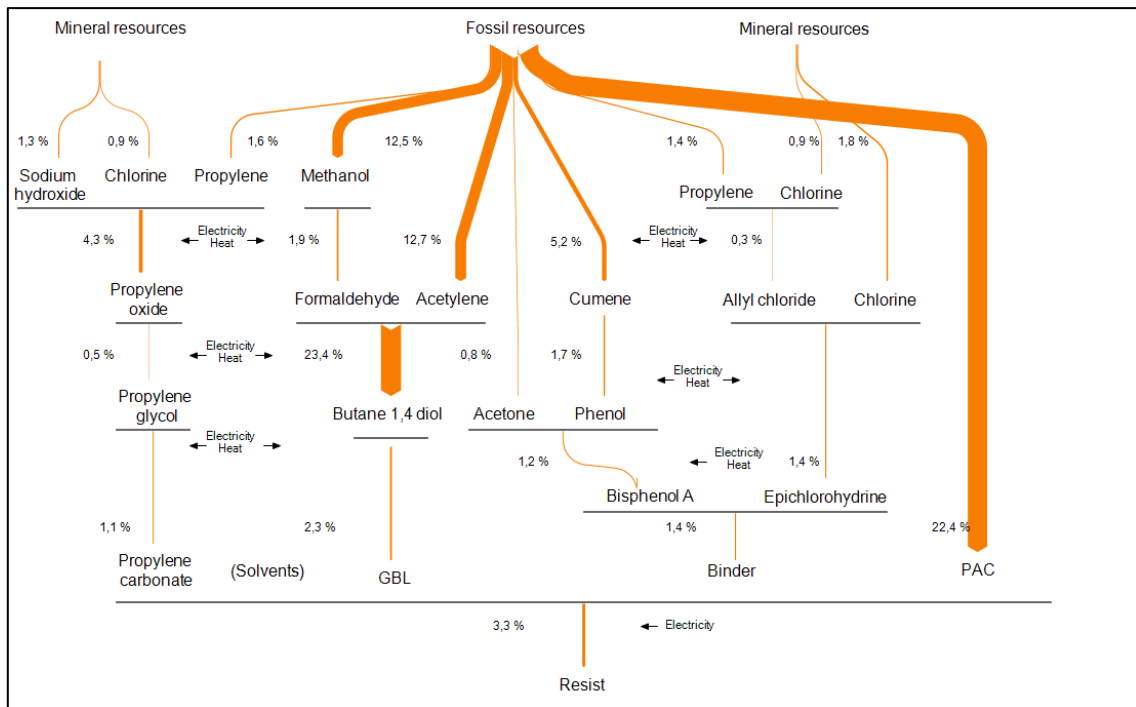


Figure 17: Relative individual contributions of processes and intermediates to the GWP of an exemplary negative resist composition

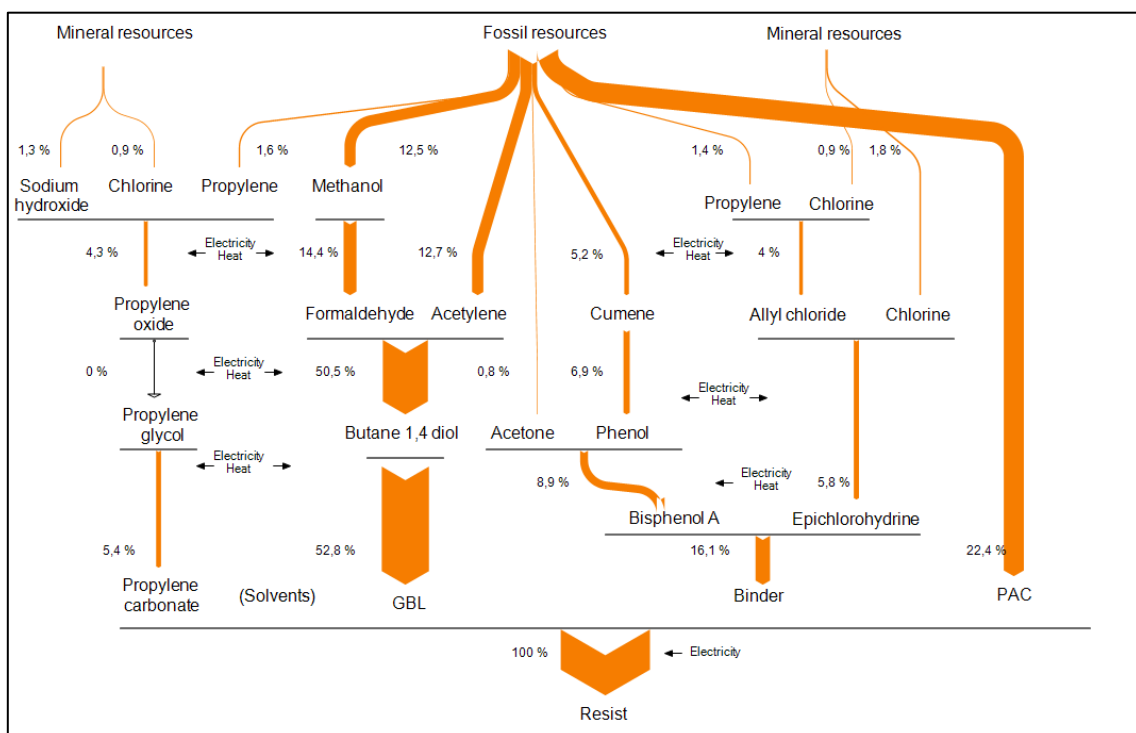


Figure 18: Relative cumulated contributions of processes and intermediates to the GWP of an exemplary negative resist composition

5.2.2. Cumulated energy demand

The cumulated energy demand (CED) of the negative resist family is between 133 and 135 MJ per kg negative resist material (Figure 19). The cumulated energy demand includes all primary energy inputs required for the production of the resist including all upstream processes. It is presented as fossil CED (coal/oil/natural gas), renewable CED (wind/sun/hydro/biomass) and nuclear CED. The fossil CED has the largest share of about 87 % or 115 MJ per kg negative resist, where the renewable CED is about 5 % and the nuclear CED about 8 %.

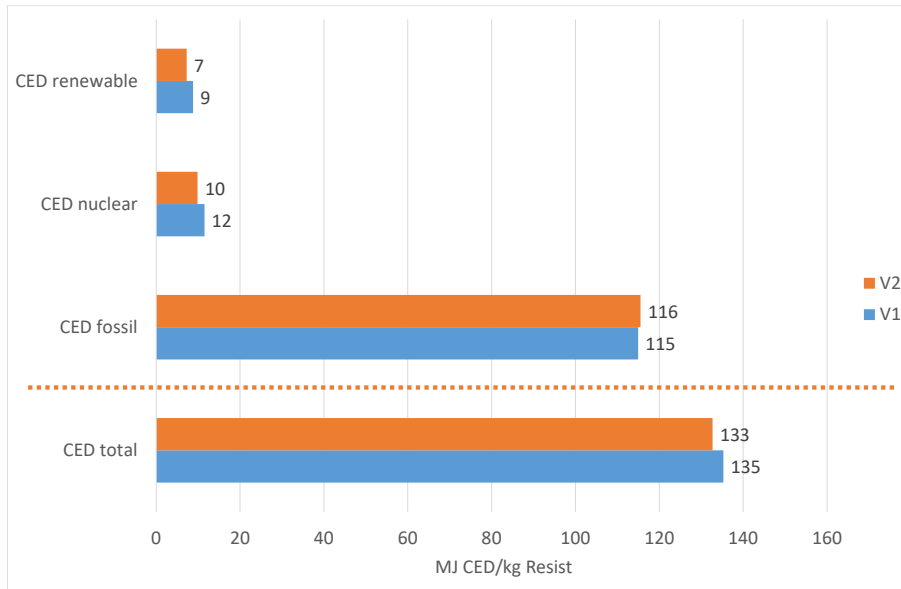


Figure 19: Cumulated Energy Demand of negative resist material family

5.2.3. Abiotic resource depletion

The abiotic resource depletion of the negative resist family is between 9.8 and 13.2 kg resources per kg positive resist material (Figure 20). It includes non-fossil-energy material resources with 6.7 to 10.0 kg per kg resist and the fossil energy resources (converted to mass unit) with 3.1 to 3.2 kg per kg resist. The range of non-fossil-energy material resources is due to the PAC and the different shares in the resist.

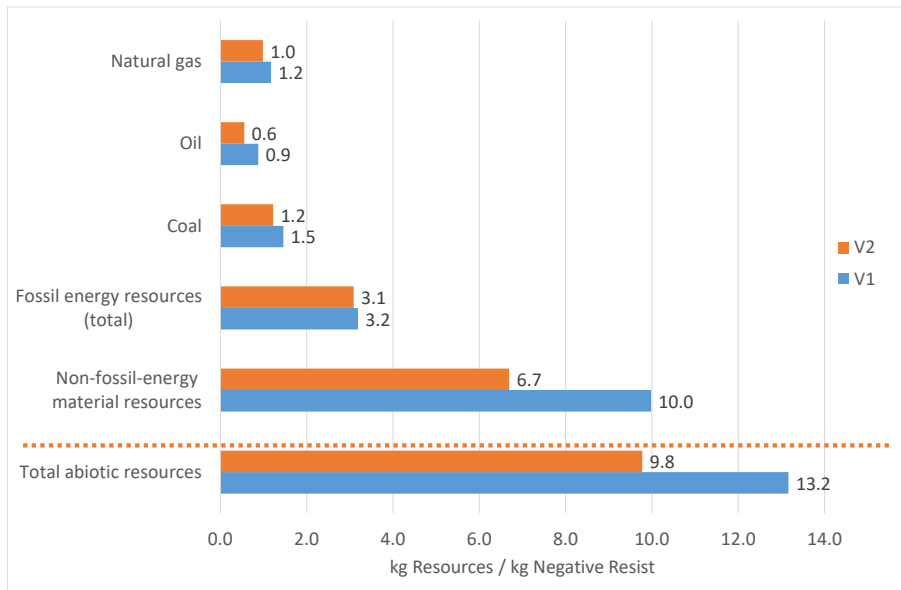


Figure 20: Abiotic resource depletion [in kg Resources] of negative resist material family

In Figure 21 the non-fossil-energy material resources are displayed as kg Sb-equivalent per kg of resist material. In comparison to other exemplary materials, such as the mineral resource concrete and the metal copper, as well as to the polymer polyethylene, the result of $7.3E-05$ to $8.5E-05$ kg Sb-e/kg resist indicates, that this impact assessment method is less meaningful for organic chemical products, as already stated in section 5.1.3.

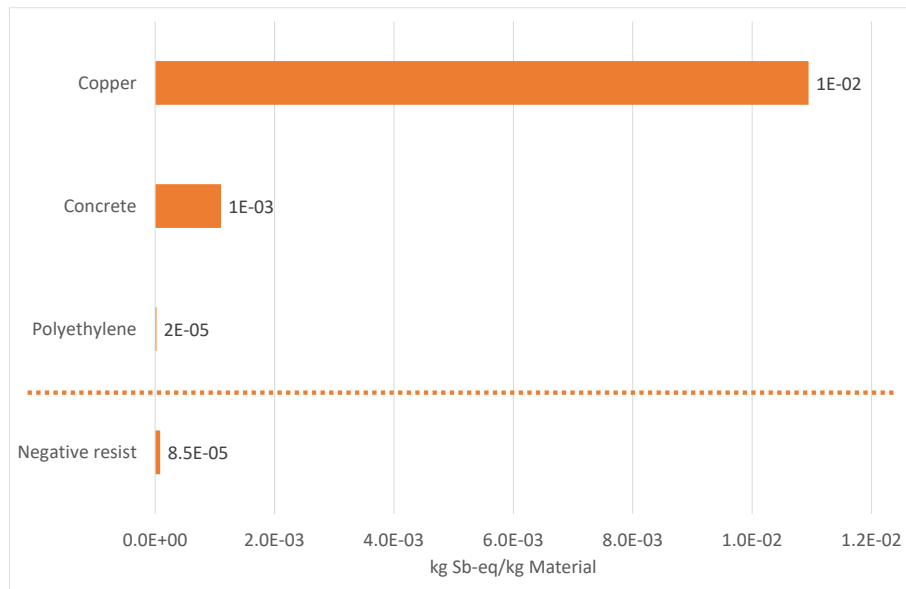


Figure 21: Abiotic resource depletion [in kg Sb-equivalent] of negative resist material family

5.3. Developer for positive resist

The component of the developer for positive resists is Tetramethylammoniumhydroxide (TMAH), dissolved in ultrapure water. The environmental impacts are:

- Global Warming Potential: 0.796 kg CO₂e/kg developer
- Cumulated Energy Demand:
 - CED total: 17.59 MJ/kg developer
 - CED fossil: 15.26 MJ/kg developer
 - CED nuclear: 1.69 MJ/kg developer
 - CED renewable: 0.65 MJ/kg developer
- Abiotic resource depletion:
 - Non fossil resources: 1.626 kg/kg developer
 - Fossil resources: 0.129 kg/kg developer
 - Material resources: metals/minerals (EF 3.1): 5.55E-06 kg Sb-e/kg developer

5.4. Developer for negative resist

The dominant component of the developer for positive resists is PGMEA Methoxypropanol acetate. The environmental impacts are:

- Global Warming Potential: 5.9 kg CO₂e/kg PGMEA
- Cumulated Energy Demand:
 - CED total: 128 MJ/kg PGMEA
 - CED fossil: 113 MJ/kg PGMEA
 - CED nuclear: 9 MJ/kg PGMEA
 - CED renewable: 6 MJ/kg PGMEA
- Abiotic resource depletion:
 - Non fossil resources: 5.1 kg/kg PGMEA
 - Fossil resources: 3.5 kg/kg PGMEA
 - Material resources: metals/minerals (EF 3.1): 7.04E-05 kg Sb-e/kg PGMEA

6. Conclusions

The goal of this first out of three LCA reports in OPTIMAL is to assess environmental impacts of first- and second-generation positive and negative tone photoresist materials and related developer materials. This deliverable lays the basis for assessing the impacts of the OPTIMAL platform and expected environmental benefits of the “First-time-right” production concept in subsequent deliverables D6.6 and D6.7.

The assessment is based on the method of LCA and includes the following relevant life cycle impact categories relevant in relation to the technical project targets: global warming potential, cumulated energy demand and abiotic resource depletion. The impacts are assessed in a cradle-to-gate LCA and calculated per kg resist respectively developer material.

In order to increase the transparency of the results, typical synthesis paths including the main upstream processes and intermediates are documented. As data source for background processes the LCA database ecoinvent (V3.10) is used. Due to confidentiality of the resist composition, foreground data are not included in this report, and impact results are presented in ranges.

The main results are summarized in Table 2:

Table 2: Summary of main LCA results of resist and developer materials

	Positive resist PR	Developer PR	Negative resist NR	Developer NR	Unit
GWP total	5.5 – 6.0	0.79	6.6 – 7.4	5.9	kg CO ₂ e/kg
CED total	132 – 135	17.59	133 – 135	128	MJ/kg
CED fossil	115 – 116	15.26	115 – 116	113	MJ/kg
Fossil resources	3.4 – 3.6	0.129	3.1 – 3.2	3.5	kg/kg
Non-fossil resources	4.1 – 4.9	1.626	6.7 – 10.0	5.1	kg/kg
Metals/Minerals	5.7 E-05 – 6.6 E-05	5.55	7.3 E-05 – 8.5 E-05	7 E-05	kg Sb-e/kg

The results of this deliverable will be used in subsequent LCA work (Deliverable 6.6 and 6.7), assessing the OPTIMAL laser lithography platform for master production as well its transfer to metal shims for series production, and the expected benefits of material waste reduction during manufacturing due the OPTIMAL “first time right” concept.

7. Degree of progress

This Deliverable describes the environmental impacts of the photoresist materials using the methodology LCA and the data provided by the OPTIMAL partner MRT. Being a public report, some confidential information concerning the synthesis and manufacturing of the photoresist material are omitted. Nevertheless, the Global Warming Potential, the Cumulated Energy Demand, the consumption of fossil and non-fossil resources and of minerals during the production of positive and negative resists are estimated. The degree of progress is 100%. In case any data updates occur related to the background processes, these will be included in D6.6 and D6.7.

8. Dissemination level

This Deliverable is available to broad public, published at the project website and at the Cordis platform.

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10. Appendix 1

Background datasets used for the life cycle inventory:

Compound	Dataset in ecoinvent V3.10
Positive resist	
Binder Novolak	Phenolic resin production phenolic resin Cutoff, U - RER
PGME	1-methoxy-2-propanol production 1-methoxy-2-propanol Cutoff, U - GLO
Acetic Acid	Acetic acid production, butane oxidation acetic acid, without water, in 98% solution state Cutoff, U - RER
Phenol	Phenol production, cumene oxidation phenol Cutoff, U - RER
Naphthalene sulfonic acid	Naphthalene sulfonic acid production naphthalene sulfonic acid Cutoff, U - RER
Thionyl chloride	Thionyl chloride production thionyl chloride Cutoff, U - RER
Electricity	market group for electricity, medium voltage electricity, medium voltage Cutoff, U - RER
Heat / Steam	Steam production, in chemical industry steam, in chemical industry Cutoff, U - RER
Developer positive resist	
Water ultrapure	Water production, ultrapure water, ultrapure Cutoff, U - RER
TMAH	Market for methylchloride methylchloride Cutoff, U - RER
	Potassium hydroxide production potassium hydroxide Cutoff, U - RER
	Market for trimethylamine trimethylamine Cutoff, U - RER
Negative resist	
Epoxy resin	Epoxy resin production, liquid epoxy resin, liquid Cutoff, U - RER
Butyrolactone	Butyrolactone production, dehydrogenation of 1,4-butanediol butyrolactone Cutoff, U - RER
Acetylene	Acetylene production acetylene Cutoff, U - RER
Propylene glycol	Propylene glycol production, liquid propylene glycol, liquid Cutoff, U - RER
PAC	Not displayed here due to confidentiality
Developer negative resist	
PGME	1-methoxy-2-propanol production 1-methoxy-2-propanol Cutoff, U - GLO
Acetic Acid	Acetic acid production, butane oxidation acetic acid, without water, in 98% solution state Cutoff, U - RER
Energy	
Electricity	market group for electricity, medium voltage electricity, medium voltage Cutoff, U - RER
Steam	Steam production, in chemical industry steam, in chemical industry Cutoff, U - RER
Heat	Market group for heat, district or industrial, natural gas heat, district or industrial, natural gas Cutoff, U - RER